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# Isodesmic reaction for accurate theoretical p$K_a$ calculations of amino acids and peptides

Supporting Information

S. Sastre,[a] R. Casasnovas,[b] F. Muñoz,[a,c] and J. Frau[a,c]

[a] Mr. Sebastià Sastre, Dr. Francisco Muñoz and Dr. Juan Frau Department de Química, Universitat de les Illes Balears Palma de Mallorca 07122, Spain
E-mail: juan.frau@uib.es
[b] Dr. Rodrigo Casasnovas
Institute of Neuroscience and Medicine INM-9, Institute for Advanced Simulations IAS-5. Computational Biomedicine, Forschungszentrum Jülich 52428, Germany
[c] Dr. Francisco Muñoz and Dr. Juan Frau
Instituto de Investigación Sanitaria de Palma (IdISPa), 07010, Palma, Spain

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**Table S1**. Absolute errors of p$K_{a1}$ of peptides calculated with the Isodesmic reaction compared to the experimental values. Alanine was used as reference species.

| | p$K_{a1}$ (exptl.[a]) | $\Delta$p$K_{a1}$ (M052X) | $\Delta$p$K_{a1}$ (M062X) | $\Delta$p$K_{a1}$ (B3LYP) | $\Delta$p$K_{a1}$ (PM6) | $\Delta$p$K_{a1}$ (ChemOffice) |
|---|---|---|---|---|---|---|
| GlyGly | 3.13 | - | - | - | - | 0.17 |
| GlyVal | 3.18 | 0.79 | 0.85 | 1.00 | 0.99 | 0.12 |
| GlyPhe | 3.23[b] | 0.63 | 0.45 | 1.28 | 0.79 | 0.39 |
| GlyAla | 3.15 | 0.46 | 0.38 | 0.89 | 0.71 | 0.10 |
| AlaGly | 3.16[c] | 1.64 | 1.57 | 1.64 | 0.46 | 0.22 |
| AlaAla | 3.32 | 0.89 | 1.28 | 1.34 | 0.06 | 0.29 |
| AsnGly | 2.90[c] | 1.29 | 1.10 | 0.02 | 1.34 | 0.24 |
| ValGly | 3.23 | 0.18 | 0.17 | 0.82 | 3.33 | 0.24 |
| SerGly | 3.10[c] | 0.58 | 0.71 | 0.22 | 2.11 | 0.07 |
| SerLeu | 3.08 | 0.48 | 0.22 | 0.74 | 0.19 | 0.01 |
| AlaHis | 2.64[d] | 0.08 | 1.09 | 0.55 | 4.31 | 0.16 |
| GlyTyr | 2.93 | 1.66 | 1.38 | 1.14 | 1.43 | 0.28 |
| HisGly | 2.40 | 3.18 | 3.24 | 1.25 | 2.30 | 0.42 |
| GlyAsp | 2.81 | 0.25 | 0.28 | 1.20 | 1.35 | 0.27 |
| CysAsn | 2.97 | 0.01 | 0.09 | 1.55 | 2.53 | 0.37 |
| PheArg | 2.66 | 0.19 | 0.22 | 0.68 | 1.81 | 0.06 |
| LysAla | 3.22[c] | 1.16 | 0.99 | 1.53 | 0.02 | 0.20 |
| LeuTyr | 3.46 | 1.47 | 1.02 | 0.89 | 1.89 | 0.85 |
| TyrGly | 2.98[e] | 2.69 | 2.22 | 0.27 | 2.51 | 0.11 |
| LysGlu | 2.93 | 0.50 | 0.12 | 0.67 | 1.51 | 1.10 |
| TyrArg | 2.65 | 2.14 | 0.44 | 0.86 | 3.32 | 0.07 |
| HisLys | 2.50[f] | 0.94 | 0.73 | 1.53 | 0.32 | 0.28 |
| AspHis | - | - | - | - | - | - |
| GlyHis | - | - | - | - | - | - |
| GlyLys | 2.96[f] | 0.01 | 0.07 | 0.31 | 0.47 | 0.04 |
| AspGly | 2.10[c] | 0.87 | 0.86 | 0.80 | 1.34 | 0.42 |
| AlaGlyGly | 3.19[c] | 0.67 | 0.67 | 1.06 | 3.27 | 0.42 |
| GlyAlaAla | 3.38 | 0.82 | 1.59 | 0.35 | 2.96 | 0.30 |
| GlySerGly | 3.32 | 0.38 | 0.50 | 0.04 | 0.77 | 0.36 |
| GlyGlyGly | 3.23 | 0.88 | 1.05 | 1.71 | 0.71 | 0.39 |
| CysGlyGly | 3.13[c] | 0.65 | 0.90 | 1.79 | 1.81 | 0.47 |
| AlaLysAla | 3.15[c] | 1.03 | 0.16 | 2.32 | 2.45 | 0.52 |
| PheAlaArg | 2.60[c] | 1.06 | 0.87 | 1.81 | 0.02 | 0.83 |
| GlyHisLys | - | - | - | - | - | - |
| MAD | | 0.94 | 0.85 | 0.98 | 1.61 | 0.32 |
| SD | | 0.76 | 0.70 | 0.60 | 1.15 | 0.25 |

[a]Experimental values taken from Reference [32] unless otherwise noted. [b]Ref. [34], [c]Ref. [33], [d]Ref. [35], [e]Ref. [36], [f]Ref. [37]

**Table S2**. Absolute errors of p$K_{a2}$ of peptides calculated with the Isodesmic reaction compared to the experimental values. Alanine was used as reference species.

| | p$K_{a2}$ (exptl.) | $\Delta$p$K_{a2}$ (M052X) | $\Delta$p$K_{a2}$ (M062X) | $\Delta$p$K_{a2}$ (B3LYP) | $\Delta$p$K_{a2}$ (PM6) | $\Delta$p$K_{a2}$ (ChemOffice) |
|---|---|---|---|---|---|---|
| GlyGly | 8.25 | - | - | - | - | 0.71 |
| GlyVal | 8.18 | 1.83 | 2.02 | 2.34 | 2.18 | 0.61 |
| GlyPhe | 8.11[b] | 1.49 | 1.80 | 1.75 | 0.50 | 0.58 |
| GlyAla | 8.33 | 0.19 | 0.50 | 0.80 | 1.41 | 0.77 |
| AlaGly | 8.24[c] | 1.81 | 1.65 | 2.42 | 0.04 | 0.57 |
| AlaAla | 8.13 | 1.56 | 1.86 | 1.80 | 0.01 | 0.43 |
| AsnGly | 7.25[c] | 0.60 | 1.02 | 1.42 | 0.71 | 0.98 |
| ValGly | 8.00 | 1.73 | 1.37 | 2.49 | 0.03 | 0.31 |
| SerGly | 7.33[c] | 0.93 | 0.85 | 0.73 | 1.69 | 0.47 |
| SerLeu | 7.45 | 1.34 | 1.26 | 1.30 | 1.54 | 0.55 |
| AlaHis | 9.40[d] | 2.17 | 1.51 | 1.73 | 0.41 | 0.37 |
| GlyTyr | 8.45 | 0.65 | 0.89 | 1.45 | 0.74 | 0.91 |
| HisGly | 7.82 | 1.11 | 2.13 | 2.17 | 2.01 | 0.36 |
| GlyAsp | 8.60 | 1.33 | 1.22 | 0.23 | 1.56 | 1.04 |
| CysAsn | 8.47 | 1.16 | 1.38 | 1.95 | 0.84 | 1.25 |
| PheArg | 7.57 | 0.60 | 1.00 | 0.97 | 2.84 | 0.16 |
| LysAla | 8.47[c] | 1.97 | 2.17 | 2.08 | 0.02 | 1.18 |
| LeuTyr | 7.84 | 2.24 | 2.70 | 2.81 | 0.52 | 0.14 |
| TyrGly | 8.00[e] | 0.78 | 1.29 | 1.02 | 2.21 | 0.56 |
| LysGlu | 7.75 | 1.96 | 1.84 | 2.65 | 0.74 | 0.64 |
| TyrArg | 7.39 | 0.95 | 1.54 | 2.26 | 1.37 | 0.05 |
| HisLys | 7.41[f] | 1.30 | 1.25 | 2.07 | 1.30 | 0.07 |
| AspHis | 7.98[c] | 1.60 | 1.57 | 3.03 | 0.17 | 0.64 |
| GlyHis | 8.20 | 2.04 | 2.01 | 2.59 | 1.07 | 0.32 |
| GlyLys | 8.01[f] | 0.66 | 0.41 | 1.11 | 1.42 | 0.46 |
| AspGly | 9.07[c] | 0.48 | 0.46 | 1.05 | 1.62 | 1.43 |
| AlaGlyGly | 8.15[c] | 0.14 | 0.17 | 0.41 | 2.10 | 0.83 |
| GlyAlaAla | 8.10 | 1.48 | 1.55 | 1.78 | 1.11 | 0.89 |
| GlySerGly | 7.99 | 1.50 | 0.99 | 3.63 | 0.95 | 0.87 |
| GlyGlyGly | 8.09 | 1.80 | 2.30 | 2.80 | 0.31 | 0.9 |
| CysGlyGly | 6.95[c] | 1.55 | 1.84 | 2.21 | 1.13 | 0.04 |
| AlaLysAla | 7.65[c] | 2.60 | 2.70 | 2.24 | 2.64 | 0.32 |
| PheAlaArg | 7.54[c] | 2.34 | 1.40 | 2.83 | 0.65 | 0.46 |
| GlyHisLys | 8.06[g] | 1.71 | 1.53 | 2.53 | 0.07 | 0.85 |
| MAD | | 1.36 | 1.46 | 1.91 | 1.06 | 0.61 |
| SD | | 0.63 | 0.62 | 0.82 | 0.77 | 0.35 |

[a]Experimental values taken from Reference [32] unless otherwise noted. [b]Ref. [34], [c]Ref. [33], [d]Ref. [35], [e]Ref. [36], [f]Ref. [37], [g]Ref. [34]

**Table S3.** Mean absolute deviation (MAD) of p$K_{a1}$ and p$K_{a2}$ of amino acids calculated with the Isodesmic reaction as a function of the amino acid used as reference species.

| Reference | MAD p$K_{a1}$ | MAD p$K_{a2}$ |
|---|---|---|
| Alanine | 0.57 | 0.49 |
| Glycine | 0.84 | 1.40 |
| Valine | 0.66 | 0.76 |
| Iso-Leucine | 0.73 | 0.64 |
| Leucine | 0.58 | 0.47 |
| Methionine | 0.53 | 0.50 |
| Proline | 0.80 | 1.68 |
| Phenylalanine | 0.55 | 0.52 |
| Tryptophan | 0.52 | 1.27 |
| Serine | 0.62 | 1.52 |
| Threonine | 0.58 | 1.66 |
| Asparagine | 0.67 | 0.60 |
| Glutamine | 0.54 | 0.48 |
| Tyrosine | 0.55 | 0.48 |
| Lysine | 0.52 | 0.48 |
| Arginine | 0.79 | 0.70 |
| Cysteine | 0.94 | 0.47 |
| Histidine | 2.09 | 0.56 |
| Aspartic acid | 1.16 | 0.62 |
| Glutamic acid | 0.66 | 0.48 |
| Average | 0.74 | 0.79 |

**Table S4** Mean absolute deviation (MAD) of p$K_{a1}$ and p$K_{a2}$ of amino acids and peptides for as a function of their size or charge.

| p$K_{a1}$ | | | | | | |
|---|---|---|---|---|---|---|
| Reference | Amino acids | Dipeptides | Tripeptides | Charge 1+ | Charge 2+ | |
| Alanine | 0.57 | 1.10 | 0.72 | 0.76 | 1.10 | |
| GlyGly | 0.87 | 1.19 | 0.42 | 0.93 | 1.18 | |
| p$K_{a2}$ | | | | Charge 1+ | Charge 0 | Charge 1- |
| Alanine | 0.49 | 1.35 | 1.76 | 1.26 | 1.10 | 0.90 |
| GlyGly | 2.10 | 0.98 | 0.91 | 0.50 | 0.82 | 2.23 |

**Table S5**. Absolute errors of p$K_{a3}$ of peptides calculated with the Isodesmic reaction and PM6 by using the minimum energy conformer as an initial structure.

| | p$K_{a3}$ (exptl.) | $\Delta$p$K_{a3}$ |
|---|---|---|
| Lysine | | |
| Lys (ref.) | 10.53[a] | - |
| LysGlu | 10.50[a] | 0.44 |
| GlyLys | 10.50[b] | 0.89 |
| HisLys | 10.49[b] | 0.88 |
| LysAla | 10.70[a] | 1.90 |
| AlaLys | 10.70[b] | 1.60 |
| AlaLysAla | 10.30[c] | 0.12 |
| LysD-Ala | 10.63[b] | 3.74 |
| GlyHisLys | 10.71[d] | 2.86 |
| GlyGlyLysAla | 11.10[e] | 5.48 |
| **MAD** | | 1.99 |
| **SD** | | 1.75 |
| Arginine | | |
| Arg (ref.) | 12.47[a] | - |
| PheArg | 12.40[a] | 3.91 |
| TyrArg | 11.62[a] | 0.22 |
| PheAlaArg | 12.43[c] | 6.10 |
| **MAD** | | 3.41 |
| **SD** | | 2.97 |
| Histidine | | |
| His (ref.) | 6.00[a] | - |
| AlaHis | 6.72[f] | 1.45 |
| HisGly | 5.80[a] | 3.85 |
| HisLys | 5.91[b] | 3.26 |
| AspHis | 6.82[a] | 3.93 |
| GlyHis | 6.77[a] | 1.80 |
| GlyHisLys | 6.60[d] | 1.73 |
| GlyHisGly | 6.62[d] | 2.74 |
| GlyGlyHisAla | 7.00[e] | 1.74 |
| TyrHisOMe | 6.41[f] | 1.28 |
| GluHisOMe | 6.44[f] | 4.29 |
| **MAD** | | 2.61 |
| **SD** | | 1.15 |
| Cysteine | | |
| Cys (ref.) | 8.18[a] | - |
| CysAsn | 7.09[a] | 2.57 |
| CysGlyGly | 6.36[c] | 0.35 |
| **MAD** | | 1.46 |
| **SD** | | 1.57 |
| Tyrosine | | |
| Tyr (ref.) | 10.60[a] | - |
| GlyTyr | 10.49[a] | 0.74 |
| TyrArg | 9.36[a] | 2.20 |
| LeuTyr | 10.09[a] | 0.97 |
| TyrGly | 10.51[g] | 1.64 |
| GlyGlyTyrAla | 10.30[e] | 2.78 |
| D-LeuTyr | 10.35[a] | 0.85 |
| TyrHisOMe | 9.69[f] | 3.62 |
| **MAD** | | 1.83 |
| **SD** | | 1.09 |
| Glu/Asp | | |
| Glu (ref.) | 4.25[a] | - |
| Asp | 3.65[a] | 0.60 |
| LysGlu | 4.47[a] | 1.09 |
| GlyGlyGluAla | 4.30[e] | 0.50 |
| GlyAsp | 4.45[a] | 3.62 |
| GlyGlyAspAla | 3.90[e] | 1.25 |
| GluHisOMe | 3.79[f] | 3.08 |
| AspGly | 4.53[c] | 0.70 |
| **MAD** | | 1.55 |
| **SD** | | 1.27 |
| All | | |
| **MAD** | | **2.13** |
| **SD** | | **1.51** |

[a]Ref. [32], [b]Ref. [36], [c]Ref. [33], [d]Ref. [37], [e]Ref. [38], [f]Ref. [39], [g]Ref. [35]

**Table S6**. Absolute errors of p$K_{a1}$ and p$K_{a2}$ of peptides calculated with the Isodesmic reaction and PM6 by using the minimum energy conformer as an initial structure. GlycylGlycine was used as reference species.

| | p$K_{a1}$ (exptl.[a]) | $\Delta$p$K_{a1}$ | p$K_{a2}$ (exptl.) | $\Delta$p$K_{a2}$ |
|---|---|---|---|---|
| GlyGly | 3.13 | - | 8.25 | - |
| GlyVal | 3.18 | 0.28 | 8.18 | 1.09 |
| GlyPhe | 3.23 | 0.21 | 8.11 | 0.76 |
| GlyAla | 3.15 | 0.86 | 8.33 | 0.25 |
| AlaGly | 3.16[b] | 0.45 | 8.24[b] | 0.30 |
| AlaAla | 3.32 | 3.17 | 8.13 | 1.81 |
| AsnGly | 2.90[b] | 3.57 | 7.25[b] | 0.22 |
| ValGly | 3.23 | 1.72 | 8.00 | 0.26 |
| SerGly | 3.10[b] | 3.77 | 7.33[b] | 0.40 |
| SerLeu | 3.08 | 0.59 | 7.45 | 4.86 |
| AlaHis | 2.64[c] | 0.87 | 9.40[c] | 4.13 |
| GlyTyr | 2.93 | 1.07 | 8.45 | 0.24 |
| HisGly | 2.40 | 2.74 | 7.82 | 0.07 |
| GlyAsp | 2.81 | 5.07 | 8.60 | 1.31 |
| CysAsn | 2.97 | 1.91 | 8.47 | 1.65 |
| PheArg | 2.66 | 1.36 | 7.57 | 1.63 |
| LysAla | 3.22[b] | 1.28 | 8.47[b] | 1.11 |
| LeuTyr | 3.46 | 2.54 | 7.84 | 1.87 |
| TyrGly | 2.98[d] | 0.20 | 8.00[d] | 0.30 |
| LysGlu | 2.93 | 4.82 | 7.75 | 3.56 |
| TyrArg | 2.65 | 0.40 | 7.39 | 0.10 |
| HisLys | 2.50[e] | 4.08 | 7.41[e] | 0.09 |
| AspHis | - | - | 7.98[b] | 1.96 |
| GlyHis | - | - | 8.20 | 1.65 |
| GlyLys | 2.96[e] | 3.30 | 8.01[e] | 3.66 |
| AspGly | 2.10[b] | 4.84 | 9.07[b] | 0.87 |
| AlaGlyGly | 3.19[b] | 2.07 | 8.15[b] | 1.89 |
| GlyAlaAla | 3.38 | 4.62 | 8.10 | 1.98 |
| GlySerGly | 3.32 | 2.40 | 7.99 | 1.05 |
| GlyGlyGly | 3.23 | 2.50 | 8.09 | 0.47 |
| CysGlyGly | 3.13[b] | 0.45 | 6.95[b] | 4.67 |
| AlaLysAla | 3.15[b] | 6.41 | 7.65[b] | 3.17 |
| PheAlaArg | 2.60[b] | 4.53 | 7.54[b] | 5.13 |
| GlyHisLys | - | - | 8.06[f] | 1.12 |
| MAD | | 2.40 | 0.91 | 1.62 |
| SD | | 1.77 | 0.79 | 1.51 |

[a]Experimental values taken from Reference [32] unless otherwise noted. [b]Ref. [33], [c]Ref. [34], [d]Ref. [35], [e]Ref. [36]

```
###
# AMINO ACIDS optimized with b3lyp
# opt(tight) freq b3lyp/6-31+G(d,p) scf=(xqc,tight) integral=ultrafine scrf(smd,solvent=water)
###
14
Ala1 b3lyp E=-324.252303318 au
N       -1.452955       -1.020541       -0.157423
H       -1.453751       -1.282289       0.835416
H       -1.114203       -1.828252       -0.690763
H       -2.420657       -0.829776       -0.438034
C       -0.602828       0.192170        -0.393345
H       -0.638620       0.396033        -1.466769
C       -1.149712       1.380218        0.397292
C       0.827139        -0.169968       -0.026374
H       -1.108316       1.187240        1.473458
H       -0.559597       2.270042        0.171533
H       -2.186240       1.568294        0.104616
O       1.157818        -1.248503       0.439042
O       1.670651        0.833653        -0.279168
H       2.576727        0.566779        -0.031918
###
12
Ala3 b3lyp E=-323.335456930 au
N       -1.437323       -1.076304       -0.377963
H       -1.008539       -1.777161       -0.980947
H       -1.389736       -1.467947       0.562601
C       -0.615852       0.142083        -0.410085
H       -0.628682       0.522967        -1.436433
C       -1.227520       1.204393        0.512015
C       0.872310        -0.058479       -0.032194
H       -1.251504       0.846645        1.548697
H       -0.648015       2.131904        0.483794
H       -2.253928       1.430226        0.205449
O       1.187294        -1.037352       0.712879
O       1.696210        0.802292        -0.482359
###
13
AlaZW b3lyp E=-323.805164065 au
N       -1.343674       -1.071093       -0.192644
H       -0.954326       -1.840963       -0.743987
H       -1.306599       -1.355983       0.791406
C       -0.554937       0.195312        -0.400672
H       -0.619752       0.418748        -1.468005
C       -1.181107       1.318603        0.420787
C       0.923950        -0.061173       -0.039157
H       -1.140679       1.091085        1.491443
H       -0.634727       2.246547        0.241048
H       -2.225286       1.473636        0.131655
O       1.215159        -1.171049       0.492960
O       1.720366        0.882047        -0.308282
H       -2.324549       -0.939859       -0.458212
###
28
Arg1 b3lyp E=-607.567288944 au
N       3.508854        -1.539645       -0.317646
H       3.635271        -1.724659       0.684576
H       4.423476        -1.285653       -0.706997
H       3.199868        -2.406209       -0.771372
C       2.497036        -0.454183       -0.535902
H       2.469965        -0.251678       -1.608013
C       1.125535        -0.946791       -0.037720
C       3.000150        0.778523        0.203905
H       0.939471        -1.908474       -0.530875
H       1.188220        -1.134804       1.040630
C       -0.028167       0.012225        -0.348360
O       3.735044        0.724142        1.176384
H       0.113177        0.964149        0.173945
H       -0.054552       0.224282        -1.423613
C       -1.360553       -0.598095       0.083392
H       -1.538814       -1.532801       -0.459998
H       -1.342698       -0.823779       1.155988
N       -2.450528       0.343414        -0.199109
H       -2.205986       1.271396        -0.525824
C       -3.741549       0.110037        0.044507
N       -4.147392       -1.067607       0.529692
N       -4.651406       1.062803        -0.222940
```

```
H       -3.503190       -1.835924       0.650987
H       -5.134539       -1.245548       0.660111
H       -4.339438       2.006441        -0.413056
H       -5.603966       0.941718        0.095368
O       2.532381        1.909338        -0.327701
H       2.842935        2.670664        0.199760
###
27
Arg2 b3lyp E=-607.121641586 au
N       3.566898        -1.454769       -0.325266
H       3.750589        -1.533655       0.682040
H       4.451729        -1.210082       -0.780047
H       3.260416        -2.363388       -0.687592
C       2.528612        -0.388758       -0.556259
H       2.506998        -0.200747       -1.630735
C       1.172683        -0.922462       -0.069341
C       2.982681        0.884863        0.194922
H       0.991716        -1.882203       -0.569973
H       1.235881        -1.122328       1.007627
C       0.005649        0.026042        -0.361232
O       3.647870        0.707837        1.257385
H       0.147788        0.975262        0.166157
H       -0.031353       0.247889        -1.434527
C       -1.321172       -0.592518       0.074589
H       -1.498223       -1.526590       -0.470454
H       -1.298263       -0.821170       1.146518
N       -2.417977       0.344074        -0.200910
H       -2.177555       1.275241        -0.521602
C       -3.707045       0.104963        0.044521
N       -4.107749       -1.075818       0.526830
N       -4.621768       1.054936        -0.219540
H       -3.459922       -1.841817       0.643416
H       -5.094159       -1.259275       0.654859
H       -5.570584       0.932116        0.109181
O       2.626179        1.989423        -0.300449
H       -4.311734       2.000934        -0.401359
###
26
Arg3 b3lyp E=-606.653503685 au
N       3.653283        -1.466313       -0.449039
H       3.807932        -1.648974       0.542022
H       3.311313        -2.339019       -0.849920
C       2.589705        -0.451285       -0.564641
H       2.488145        -0.192118       -1.622641
C       1.220512        -0.954590       -0.056466
C       3.018838        0.823055        0.187602
H       1.009880        -1.898987       -0.576282
H       1.303993        -1.188947       1.013106
C       0.061166        0.019879        -0.294837
O       3.501414        0.681173        1.354528
H       0.221103        0.946396        0.269916
H       0.021686        0.290202        -1.357773
C       -1.278601       -0.586966       0.115751
H       -1.461734       -1.506851       -0.451245
H       -1.271877       -0.839565       1.182480
N       -2.363827       0.366812        -0.152669
H       -2.108962       1.301045        -0.452567
C       -3.661581       0.123085        0.030268
N       -4.080465       -1.065402       0.478277
N       -4.567318       1.075580        -0.261202
H       -3.435318       -1.831259       0.611048
H       -5.071137       -1.258750       0.543257
H       -4.248630       2.024953        -0.407876
H       -5.523123       0.953618        0.047452
O       2.844186        1.940634        -0.392604
###
25
Arg4 b3lyp E=-606.172121830 au
N       -3.609378       1.531172        0.007584
H       -3.657186       1.509041        1.025990
H       -3.315128       2.475372        -0.240192
C       -2.559786       0.587159        -0.422393
H       -2.541567       0.587810        -1.516092
C       -1.155717       0.969857        0.092539
C       -2.943234       -0.833098       0.035557
H       -0.941791       1.985377        -0.268077
```

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H       -1.188527       1.020131        1.189166
C       -0.032111       0.024092        -0.350207
O       -3.249234       -0.991358       1.258942
H       -0.184208       -0.968603       0.094280
H       -0.060232       -0.105347       -1.439782
C       1.343993        0.545549        0.059525
H       1.537798        1.488787        -0.460557
H       1.355756        0.756029        1.138990
N       2.387227        -0.430363       -0.291946
H       2.110460        -1.389437       -0.108981
C       3.717394        -0.237344       0.028966
N       4.137220        1.078220        0.090811
N       4.474118        -1.271215       0.265062
H       3.627466        1.756187        -0.462715
H       5.141024        1.207742        0.060962
H       5.441814        -0.971416       0.385719
O       -2.909919       -1.764100       -0.829344
###
18
Asn1 b3lyp E=-492.977702442 au
N       -1.726531       -1.652413       0.009532
H       -2.584116       -1.492593       0.550193
H       -1.356995       -2.577907       0.252957
H       -1.985942       -1.661379       -0.984077
C       -0.706149       -0.597852       0.298177
H       -0.472794       -0.664984       1.364167
C       0.559405        -0.852453       -0.531226
C       -1.354137       0.753747        0.031389
H       0.767513        -1.929175       -0.514139
H       0.406003        -0.562752       -1.574133
C       1.792577        -0.181788       0.062399
O       -2.512341       0.888141        -0.324956
O       1.980699        -0.141192       1.292154
N       2.676344        0.302156        -0.823715
H       3.547942        0.697822        -0.492165
H       2.501637        0.267370        -1.819160
O       -0.502620       1.757610        0.243190
H       -0.948021       2.608995        0.068107
###
16
Asn3 b3lyp E=-492.065243637 au
N       -1.859223       1.640078        0.010031
H       -2.667588       1.456867        -0.583151
H       -2.168954       1.429933        0.958986
C       -0.799626       0.686646        -0.346613
H       -0.546250       0.843322        -1.397779
C       0.449990        0.990642        0.509603
C       -1.196264       -0.801592       -0.174764
H       0.674622        2.057818        0.412549
H       0.231825        0.784077        1.562495
C       1.687550        0.240176        0.055157
O       -1.930925       -1.111100       0.813082
O       2.196088        0.445201        -1.067947
N       2.222608        -0.634890       0.925402
H       3.045009        -1.164865       0.663743
H       1.793833        -0.810642       1.823619
O       -0.734674       -1.625107       -1.026233
###
17
AsnZW b3lyp E=-492.532462115 au
N       1.769420        1.575284        -0.107468
H       2.675154        1.258290        0.257766
H       1.544064        2.499470        0.272128
H       1.870850        1.662067        -1.124285
C       0.721558        0.559926        0.251906
H       0.523133        0.698373        1.317910
C       -0.552909       0.826580        -0.551233
C       1.313358        -0.857746       0.062659
H       -0.751749       1.906001        -0.557489
H       -0.427859       0.507018        -1.589658
C       -1.780939       0.189253        0.079909
O       2.568229        -0.942139       -0.072744
O       -1.993094       0.262200        1.306516
N       -2.650465       -0.387435       -0.765954
H       -3.507066       -0.789135       -0.404773
H       -2.451881       -0.465760       -1.754023
```

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O       0.485647        -1.807479       0.095845
###
17
Asp1 b3lyp E=-512.836601727 au
N       1.727720        1.644025        0.071454
H       2.573171        1.453484        0.621636
H       1.370031        2.568347        0.337318
H       2.003668        1.677614        -0.917394
C       0.687592        0.597455        0.314396
H       0.434457        0.646184        1.376188
C       -0.547050       0.885931        -0.554842
C       1.323502        -0.758352       0.032735
H       -0.785816       1.953628        -0.467781
H       -0.344253       0.672071        -1.606082
C       -1.806158       0.151579        -0.152378
O       2.491347        -0.901770       -0.283695
O       -1.993095       0.097533        1.176054
O       -2.609969       -0.294053       -0.956858
O       0.445275        -1.749385       0.183725
H       0.878238        -2.605877       0.001670
H       -2.839310       -0.351902       1.360996
###
16
Asp2 b3lyp E=-512.392810622 au
N       1.817075        1.540818        -0.026325
H       2.708366        1.116428        0.262271
H       1.682419        2.436343        0.452073
H       1.881533        1.719570        -1.034560
C       0.718929        0.565398        0.288356
H       0.532858        0.658388        1.361155
C       -0.534965       0.928138        -0.510863
C       1.240807        -0.869716       0.026253
H       -0.772571       1.988298        -0.351369
H       -0.368758       0.774612        -1.579512
C       -1.772790       0.160992        -0.117510
O       2.494893        -1.015242       -0.043517
O       -1.964450       0.101131        1.214221
O       -2.577112       -0.297172       -0.917307
O       0.359500        -1.765535       -0.057720
H       -2.797911       -0.373693       1.391382
###
15
Asp3 b3lyp E=-511.937248848 au
N       1.650179        1.624847        -0.021635
H       2.568612        1.323798        0.324762
H       1.382516        2.512181        0.413115
H       1.745353        1.777324        -1.031050
C       0.642750        0.544256        0.269817
H       0.424898        0.618509        1.338413
C       -0.629550       0.792746        -0.538761
C       1.316279        -0.826446       0.021518
H       -0.853551       1.867857        -0.515187
H       -0.478765       0.513828        -1.585071
C       -1.884084       0.093762        0.013167
O       2.578704        -0.832016       -0.087832
O       -2.029271       0.031484        1.272041
O       -2.727534       -0.323334       -0.839683
O       0.551515        -1.827801       -0.018025
###
14
Asp4 b3lyp E=-511.466984769 au
N       -1.770800       1.675380        -0.095257
H       -2.583236       1.465689        -0.674356
H       -2.085624       1.539655        0.865455
C       -0.727745       0.676624        -0.378697
H       -0.455881       0.768868        -1.433269
C       0.516034        0.990381        0.479284
C       -1.174150       -0.786683       -0.139210
H       0.779925        2.039830        0.306785
H       0.263385        0.871589        1.537945
C       1.745615        0.136778        0.141751
O       -1.955809       -1.022650       0.834265
O       2.266650        0.286853        -1.009871
O       2.189415        -0.656476       1.032430
O       -0.710442       -1.672214       -0.926139
###
```

```
15
Cys1 b3lyp E=-722.433244805 au
N       -1.366173       1.719414        -0.287649
H       -2.208879       1.577051        -0.856708
H       -0.932243       2.603104        -0.578364
H       -1.658331       1.808100        0.693591
C       -0.396492       0.584121        -0.460323
H       -0.187207       0.502712        -1.527176
C       0.876498        0.923652        0.335469
C       -1.090578       -0.678895       0.042555
H       1.219415        1.916296        0.035774
H       0.650323        0.948989        1.405106
S       2.251263        -0.272419       0.139065
O       -1.815235       -0.687457       1.023421
H       2.522172        0.008295        -1.153685
O       -0.805042       -1.747328       -0.700618
H       -1.236605       -2.536713       -0.318679
###
14
Cys2 b3lyp E=-721.986475273 au
N       -1.505287       1.583593        -0.257849
H       -1.891264       1.483321        0.688989
H       -2.279845       1.456698        -0.916932
H       -1.134343       2.531589        -0.377809
C       -0.450299       0.532370        -0.475346
H       -0.239540       0.512319        -1.545129
C       0.791955        0.953320        0.319377
C       -1.032863       -0.829915       -0.019374
H       1.107038        1.944552        -0.014988
H       0.555895        0.994550        1.386055
S       2.199167        -0.213795       0.041250
O       -1.909772       -0.791220       0.891454
H       3.142036        0.633629        0.502506
O       -0.560527       -1.853247       -0.582165
###
13
Cys3 b3lyp E=-721.513436184 au
N       -1.382271       1.644379        -0.254123
H       -1.685929       1.630099        0.726199
H       -2.212941       1.526239        -0.842304
H       -0.969179       2.559333        -0.458911
C       -0.376140       0.530197        -0.480170
H       -0.202074       0.486412        -1.555399
C       0.908341        0.898721        0.273207
C       -1.047285       -0.773031       0.012649
H       1.208016        1.895367        -0.074105
H       0.661308        0.987852        1.338094
S       2.301991        -0.286698       0.036088
O       -1.581266       -0.720097       1.162150
O       -1.026816       -1.772917       -0.757929
###
12
Cys4 b3lyp E=-721.041933997 au
N       -1.401918       1.720404        -0.267069
H       -1.585329       1.810832        0.732291
H       -0.961680       2.595994        -0.548907
C       -0.418914       0.625576        -0.456576
H       -0.230063       0.537039        -1.529890
C       0.915865        0.893935        0.260734
C       -1.085201       -0.680490       0.013814
H       1.274726        1.870429        -0.090012
H       0.708758        0.998068        1.333614
S       2.239696        -0.378625       -0.006518
O       -1.424018       -0.754336       1.238563
O       -1.288310       -1.599578       -0.842458
###
21
Gln1 b3lyp E=-532.297465068 au
N       -2.096486       1.716227        -0.448324
H       -2.254571       1.934505        0.542810
H       -3.013924       1.606376        -0.894301
H       -1.624778       2.516018        -0.884540
C       -1.263488       0.476796        -0.593556
H       -1.216982       0.244323        -1.658989
C       0.143403        0.757059        -0.032859
C       -1.995592       -0.638343       0.140135
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H       0.505272        1.662865        -0.532145
H       0.065827        0.973312        1.036959
C       1.135443        -0.384748       -0.280811
O       -2.791298       -0.438349       1.043491
H       0.846400        -1.277819       0.285216
H       1.148436        -0.659785       -1.339423
C       2.534077        -0.019317       0.183958
O       2.733413        0.593223        1.253424
N       3.546701        -0.419506       -0.605268
H       4.503145        -0.248138       -0.320053
H       3.376604        -0.909552       -1.472957
O       -1.654913       -1.846895       -0.310423
H       -2.107596       -2.531663       0.219421
###
19
Gln3 b3lyp E=-531.382727233 au
N       -2.225714       1.729351        -0.357334
H       -2.319288       1.867189        0.648619
H       -1.755753       2.559942        -0.715861
C       -1.352202       0.562071        -0.578917
H       -1.307258       0.377515        -1.656014
C       0.082319        0.784870        -0.053640
C       -1.991571       -0.673842       0.083987
H       0.473097        1.692240        -0.531910
H       0.036739        0.978023        1.024064
C       1.039548        -0.386124       -0.334962
O       -2.358092       -0.561202       1.295102
H       0.694455        -1.288490       0.184615
H       1.059070        -0.611370       -1.405867
C       2.440387        -0.106685       0.170971
O       2.658075        0.202121        1.363246
N       3.442200        -0.214464       -0.721571
H       4.397508        -0.053336       -0.426558
H       3.265558        -0.461469       -1.685545
O       -2.096284       -1.734193       -0.609328
###
20
GlnZW b3lyp E=-531.851249126 au
N       -2.170031       1.628981        -0.459584
H       -2.404072       1.736066        0.535121
H       -3.051231       1.525799        -0.972280
H       -1.701098       2.476951        -0.793426
C       -1.301667       0.408950        -0.624984
H       -1.275419       0.182574        -1.691734
C       0.103358        0.748548        -0.104241
C       -1.971027       -0.754803       0.144115
H       0.461017        1.627625        -0.653974
H       0.035538        1.024766        0.953151
C       1.103987        -0.399704       -0.282649
O       -2.650106       -0.442544       1.165758
H       0.803221        -1.264350       0.320707
H       1.132704        -0.727663       -1.325820
C       2.495225        -0.013726       0.184568
O       2.684290        0.601152        1.255388
N       3.517631        -0.394581       -0.602396
H       4.469954        -0.204609       -0.315266
H       3.359078        -0.889087       -1.469640
O       -1.764452       -1.916666       -0.302875
###
20
Glu1 b3lyp E=-552.155370570 au
N       -2.017941       1.812075        0.056700
H       -2.948877       1.850511        -0.373016
H       -1.528433       2.686248        -0.163098
H       -2.146482       1.757709        1.074285
C       -1.235334       0.636611        -0.447509
H       -1.228631       0.696627        -1.537281
C       0.196606        0.722770        0.113344
C       -1.980504       -0.616362       -0.006512
H       0.571458        1.723532        -0.126921
H       0.158968        0.628682        1.204093
C       1.145008        -0.331871       -0.490358
O       -2.734794       -0.644302       0.951791
H       0.844318        -1.340129       -0.189221
H       1.132193        -0.273327       -1.580505
C       2.569672        -0.100704       -0.040202
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O       2.880829        -0.441381       1.231559
O       3.445647        0.377280        -0.745463
O       -1.698868       -1.665680       -0.779677
H       -2.163757       -2.455601       -0.441005
H       2.119640        -0.828774       1.697523
###
19
Glu2 b3lyp E=-551.709857068 au
N       -2.091050       1.736135        0.092622
H       -2.275830       1.560044        1.087721
H       -2.997439       1.800791        -0.381406
H       -1.609786       2.635350        -0.009275
C       -1.273811       0.601252        -0.464991
H       -1.279947       0.711933        -1.550013
C       0.154697        0.727161        0.086203
C       -1.959241       -0.727111       -0.063623
H       0.533712        1.720021        -0.181967
H       0.125055        0.664537        1.180031
C       1.102346        -0.348192       -0.482118
O       -2.556295       -0.741472       1.051772
H       0.799392        -1.342979       -0.140189
H       1.083298        -0.333035       -1.573831
C       2.528034        -0.098134       -0.050011
O       2.855513        -0.414116       1.224907
O       3.393810        0.379642        -0.769234
O       -1.837470       -1.686229       -0.874364
H       2.102286        -0.802070       1.703170
###
18
Glu3 b3lyp E=-551.254629184 au
N       -2.071754       1.693904        -0.303828
H       -2.288239       1.731530        0.699536
H       -2.963297       1.653335        -0.807429
H       -1.584886       2.552269        -0.579644
C       -1.235954       0.470609        -0.578749
H       -1.214811       0.341808        -1.661916
C       0.177722        0.721104        -0.031140
C       -1.939222       -0.737780       0.081521
H       0.547055        1.650161        -0.484002
H       0.117762        0.884170        1.050481
C       1.160780        -0.415951       -0.342743
O       -2.592038       -0.503696       1.141133
H       0.853854        -1.328553       0.181764
H       1.158436        -0.632618       -1.414644
C       2.592329        -0.088188       0.103613
O       2.772020        0.250734        1.316505
O       3.521293        -0.190240       -0.760123
O       -1.783466       -1.857822       -0.479060
###
17
Glu4 b3lyp E=-550.784308367 au
N       -2.142615       1.775077        -0.182060
H       -2.216728       1.829986        0.833435
H       -1.659335       2.623782        -0.474422
C       -1.288792       0.616603        -0.513462
H       -1.256826       0.529060        -1.603249
C       0.154371        0.765798        0.010688
C       -1.951511       -0.660666       0.039093
H       0.551213        1.709070        -0.388530
H       0.125098        0.865026        1.102304
C       1.091995        -0.388269       -0.387783
O       -2.268098       -0.667199       1.270138
H       0.747335        -1.320931       0.076444
H       1.070971        -0.528829       -1.472985
C       2.536916        -0.147889       0.062585
O       2.756826        -0.048166       1.312996
O       3.439503        -0.057017       -0.831662
O       -2.130892       -1.633388       -0.759635
###
11
Gly1 b3lyp E=-284.932558978 au
N       1.847942        0.081368        0.000003
H       1.877311        0.686261        -0.828054
C       0.629980        -0.770744       -0.000001
H       2.689925        -0.503962       -0.000032
H       1.877344        0.686206        0.828099
```

```
C       -0.602919       0.099674        0.000000
H       0.644850        -1.405218       -0.887941
H       0.644849        -1.405227       0.887933
O       -0.575375       1.318896        -0.000016
O       -1.716697       -0.637868       0.000012
H       -2.495664       -0.049442       0.000008
###
Gly3 b3lyp E=-284.017801773 au
###
10
GlyZW b3lyp E=-284.485826830 au
N       -1.787000       0.081308        0.020240
C       -0.567125       -0.782314       -0.028871
C       0.714607        0.058442        -0.001554
O       1.791834        -0.602751       0.021627
O       0.591926        1.316171        -0.013458
H       -1.826419       0.604755        0.899984
H       -0.612008       -1.369162       -0.947690
H       -0.599218       -1.459668       0.825279
H       -1.767772       0.769834        -0.738185
H       -2.640553       -0.479044       -0.063871
###
22
His1 b3lyp E=-549.753163905 au
N       2.576102        -1.481287       -0.003998
H       3.340061        -1.288960       -0.661799
H       2.326529        -2.473473       -0.083363
H       2.934653        -1.313669       0.943691
C       1.384245        -0.623765       -0.293498
H       1.067931        -0.849377       -1.313610
C       0.256421        -0.973582       0.710608
C       1.833365        0.828524        -0.217557
H       0.228133        -2.063959       0.797094
H       0.504830        -0.572047       1.697989
C       -1.101088       -0.506257       0.294134
O       2.904534        1.178763        0.247544
N       -1.763222       0.548506        0.904939
C       -1.957469       -0.980845       -0.661312
H       -1.391640       1.119052        1.659054
C       -2.965061       0.719235        0.352477
N       -3.095848       -0.201993       -0.603178
H       -1.854284       -1.794673       -1.360958
H       -3.695996       1.461819        0.630197
O       0.910853        1.655301        -0.709934
H       1.216659        2.578625        -0.618990
H       -3.921663       -0.312284       -1.183639
###
21
His2 b3lyp E=-549.313934765 au
N       -2.448772       1.550848        -0.253264
H       -3.306084       1.084788        -0.579758
H       -2.257335       2.381822        -0.820431
H       -2.618001       1.853084        0.712417
C       -1.322859       0.558705        -0.323378
H       -0.997094       0.546953        -1.367377
C       -0.177286       1.039199        0.590897
C       -1.910160       -0.845569       -0.006839
H       -0.112676       2.129318        0.531184
H       -0.418249       0.785332        1.630348
C       1.172387        0.504324        0.232787
O       -3.163397       -0.957447       -0.059443
N       1.419334        -0.846948       0.060495
C       2.371519        1.138042        0.054666
H       0.634369        -1.524862       0.101643
C       2.706128        -1.041988       -0.219066
N       3.303566        0.153328        -0.219285
H       2.637969        2.181553        0.101923
H       3.183406        -1.989584       -0.413932
O       -1.085836       -1.775970       0.236742
H       4.290290        0.302048        -0.404421
###
20
His3 b3lyp E=-548.851629277 au
N       -2.702579       -1.253178       -0.011575
H       -3.053024       -0.813922       -0.872431
H       -3.417110       -1.124819       0.711253
```

```
H       -2.579173       -2.258737       -0.167200
C       -1.410436       -0.585840       0.378620
H       -1.210787       -0.859102       1.415080
C       -0.300024       -1.124424       -0.550284
C       -1.610431       0.942099        0.259589
H       -0.274061       -2.213293       -0.427163
H       -0.579596       -0.916210       -1.588396
C       1.060745        -0.554947       -0.283311
O       -2.416585       1.339622        -0.632417
N       1.625616        0.420887        -1.091700
C       1.932071        -0.878366       0.731536
C       2.813005        0.676511        -0.562389
N       3.039983        -0.081919       0.540306
H       1.865218        -1.582230       1.547332
H       3.536171        1.385476        -0.938402
O       -0.935651       1.661064        1.046380
H       3.879532        -0.073381       1.106436
###
19
His4 b3lyp E=-548.382510258 au
N       2.683659        -1.263477       -0.609307
H       2.497015        -2.096070       -1.167081
H       2.879733        -1.597649       0.334245
C       1.452120        -0.447254       -0.563821
H       1.243215        -0.119295       -1.585358
C       0.244445        -1.236356       -0.023313
C       1.759739        0.806562        0.284345
H       0.162746        -2.158837       -0.615922
H       0.464184        -1.550750       1.004256
C       -1.073125       -0.515053       -0.044624
O       1.997183        0.625225        1.519589
N       -2.161214       -0.996166       0.674647
C       -1.443943       0.620180        -0.729312
C       -3.157921       -0.160920       0.421805
N       -2.773868       0.830665        -0.420046
H       -0.904708       1.282589        -1.387815
H       -4.160022       -0.228967       0.819919
O       1.783352        1.934646        -0.299122
H       -3.354376       1.589896        -0.753518
###
23
Ile1 b3lyp E=-442.199166753 au
N       1.345115        -1.668215       -0.710078
H       1.578439        -1.985601       0.237434
H       2.227172        -1.573906       -1.225430
H       0.784684        -2.396211       -1.165836
C       0.588387        -0.369686       -0.686607
H       0.469072        -0.066181       -1.728701
C       -0.815594       -0.570280       -0.046226
C       1.481380        0.642259        0.016974
H       -1.206283       -1.476133       -0.530790
C       -0.753682       -0.814813       1.469457
C       -1.763667       0.587649        -0.424626
O       2.439681        0.331018        0.706524
H       -0.430327       0.085091        2.005346
H       -1.742551       -1.088951       1.845449
H       -0.075614       -1.633041       1.735140
H       -1.646430       0.803078        -1.493834
H       -1.469402       1.494796        0.115181
C       -3.238373       0.280770        -0.141160
H       -3.432584       0.138832        0.926843
H       -3.869451       1.108325        -0.482562
H       -3.562494       -0.625613       -0.666418
O       1.096416        1.899947        -0.207909
H       1.680482        2.509911        0.282928
###
22
Ile2 b3lyp E=-441.751675120 au
N       1.419647        -1.549627       -0.774484
H       1.872006        -1.699963       0.135610
H       2.166426        -1.474623       -1.471374
H       0.838795        -2.359501       -1.011577
C       0.614925        -0.273407       -0.716694
H       0.489479        0.053986        -1.749852
C       -0.778573       -0.558362       -0.098159
C       1.458988        0.773038        0.049850
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H       -1.157278       -1.440501       -0.635764
C       -0.708442       -0.901111       1.398446
C       -1.756137       0.597507        -0.395722
O       2.360063        0.329919        0.822049
H       -0.406837       -0.029557       1.990700
H       -1.686653       -1.229421       1.760537
H       -0.001662       -1.712250       1.605456
H       -1.661475       0.871765        -1.453892
H       -1.464468       1.481092        0.183799
C       -3.221614       0.254785        -0.104302
H       -3.397450       0.062615        0.959161
H       -3.873038       1.085031        -0.398617
H       -3.540500       -0.633679       -0.662998
O       1.168717        1.984793        -0.150840
###
21
Ile3 b3lyp E=-441.280908754 au
N       1.463289        -1.518559       -0.976080
H       1.773286        -1.862497       -0.069062
H       0.856579        -2.238873       -1.366144
C       0.670513        -0.293500       -0.767108
H       0.521383        0.172297        -1.746404
C       -0.754600       -0.557794       -0.180163
C       1.478786        0.704883        0.085801
H       -1.173202       -1.339593       -0.833652
C       -0.727943       -1.112999       1.251648
C       -1.675701       0.672293        -0.308799
O       2.235995        0.241869        0.994787
H       -0.421472       -0.344795       1.971637
H       -1.718147       -1.471070       1.550534
H       -0.037425       -1.957985       1.346503
H       -1.571026       1.083206        -1.321683
H       -1.337651       1.457629        0.379297
C       -3.157992       0.376399        -0.047903
H       -3.339135       0.064807        0.986373
H       -3.770180       1.266445        -0.233099
H       -3.525221       -0.421242       -0.705783
O       1.326606        1.943867        -0.160639
###
23
Leu1 b3lyp E=-442.200966706 au
N       1.665507        1.716762        0.456668
H       1.933504        1.933481        -0.510804
H       2.525990        1.567022        0.995005
H       1.181754        2.532154        0.848060
C       0.768641        0.512950        0.500353
H       0.598701        0.285591        1.553046
C       -0.546346       0.858646        -0.227478
C       1.529307        -0.630414       -0.154779
H       -0.931591       1.773167        0.241496
H       -0.300440       1.102549        -1.268279
C       -1.650746       -0.215886       -0.197396
O       2.388175        -0.465181       -1.006675
H       -1.255920       -1.134770       -0.649045
C       -2.121187       -0.538334       1.228179
C       -2.827051       0.259557        -1.063073
H       -2.499875       0.363286        1.726185
H       -2.933015       -1.273657       1.204159
H       -1.320453       -0.954975       1.847876
H       -2.511884       0.456610        -2.094008
H       -3.617174       -0.498595       -1.090792
H       -3.262923       1.182879        -0.661060
O       1.137014        -1.822837       0.297399
H       1.617551        -2.527045       -0.179148
###
21
Leu3 b3lyp E=-441.284355411 au
N       -1.709448       1.700182        -0.664660
H       -2.597753       1.428074        -1.084094
H       -1.936302       2.005869        0.281724
C       -0.844380       0.507459        -0.569536
H       -0.675861       0.150226        -1.588531
C       0.497092        0.912090        0.066118
C       -1.496534       -0.650078       0.222808
H       0.909554        1.742110        -0.523569
H       0.286358        1.310737        1.068264
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C       1.564475        -0.194015       0.181679
O       -1.976098       -0.386647       1.371030
H       1.123465        -1.046423       0.718357
C       2.039529        -0.691768       -1.192188
C       2.755168        0.309122        1.011297
H       2.477967        0.131131        -1.771940
H       2.806920        -1.467061       -1.082305
H       1.222134        -1.119210       -1.781785
H       2.439659        0.627715        2.011742
H       3.512214        -0.474694       1.131592
H       3.238736        1.166022        0.524189
O       -1.515534       -1.802431       -0.317541
###
22
LeuZW b3lyp E=-441.753760538 au
N       1.737865        1.615167        0.496742
H       2.091145        1.730670        -0.460521
H       2.547739        1.457747        1.103777
H       1.272720        2.477878        0.795512
C       0.796393        0.438265        0.531011
H       0.624695        0.212165        1.583420
C       -0.504561       0.853713        -0.177541
C       1.507563        -0.749469       -0.156507
H       -0.880083       1.757544        0.322125
H       -0.254016       1.134667        -1.208580
C       -1.629835       -0.198881       -0.200062
O       2.325203        -0.462098       -1.080343
H       -1.241915       -1.106682       -0.679663
C       -2.118989       -0.568342       1.208215
C       -2.792465       0.322934        -1.057329
H       -2.492568       0.318827        1.735655
H       -2.938891       -1.293319       1.151793
H       -1.327561       -1.015466       1.818262
H       -2.466103       0.551513        -2.078429
H       -3.595239       -0.420263       -1.119110
H       -3.217822       1.238980        -0.627626
O       1.195324        -1.905371       0.242776
###
26
Lys1 b3lyp E=-498.028665004 au
N       2.674510        -1.651154       -0.164260
H       2.808386        -1.743424       0.849609
H       3.592691        -1.479591       -0.588590
H       2.319661        -2.543989       -0.524879
C       1.706073        -0.548839       -0.481276
H       1.659310        -0.467837       -1.568293
C       0.326496        -0.913058       0.098392
C       2.277028        0.734443        0.103254
H       0.074456        -1.904763       -0.296367
H       0.414133        -1.003420       1.187750
C       -0.787981       0.073631        -0.269379
O       2.981916        0.764759        1.099138
H       -0.602935       1.046446        0.199932
H       -0.791542       0.234834        -1.354437
C       -2.159404       -0.452792       0.172788
H       -2.362919       -1.411580       -0.321082
H       -2.157055       -0.636156       1.254840
C       -3.267041       0.534700        -0.168995
H       -3.149702       1.480179        0.363139
H       -3.317434       0.734651        -1.240789
N       -4.611759       -0.013668       0.225591
H       -4.649692       -0.211242       1.230925
H       -5.360181       0.650764        0.005779
H       -4.811201       -0.887840       -0.271210
O       1.903189        1.811729        -0.590558
H       2.242906        2.616306        -0.152992
###
25
Lys2 b3lyp E=-497.582784670 au
N       2.762379        -1.545968       -0.100785
H       2.976951        -1.426369       0.897200
H       3.639574        -1.436256       -0.618920
H       2.409337        -2.494627       -0.259992
C       1.755852        -0.499573       -0.505165
H       1.754785        -0.465662       -1.595363
C       0.378941        -0.922347       0.029691
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C       2.233570        0.855611        0.065921
H       0.152294        -1.913458       -0.384127
H       0.442060        -1.030219       1.120097
C       -0.751045       0.049043        -0.330002
O       2.843054        0.817379        1.175506
H       -0.567099       1.023466        0.136273
H       -0.766403       0.211787        -1.415024
C       -2.116470       -0.479320       0.128006
H       -2.334326       -1.432979       -0.369792
H       -2.094667       -0.671700       1.208547
C       -3.225279       0.517508        -0.180605
H       -3.072249       1.467302        0.334688
H       -3.318509       0.706661        -1.251532
N       -4.559200       -0.007082       0.277425
H       -4.553101       -0.197757       1.284790
H       -5.306891       0.667095        0.087325
H       -4.792861       -0.881115       -0.204421
O       1.951376        1.885077        -0.607170
###
23
Lys3 b3lyp E=-496.644981775 au
N       -2.732084       1.645931        -0.115653
H       -3.660544       1.370873        -0.433929
H       -2.793908       1.694155        0.901271
C       -1.769332       0.584825        -0.469716
H       -1.759135       0.502185        -1.560774
C       -0.367747       0.993984        0.009710
C       -2.164341       -0.802346       0.089326
H       -0.134368       1.964824        -0.445717
H       -0.403529       1.153788        1.096607
C       0.747843        -0.004706       -0.324203
O       -2.416290       -0.892218       1.332980
H       0.547811        -0.965664       0.168336
H       0.748218        -0.202667       -1.405312
C       2.133528        0.497476        0.100289
H       2.345880        1.455285        -0.393724
H       2.131467        0.695739        1.182258
C       3.254231        -0.489484       -0.219064
H       3.013180        -1.464258       0.233066
H       3.306869        -0.648541       -1.302034
N       4.565291        0.023725        0.225710
H       4.564200        0.086104        1.243229
H       5.286069        -0.656390       -0.008927
O       -2.212429       -1.776722       -0.728330
###
24
LysZW b3lyp E=-497.114042997 au
N       -2.867886       1.566371        -0.130439
H       -2.936795       1.612615        0.885918
H       -2.549991       2.487160        -0.431589
C       -1.825893       0.577745        -0.473006
H       -1.786784       0.502858        -1.563513
C       -0.425883       0.971101        0.042603
C       -2.248134       -0.800677       0.071774
H       -0.186894       1.957059        -0.379235
H       -0.476715       1.094070        1.132974
C       0.690035        -0.018871       -0.315787
O       -2.546777       -0.875852       1.305152
H       0.492844        -0.988470       0.159398
H       0.692073        -0.194134       -1.399947
C       2.074581        0.478297        0.119433
H       2.306173        1.424257        -0.387253
H       2.073521        0.678394        1.198976
C       3.158278        -0.542725       -0.198769
H       2.996622        -1.484622       0.328395
H       3.228222        -0.743937       -1.269299
N       4.511521        -0.041025       0.229589
H       4.527366        0.160203        1.234720
H       5.242221        -0.731856       0.033634
H       4.753984        0.823283        -0.265283
O       -2.255623       -1.782088       -0.736331
###
21
Met1 b3lyp E=-801.070782752 au
N       -2.394327       -1.632402       0.275866
H       -2.552810       -1.777663       -0.728363
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H       -3.304717       -1.450718       0.712755
H       -2.018044       -2.500542       0.672986
C       -1.436903       -0.503290       0.513754
H       -1.345327       -0.383671       1.595101
C       -0.075573       -0.872843       -0.109428
C       -2.061581       0.748061        -0.085478
H       0.175401        -1.870603       0.268444
H       -0.190098       -0.947049       -1.196472
C       1.045470        0.103077        0.251799
O       -2.910506       0.721885        -0.961726
H       0.886622        1.080070        -0.210780
H       1.103845        0.235333        1.336708
S       2.651415        -0.567195       -0.346655
C       3.753093        0.795116        0.170162
H       3.722570        0.932364        1.254454
H       4.768369        0.517134        -0.123343
H       3.481641        1.728561        -0.330005
O       -1.562511       1.862808        0.450722
H       -1.952695       2.640444        0.007106
###
19
Met3 b3lyp E=-800.156354440 au
N       2.584193        -1.550311       -0.321039
H       2.743161        -1.627634       0.682923
H       2.216842        -2.451997       -0.623052
C       1.551524        -0.523253       -0.541959
H       1.447088        -0.377592       -1.620956
C       0.172225        -0.931348       0.031633
C       2.014582        0.812687        0.070032
H       -0.081560       -1.907512       -0.401369
H       0.270694        -1.071897       1.115503
C       -0.944636       0.068788        -0.272194
O       2.529188        0.779141        1.231159
H       -0.757620       1.029773        0.216006
H       -1.022568       0.241917        -1.350923
S       -2.566489       -0.565456       0.327523
C       -3.639494       0.831711        -0.159779
H       -3.615378       0.983923        -1.242481
H       -4.660032       0.579390        0.139135
H       -3.337790       1.751722        0.348468
O       1.826615        1.870592        -0.609003
###
20
MetZW b3lyp E=-800.624649758 au
N       2.494451        -1.523989       -0.240723
H       2.729620        -1.481833       0.758611
H       3.361130        -1.373138       -0.766566
H       2.140122        -2.458911       -0.466625
C       1.482544        -0.452665       -0.548568
H       1.434283        -0.364491       -1.634536
C       0.126647        -0.897436       0.025056
C       1.992184        0.869790        0.071319
H       -0.113031       -1.875824       -0.409652
H       0.227502        -1.031284       1.108717
C       -0.999945       0.089730        -0.282133
O       2.646417        0.770768        1.150378
H       -0.826558       1.050354        0.209547
H       -1.079259       0.261050        -1.360377
S       -2.601578       -0.585333       0.323903
C       -3.700001       0.802025        -0.129941
H       -3.689465       0.971294        -1.210113
H       -4.712512       0.527079        0.175857
H       -3.407858       1.717693        0.391297
O       1.690026        1.932057        -0.538871
###
24
Phe1 b3lyp E=-555.315735794 au
N       2.941577        -1.290218       0.161162
H       3.298443        -0.874949       1.030332
H       3.664145        -1.175620       -0.558253
H       2.803762        -2.295175       0.315277
C       1.651888        -0.645011       -0.251586
H       1.393591        -1.042957       -1.233955
C       0.564067        -1.003378       0.790232
C       1.909586        0.851617        -0.353126
H       0.569644        -2.095738       0.875363
```

```
H       0.863869        -0.592316       1.759562
C       -0.829319       -0.531926       0.432000
O       2.795489        1.424549        0.260445
C       -1.422004       0.532138        1.126184
C       -1.558804       -1.166104       -0.585834
H       -0.869135       1.026604        1.920820
C       -2.716655       0.957259        0.810179
C       -2.850661       -0.741067       -0.906325
H       -1.114721       -1.998642       -1.126024
H       -3.162681       1.780432        1.361051
C       -3.433890       0.322716        -0.208096
H       -3.403787       -1.243062       -1.695060
H       -4.440162       0.650242        -0.452947
O       1.044299        1.452770        -1.170565
H       1.202437        2.416687        -1.165112
###
22
Phe3 b3lyp E=-554.401485469 au
N       -2.992406       -1.305968       -0.244225
H       -3.703500       -1.149879       0.469252
H       -3.315208       -0.797977       -1.067915
C       -1.727846       -0.695391       0.203450
H       -1.442057       -1.173774       1.144125
C       -0.636387       -0.984487       -0.852424
C       -1.844500       0.824174        0.470197
H       -0.623563       -2.068612       -1.010342
H       -0.940368       -0.519537       -1.797823
C       0.752260        -0.513795       -0.475462
O       -2.386786       1.540896        -0.428851
C       1.290919        0.666038        -1.012019
C       1.536526        -1.253505       0.426084
H       0.702610        1.248633        -1.716558
C       2.573617        1.098612        -0.657072
C       2.817651        -0.825418       0.784544
H       1.140387        -2.174928       0.846491
H       2.972025        2.013323        -1.087464
C       3.341593        0.354542        0.243547
H       3.408647        -1.414596       1.480528
H       4.339012        0.686544        0.517511
O       -1.389982       1.267600        1.572190
###
23
PheZW b3lyp E=-554.869186056 au
N       -2.950130       -1.243469       -0.172648
H       -3.322967       -0.712998       -0.969054
H       -3.647108       -1.195704       0.576889
H       -2.835312       -2.225664       -0.442622
C       -1.646228       -0.628419       0.262791
H       -1.379598       -1.093360       1.212435
C       -0.587556       -0.940039       -0.816812
C       -1.877482       0.888016        0.457219
H       -0.590662       -2.024922       -0.975503
H       -0.898799       -0.467743       -1.755168
C       0.811710        -0.491673       -0.451778
O       -2.753486       1.424691        -0.282708
C       1.368970        0.660725        -1.024674
C       1.582411        -1.230081       0.460538
H       0.785306        1.239920        -1.735646
C       2.664832        1.069959        -0.692603
C       2.876107        -0.822692       0.796916
H       1.167828        -2.130757       0.906833
H       3.080892        1.963805        -1.148849
C       3.422015        0.329979        0.220394
H       3.459417        -1.407199       1.502926
H       4.429350        0.644887        0.477392
O       -1.157277       1.462729        1.318576
###
18
Pro1 b3lyp E=-401.670407657 au
N       0.740688        -1.065866       0.470010
H       0.223088        -1.811796       -0.012930
H       0.944893        -1.393363       1.417892
C       2.031936        -0.717964       -0.258904
C       -0.115916       0.182767        0.540884
H       1.906362        -1.034318       -1.295010
H       2.847989        -1.272276       0.202448
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C       2.118735        0.798639        -0.131834
C       0.658018        1.248281        -0.267847
H       -0.197798       0.470469        1.590410
C       -1.494995       -0.127454       -0.001913
H       2.760422        1.224947        -0.906001
H       2.519587        1.078946        0.847754
H       0.346027        1.224524        -1.316685
H       0.468832        2.245073        0.132266
O       -1.794821       -1.184246       -0.535247
O       -2.329308       0.901689        0.159899
H       -3.197850       0.683690        -0.229745
###
16
Pro3 b3lyp E=-400.747671121 au
N       0.742103        -0.968092       0.805235
H       1.230435        -0.831594       1.688673
C       1.763690        -0.839259       -0.258275
C       -0.156604       0.204068        0.647468
H       1.356549        -1.237682       -1.195002
H       2.651088        -1.424367       -0.002580
C       2.026520        0.665946        -0.388864
C       0.620758        1.269488        -0.207058
H       -0.382623       0.602357        1.639757
C       -1.505902       -0.106682       -0.021439
H       2.483779        0.944519        -1.344228
H       2.696071        0.992285        0.416305
H       0.137977        1.405590        -1.180962
H       0.638410        2.243974        0.287995
O       -1.655262       -1.170689       -0.695247
O       -2.406886       0.785713        0.123048
###
17
ProZW b3lyp E=-401.224197523 au
N       0.652411        -1.047625       0.490984
H       0.067437        -1.743920       0.003748
H       0.844534        -1.387867       1.435426
C       1.945658        -0.762102       -0.249030
C       -0.169225       0.231743        0.550178
H       1.801469        -1.081641       -1.282268
H       2.747356        -1.342909       0.205909
C       2.095789        0.752326        -0.139520
C       0.650407        1.255093        -0.263073
H       -0.236662       0.526322        1.598356
C       -1.580171       -0.033097       -0.005508
H       2.749554        1.144865        -0.922081
H       2.518021        1.024076        0.833991
H       0.333697        1.241425        -1.311533
H       0.509270        2.264523        0.126530
O       -1.787357       -1.160055       -0.547318
O       -2.407180       0.913145        0.111912
###
15
Ser1 b3lyp E=-399.470129598 au
N       -0.352465       1.904389        -0.269517
H       -0.605436       2.091863        0.708612
H       -1.188472       2.065760        -0.842406
H       0.364875        2.580695        -0.554697
C       0.153321        0.507283        -0.436762
H       0.369945        0.359101        -1.496257
C       1.444834        0.353142        0.386725
C       -0.952405       -0.440439       0.008133
H       2.102380        1.195301        0.137713
H       1.212359        0.389746        1.457538
O       2.046238        -0.884712       0.028676
O       -1.850860       -0.109145       0.764267
H       2.755522        -1.067998       0.662160
O       -0.808893       -1.658527       -0.513422
H       -1.510302       -2.246040       -0.170787
###
13
Ser3 b3lyp E=-398.559129971 au
N       -0.210136       1.949899        -0.314629
H       -0.398854       2.113152        0.673943
H       0.591935        2.531016        -0.555823
C       0.155844        0.533710        -0.487141
H       0.308771        0.345199        -1.553078
```

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C       1.449287        0.191690        0.259943
C       -1.005239       -0.358025       -0.002851
H       2.253384        0.840331        -0.112016
H       1.314967        0.381360        1.333030
O       1.786502        -1.189298       0.036876
O       -1.460078       -0.134160       1.161738
H       2.608346        -1.378889       0.512318
O       -1.427292       -1.262256       -0.788074
###
14
SerZW b3lyp E=-399.024330185 au
N       -0.531323       1.816980        -0.283220
H       -0.944136       1.867643        0.656347
H       -1.291305       1.955930        -0.956383
H       0.145397        2.577859        -0.403295
C       0.098372        0.467610        -0.470803
H       0.326971        0.359062        -1.531654
C       1.393268        0.437494        0.350886
C       -0.920650       -0.607430       -0.020206
H       2.013314        1.297506        0.065616
H       1.158968        0.513436        1.420480
O       2.068755        -0.785710       0.062921
O       -1.722488       -0.267587       0.898280
H       2.880545        -0.809487       0.590286
O       -0.845821       -1.730059       -0.588467
###
18
Thr1 b3lyp E=-438.795404006 au
N       0.175312        1.734925        -0.090928
H       -0.652648       2.310542        -0.278854
H       0.978578        2.168760        -0.557584
H       0.344492        1.751683        0.922210
C       -0.026284       0.329496        -0.567218
H       -0.002557       0.342684        -1.659461
C       1.085841        -0.597435       -0.046845
C       -1.415651       -0.111250       -0.122929
H       0.832174        -1.602697       -0.400553
C       2.477576        -0.229954       -0.550366
O       0.992319        -0.545196       1.384227
O       -2.170636       0.590401        0.528414
H       2.798157        0.757636        -0.203348
H       3.196418        -0.966692       -0.178026
H       2.504405        -0.249983       -1.644443
H       1.721854        -1.060985       1.760159
O       -1.705795       -1.339655       -0.554973
H       -2.604056       -1.584973       -0.260811
###
16
Thr3 b3lyp E=-437.880421036 au
N       0.060363        1.796016        -0.236757
H       1.016808        2.101237        -0.403232
H       -0.119111       1.910277        0.758449
C       -0.073353       0.376366        -0.581449
H       -0.021504       0.282051        -1.670932
C       1.033311        -0.556573       -0.031949
C       -1.453170       -0.173520       -0.156331
H       0.787560        -1.575388       -0.358007
C       2.432253        -0.208307       -0.531232
O       0.971405        -0.505098       1.411492
O       -2.105795       0.438789        0.741167
H       2.739119        0.796856        -0.222252
H       3.161001        -0.921206       -0.128758
H       2.472859        -0.266016       -1.624485
H       1.672650        -1.073981       1.761810
O       -1.836381       -1.240409       -0.733849
###
17
ThrZW b3lyp E=-438.350095408 au
N       0.022789        1.684669        0.016928
H       -0.942531       2.003242        0.195956
H       0.504188        2.328600        -0.615117
H       0.519368        1.673487        0.915243
C       -0.081476       0.292702        -0.543142
H       -0.055594       0.377128        -1.632009
C       1.100091        -0.561342       -0.078771
C       -1.473613       -0.278113       -0.156450
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H       0.907718        -1.578680       -0.435420
C       2.448113        -0.082505       -0.609567
O       1.060736        -0.538415       1.361363
O       -2.292383       0.534826        0.365317
H       2.674618        0.940119        -0.288555
H       3.242604        -0.739155       -0.239338
H       2.459435        -0.118204       -1.703723
H       1.859302        -0.971876       1.697403
O       -1.679268       -1.487885       -0.437349
###
28
Trp1 b3lyp E=-686.900184663 au
N       3.306101        1.536431        -0.539212
H       3.918997        0.895961        -1.058204
H       3.851835        1.939115        0.230722
H       3.028755        2.298971        -1.167073
C       2.092458        0.814102        -0.031047
H       1.536619        1.513879        0.593312
C       1.243668        0.353613        -1.244691
C       2.582311        -0.358157       0.804493
H       1.029645        1.256456        -1.830038
H       1.864369        -0.302828       -1.864404
C       -0.031781       -0.341692       -0.876531
O       3.630119        -0.945415       0.585324
C       -0.273725       -1.694360       -0.965982
C       -1.238497       0.255503        -0.356215
H       0.374527        -2.487966       -1.311611
N       -1.553031       -1.975505       -0.536264
C       -2.171388       -0.802491       -0.154741
C       -1.627386       1.574603        -0.048462
H       -1.971280       -2.895576       -0.515155
C       -3.462211       -0.578694       0.341202
C       -2.909960       1.801887        0.443947
H       -0.937780       2.401881        -0.193096
H       -4.157717       -1.400106       0.486945
C       -3.817438       0.734904        0.638873
H       -3.221488       2.814354        0.684640
H       -4.810651       0.943513        1.025999
O       1.727035        -0.678049       1.776551
H       2.049139        -1.471734       2.246236
###
26
Trp3 b3lyp E=-685.984940808 au
N       -3.310456       -1.586246       -0.654413
H       -3.854876       -1.983533       0.110014
H       -3.923752       -0.904112       -1.100861
C       -2.156389       -0.863983       -0.089905
H       -1.557744       -1.584234       0.473891
C       -1.304322       -0.301180       -1.251167
C       -2.560663       0.269247        0.880982
H       -1.065040       -1.143796       -1.911557
H       -1.930320       0.389760        -1.829208
C       -0.039908       0.395901        -0.835635
O       -3.446978       1.093145        0.489439
C       0.183608        1.754247        -0.811360
C       1.182036        -0.218594       -0.369682
H       -0.477282       2.565158        -1.085756
N       1.463630        2.022827        -0.361809
C       2.101532        0.832938        -0.083685
C       1.594207        -1.552314       -0.174813
H       1.867078        2.944072        -0.263264
C       3.398181        0.587472        0.387257
C       2.882610        -1.801567       0.291864
H       0.916095        -2.375322       -0.383773
H       4.082107        1.404257        0.599726
C       3.775602        -0.741036       0.571514
H       3.210179        -2.825902       0.446091
H       4.773807        -0.965983       0.936373
O       -1.984452       0.313952        2.014268
###
27
TrpZW b3lyp E=-686.453191009 au
N       3.281089        1.552068        -0.517481
H       3.959086        0.880593        -0.898773
H       3.750496        2.072087        0.230184
H       3.006581        2.215964        -1.248280
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C       2.095819        0.790133        0.015782
H       1.529707        1.480159        0.641601
C       1.251367        0.314306        -1.189259
C       2.634711        -0.386622       0.859983
H       1.027161        1.199154        -1.799151
H       1.869828        -0.352996       -1.800385
C       -0.026059       -0.376599       -0.814956
O       3.735840        -0.888573       0.484195
C       -0.271205       -1.729984       -0.871947
C       -1.241040       0.235819        -0.331989
H       0.380349        -2.534884       -1.183463
N       -1.559909       -1.997814       -0.456228
C       -2.180784       -0.813850       -0.116986
C       -1.632546       1.563991        -0.069514
H       -1.978483       -2.916610       -0.409387
C       -3.479974       -0.572451       0.348178
C       -2.923477       1.808984        0.391958
H       -0.938032       2.385292        -0.224500
H       -4.180678       -1.387588       0.504346
C       -3.837390       0.750141        0.600904
H       -3.236337       2.828768        0.597731
H       -4.837156       0.972099        0.963081
O       1.921996        -0.764557       1.829558
###
25
Tyr1 b3lyp E=-630.549306754 au
N       3.398894        -1.190726       0.026566
H       4.068913        -1.028898       -0.733720
H       3.309100        -2.203366       0.163805
H       3.792338        -0.780904       0.882671
C       2.060756        -0.590200       -0.290032
H       1.763450        -0.970887       -1.267910
C       1.042981        -1.018428       0.796651
C       2.250180        0.917905        -0.354473
H       1.118950        -2.109139       0.875162
H       1.358598        -0.594286       1.755379
C       -0.386331       -0.626329       0.491881
O       3.121094        1.510914        0.261955
C       -1.009161       0.425804        1.176053
C       -1.126806       -1.316045       -0.481663
H       -0.459413       0.972591        1.937617
C       -2.331126       0.787027        0.901471
C       -2.445606       -0.967029       -0.769893
H       -0.669067       -2.141539       -1.020934
H       -2.805536       1.602756        1.440913
C       -3.046774       0.087823        -0.074196
H       -3.013277       -1.507055       -1.521472
O       -4.356977       0.395359        -0.388035
H       -4.664091       1.126224        0.170746
O       1.347230        1.505255        -1.140530
H       1.468327        2.474189        -1.110133
###
23
Tyr3 b3lyp E=-629.634669352 au
N       -3.471799       -1.179434       -0.092227
H       -4.144294       -0.924801       0.630063
H       -3.791253       -0.709675       -0.939613
C       -2.156399       -0.622958       0.271510
H       -1.859356       -1.068517       1.225028
C       -1.128731       -1.030977       -0.808375
C       -2.172281       0.912347        0.460352
H       -1.191195       -2.120084       -0.912733
H       -1.443292       -0.594505       -1.764073
C       0.300249        -0.631435       -0.509641
O       -2.715765       1.613787        -0.450215
C       0.882907        0.501632        -1.095445
C       1.087480        -1.387770       0.375055
H       0.302669        1.105277        -1.788606
C       2.200885        0.875096        -0.812504
C       2.403760        -1.030846       0.670337
H       0.666520        -2.276074       0.839743
H       2.639157        1.754163        -1.278436
C       2.959123        0.105222        0.072868
H       3.003351        -1.626832       1.351976
O       4.270065        0.420998        0.389373
H       4.535418        1.221741        -0.088893
```

```
O       -1.638938       1.384400        1.514115
###
22
Tyr4 b3lyp E=-629.156751877 au
N       -3.425065       -1.202652       -0.102082
H       -4.109376       -0.942434       0.607008
H       -3.736044       -0.746883       -0.960197
C       -2.116120       -0.633359       0.270042
H       -1.824286       -1.072967       1.228112
C       -1.073635       -1.034373       -0.798531
C       -2.150420       0.901129        0.454971
H       -1.132582       -2.124991       -0.900163
H       -1.391356       -0.606698       -1.758216
C       0.352407        -0.621643       -0.500774
O       -2.684231       1.596246        -0.467022
C       0.937174        0.512716        -1.088599
C       1.155244        -1.360662       0.386953
H       0.351402        1.109380        -1.786427
C       2.251348        0.896806        -0.809707
C       2.468523        -0.990949       0.678509
H       0.742688        -2.251982       0.858361
H       2.670709        1.779106        -1.289907
C       3.075034        0.158641        0.089486
H       3.061166        -1.592091       1.365816
O       4.320950        0.508449        0.356055
O       -1.643494       1.382592        1.517977
###
24
TyrZW b3lyp E=-630.102611176 au
N       3.424960        -1.122567       0.071257
H       3.802731        -0.576442       0.854884
H       4.086888        -1.038907       -0.706256
H       3.368294        -2.109869       0.340710
C       2.074137        -0.571175       -0.305033
H       1.803912        -1.022957       -1.259998
C       1.068789        -0.975620       0.795508
C       2.211946        0.961135        -0.458873
H       1.141199        -2.063207       0.918788
H       1.384139        -0.517134       1.739364
C       -0.364115       -0.596093       0.491603
O       3.067079        1.528190        0.283213
C       -0.969245       0.504142        1.113648
C       -1.129310       -1.344475       -0.417467
H       -0.400983       1.098654        1.824201
C       -2.294711       0.855129        0.841507
C       -2.452290       -1.007145       -0.703116
H       -0.687359       -2.207597       -0.908958
H       -2.753532       1.708226        1.334740
C       -3.033892       0.096361        -0.069712
H       -3.037620       -1.593551       -1.404881
O       -4.349923       0.390737        -0.377733
H       -4.637548       1.167240        0.127199
O       1.443758        1.516069        -1.291352
###
20
Val1 b3lyp E=-402.883754347 au
N       -0.639197       1.799317        -0.658579
H       -0.776852       2.126734        0.303920
H       -1.538666       1.885016        -1.143974
H       0.033150        2.422176        -1.118637
C       -0.137818       0.383354        -0.692881
H       -0.124140       0.087177        -1.743579
C       1.305730        0.304562        -0.118406
C       -1.162389       -0.464349       0.045683
H       1.838619        1.129223        -0.609758
C       1.371621        0.515260        1.401291
C       1.998857        -0.999465       -0.535344
O       -1.994028       -0.003447       0.811563
H       0.881377        -0.304965       1.938724
H       2.418827        0.540729        1.717732
H       0.910851        1.456556        1.720703
H       1.939510        -1.157539       -1.617343
H       3.056219        -0.948685       -0.257568
H       1.562665        -1.869005       -0.034830
O       -1.042341       -1.762466       -0.240215
H       -1.692237       -2.271508       0.281810
```

```
###
18
Val3 b3lyp E=-401.965673848 au
N       -0.622355       1.715129        -0.942200
H       -0.840318       2.099482        -0.024657
H       0.157436        2.260526        -1.307167
C       -0.184718       0.318771        -0.766479
H       -0.178578       -0.155191       -1.753255
C       1.266111        0.186872        -0.202958
C       -1.216339       -0.443745       0.089220
H       1.867278        0.839159        -0.854222
C       1.419934        0.698612        1.236114
C       1.830049        -1.234104       -0.340698
O       -1.816984       0.189719        1.012270
H       0.906829        0.043748        1.950179
H       2.479108        0.726936        1.516241
H       1.018724        1.710801        1.358204
H       1.722421        -1.611283       -1.364407
H       2.897158        -1.245135       -0.090208
H       1.325018        -1.936551       0.331613
O       -1.394117       -1.676821       -0.169534
###
19
ValZW b3lyp E=-402.436292916 au
N       -0.770155       1.688883        -0.699903
H       -1.648069       1.712931        -1.227101
H       -0.992087       1.973625        0.259764
C       -0.180029       0.300133        -0.706245
H       -0.140398       -0.002750       -1.754053
C       1.260724        0.349631        -0.135844
C       -1.149000       -0.634824       0.053917
H       1.744986        1.193457        -0.646841
C       1.311640        0.612685        1.376852
C       2.050376        -0.913252       -0.505587
O       -1.976376       -0.091313       0.843106
H       0.881746        -0.222972       1.940671
H       2.352693        0.728127        1.695546
H       0.778861        1.525570        1.665822
H       2.018872        -1.103427       -1.583965
H       3.098731        -0.788128       -0.215166
H       1.662028        -1.797292       0.009098
O       -1.023983       -1.870848       -0.171803
H       -0.125675       2.369720        -1.113440
###
# PEPTIDES optimized with b3lyp
# opt(tight) freq b3lyp/6-31+G(d,p) scf=(xqc,tight) integral=ultrafine scrf(smd,solvent=water)
###
24
AlaAla1 b3lyp E=-571.608330726 au
N       -3.463049       -0.566697       -0.322800
H       -3.553927       -0.938508       0.630129
H       -3.326676       -1.363616       -0.953300
H       -4.337008       -0.097338       -0.580459
C       -2.309343       0.391185        -0.392424
H       -2.165701       0.631024        -1.447584
C       -2.638063       1.649504        0.408462
C       -1.086094       -0.350300       0.160293
H       -2.797421       1.412713        1.464919
H       -1.813036       2.360769        0.327129
H       -3.538738       2.122841        0.006773
O       -1.228205       -1.256340       1.000689
N       0.098768        0.067121        -0.305843
H       0.129659        0.811478        -0.995628
C       1.368674        -0.496208       0.134653
H       1.272425        -0.772949       1.189264
C       1.760527        -1.741981       -0.682921
C       2.434615        0.588246        0.028644
H       1.908767        -1.481828       -1.735041
H       2.679146        -2.190805       -0.294725
H       0.958888        -2.480776       -0.608918
O       2.278390        1.636999        -0.575031
O       3.615633        0.338718        0.620297
H       3.625154        -0.513660       1.090058
###
23
AlaAla2 b3lyp E=-571.159484891 au
```

```
N       3.430634        0.493283        -0.377867
H       3.503268        0.955344        0.536750
H       3.341460        1.226063        -1.089332
H       4.294965        -0.027060       -0.557584
C       2.245299        -0.427575       -0.387170
H       2.095223        -0.735116       -1.423375
C       2.532240        -1.635973       0.502886
C       1.046762        0.385872        0.117224
H       2.691343        -1.329163       1.541260
H       1.688151        -2.328247       0.465648
H       3.421840        -2.161913       0.143557
O       1.232449        1.354848        0.882153
N       -0.151251       -0.039539       -0.288061
H       -0.224818       -0.878682       -0.857869
C       -1.423541       0.496561        0.199248
H       -1.310842       0.725450        1.263228
C       -1.825409       1.775666        -0.551169
C       -2.515365       -0.590206       0.061714
H       -1.980265       1.568674        -1.615375
H       -2.752028       2.180035        -0.135211
H       -1.044221       2.534817        -0.453699
O       -2.250356       -1.616900       -0.632857
O       -3.612050       -0.354507       0.649091
###
22
AlaAla3 b3lyp E=-570.696499977 au
N       -3.285586       0.404856        0.978137
H       -2.840623       0.926282        1.732400
H       -3.590768       1.097014        0.294302
C       -2.295264       -0.478484       0.345412
H       -1.938591       -1.174028       1.111013
C       -2.946311       -1.276405       -0.786841
C       -1.090797       0.297051        -0.207212
H       -3.351582       -0.603462       -1.550636
H       -2.221121       -1.942382       -1.265550
H       -3.765297       -1.884558       -0.391442
O       -1.252577       1.258422        -0.995267
N       0.119164        -0.120164       0.192728
H       0.198916        -0.927232       0.803220
C       1.391276        0.440030        -0.261022
H       1.326621        0.617238        -1.338945
C       1.721414        1.764417        0.448035
C       2.517074        -0.588764       -0.013235
H       1.840429        1.605858        1.525265
H       2.650780        2.183131        0.052103
H       0.920960        2.492065        0.289203
O       2.277934        -1.558256       0.768456
O       3.618503        -0.366395       -0.599166
###
21
AlaGly1 b3lyp E=-532.293202855 au
N       -3.312483       -0.397962       -0.624984
H       -3.487077       -1.054811       0.144530
H       -3.149937       -0.949903       -1.473743
H       -4.152170       0.172807        -0.767259
C       -2.135638       0.476464        -0.306350
H       -1.929745       1.061158        -1.204937
C       -2.478461       1.391342        0.868676
C       -0.961206       -0.455681       0.004473
H       -2.699963       0.807809        1.767678
H       -1.633562       2.052314        1.075651
H       -3.345496       2.010050        0.619156
O       -1.160551       -1.615929       0.407124
N       0.257866        0.070544        -0.165935
H       0.358844        1.028759        -0.486458
C       1.463190        -0.668483       0.159891
C       2.680464        0.189499        -0.074819
H       1.461025        -0.987330       1.208168
H       1.549339        -1.573117       -0.451783
O       2.653665        1.346585        -0.464259
O       3.810062        -0.478140       0.201316
H       4.575555        0.105209        0.040753
###
20
AlaGly2 b3lyp E=-531.842630284 au
N       -3.247838       -0.374285       -0.642038
```

```
H       -3.433343       -1.035462       0.121226
H       -3.087042       -0.921826       -1.493839
H       -4.079911       0.207207        -0.784459
C       -2.059892       0.480667        -0.308719
H       -1.835644       1.063968        -1.203634
C       -2.402181       1.398345        0.863712
C       -0.903281       -0.472054       0.013860
H       -2.643065       0.817030        1.759276
H       -1.548878       2.044850        1.081676
H       -3.256500       2.031898        0.606987
O       -1.136866       -1.625018       0.431813
N       0.321756        0.023945        -0.161957
H       0.452072        0.978869        -0.484945
C       1.539329        -0.702955       0.168889
C       2.784433        0.165738        -0.061403
H       1.523547        -1.017827       1.217838
H       1.621490        -1.608594       -0.440531
O       2.619367        1.363533        -0.437380
O       3.894925        -0.404287       0.154359
###
19
AlaGly3 b3lyp E=-531.379844469 au
N       3.135779        0.012935        -1.109606
H       2.701822        0.249441        -2.000713
H       3.481401        0.890060        -0.720865
C       2.119046        -0.534892       -0.202698
H       1.728700        -1.450868       -0.656521
C       2.751143        -0.879236       1.149227
C       0.949101        0.433494        0.017456
H       3.178122        0.016673        1.613835
H       2.010432        -1.302014       1.835440
H       3.551677        -1.611952       1.009822
O       1.150106        1.636765        0.306051
N       -0.284341       -0.077307       -0.102301
H       -0.413766       -1.055145       -0.341114
C       -1.502378       0.684107        0.125912
C       -2.753817       -0.189508       -0.039801
H       -1.506154       1.108633        1.135701
H       -1.569152       1.523260        -0.575025
O       -2.601092       -1.410975       -0.338598
O       -3.861729       0.399052        0.142823
###
32
AlaHis1 b3lyp E=-797.112722708 au
N       -4.389398       -1.524787       -0.476215
H       -4.331023       -2.003974       0.430367
H       -3.958975       -2.133661       -1.180121
H       -5.378053       -1.402997       -0.719001
C       -3.700503       -0.193006       -0.400181
H       -3.675827       0.205379        -1.415662
C       -4.482803       0.732159        0.531034
C       -2.280608       -0.451476       0.113487
H       -4.517131       0.325533        1.546430
H       -4.003589       1.713358        0.559290
H       -5.503547       0.857811        0.158298
O       -2.051591       -1.394878       0.888025
N       -1.351497       0.423769        -0.305421
H       -1.612542       1.156648        -0.958016
C       0.029717        0.389263        0.149916
H       0.047327        -0.016090       1.163926
C       0.886679        -0.525632       -0.778968
C       0.556052        1.825185        0.157553
H       0.384677        -1.496459       -0.801724
H       0.873172        -0.118254       -1.793416
C       2.301413        -0.712508       -0.334867
O       0.178776        2.667935        -0.639149
O       1.492702        2.141734        1.064473
N       3.386112        -0.235473       -1.057880
C       2.831476        -1.317081       0.772483
H       3.330802        0.262110        -1.942186
C       4.525766        -0.535046       -0.432197
N       4.204007        -1.190452       0.683587
H       2.356342        -1.822267       1.597823
H       5.522135        -0.296622       -0.769348
H       1.681044        1.414622        1.684420
H       4.878380        -1.546021       1.354069
```

```
###
31
AlaHis2 b3lyp E=-796.666927720 au
N       4.339273        -1.456704       0.649123
H       4.235746        -2.084585       -0.157423
H       3.913045        -1.917091       1.460692
H       5.338153        -1.328927       0.841410
C       3.681984        -0.137561       0.357049
H       3.671305        0.421320        1.293832
C       4.482070        0.606961        -0.709725
C       2.254299        -0.444832       -0.108651
H       4.511579        0.039951        -1.645094
H       4.019942        1.578405        -0.900063
H       5.504828        0.775582        -0.359782
O       2.022024        -1.475222       -0.770545
N       1.336288        0.470950        0.216948
H       1.605610        1.289531        0.756213
C       -0.055819       0.437372        -0.219961
H       -0.097323       0.032540        -1.233075
C       -0.880389       -0.486849       0.725397
C       -0.611634       1.881570        -0.230711
H       -0.384148       -1.460389       0.746769
H       -0.850737       -0.076605       1.739476
C       -2.301983       -0.693736       0.317764
O       -0.075716       2.715782        0.557507
O       -1.579459       2.106568        -1.012509
N       -3.361951       0.001644        0.884353
C       -2.864912       -1.536200       -0.602115
H       -3.278024       0.718259        1.599273
C       -4.515595       -0.386196       0.338042
N       -4.230142       -1.320870       -0.568814
H       -2.415948       -2.258724       -1.264357
H       -5.497189       -0.015023       0.587043
H       -4.924031       -1.799590       -1.134350
###
30
AlaHis3 b3lyp E=-796.206811273 au
N       -4.323350       -1.531287       -0.494824
H       -4.250145       -2.031490       0.399024
H       -3.893957       -2.120082       -1.215899
H       -5.314526       -1.410559       -0.726235
C       -3.638877       -0.198409       -0.392458
H       -3.622118       0.222082        -1.399227
C       -4.422251       0.702839        0.560114
C       -2.212652       -0.466058       0.104517
H       -4.447891       0.278007        1.568412
H       -3.948867       1.686344        0.603998
H       -5.446599       0.829790        0.197256
O       -1.978918       -1.460562       0.820746
N       -1.300775       0.441706        -0.254647
H       -1.574425       1.224577        -0.841536
C       0.095405        0.430981        0.183458
H       0.137411        -0.000270       1.185005
C       0.946756        -0.444490       -0.782748
C       0.604507        1.889148        0.241934
H       0.444245        -1.415076       -0.847480
H       0.915830        0.007033        -1.779405
C       2.375565        -0.646027       -0.376129
O       0.128885        2.703023        -0.606602
O       1.475963        2.155608        1.119826
N       3.424772        0.030119        -0.984582
C       2.872266        -1.490177       0.591711
C       4.524196        -0.401401       -0.384315
N       4.240222        -1.319016       0.574699
H       2.389934        -2.177920       1.269720
H       5.534406        -0.091451       -0.608956
H       4.913679        -1.794623       1.162534
###
29
AlaHis4 b3lyp E=-795.744001118 au
N       -4.277337       -1.403696       -0.954305
H       -3.675756       -1.733488       -1.707938
H       -4.277434       -2.141009       -0.249704
C       -3.695891       -0.191519       -0.362068
H       -3.653909       0.572937        -1.143909
C       -4.580689       0.313691        0.780606
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C       -2.271653       -0.423732       0.162699
H       -4.673184       -0.448123       1.562736
H       -4.162728       1.219589        1.231331
H       -5.580709       0.545548        0.402454
O       -2.011938       -1.388210       0.918460
N       -1.346584       0.470250        -0.223440
H       -1.616502       1.225685        -0.844200
C       0.054506        0.454493        0.193115
H       0.106929        0.048305        1.204563
C       0.886582        -0.455406       -0.758571
C       0.588425        1.903905        0.208449
H       0.374484        -1.422519       -0.790724
H       0.848174        -0.031229       -1.767055
C       2.317575        -0.660650       -0.361182
O       0.157486        2.691602        -0.687966
O       1.436869        2.194387        1.102770
N       3.366968        0.007710        -0.978478
C       2.815605        -1.499660       0.610510
C       4.467344        -0.423472       -0.379592
N       4.184218        -1.333744       0.586633
H       2.333506        -2.180803       1.295330
H       5.477786        -0.118989       -0.610693
H       4.858321        -1.807681       1.175026
###
34
AlaLys3 b3lyp E=-744.475144058 au
N       -3.960790       -2.179177       -0.748711
H       -3.900421       -2.727067       0.109199
H       -3.227828       -2.532060       -1.362710
C       -3.690395       -0.771821       -0.425614
H       -3.700960       -0.208060       -1.363595
C       -4.783323       -0.222559       0.495294
C       -2.321330       -0.577219       0.242948
H       -4.817466       -0.787482       1.433528
H       -4.604395       0.830795        0.733415
H       -5.758015       -0.306170       0.005311
O       -1.978514       -1.276452       1.224667
N       -1.541620       0.384789        -0.274697
H       -1.873632       0.918042        -1.071144
C       -0.239082       0.783236        0.261470
H       -0.268205       0.663626        1.347102
C       0.884821        -0.108513       -0.318298
C       -0.006709       2.275761        -0.065181
H       0.593181        -1.150712       -0.142273
H       0.919440        0.036568        -1.405614
C       2.271559        0.136025        0.286923
O       -0.470802       2.710414        -1.163255
O       0.654633        2.954503        0.775788
H       2.596842        1.162465        0.082435
H       2.217563        0.031879        1.378723
C       3.317508        -0.840662       -0.266785
H       3.010548        -1.874310       -0.060798
H       3.385124        -0.730701       -1.357106
C       4.687537        -0.593818       0.348231
H       5.048102        0.417478        0.152055
H       4.687765        -0.767636       1.425730
N       5.709916        -1.531569       -0.235877
H       5.818612        -1.372771       -1.242607
H       6.625323        -1.403699       0.204849
H       5.429817        -2.508792       -0.103031
###
33
AlaLys4 b3lyp E=-744.005463419 au
N       -3.899102       -2.157678       -0.776165
H       -3.827910       -2.728668       0.065720
H       -3.165505       -2.484847       -1.403646
C       -3.642510       -0.756733       -0.415150
H       -3.666218       -0.167245       -1.336955
C       -4.734352       -0.246504       0.528534
C       -2.270315       -0.567119       0.248217
H       -4.754993       -0.837210       1.451189
H       -4.564581       0.801741        0.794601
H       -5.712013       -0.327189       0.043998
O       -1.920462       -1.279605       1.218161
N       -1.495881       0.403369        -0.260677
H       -1.831580       0.943036        -1.051183
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C       -0.182606       0.786888        0.261444
H       -0.198016       0.657088        1.346185
C       0.927108        -0.107610       -0.341641
C       0.054789        2.280674        -0.053473
H       0.631241        -1.148678       -0.164420
H       0.940515        0.040610        -1.429180
C       2.328137        0.122732        0.236662
O       -0.416382       2.727787        -1.143806
O       0.725851        2.949442        0.787956
H       2.666026        1.140472        0.005822
H       2.285200        0.047885        1.332007
C       3.354251        -0.882457       -0.302626
H       3.029672        -1.903636       -0.054881
H       3.392531        -0.821020       -1.398762
C       4.756359        -0.658305       0.258095
H       5.113683        0.335973        -0.032722
H       4.708891        -0.668814       1.358373
N       5.711722        -1.652236       -0.268847
H       6.633094        -1.468300       0.123754
H       5.445569        -2.575777       0.071056
###
25
AsnGly1 b3lyp E=-701.016738556 au
N       -2.637373       -2.018065       -0.382376
H       -2.285253       -2.792455       -0.954813
H       -3.572059       -1.765901       -0.720948
H       -2.719186       -2.364756       0.580010
C       -1.716480       -0.838845       -0.454714
H       -1.655275       -0.554892       -1.506622
C       -2.315293       0.310907        0.367941
C       -0.342712       -1.323654       0.035370
H       -3.389505       0.374265        0.151847
H       -2.214579       0.115511        1.440879
C       -1.718833       1.669155        0.024042
O       -0.233043       -2.420108       0.613045
O       -0.965177       1.833565        -0.956120
N       -2.078658       2.675982        0.833120
H       -1.748733       3.613848        0.641549
H       -2.688484       2.523794        1.626000
N       0.688116        -0.504500       -0.202750
H       0.522832        0.393627        -0.656023
C       2.028659        -0.830403       0.244704
C       2.975130        0.309620        -0.054436
H       2.047570        -1.022852       1.324126
H       2.401587        -1.734720       -0.250559
O       2.634072        1.368895        -0.552676
O       4.265429        0.109616        0.267050
H       4.423422        -0.775815       0.640764
###
24
AsnGly2 b3lyp E=-700.568617408 au
N       -2.324812       -2.122113       -0.700818
H       -1.838520       -2.774527       -1.325658
H       -3.263714       -1.957413       -1.078602
H       -2.409150       -2.576311       0.217352
C       -1.561755       -0.837268       -0.567731
H       -1.352679       -0.484378       -1.577956
C       -2.427119       0.181795        0.187066
C       -0.270492       -1.177306       0.191161
H       -3.425171       0.194236        -0.267976
H       -2.541272       -0.112377       1.233942
C       -1.888645       1.600327        0.061449
O       -0.300550       -2.033539       1.098689
O       -1.437496       2.029821        -1.017272
N       -1.970602       2.358885        1.165194
H       -1.691316       3.331616        1.125133
H       -2.339506       1.991133        2.032189
N       0.820964        -0.503532       -0.169058
H       0.781455        0.185246        -0.916147
C       2.104952        -0.639428       0.504907
C       3.164805        0.273752        -0.127877
H       2.007779        -0.388211       1.566192
H       2.453882        -1.675535       0.446591
O       2.827855        0.987808        -1.117448
O       4.311301        0.231236        0.409015
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```

```
23
AsnGly3 b3lyp E=-700.109084985 au
N       1.837208        2.393398        -0.852938
H       1.055907        2.936684        -1.217414
H       2.081608        2.810716        0.044714
C       1.395935        1.009641        -0.630606
H       1.083052        0.601524        -1.594504
C       2.580966        0.183927        -0.101926
C       0.213851        0.943038        0.350857
H       3.423130        0.333724        -0.786570
H       2.880744        0.552065        0.883979
C       2.311389        -1.309882       -0.067663
O       0.313047        1.415278        1.507458
O       1.885811        -1.917678       -1.072343
N       2.580880        -1.945873       1.085382
H       2.446780        -2.947744       1.148030
H       2.915269        -1.446094       1.897754
N       -0.914909       0.384056        -0.104736
H       -0.955764       0.013451        -1.048727
C       -2.131753       0.255454        0.681773
C       -3.268058       -0.375706       -0.135600
H       -1.953718       -0.362654       1.568487
H       -2.461607       1.237844        1.036088
O       -3.036797       -0.700724       -1.337628
O       -4.368517       -0.520551       0.476662
###
24
AspGly1 b3lyp E=-720.879235414 au
N       -2.629593       -2.004785       -0.436783
H       -2.281637       -2.758556       -1.038919
H       -3.566458       -1.741045       -0.761062
H       -2.704155       -2.385241       0.513726
C       -1.705693       -0.827143       -0.471468
H       -1.628919       -0.520712       -1.516197
C       -2.313632       0.304420        0.371604
C       -0.342062       -1.324813       0.036972
H       -3.390294       0.371144        0.169620
H       -2.203961       0.107167        1.443371
C       -1.737584       1.663808        0.058910
O       -0.260134       -2.398236       0.659314
O       -2.259246       2.612603        0.851607
O       -0.910235       1.902335        -0.809876
N       0.705664        -0.538337       -0.231710
H       0.560452        0.345751        -0.714994
C       2.035404        -0.850236       0.259888
C       2.984758        0.276862        -0.058886
H       2.028193        -1.007497       1.343926
H       2.421961        -1.768583       -0.195782
O       2.676604        1.303310        -0.644081
O       4.224543        0.012943        0.379089
H       -1.876816       3.477571        0.610963
H       4.809751        0.760816        0.154252
###
23
AspGly2 b3lyp E=-720.428745461 au
N       2.328658        -2.129277       0.686343
H       1.881302        -2.766873       1.353849
H       3.283152        -1.943668       1.012361
H       2.370707        -2.611244       -0.220854
C       1.544567        -0.859089       0.554413
H       1.366975        -0.487859       1.564233
C       2.367963        0.151114        -0.255476
C       0.228353        -1.233685       -0.146222
H       3.410470        0.129730        0.086285
H       2.375501        -0.101373       -1.319918
C       1.896147        1.573845        -0.076960
O       0.219639        -2.169370       -0.971694
O       2.439711        2.393156        -0.994336
O       1.139135        1.964479        0.798603
N       -0.835798       -0.497537       0.167059
H       -0.757817       0.255040        0.846787
C       -2.138134       -0.663294       -0.463283
C       -3.158023       0.344224        0.086207
H       -2.056443       -0.526934       -1.546572
H       -2.517696       -1.675771       -0.290821
O       -2.785990       1.140251        0.997535
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O       -4.311814       0.287863        -0.433786
H       2.143141        3.306911        -0.821821
###
22
AspGly3 b3lyp E=-719.975825276 au
N       -2.674754       -1.891675       -0.402217
H       -2.358119       -2.659015       -1.003484
H       -3.600570       -1.589574       -0.722526
H       -2.762650       -2.268002       0.547735
C       -1.707509       -0.743545       -0.438049
H       -1.639987       -0.431608       -1.481387
C       -2.252962       0.407927        0.418014
C       -0.352340       -1.296279       0.028941
H       -3.333043       0.492714        0.246583
H       -2.116808       0.194071        1.483341
C       -1.655682       1.791744        0.103926
O       -0.285294       -2.430639       0.549846
O       -2.034789       2.738627        0.855264
O       -0.854620       1.903841        -0.873305
N       0.701000        -0.501724       -0.160678
H       0.555798        0.431790        -0.548369
C       2.046453        -0.869620       0.256458
C       3.059226        0.248465        -0.025532
H       2.066039        -1.091850       1.329110
H       2.371625        -1.775633       -0.265468
O       2.637826        1.337237        -0.513086
O       4.263237        -0.021724       0.267804
###
21
AspGly4 b3lyp E=-719.508537381 au
N       -2.736749       -1.927467       -0.312006
H       -2.383190       -2.752154       -0.792456
H       -3.575404       -1.635798       -0.810161
C       -1.750660       -0.840457       -0.420082
H       -1.625880       -0.501155       -1.457167
C       -2.248296       0.355948        0.414710
C       -0.376405       -1.355867       0.032832
H       -3.332089       0.436490        0.261784
H       -2.109316       0.157611        1.483559
C       -1.676754       1.745827        0.099303
O       -0.223522       -2.506443       0.503918
O       -2.059575       2.690319        0.859303
O       -0.888270       1.891624        -0.886794
N       0.654198        -0.512758       -0.128212
H       0.476561        0.421012        -0.498849
C       2.015308        -0.855559       0.251005
C       3.005170        0.282496        -0.029197
H       2.068531        -1.099252       1.318351
H       2.351660        -1.745112       -0.293025
O       2.566642        1.367724        -0.510199
O       4.216826        0.032477        0.256030
###
35
AspHis0 b3lyp E=-985.701128743 au
N       -3.189809       -2.689486       -0.534946
H       -2.593764       -3.186690       -1.205890
H       -4.167862       -2.822086       -0.814914
H       -3.048942       -3.121762       0.386128
C       -2.844489       -1.231225       -0.495279
H       -2.915274       -0.864999       -1.519959
C       -3.852095       -0.504196       0.405757
C       -1.400266       -1.134577       0.023752
H       -4.866230       -0.860182       0.183997
H       -3.665768       -0.714294       1.463631
C       -3.872039       0.989373        0.187425
O       -0.960329       -1.995401       0.802370
O       -4.618216       1.611502        1.115355
O       -3.310750       1.580008        -0.723267
N       -0.696260       -0.080248       -0.413467
H       -1.145346       0.604561        -1.016347
C       0.651966        0.208042        0.052986
H       0.732839        -0.073049       1.105832
C       1.703308        -0.600898       -0.768049
C       0.879909        1.707550        -0.071659
H       1.363049        -1.639623       -0.768059
H       1.698923        -0.251604       -1.804091
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C       3.093586        -0.544921       -0.222523
O       0.230075        2.437563        -0.803228
O       1.889766        2.130911        0.696649
N       4.154794        0.014115        -0.920836
C       3.621633        -0.990529       0.958550
H       4.096655        0.436214        -1.843197
C       5.278360        -0.079193       -0.206527
N       4.968717        -0.685340       0.939868
H       3.160107        -1.489038       1.795481
H       6.254874        0.269162        -0.503706
H       5.634558        -0.888753       1.679047
H       -4.632501       2.569023        0.927248
H       2.028990        3.086620        0.550828
###
34
AspHis2 b3lyp E=-985.253128095 au
N       3.181759        2.667130        -0.576484
H       2.601825        3.149212        -1.271934
H       4.165864        2.789763        -0.838247
H       3.019792        3.121804        0.330218
C       2.826047        1.212496        -0.504630
H       2.902032        0.820932        -1.519375
C       3.821599        0.501306        0.422043
C       1.376742        1.139632        0.007466
H       4.839148        0.853491        0.209400
H       3.620721        0.728197        1.473612
C       3.848689        -0.995466       0.227252
O       0.945113        2.033424        0.759651
O       4.555520        -1.604476       1.194923
O       3.328082        -1.599838       -0.698052
N       0.671155        0.079289        -0.395409
H       1.112546        -0.633738       -0.971448
C       -0.676790       -0.225781       0.077010
H       -0.758905       0.079209        1.122415
C       -1.722112       0.570560        -0.761732
C       -0.910556       -1.752046       -0.023393
H       -1.407350       1.616867        -0.770440
H       -1.701227       0.209083        -1.794878
C       -3.121272       0.521729        -0.243008
O       -0.228843       -2.391361       -0.877672
O       -1.791063       -2.235102       0.744824
N       -4.048431       -0.440008       -0.622481
C       -3.783492       1.347722        0.624076
H       -3.859222       -1.223702       -1.240202
C       -5.215842       -0.224051       -0.015202
N       -5.072017       0.861926        0.745818
H       -3.452046       2.229440        1.148494
H       -6.111118       -0.815871       -0.122378
H       -5.808235       1.263151        1.317739
H       4.580365        -2.563961       1.018236
###
33
AspHis3 b3lyp E=-984.800791634 au
N       -3.309373       2.664127        0.251837
H       -2.695126       3.297318        0.773490
H       -4.265570       2.772008        0.604219
H       -3.287611       2.960350        -0.730018
C       -2.863949       1.237072        0.389614
H       -2.911225       1.002669        1.454269
C       -3.829249       0.334986        -0.391056
C       -1.403871       1.183540        -0.087525
H       -4.851397       0.700312        -0.233994
H       -3.632033       0.399447        -1.466374
C       -3.830646       -1.145795       0.029928
O       -0.896797       2.173275        -0.653833
O       -4.589199       -1.907039       -0.640309
O       -3.106903       -1.503801       1.008666
N       -0.757100       0.038000        0.150275
H       -1.269127       -0.730530       0.588786
C       0.626064        -0.194552       -0.252707
H       0.792082        0.279742        -1.222251
C       1.595031        0.445282        0.786865
C       0.888306        -1.712222       -0.387267
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C       3.027363        0.464760        0.361101
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O 0.177636 -2.494231 0.308752
O 1.827836 -2.050696 -1.165601
N 4.007823 -0.319021 0.954074
C 3.670698 1.187313 -0.607210
H 3.854605 -0.974960 1.714310
C 5.191877 -0.095980 0.379172
N 5.001691 0.817504 -0.573279
H 3.299191 1.918890 -1.306346
H 6.127529 -0.564510 0.640300
H 5.734764 1.179932 -1.174462
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32
AspHis4 b3lyp E=-984.339955021 au
N 3.332864 2.641154 -0.222795
H 2.737679 3.295928 -0.739878
H 4.293656 2.731523 -0.567499
H 3.310726 2.924497 0.762843
C 2.854126 1.227304 -0.382754
H 2.890038 1.010785 -1.451542
C 3.802810 0.290022 0.376295
C 1.396032 1.196585 0.104552
H 4.833197 0.626293 0.208103
H 3.621480 0.349464 1.454640
C 3.756136 -1.185790 -0.059781
O 0.920378 2.182643 0.705703
O 4.480570 -1.980596 0.609605
O 3.031711 -1.507905 -1.050406
N 0.723184 0.073471 -0.158633
H 1.216492 -0.684831 -0.633770
C -0.666729 -0.146275 0.244000
H -0.826264 0.345526 1.205134
C -1.636189 0.473674 -0.804455
C -0.914000 -1.662159 0.409891
H -1.318857 1.510883 -0.954266
H -1.504000 -0.049163 -1.756736
C -3.084309 0.437863 -0.415788
O -0.338505 -2.437116 -0.411244
O -1.698026 -2.016666 1.339658
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N -5.042200 0.786791 0.521668
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H -5.788383 1.141077 1.107220
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31
AspHis5 b3lyp E=-983.875034120 au
N 4.877767 -0.729167 1.144227
C 3.528246 -1.010777 1.120048
C 3.081289 -0.604549 -0.117626
N 4.143217 -0.084831 -0.846163
C 5.200756 -0.177887 -0.053241
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O 1.820482 2.388153 0.402286
N -0.670206 0.062048 -0.560194
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C -3.991727 -0.657435 0.263313
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O -4.108149 1.705166 -0.156772
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H -3.863009 -2.450326 -1.757023
H -2.976890 -3.027574 -0.516965
H -2.915387 -0.300571 -1.574763
H -4.942724 -0.845289 -0.249610
H -3.929650 -1.330492 1.123180
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H 1.280706 -1.685609 -0.496977
H 1.723369 -0.532756 -1.755620

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H       3.021997        -1.461996       1.959917
H       6.207396        0.128643        -0.297702
H       5.515625        -0.907605       1.910038
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34
AspHis b3lyp E=-985.251161444 au
N       3.454364        2.620077        -0.072747
H       2.874697        3.331650        -0.529674
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H       3.453695        2.829393        0.931676
C       2.927790        1.239897        -0.338915
H       2.946397        1.109343        -1.422712
C       3.850719        0.211076        0.331629
C       1.471087        1.224921        0.150123
H       4.889600        0.529497        0.187232
H       3.674299        0.187178        1.412739
C       3.753073        -1.224594       -0.216054
O       1.001805        2.204370        0.757555
O       4.547375        -2.064627       0.296039
O       2.909452        -1.475386       -1.133081
N       0.784408        0.108356        -0.131257
H       1.282824        -0.644667       -0.619802
C       -0.601897       -0.069344       0.266756
H       -0.781466       0.489775        1.186678
C       -1.561709       0.471982        -0.840936
C       -0.846828       -1.546497       0.536597
H       -1.246976       1.498828        -1.042456
H       -1.417136       -0.108919       -1.756240
C       -3.008189       0.481205        -0.469597
O       -0.248228       -2.455498       -0.015252
O       -1.825617       -1.737497       1.432485
N       -3.916575       -0.470700       -0.913944
C       -3.728104       1.340680        0.314300
H       -3.695307       -1.259344       -1.515221
C       -5.131058       -0.213183       -0.425516
N       -5.032110       0.885002        0.324824
H       -3.425470       2.224106        0.853215
H       -6.027309       -0.784880       -0.608368
H       -5.810166       1.319013        0.811993
H       -1.989559       -2.694938       1.533336
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29
CysAsn1 b3lyp E=-1138.52079934 au
N       -3.246292       -2.269735       -0.041430
H       -2.726872       -3.082410       -0.391834
H       -4.200644       -2.315705       -0.414959
H       -3.289273       -2.341150       0.982783
C       -2.578107       -0.986846       -0.449779
H       -2.443670       -1.030408       -1.531133
C       -3.501263       0.180039        -0.060006
C       -1.231720       -0.941108       0.284506
H       -4.482971       0.010369        -0.511188
H       -3.625940       0.221901        1.024762
S       -2.960342       1.816226        -0.689879
O       -1.158255       -1.321969       1.461767
H       -1.914432       1.987140        0.146789
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H       -0.368076       -0.166452       -1.389484
C       1.124483        -0.207536       0.126063
H       1.201933        -0.784602       1.052159
C       2.212099        -0.651748       -0.854391
C       1.278385        1.266162        0.524345
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H       2.176211        -0.053496       -1.769131
C       3.605060        -0.630777       -0.245657
O       0.247236        1.703996        1.260785
O       2.238482        1.959523        0.233130
O       3.799805        -0.914579       0.952898
N       4.611987        -0.350019       -1.089466
H       5.567468        -0.381079       -0.755842
H       4.438819        -0.104694       -2.054953
H       0.393431        2.639065        1.499119
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28
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H -4.572003 -0.365205 -0.121074
H -3.570898 -0.776907 1.280575
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O -0.854563 -1.617957 0.893014
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27
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O -2.621599 1.593196 -1.336576
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26
CysAsn4 b3lyp E=-1137.13302879 au
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H 3.500934 -2.160807 -1.225673
C 2.653451 -1.027919 0.241043
H 2.651494 -1.041366 1.338880
C 3.405623 0.236325 -0.216387
C 1.165366 -1.074268 -0.172781
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N       -4.192976       -0.261944       1.264068
H       -5.162336       -0.501112       1.095086
H       -3.970577       0.373213        2.018147
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42
DLeuTyr3 b3lyp E=-994.940188427 au
C       1.565054        -1.544103       0.804861
C       2.762683        -2.099399       -0.001963
C       0.737284        -0.578640       -0.057098
H       3.307201        -2.791945       0.654864
H       2.336831        -2.709704       -0.805428
C       3.760777        -1.106251       -0.635710
O       0.213149        -0.986981       -1.121046
H       3.186490        -0.348678       -1.187939
C       4.648543        -0.378193       0.386012
C       4.636922        -1.853356       -1.654689
H       5.214373        -1.097319       0.992880
H       5.373323        0.264922        -0.127043
H       4.066877        0.251286        1.064278
H       4.030226        -2.319755       -2.439409
H       5.346973        -1.171423       -2.136423
H       5.217276        -2.646141       -1.164528
N       0.618802        0.672254        0.403227
H       1.143551        0.881718        1.248644
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H       -0.194553       1.510454        -1.310500
C       -1.510321       1.990262        0.349458
C       0.713219        3.076451        -0.137836
H       -1.397180       2.227332        1.413239
H       -1.923793       2.876814        -0.142583
C       -2.462107       0.826636        0.181994
O       1.561023        3.178444        0.798066
O       0.431927        3.979996        -0.981943
C       -2.742753       -0.046563       1.241988
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H       -2.283889       0.123029        2.212626
C       -3.608404       -1.134159       1.083341
C       -3.956077       -0.496245       -1.228909
H       -2.899519       1.247984        -1.889853
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H       -4.436844       -0.673830       -2.186301
O       -5.076592       -2.416712       -0.374913
H       -5.172601       -2.930683       0.441894
N       1.951401        -0.940121       2.093370
H       1.253533        -1.165173       2.798186
H       2.828256        -1.342894       2.412713
H       0.893139        -2.398137       0.967375
###
41
DLeuTyr4 b3lyp E=-994.462792481 au
C       1.543415        -1.569376       0.735440
C       2.778716        -2.071285       -0.049350
C       0.724096        -0.587473       -0.116267
H       3.311844        -2.781136       0.598355
H       2.393098        -2.655356       -0.891733
C       3.780834        -1.036800       -0.606318
O       0.229335        -0.970878       -1.203970
H       3.213277        -0.268316       -1.150312
C       4.617310        -0.334399       0.474895
C       4.707061        -1.728103       -1.620322
H       5.177878        -1.066825       1.070718
H       5.344728        0.344697        0.014521
H       3.999663        0.254063        1.158354
H       4.137261        -2.177476       -2.441765
H       5.418464        -1.015344       -2.053053
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H       -1.432996       2.156725        1.439853
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O       1.504765        3.159694        0.810460
O       0.345196        3.981833        -0.939628
C       -2.769038       -0.133198       1.240289
C       -3.158101       0.535590        -1.026425
H       -2.293759       0.020726        2.208003
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C       -4.295788       -1.472939       -0.158119
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O       -5.120474       -2.492365       -0.320178
N       1.874588        -1.006410       2.057281
H       1.151729        -1.261115       2.725917
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H       0.883724        -2.441357       0.843454
###
41
GluHisOMe2 b3lyp E=-1064.32012939 au
N       2.897457        3.311645        -0.143316
H       2.917031        3.430780        0.877152
H       2.273135        4.025616        -0.533768
H       3.841502        3.480400        -0.507128
C       2.436736        1.927183        -0.498174
H       2.309982        1.906236        -1.582019
C       3.515330        0.925479        -0.056400
C       1.102176        1.701257        0.223347
H       4.441497        1.187234        -0.577266
H       3.690082        1.039551        1.018733
C       3.132527        -0.519838       -0.376294
O       0.981406        2.018724        1.416281
H       2.255927        -0.843669       0.195101
H       2.869533        -0.631870       -1.436748
C       4.244768        -1.500167       -0.094761
O       5.394618        -1.203237       0.190012
O       3.920484        -2.811959       -0.185545
N       0.125880        1.143940        -0.518063
H       0.348019        0.854470        -1.465515
C       -1.126411       0.668032        0.053629
H       -1.364917       1.288472        0.917745
C       -2.252581       0.806965        -1.003450
C       -1.014035       -0.771649       0.570773
H       -2.277854       1.856290        -1.309158
H       -2.004141       0.209777        -1.886504
C       -3.606319       0.413219        -0.503430
O       -1.594143       -1.163622       1.572989
N       -4.284693       -0.707840       -0.961669
C       -4.432145       0.993467        0.420080
C       -5.466836       -0.813337       -0.352446
N       -5.568802       0.212474        0.493329
H       -4.307413       1.880010        1.020638
H       -6.202891       -1.584322       -0.516462
H       -6.373062       0.387865        1.087832
O       -0.251273       -1.540616       -0.205729
C       -0.067418       -2.922675       0.200868
H       0.356561        -2.961037       1.205610
H       -1.023869       -3.448003       0.171538
H       0.622771        -3.345889       -0.527629
H       -3.940564       -1.357742       -1.662416
H       2.976289        -2.937646       -0.388229
###
40
GluHisOMe3 b3lyp E=-1063.86550030 au
N       -2.898013       -3.251745       -0.357406
H       -2.928340       -3.454509       0.649254
H       -2.244759       -3.911988       -0.792577
H       -3.830272       -3.417825       -0.750264
C       -2.478393       -1.825540       -0.586587
H       -2.342864       -1.707531       -1.663151
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H       -3.731732       -1.082210       1.001406
C       -3.293668       0.583024        -0.320892
O       -1.033346       -2.068284       1.319530
H       -2.402056       0.907197        0.228906
H       -3.075804       0.752684        -1.382636
C       -4.429756       1.540518        0.070061
O       -5.498122       1.067440        0.563796
O       -4.212722       2.778588        -0.134442
N       -0.195229       -0.973097       -0.509478
H       -0.407284       -0.624082       -1.438942
C       1.062443        -0.549973       0.096008
H       1.177739        -1.094170       1.032737
C       2.233598        -0.876411       -0.855941
C       0.999359        0.939752        0.458707
H       2.209415        -1.954320       -1.046628
H       2.079277        -0.371342       -1.814317
C       3.574452        -0.493997       -0.310736
O       1.175283        1.368351        1.589374
N       4.535346        0.134887        -1.090415
C       4.151599        -0.667418       0.918085
C       5.647723        0.336397        -0.381470
N       5.428149        -0.143817       0.842473
H       3.770327        -1.110494       1.823637
H       6.552627        0.806629        -0.732460
H       6.106063        -0.120225       1.597972
O       0.731660        1.705044        -0.601325
C       0.614048        3.135696        -0.374752
H       -0.189210       3.332441        0.337268
H       1.560873        3.531614        -0.003358
H       0.376536        3.558924        -1.349052
H       4.417837        0.405328        -2.062570
###
39
GluHisOMe4 b3lyp E=-1063.40825645 au
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H       -2.317751       -3.951159       -0.515286
H       -3.881548       -3.391920       -0.486418
C       -2.465986       -1.847598       -0.494756
H       -2.331365       -1.840260       -1.577853
C       -3.542218       -0.835252       -0.073077
C       -1.132493       -1.633995       0.229700
H       -4.472426       -1.127979       -0.570788
H       -3.704906       -0.920012       1.007050
C       -3.190358       0.605141        -0.449668
O       -1.010410       -1.978093       1.416580
H       -2.318254       0.957687        0.112907
H       -2.914180       0.663793        -1.510216
C       -4.316969       1.625389        -0.220436
O       -5.444267       1.222913        0.199733
O       -4.033743       2.839257        -0.480363
N       -0.152630       -1.070134       -0.500078
H       -0.367677       -0.761548       -1.443224
C       1.137523        -0.671750       0.062647
H       1.367818        -1.357885       0.877974
C       2.222040        -0.744913       -1.025734
C       1.023708        0.723448        0.693579
H       2.226637        -1.771972       -1.410407
H       1.944605        -0.092837       -1.860021
C       3.591230        -0.362865       -0.541901
O       1.137642        0.938396        1.892061
N       4.518572        0.209648        -1.400653
C       4.153392        -0.526268       0.704250
C       5.615544        0.381014        -0.677579
N       5.441864        -0.046469       0.597956
H       3.771635        -0.929307       1.629494
H       6.544271        0.809386        -1.025088
H       6.131524        -0.011285       1.338749
O       0.765099        1.669194        -0.212776
C       0.599665        3.025747        0.277408
H       -0.256499       3.074819        0.952782
H       1.507934        3.349523        0.788825
H       0.422326        3.630340        -0.610325
```

```
###
21
GlyAla1 b3lyp E=-532.290818003 au
N       -3.802091       -0.200149       0.036357
H       -3.855154       0.300239        -0.858489
C       -2.485677       -0.882656       0.172179
H       -3.944796       0.488912        0.782215
H       -4.565120       -0.882491       0.079366
C       -1.371148       0.100169        -0.164926
H       -2.400118       -1.271695       1.186971
H       -2.466581       -1.715246       -0.534898
O       -1.619277       1.149799        -0.783646
N       -0.145907       -0.280007       0.221993
H       -0.031881       -1.156488       0.721975
C       1.059970        0.478139        -0.091795
H       0.950502        0.900817        -1.095056
C       1.320795        1.617810        0.910171
C       2.229805        -0.491221       -0.125817
H       1.479026        1.220154        1.916980
H       2.201216        2.191552        0.610933
H       0.457680        2.287467        0.925032
O       2.188523        -1.643951       0.277221
O       3.333591        0.073579        -0.635268
H       4.066048        -0.570993       -0.608803
###
20
GlyAla2 b3lyp E=-531.839830055 au
N       -3.715283       -0.364171       -0.236859
H       -3.842355       0.654609        -0.220102
C       -2.445978       -0.733479       0.450290
H       -4.518613       -0.808973       0.217529
H       -3.701997       -0.654541       -1.220197
C       -1.326353       0.171164        -0.052924
H       -2.588456       -0.573762       1.521385
H       -2.246296       -1.789539       0.268348
O       -1.603482       1.258341        -0.599269
N       -0.088422       -0.272693       0.172568
H       0.060272        -1.201138       0.559179
C       1.129363        0.471711        -0.155461
H       1.010405        0.899211        -1.155584
C       1.395522        1.604781        0.848841
C       2.323052        -0.509361       -0.200057
H       1.556022        1.201871        1.854349
H       2.284244        2.167521        0.551441
H       0.546949        2.293696        0.879969
O       2.159272        -1.671795       0.278365
O       3.395725        -0.056522       -0.697897
###
19
GlyAla3 b3lyp E=-531.377666368 au
N       -3.836663       -0.328354       0.199278
H       -3.838019       0.316478        0.987973
C       -2.500600       -0.897367       0.051783
H       -4.048732       0.237196        -0.620680
C       -1.384000       0.113991        -0.216474
H       -2.255940       -1.482329       0.942465
H       -2.501637       -1.595760       -0.793397
O       -1.619751       1.213630        -0.766307
N       -0.150112       -0.273053       0.142491
H       -0.013419       -1.195373       0.544576
C       1.071430        0.483118        -0.127516
H       0.981704        0.937054        -1.118990
C       1.296511        1.593207        0.913201
C       2.280668        -0.478253       -0.155231
H       1.424805        1.164782        1.913119
H       2.189831        2.172205        0.662878
H       0.440073        2.273048        0.933534
O       2.136480        -1.638240       0.336015
O       3.351359        -0.013595       -0.649514
###
24
GlyAsp1 b3lyp E=-720.880849639 au
N       4.377159        -0.610388       -0.296382
H       4.130579        -1.601564       -0.398466
C       3.338672        0.103301        0.497031
H       4.459515        -0.215300       -1.238983
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C       1.964637        -0.228761       -0.069395
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O       1.798610        -1.229483       -0.785511
N       0.982413        0.610903        0.293534
H       1.204050        1.447512        0.825196
C       -0.400090       0.433072        -0.119388
H       -0.412779       0.118604        -1.168805
C       -1.099550       -0.657502       0.737015
C       -1.086126       1.803590        -0.049555
H       -0.388337       -1.464055       0.924117
H       -1.394672       -0.255274       1.714313
C       -2.327419       -1.250498       0.099288
O       -0.516886       2.806986        0.355807
O       -2.347310       1.858291        -0.469223
O       -3.048676       -0.667655       -0.712266
O       -2.585207       -2.490290       0.514719
H       5.291299        -0.542108       0.161290
H       -3.415444       -2.805824       0.108155
H       -2.691981       0.947891        -0.702864
###
23
GlyAsp2 b3lyp E=-720.430271367 au
N       4.407443        -0.561397       -0.189915
H       4.154457        -1.549439       -0.314315
C       3.340168        0.137317        0.580405
H       4.518696        -0.151621       -1.123064
C       1.984022        -0.275030       0.020703
H       3.413249        -0.185545       1.621228
H       3.513473        1.212063        0.523897
O       1.861601        -1.367173       -0.566604
N       0.982019        0.579447        0.248786
H       1.177466        1.505034        0.621590
C       -0.388943       0.364101        -0.197508
H       -0.364469       -0.038773       -1.215220
C       -1.129187       -0.639165       0.715186
C       -1.134568       1.721627        -0.243897
H       -0.483101       -1.509485       0.878633
H       -1.348619       -0.191529       1.686524
C       -2.389733       -1.175976       0.087215
O       -0.488677       2.767214        0.056368
O       -2.351694       1.662253        -0.580087
O       -2.465403       -1.634489       -1.045828
O       -3.442819       -1.170098       0.931078
H       5.307946        -0.503551       0.294988
H       -4.209944       -1.572416       0.481609
###
22
GlyAsp3 b3lyp E=-719.972102995 au
N       4.365949        -0.506007       -0.185038
H       4.122717        -1.493893       -0.329654
C       3.278818        0.169653        0.578860
H       5.257975        -0.448482       0.315293
H       4.488258        -0.080409       -1.109586
C       1.935463        -0.251971       -0.005563
H       3.341209        -0.167706       1.615798
H       3.440467        1.246769        0.540077
O       1.835892        -1.346413       -0.596984
N       0.925903        0.594242        0.202787
H       1.096516        1.502104        0.627586
C       -0.455090       0.349011        -0.211036
H       -0.445633       -0.085955       -1.213712
C       -1.165193       -0.629707       0.752519
C       -1.202486       1.701615        -0.267393
H       -0.475858       -1.457334       0.957661
H       -1.376059       -0.130002       1.702146
C       -2.448778       -1.260146       0.191740
O       -0.643758       2.711415        0.258203
O       -2.341049       1.688962        -0.818593
O       -2.395438       -1.774433       -0.969097
O       -3.474267       -1.276214       0.943394
###
21
GlyAsp4 b3lyp E=-719.509025587 au
N       4.500625        -0.607322       0.066325
H       4.350032        -1.501666       0.529596
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C       2.001365        -0.232530       -0.086793
H       3.340242        0.467259        1.432952
H       3.549142        1.245691        -0.124729
O       1.856591        -1.339685       -0.649577
N       0.975239        0.595726        0.167743
H       1.153703        1.508608        0.575685
C       -0.411308       0.349401        -0.218961
H       -0.424988       -0.070787       -1.228474
C       -1.098774       -0.650952       0.741019
C       -1.173520       1.694872        -0.242878
H       -0.402901       -1.481827       0.906117
H       -1.281916       -0.173701       1.707944
C       -2.397438       -1.269036       0.203647
O       -0.621766       2.703736        0.292758
O       -2.318621       1.682323        -0.783114
O       -2.371518       -1.779154       -0.960622
O       -3.410030       -1.280689       0.973533
###
18
GlyGly1 b3lyp E=-492.973394073 au
N       -3.650841       0.215681        0.192919
H       -3.689568       -0.007174       1.193289
C       -2.341547       0.822757        -0.175353
H       -3.795856       -0.660221       -0.322153
C       -1.253870       -0.238507       -0.075409
H       -2.414100       1.177088        -1.205985
H       -2.155779       1.671661        0.482499
O       -1.543871       -1.447952       -0.080563
N       -0.001494       0.229587        -0.011519
H       0.168651        1.230603        -0.001777
C       1.152663        -0.648546       0.011329
C       2.419472        0.169117        0.023217
H       1.145184        -1.290128       0.899498
H       1.167764        -1.306552       -0.864251
O       2.459449        1.389774        0.020258
H       -4.419808       0.857548        -0.023721
O       3.508380        -0.612513       0.038338
H       4.307884        -0.053110       0.045829
###
17
GlyGly2 b3lyp E=-492.522793967 au
N       -3.580644       0.243803        0.197453
H       -3.624171       0.037445        1.200996
C       -2.262391       0.828474        -0.177490
H       -3.729052       -0.639807       -0.303264
C       -1.192013       -0.251970       -0.076521
H       -2.334249       1.178588        -1.209556
H       -2.062116       1.677599        0.475530
O       -1.514074       -1.457665       -0.097210
N       0.063413        0.189524        0.003223
H       0.263063        1.186406        0.014645
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H       1.213294        -1.322451       0.911909
H       1.226287        -1.342570       -0.852567
O       2.441170        1.395572        0.003125
O       3.598726        -0.543674       0.048237
H       -4.342914       0.888639        -0.032517
###
16
GlyGly3 b3lyp E=-492.060751234 au
N       3.677966        -0.393062       0.234118
H       3.639205        -0.130703       1.218035
C       2.346814        -0.804479       -0.201613
H       3.941216        0.453203        -0.267801
C       1.261816        0.266608        -0.085952
H       2.391451        -1.091877       -1.258740
H       2.039981        -1.695928       0.351966
O       1.539126        1.486644        -0.132815
N       0.003868        -0.182095       0.034001
H       -0.181440       -1.179949       0.054758
C       -1.168194       0.678568        0.052615
C       -2.467788       -0.137649       0.024540
H       -1.173242       1.307740        0.949505
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H       -1.163359       1.351266        -0.811861
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O       -3.540457       0.537832        0.061773
###
27
GlyHis2 b3lyp E=-756.887108515 au
N       -4.896260       -0.997634       0.067936
H       -4.564619       -1.967922       0.026218
C       -3.893100       -0.080274       -0.541448
H       -5.053085       -0.771559       1.055599
C       -2.518545       -0.378492       0.048770
H       -3.880976       -0.265822       -1.617621
H       -4.207575       0.947559        -0.359015
O       -2.317719       -1.445030       0.662688
N       -1.593881       0.560665        -0.169319
H       -1.845921       1.409521        -0.667813
C       -0.193601       0.456083        0.242717
H       -0.155368       -0.056113       1.205768
C       0.613458        -0.365136       -0.804749
C       0.370460        1.884954        0.408226
H       0.076286        -1.308287       -0.947989
H       0.592015        0.172592        -1.758004
C       2.037158        -0.646512       -0.428442
O       -0.075430       2.774621        -0.378491
O       1.250538        2.057394        1.300793
N       3.104577        0.024794        -1.009593
C       2.510910        -1.558103       0.488492
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N       3.884033        -1.433183       0.467989
H       2.009805        -2.263011       1.134503
H       5.211598        -0.191744       -0.662702
H       4.545213        -1.964285       1.021489
H       -5.792829       -0.931555       -0.423395
###
28
GlyHis3 b3lyp E=-757.347163348 au
N       4.796124        -1.220972       0.253799
H       4.608319        -1.811365       -0.564935
C       3.979150        0.022754        0.183683
H       4.566614        -1.771231       1.088002
H       5.795437        -0.996344       0.281704
C       2.541600        -0.340464       -0.168527
H       4.055765        0.544778        1.137151
H       4.398287        0.652047        -0.604721
O       2.287927        -1.426294       -0.724615
N       1.632480        0.594778        0.125293
H       1.920923        1.464714        0.565617
C       0.224572        0.517133        -0.249314
H       0.146892        0.027767        -1.222531
C       -0.558564       -0.328197       0.800067
C       -0.344276       1.951864        -0.359126
H       -0.005092       -1.258732       0.949112
H       -0.570829       0.206140        1.755199
C       -1.954913       -0.676978       0.400563
O       0.250016        2.864734        0.287537
O       -1.379672       2.093926        -1.070457
N       -3.076374       0.002957        0.857195
C       -2.431565       -1.659986       -0.423831
H       -3.060613       0.805456        1.479502
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N       -3.808006       -1.538475       -0.447396
H       -1.915434       -2.423248       -0.983444
H       -5.196217       -0.198506       0.514512
H       -4.449427       -2.130763       -0.965284
###
26
GlyHis4 b3lyp E=-756.425127791 au
N       -5.052459       -0.932123       0.017048
H       -4.826311       -1.924397       -0.021727
C       -3.948832       -0.171071       -0.557379
H       -5.131906       -0.706368       1.007173
C       -2.570977       -0.443148       0.052637
H       -3.871844       -0.403118       -1.626030
H       -4.168413       0.898015        -0.486582
O       -2.330812       -1.492191       0.689570
N       -1.647843       0.508107        -0.168626
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33
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32
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N -4.779528 -1.687488 0.107876
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H       -4.287993       -2.467219       0.561262
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31
GlyLys3 b3lyp E=-705.153491452 au
N       -4.909419       -1.618643       0.107499
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H       -5.631741       -1.948716       -0.528129
H       -5.329010       -0.867198       0.652299
C       -2.570704       -0.775471       0.154032
H       -3.495638       -1.848323       -1.409472
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O       -2.233718       -1.483732       1.128126
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H       -2.185000       0.833299        -1.043697
C       -0.567856       0.694197        0.308121
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C       1.966382        0.128476        0.290182
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H       2.261732        1.169921        0.117931
H       1.926911        -0.014801       1.378079
C       3.030966        -0.800794       -0.308050
H       2.756022        -1.847984       -0.126508
H       3.076654        -0.658774       -1.395779
C       4.404304        -0.533924       0.290633
H       4.742652        0.486317        0.101259
H       4.423405        -0.720144       1.365908
N       5.435794        -1.445806       -0.318766
H       5.521991        -1.278771       -1.326369
H       6.356409        -1.300037       0.105052
H       5.179695        -2.429657       -0.186707
###
30
GlyLys4 b3lyp E=-704.683728305 au
N       -4.870536       -1.585317       0.155232
C       -3.789101       -1.042038       -0.670405
H       -5.627838       -1.873985       -0.459564
H       -5.247857       -0.846027       0.745674
C       -2.519108       -0.781562       0.134637
H       -3.523256       -1.790417       -1.425897
H       -4.065332       -0.127631       -1.212233
O       -2.156355       -1.528736       1.069671
N       -1.806712       0.287068        -0.260394
H       -2.157632       0.868204        -1.013938
C       -0.507943       0.675834        0.292525
H       -0.520967       0.473619        1.365946
C       0.634240        -0.137584       -0.362724
C       -0.319473       2.194687        0.080945
H       0.377649        -1.198106       -0.251805
H       0.642920        0.078690        -1.438835
C       2.025660        0.108544        0.232255
O       -0.794832       2.697531        -0.983172
O       0.318829        2.827904        0.973668
H       2.329472        1.148073        0.057451
H       1.983671        -0.026270       1.321834
C       3.086110        -0.831467       -0.355769
H       2.800970        -1.874152       -0.153343
H       3.116492        -0.719116       -1.448110
C       4.481542        -0.580065       0.210183
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H       4.437389        -0.630529       1.309495
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N       5.468466        -1.522346       -0.352384
H       6.384192        -1.319923       0.044077
H       5.234954        -2.465358       -0.043290
###
31
GlyPhe1 b3lyp E=-763.355718384 au
N       5.104774        -1.139554       -0.044989
H       4.742430        -2.098308       0.005402
C       4.141946        -0.185143       0.570056
H       6.008008        -1.101157       0.437631
H       5.260119        -0.922816       -1.035092
C       2.756548        -0.425223       -0.016005
H       4.123694        -0.372535       1.645956
H       4.496092        0.829960        0.389057
O       2.499316        -1.477758       -0.624062
N       1.874670        0.562158        0.200519
H       2.172417        1.389012        0.708972
C       0.474207        0.482474        -0.194707
H       0.406156        -0.092692       -1.119723
C       -0.377845       -0.214474       0.911187
C       -0.014632       1.898097        -0.457954
H       0.137396        -1.155909       1.127335
H       -0.337242       0.401454        1.814917
C       -1.814567       -0.494788       0.528582
O       0.439332        2.890871        0.092113
C       -2.865572       0.251498        1.081689
C       -2.123609       -1.516657       -0.384345
H       -2.642327       1.042948        1.792759
C       -4.194054       -0.013326       0.731576
C       -3.448894       -1.782164       -0.738492
H       -1.321128       -2.109635       -0.816344
H       -4.994929       0.573104        1.173172
C       -4.489766       -1.030049       -0.181302
H       -3.669465       -2.577885       -1.444561
H       -5.520625       -1.237919       -0.453439
O       -1.019327       1.936428        -1.341055
H       -1.333850       2.856354        -1.432436
###
30
GlyPhe2 b3lyp E=-762.905312419 au
N       -0.669033       4.003925        -0.368096
C       -0.905812       2.849608        0.544999
H       0.142830        3.810114        -0.967151
H       -0.497083       4.861622        0.164558
C       -0.751541       1.553096        -0.244755
H       -0.148088       2.885382        1.330941
H       -1.893814       2.954768        0.992840
O       -0.106036       1.551604        -1.311184
N       -1.320970       0.481426        0.314207
H       -1.900333       0.607391        1.138662
C       -1.263126       -0.876881       -0.219488
H       -1.032677       -0.810050       -1.283999
C       -0.179942       -1.738965       0.488200
C       -2.638908       -1.566445       -0.051362
H       -0.427794       -1.795038       1.553849
H       -0.260259       -2.749803       0.075978
C       1.233253        -1.228537       0.314485
O       -3.418923       -1.121948       0.842402
C       1.859420        -0.474951       1.318900
C       1.947724        -1.493209       -0.865919
H       1.327858        -0.271928       2.245094
C       3.161337        0.009604        1.147681
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C       3.859261        -0.255905       -0.034146
H       3.784959        -1.231344       -1.959887
H       4.870971        0.116458        -0.167875
O       -2.861225       -2.559041       -0.805630
H       -1.474054       4.163321        -0.982594
###
29
GlyPhe3 b3lyp E=-762.441180565 au
N       -1.601743       3.875307        -0.466177
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H       -0.771804       4.016035        -1.039937
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H -1.735621 4.738323 0.056777
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32
GlyTyr1 b3lyp E=-838.589251242 au
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H 6.540144 -0.758393 0.044034
H 5.701711 0.516826 -0.619289
C 3.216167 -0.342422 -0.141275
H 4.513273 -1.845872 0.727451
H 4.682431 -0.231824 1.452239
O 3.208750 0.160070 -1.277020
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C -0.284141 -0.653332 1.119840
C 0.627956 1.259752 -0.271725
H -0.073635 -1.702893 1.351513
H -0.129071 -0.073506 2.035334
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31
GlyTyr2 b3lyp E=-838.138665802 au
N -0.902070 4.006971 -0.388382
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O       -3.240095       -2.517693       -0.790570
C       1.500935        -0.515277       1.337651
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H       3.299606        0.515013        1.963768
C       3.514102        -0.371813       0.010835
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O       4.818757        0.040000        -0.201731
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30
GlyTyr3 b3lyp E=-837.676404469 au
N       -1.098584       4.133182        -0.287179
H       -0.212500       4.114476        -0.789154
C       -1.217769       2.915050        0.508205
H       -1.821550       4.132852        -1.004999
C       -1.074918       1.605282        -0.272498
H       -0.433585       2.911458        1.273992
H       -2.173906       2.919189        1.039050
O       -0.450560       1.558628        -1.354557
N       -1.640799       0.530739        0.304085
H       -2.201008       0.669631        1.138033
C       -1.601331       -0.831162       -0.215853
H       -1.361135       -0.776680       -1.278966
C       -0.534501       -1.706147       0.502982
C       -2.983236       -1.508244       -0.057855
H       -0.789984       -1.750964       1.567648
H       -0.628172       -2.719929       0.099806
C       0.888113        -1.221056       0.337365
O       -3.758785       -1.076183       0.846783
O       -3.220094       -2.485655       -0.829834
C       1.525218        -0.472188       1.336681
C       1.612831        -1.502495       -0.833081
H       0.996017        -0.246386       2.258724
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H       1.147039        -2.085910       -1.623529
H       3.319691        0.562641        1.966931
C       3.533859        -0.306538       0.005956
H       3.474512        -1.283167       -1.912869
O       4.836967        0.111868        -0.205046
H       5.152266        0.603184        0.569513
###
29
GlyTyr4 b3lyp E=-837.198628873 au
N       5.509045        -1.297405       -0.039830
H       5.183792        -2.259882       0.032969
C       4.499824        -0.413101       0.534953
H       5.586486        -1.107446       -1.037751
C       3.084638        -0.584042       -0.021228
H       4.435479        -0.599166       1.613626
H       4.816527        0.626241        0.414113
O       2.704412        -1.669884       -0.513757
N       2.286839        0.491340        0.082517
H       2.654033        1.343630        0.493460
C       0.865901        0.514242        -0.268265
H       0.727651        -0.067306       -1.181871
C       0.009257        -0.118132       0.870700
C       0.448518        1.975046        -0.536529
H       0.470713        -1.085258       1.100111
H       0.117962        0.510888        1.761780
C       -1.455684       -0.310536       0.549242
O       1.006220        2.875905        0.163699
O       -0.439311       2.172462        -1.417867
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H       -2.136753       1.417972        1.642688
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H       -1.166175       -2.099456       -0.623283
H       -4.527445       1.097369        1.129571
C       -4.255744       -0.691517       -0.061152
H       -3.551072       -2.427008       -1.150396
O       -5.535542       -0.873483       -0.329657
###
27
GlyVal1 b3lyp E=-610.921215365 au
N       4.210426        -0.085468       -0.031777
H       4.216875        -1.078608       -0.286717
C       2.955804        0.274034        0.684186
H       5.026143        0.105490        0.558469
H       4.305928        0.452124        -0.900066
C       1.760589        -0.051274       -0.202101
H       2.915016        -0.301529       1.610738
H       2.993639        1.336964        0.927641
O       1.921111        -0.613981       -1.298053
N       0.570069        0.313142        0.303674
H       0.544529        0.728166        1.228960
C       -0.695797       -0.000340       -0.353436
H       -0.471103       -0.202950       -1.401587
C       -1.364009       -1.280313       0.249112
C       -1.636094       1.195131        -0.345074
H       -0.546296       -2.011466       0.265971
C       -1.863508       -1.078652       1.684988
C       -2.470088       -1.830445       -0.659248
O       -2.526691       1.347985        -1.167770
H       -2.721400       -0.396647       1.718738
H       -2.188638       -2.037760       2.101440
H       -1.084973       -0.679582       2.344135
H       -2.113008       -1.969056       -1.685578
H       -2.804287       -2.803236       -0.283229
H       -3.341626       -1.168146       -0.686734
O       -1.424005       2.052127        0.667645
H       -2.078961       2.774623        0.619411
###
26
GlyVal2 b3lyp E=-610.470692122 au
N       4.168495        0.005216        -0.121684
H       4.123112        -0.990959       -0.366053
C       2.932143        0.412334        0.603618
H       4.999660        0.172772        0.453100
H       4.272505        0.528325        -0.997364
C       1.715747        -0.120430       -0.147255
H       2.970619        -0.025171       1.603365
H       2.923224        1.498900        0.690839
O       1.854017        -1.031879       -0.988426
N       0.551045        0.439789        0.186143
H       0.530653        1.211464        0.846907
C       -0.740079       0.067720        -0.399067
H       -0.572605       -0.161196       -1.454704
C       -1.326707       -1.207186       0.284619
C       -1.684073       1.290675        -0.320779
H       -0.483368       -1.907602       0.333123
C       -1.810973       -0.948851       1.717791
C       -2.420878       -1.870754       -0.561655
O       -2.661463       1.303631        -1.125668
H       -2.693229       -0.297643       1.730990
H       -2.091704       -1.893707       2.195975
H       -1.036581       -0.480891       2.335049
H       -2.080997       -2.045463       -1.588821
H       -2.690312       -2.839728       -0.126722
H       -3.328873       -1.260595       -0.603926
O       -1.426300       2.182674        0.543268
###
25
GlyVal3 b3lyp E=-610.008514032 au
N       4.284957        0.129545        -0.057068
H       4.388681        -0.848838       -0.320424
C       3.005159        0.303407        0.621898
H       4.272297        0.651901        -0.931788
C       1.776504        -0.169273       -0.159501
H       3.020383        -0.265998       1.558606
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H       2.877986        1.354441        0.896417
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H       0.607307        1.135136        0.889605
C       -0.687146       0.066938        -0.395596
H       -0.526158       -0.154435       -1.453667
C       -1.306856       -1.202961       0.269122
C       -1.608897       1.305005        -0.305881
H       -0.482969       -1.927534       0.297971
C       -1.773149       -0.958849       1.710840
C       -2.427654       -1.818672       -0.578597
O       -2.562681       1.366361        -1.138440
H       -2.642470       -0.291086       1.742579
H       -2.067765       -1.905612       2.177031
H       -0.984688       -0.515223       2.328266
H       -2.102668       -1.985553       -1.611932
H       -2.723694       -2.786627       -0.158681
H       -3.317139       -1.180509       -0.602273
O       -1.363380       2.164172        0.594749
###
29
HisGly1 b3lyp E=-757.793205229 au
N       -1.823001       -2.972688       -0.602339
H       -1.197383       -3.595669       -1.125549
H       -2.747891       -3.001220       -1.045825
H       -1.905054       -3.341523       0.353290
C       -1.288379       -1.570590       -0.577001
H       -1.114291       -1.280535       -1.613915
C       -2.356145       -0.656288       0.064985
C       0.020627        -1.603212       0.222406
H       -3.287167       -0.792515       -0.494609
H       -2.535550       -0.975718       1.096212
C       -1.984376       0.791605        0.045225
O       0.104789        -2.287514       1.256524
N       -1.658546       1.502723        1.191411
C       -1.881233       1.682988        -0.987214
H       -1.645199       1.125681        2.134992
C       -1.369340       2.767435        0.881596
N       -1.497696       2.891155        -0.440092
H       -2.048234       1.560382        -2.045315
H       -1.090174       3.546062        1.573573
H       -1.344031       3.753956        -0.953292
N       1.012946        -0.848869       -0.263309
H       0.870443        -0.308503       -1.111622
C       2.276564        -0.685535       0.430528
C       3.107230        0.370392        -0.265901
H       2.114150        -0.384935       1.471621
H       2.845204        -1.623119       0.446989
O       2.759544        0.942764        -1.285397
O       4.291132        0.666115        0.293522
H       4.455852        0.159721        1.108813
###
28
HisGly2 b3lyp E=-757.346299454 au
N       1.128049        3.169455        -0.616241
H       0.327492        3.645307        -1.047914
H       1.967806        3.411395        -1.153828
H       1.236017        3.534042        0.338457
C       0.917313        1.681135        -0.587616
H       0.719105        1.369358        -1.613360
C       2.214525        1.025711        -0.064360
C       -0.293383       1.424317        0.319592
H       3.031384        1.326150        -0.727014
H       2.434121        1.411378        0.936597
C       2.160902        -0.466886       -0.023011
O       -0.333459       1.944126        1.453000
N       1.809838        -1.179983       1.116585
C       2.423212        -1.405529       -0.982460
H       1.552238        -0.769145       2.009768
C       1.852534        -2.489659       0.870213
N       2.222718        -2.642712       -0.401758
H       2.735178        -1.297218       -2.008781
H       1.631173        -3.279140       1.570858
H       2.341690        -3.541688       -0.858528
N       -1.244855       0.637587        -0.181664
H       -1.153981       0.242931        -1.114235
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C       -2.427380       0.230017        0.563524
C       -3.283428       -0.749594       -0.252847
H       -2.136227       -0.251801       1.502615
H       -3.036200       1.102962        0.820663
O       -2.882445       -1.074837       -1.409112
O       -4.339822       -1.155793       0.314617
###
27
HisGly3 b3lyp E=-756.889918092 au
N       1.744320        2.960944        -0.628888
H       1.117535        3.557558        -1.179881
H       2.675831        2.991367        -1.056347
H       1.802309        3.357584        0.316992
C       1.234712        1.547656        -0.565317
H       1.067445        1.228047        -1.594687
C       2.312155        0.665730        0.103161
C       -0.077339       1.586870        0.224430
H       3.243669        0.824433        -0.451987
H       2.472824        1.015376        1.127813
C       1.967032        -0.793484       0.121962
O       -0.173229       2.320782        1.230121
N       1.581509        -1.445530       1.283773
C       1.968901        -1.680945       -0.930490
C       1.355222        -2.700975       0.927240
N       1.574600        -2.888820       -0.399525
H       2.208610        -1.563936       -1.976512
H       1.042154        -3.500645       1.582437
N       -1.054888       0.800254        -0.225323
H       -0.903057       0.206199        -1.036235
C       -2.324678       0.619480        0.464224
C       -3.183529       -0.450255       -0.226096
H       -2.152821       0.319172        1.502992
H       -2.885201       1.559906        0.485908
O       -2.723831       -1.008059       -1.265764
O       -4.302646       -0.685841       0.317764
H       1.474725        -3.762515       -0.902416
###
26
HisGly4 b3lyp E=-756.428473121 au
N       1.066658        3.178017        -0.758443
H       0.215416        3.575379        -1.153863
H       1.174010        3.600482        0.163778
C       0.892857        1.727400        -0.594904
H       0.693898        1.301467        -1.582627
C       2.205515        1.117898        -0.052532
C       -0.288495       1.402306        0.328219
H       3.003329        1.456580        -0.720973
H       2.407461        1.542843        0.937372
C       2.224312        -0.379677       0.033479
O       -0.356316       1.886440        1.482664
N       1.926059        -1.067388       1.202937
C       2.508500        -1.280111       -0.969104
C       2.028989        -2.352663       0.898340
N       2.378106        -2.530061       -0.401382
H       2.785919        -1.145808       -2.003750
H       1.869210        -3.180405       1.573990
N       -1.242049       0.604595        -0.171889
H       -1.144593       0.215856        -1.104228
C       -2.411776       0.172917        0.577092
C       -3.275586       -0.801128       -0.236136
H       -2.110179       -0.323129       1.506149
H       -3.027702       1.033706        0.859025
O       -2.892651       -1.120017       -1.400705
O       -4.325418       -1.215808       0.340942
H       2.521003        -3.419685       -0.863364
###
44
HisLys0 b3lyp E=-970.887507171 au
N       1.965311        3.412020        -0.492525
H       1.142147        3.686710        -1.040302
H       1.830872        3.741561        0.471391
C       2.161262        1.922295        -0.515888
H       2.203685        1.624647        -1.563841
C       3.495893        1.607118        0.193388
C       0.949430        1.307299        0.198288
H       4.283590        2.175544        -0.309669
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H       3.442322        1.952794        1.230444
C       3.871764        0.162149        0.161164
O       0.626040        1.718505        1.325166
N       3.562600        -0.728780       1.180942
C       4.554591        -0.565490       -0.773775
C       4.029520        -1.942983       0.886817
N       4.634337        -1.859679       -0.298746
H       4.987798        -0.272574       -1.716618
H       3.938341        -2.827152       1.497870
H       5.089774        -2.638386       -0.765446
N       0.316906        0.332849        -0.469320
H       0.619335        0.096617        -1.409283
C       -0.836380       -0.386017       0.065467
H       -0.764712       -0.371674       1.155706
C       -2.161474       0.284417        -0.374605
C       -0.752488       -1.825260       -0.438864
H       -2.110982       1.318914        -0.017767
H       -2.187487       0.314476        -1.469984
C       -3.427516       -0.388731       0.166686
O       -0.348340       -2.112826       -1.554007
O       -1.176457       -2.799825       0.381351
H       -3.547617       -1.384001       -0.278108
H       -3.335040       -0.532180       1.251374
C       -4.676207       0.451261        -0.131200
H       -4.582691       1.433215        0.349877
H       -4.759820       0.623465        -1.212221
C       -5.941573       -0.234539       0.364165
H       -6.114787       -1.187733       -0.138516
H       -5.921454       -0.400679       1.442801
N       -7.148801       0.619221        0.086075
H       -7.244308       0.805293        -0.917536
H       -8.007194       0.160336        0.405679
H       -7.078239       1.523120        0.564841
H       2.782626        3.891274        -0.887794
H       3.049968        -0.500050       2.028149
H       -1.439476       -2.458905       1.254019
###
43
HisLys1 b3lyp E=-970.440817615 au
N       2.086409        3.440618        -0.471265
H       1.296655        3.763980        -1.040917
H       1.938337        3.774486        0.489155
C       2.185073        1.942602        -0.489298
H       2.233629        1.640502        -1.535847
C       3.480201        1.535158        0.249286
C       0.916177        1.410661        0.191464
H       4.309461        2.087517        -0.202608
H       3.410372        1.836019        1.299184
C       3.784345        0.074796        0.156667
O       0.505331        1.960960        1.232725
N       3.496290        -0.832924       1.167572
C       4.371415        -0.654262       -0.840549
C       3.882291        -2.057981       0.808646
N       4.416014        -1.965427       -0.409948
H       4.758110        -0.352425       -1.800641
H       3.784484        -2.956132       1.397767
H       4.802761        -2.749055       -0.927068
N       0.344990        0.356726        -0.393100
H       0.756637        -0.036789       -1.235095
C       -0.805893       -0.370290       0.150090
H       -0.757762       -0.316400       1.240100
C       -2.126260       0.272317        -0.337491
C       -0.686748       -1.850880       -0.280837
H       -2.085090       1.335857        -0.073785
H       -2.160993       0.212552        -1.432477
C       -3.394703       -0.349294       0.256706
O       -0.137171       -2.085375       -1.399599
O       -1.165938       -2.717253       0.507123
H       -3.470789       -1.401556       -0.039810
H       -3.335039       -0.331663       1.352808
C       -4.659506       0.392257        -0.196659
H       -4.615731       1.439760        0.128420
H       -4.716369       0.391922        -1.293110
C       -5.912705       -0.259819       0.370252
H       -6.017183       -1.294451       0.039065
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N       -7.151026       0.462507        -0.090225
H       -7.226640       0.449156        -1.112359
H       -7.995242       0.028037        0.294770
H       -7.136341       1.442957        0.209102
H       2.941939        3.870102        -0.840803
H       3.044810        -0.609349       2.049949
###
42
HisLys2 b3lyp E=-969.984957727 au
N       2.051388        3.446082        -0.464620
H       1.280684        3.764970        -1.061329
H       1.858794        3.764722        0.492858
C       2.177895        1.948202        -0.488163
H       2.238480        1.653501        -1.536412
C       3.470458        1.553707        0.259251
C       0.907812        1.396271        0.170243
H       4.289931        2.119091        -0.198677
H       3.390239        1.874023        1.302694
C       3.770542        0.085220        0.207305
O       0.432523        1.975343        1.169026
N       3.646878        -0.733532       1.319739
C       4.195310        -0.657168       -0.871440
C       3.991613        -1.944896       0.908884
N       4.327783        -1.946651       -0.406599
H       4.410550        -0.391325       -1.895277
H       4.015997        -2.838657       1.515020
H       4.624738        -2.750992       -0.945772
N       0.396777        0.295273        -0.383553
H       0.857293        -0.125281       -1.185756
C       -0.759760       -0.434024       0.143383
H       -0.740623       -0.360938       1.233431
C       -2.075481       0.184668        -0.388431
C       -0.623250       -1.920090       -0.259735
H       -2.018485       1.265459        -0.213557
H       -2.119339       0.035805        -1.474789
C       -3.346674       -0.362619       0.269078
O       -0.030005       -2.172770       -1.352003
O       -1.137927       -2.774490       0.519325
H       -3.439390       -1.437428       0.077063
H       -3.275223       -0.239225       1.357731
C       -4.605733       0.350647        -0.241974
H       -4.527214       1.428957        -0.051754
H       -4.694780       0.215759        -1.327783
C       -5.857137       -0.188593       0.435249
H       -6.005329       -1.250429       0.230860
H       -5.833240       -0.035342       1.515501
N       -7.088075       0.517900        -0.067809
H       -7.191889       0.396386        -1.080255
H       -7.932444       0.151046        0.381856
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H       2.915784        3.890044        -0.792292
###
41
HisLys3 b3lyp E=-969.523579555 au
N       -2.164010       3.426349        0.662027
H       -1.321626       3.680300        1.176262
H       -2.051238       3.815169        -0.274078
C       -2.245222       1.963142        0.557445
H       -2.301565       1.559490        1.572499
C       -3.541063       1.578826        -0.194366
C       -1.013962       1.369850        -0.142774
H       -4.363177       2.080794        0.325359
H       -3.494021       1.993465        -1.207773
C       -3.820565       0.106955        -0.270556
O       -0.637889       1.806538        -1.255296
N       -3.483782       -0.664785       -1.375377
C       -4.409293       -0.691242       0.684713
C       -3.863567       -1.899190       -1.078949
N       -4.427074       -1.963882       0.154414
H       -4.808510       -0.473073       1.663756
H       -3.760092       -2.765887       -1.715478
H       -4.803012       -2.793947       0.596105
N       -0.376707       0.383522        0.507289
H       -0.752922       0.049752        1.388418
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H       0.667238        -0.390519       -1.116301
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C       0.683225        -1.818563       0.503505
H       2.026334        1.359845        0.038772
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C       3.337027        -0.326807       -0.277479
O       0.233613        -1.983765       1.678698
O       1.097349        -2.737646       -0.263594
H       3.431240        -1.368024       0.051810
H       3.223795        -0.348220       -1.369412
C       4.620281        0.430335        0.089123
H       4.557241        1.468181        -0.262551
H       4.730558        0.461123        1.181124
C       5.848022        -0.234314       -0.516907
H       5.956737        -1.267232       -0.181637
H       5.827830        -0.216073       -1.607994
N       7.104727        0.483208        -0.100896
H       7.208197        0.480745        0.918957
H       7.934984        0.039073        -0.504657
H       7.088499        1.460444        -0.410504
###
40
HisLys4 b3lyp E=-969.053988425 au
N       -1.990314       3.344622        0.844546
H       -1.138460       3.514993        1.377317
H       -1.848131       3.780073        -0.066647
C       -2.162306       1.897093        0.654186
H       -2.260881       1.440683        1.643482
C       -3.462829       1.639512        -0.138618
C       -0.955666       1.272222        -0.061002
H       -4.266477       2.148711        0.403290
H       -3.377301       2.119757        -1.119513
C       -3.811587       0.191950        -0.329029
O       -0.582320       1.699383        -1.178352
N       -3.644301       -0.463022       -1.542716
C       -4.318002       -0.688338       0.601294
C       -4.041817       -1.709807       -1.334785
N       -4.455132       -1.893270       -0.055235
H       -4.585914       -0.568620       1.640192
H       -4.053639       -2.503071       -2.068111
H       -4.811656       -2.755965       0.337500
N       -0.334637       0.271062        0.581543
H       -0.678862       -0.023072       1.489206
C       0.819931        -0.465488       0.061380
H       0.703552        -0.554720       -1.021114
C       2.137726        0.283429        0.371184
C       0.816174        -1.882600       0.677232
H       2.034901        1.299174        -0.029130
H       2.239301        0.375757        1.460038
C       3.393964        -0.369789       -0.216923
O       0.465721        -1.986201       1.892815
O       1.187532        -2.838802       -0.066222
H       3.545713        -1.358088       0.235106
H       3.247302        -0.537649       -1.292713
C       4.653463        0.479690        -0.002065
H       4.519636        1.459036        -0.484116
H       4.790958        0.672491        1.070534
C       5.912632        -0.180624       -0.558519
H       6.093214        -1.126656       -0.035993
H       5.745324        -0.430391       -1.617961
N       7.101314        0.673716        -0.367858
H       7.916127        0.197066        -0.750324
H       6.989212        1.520199        -0.924945
###
44
LeuTyr1 b3lyp E=-995.858252349 au
N       3.849092        2.671711        0.008663
H       3.853182        2.779571        1.030211
H       3.240581        3.397915        -0.384029
H       4.801227        2.831701        -0.336885
C       3.380521        1.291431        -0.368763
H       3.280834        1.291693        -1.454448
C       4.434505        0.278240        0.102754
C       2.018680        1.102892        0.309859
H       5.390042        0.567750        -0.353893
H       4.544927        0.382376        1.188947
C       4.138835        -1.193712       -0.244648
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O 1.870671 1.398375 1.508269
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43
LeuTyr2 b3lyp E=-995.407691305 au
N -0.529063 -2.728849 -0.686633
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H -0.995359 -3.522693 -1.138282
C -1.475261 -1.562618 -0.550188
H -1.702168 -1.237723 -1.565757
C -2.733148 -2.042576 0.186835
C -0.700085 -0.482780 0.218071
H -3.147046 -2.885518 -0.382402
H -2.426728 -2.428989 1.166490
C -3.830845 -0.977690 0.376879
O -0.114267 -0.791644 1.274791
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C -4.375461 -0.451076 -0.958851
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H -3.607105 0.062865 -1.546432
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H -5.736125 -0.814173 1.423081
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C -0.889890 3.171012 0.008826
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H 1.782412 3.043711 -0.013441
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O -1.781068 3.134967 -0.890764
O -0.605679 4.168077 0.735825
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42
LeuTyr3 b3lyp E=-994.944877204 au
N       -0.761973       -2.497459       -1.353680
H       -0.359460       -3.002029       -0.563759
H       0.025062        -2.078970       -1.848800
C       -1.632425       -1.425927       -0.832052
H       -2.029029       -0.883856       -1.695096
C       -2.785399       -2.046195       -0.031373
C       -0.824298       -0.447243       0.034102
H       -3.283317       -2.777843       -0.680554
H       -2.349658       -2.608125       0.805228
C       -3.837385       -1.061472       0.516375
O       -0.294126       -0.824706       1.103951
H       -3.315062       -0.275833       1.081431
C       -4.644285       -0.386104       -0.603037
C       -4.774539       -1.787199       1.492921
H       -5.177807       -1.135334       -1.202377
H       -5.390238       0.299680        -0.184792
H       -4.008872       0.194865        -1.280036
H       -4.215889       -2.233927       2.323566
H       -5.514069       -1.097824       1.916399
H       -5.321234       -2.592818       0.985605
N       -0.695345       0.799748        -0.451290
H       -1.226053       1.054828        -1.276914
C       0.036262        1.890554        0.183766
H       0.119035        1.669400        1.249851
C       1.463079        2.069285        -0.410569
C       -0.744047       3.217519        0.018136
H       1.364391        2.274988        -1.482314
H       1.892310        2.961410        0.057091
C       2.387010        0.890378        -0.198779
O       -1.610372       3.287126        -0.904087
O       -0.424165       4.157761        0.805320
C       2.659674        -0.020087       -1.229224
C       2.995699        0.669592        1.048450
H       2.215553        0.130223        -2.209853
C       3.499418        -1.121328       -1.028610
C       3.833451        -0.423382       1.268422
H       2.810341        1.363062        1.865072
H       3.701058        -1.817265       -1.838942
C       4.080623        -1.322642       0.225283
H       4.297519        -0.584329       2.236931
O       4.915253        -2.395617       0.489550
H       4.996891        -2.947345       -0.303679
###
41
LeuTyr4 b3lyp E=-994.467107821 au
N       -3.374937       -2.076682       -1.825661
H       -3.214100       -2.903461       -1.250338
H       -2.638926       -2.073278       -2.530813
C       -3.243768       -0.877600       -0.977836
H       -3.355898       -0.008315       -1.631154
C       -4.353683       -0.879341       0.084364
C       -1.857732       -0.819285       -0.319916
H       -5.312441       -0.962344       -0.443470
H       -4.242126       -1.791686       0.685295
C       -4.401052       0.340719        1.025346
O       -1.481456       -1.719508       0.467493
H       -3.417267       0.446688        1.505246
C       -4.707107       1.646528        0.275699
C       -5.433448       0.103252        2.137623
H       -5.675333       1.581288        -0.237642
H       -4.754372       2.491794        0.971974
H       -3.945018       1.881221        -0.474991
H       -5.199183       -0.798909       2.714609
H       -5.463214       0.949226        2.833947
H       -6.440376       -0.019261       1.717824
N       -1.080073       0.221935        -0.655948
H       -1.440677       0.928105        -1.288713
C       0.279176        0.437787        -0.159809
H       0.322394        0.102711        0.878514
C       1.305360        -0.384082       -0.999894
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C       0.592750        1.947439        -0.214651
H       0.910229        -1.404866       -1.053461
H       1.303361        0.016817        -2.020135
C       2.714594        -0.408375       -0.452393
O       0.077732        2.613593        -1.165241
O       1.363878        2.411612        0.676124
C       3.069459        -1.258112       0.610980
C       3.727281        0.414217        -0.973816
H       2.315224        -1.918743       1.036770
C       4.362065        -1.283445       1.135094
C       5.027237        0.399377        -0.463725
H       3.492903        1.081800        -1.801811
H       4.601073        -1.956892       1.956164
C       5.399295        -0.449206       0.619989
H       5.786327        1.048590        -0.896272
O       6.623589        -0.466508       1.113799
###
36
LysAla1 b3lyp E=-745.385742171 au
N       0.013435        3.473400        -0.450734
H       -0.027037       3.738078        0.540961
H       -0.859727       3.774921        -0.896707
H       0.788393        3.981873        -0.890045
C       0.217084        1.988497        -0.580877
H       0.110064        1.750428        -1.640729
C       1.626815        1.638658        -0.083901
C       -0.886821       1.323987        0.250819
H       2.333879        2.247576        -0.660054
H       1.716886        1.935815        0.967795
C       1.977508        0.155708        -0.247561
O       -1.130769       1.739288        1.397998
H       1.316189        -0.457408       0.375891
H       1.811041        -0.147384       -1.289016
C       3.435191        -0.121661       0.141392
H       4.106884        0.482149        -0.482208
H       3.602069        0.173923        1.185056
C       3.781420        -1.594204       -0.028187
H       3.167395        -2.234851       0.607309
H       3.677893        -1.919189       -1.064894
N       5.211641        -1.853666       0.361340
H       5.371239        -1.620404       1.346841
H       5.457573        -2.838942       0.227132
H       5.856564        -1.288669       -0.200988
N       -1.528970       0.303212        -0.333242
H       -1.259574       0.011950        -1.267950
C       -2.549368       -0.484251       0.349228
H       -2.267276       -0.572561       1.403433
C       -3.945420       0.160883        0.252250
C       -2.552743       -1.882098       -0.257118
H       -4.281485       0.203124        -0.787732
H       -4.672831       -0.406600       0.839421
H       -3.897114       1.175722        0.653799
O       -1.988835       -2.169064       -1.300478
O       -3.244098       -2.828235       0.400728
H       -3.636158       -2.499197       1.228868
###
35
LysAla2 b3lyp E=-744.937712574 au
N       0.095926        3.444393        0.511831
H       0.146832        3.732086        -0.472946
H       0.973582        3.715477        0.967853
H       -0.669994       3.957348        0.961150
C       -0.136021       1.959773        0.601048
H       -0.028543       1.690549        1.653100
C       -1.555449       1.650590        0.105538
C       0.951363        1.296029        -0.254837
H       -2.248023       2.260564        0.698273
H       -1.646171       1.970407        -0.939532
C       -1.932579       0.171375        0.242932
O       1.196978        1.749354        -1.391926
H       -1.283649       -0.442208       -0.392960
H       -1.767717       -0.153004       1.278260
C       -3.395911       -0.075921       -0.144320
H       -4.055635       0.531364        0.488696
H       -3.561701       0.234299        -1.183925
C       -3.764713       -1.544697       0.009777
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H       -3.160694       -2.187381       -0.633124
H       -3.664554       -1.882193       1.042802
N       -5.199113       -1.779237       -0.380506
H       -5.357264       -1.527052       -1.361538
H       -5.456990       -2.763567       -0.262531
H       -5.835439       -1.215853       0.193056
N       1.569662        0.247665        0.292570
H       1.267666        -0.098989       1.199698
C       2.539547        -0.594935       -0.410404
H       2.207034        -0.704186       -1.447061
C       3.946300        0.024243        -0.395442
C       2.553743        -1.998927       0.236754
H       4.322959        0.106398        0.629569
H       4.634574        -0.597431       -0.974040
H       3.925895        1.022926        -0.840540
O       1.986068        -2.142045       1.360950
O       3.161308        -2.902868       -0.408749
###
34
LysAla3 b3lyp E=-744.476220140 au
N       0.025271        3.337651        0.695835
H       0.982094        3.514113        0.999786
H       -0.044868       3.706581        -0.252443
C       -0.211174       1.883789        0.656445
H       -0.056531       1.499501        1.669596
C       -1.661905       1.605056        0.239492
C       0.776777        1.186706        -0.289981
H       -2.309768       2.140482        0.943306
H       -1.835653       2.042496        -0.752465
C       -2.040762       0.118889        0.224654
O       0.802446        1.469573        -1.511424
H       -1.455485       -0.410787       -0.537955
H       -1.785216       -0.334309       1.191588
C       -3.534413       -0.092280       -0.052422
H       -4.127981       0.403320        0.726936
H       -3.803979       0.369688        -1.011129
C       -3.893648       -1.571230       -0.090058
H       -3.382014       -2.096389       -0.898481
H       -3.669323       -2.069854       0.854670
N       -5.369167       -1.753695       -0.329055
H       -5.652697       -1.321188       -1.214197
H       -5.620175       -2.746149       -0.365704
H       -5.917252       -1.317364       0.419431
N       1.611369        0.295321        0.265712
H       1.515162        0.058378        1.248037
C       2.598076        -0.492386       -0.471977
H       2.153306        -0.791731       -1.425785
C       3.880979        0.308716        -0.751259
C       2.927765        -1.776670       0.321440
H       4.375177        0.592003        0.184103
H       4.575873        -0.289492       -1.347090
H       3.645239        1.219259        -1.309346
O       2.578278        -1.835304       1.538872
O       3.555728        -2.677649       -0.310987
###
33
LysAla4 b3lyp E=-744.007310435 au
N       -0.074715       3.307166        0.702973
H       0.882193        3.493707        1.000802
H       -0.156075       3.680107        -0.242838
C       -0.294910       1.850470        0.657020
H       -0.135901       1.463320        1.668603
C       -1.741662       1.555016        0.237908
C       0.703800        1.171823        -0.291078
H       -2.395494       2.086940        0.939328
H       -1.917671       1.990585        -0.754818
C       -2.109387       0.065713        0.224229
O       0.724344        1.456522        -1.512298
H       -1.510299       -0.459577       -0.531967
H       -1.849672       -0.381389       1.193982
C       -3.597368       -0.176016       -0.060126
H       -4.204021       0.324811        0.708129
H       -3.867934       0.281063        -1.022954
C       -3.968647       -1.661955       -0.094790
H       -3.376789       -2.168237       -0.866046
H       -3.700421       -2.128096       0.860382
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N       -5.391130       -1.950807       -0.354193
H       -5.658115       -1.510890       -1.234519
H       -5.952884       -1.488510       0.360254
N       1.555228        0.295223        0.262978
H       1.469565        0.062811        1.247146
C       2.565891        -0.461912       -0.474122
H       2.131782        -0.773205       -1.428791
C       3.825706        0.377133        -0.749872
C       2.936474        -1.734862       0.318601
H       4.311907        0.669379        0.186930
H       4.537269        -0.198308       -1.348560
H       3.564098        1.283492        -1.303175
O       2.613079        -1.794327       1.543211
O       3.573002        -2.624886       -0.321014
###
34
LysDAla3 b3lyp E=-744.475997810 au
N       -0.047288       3.302376        -0.271426
H       -1.028596       3.490047        -0.473201
H       0.095833        3.557019        0.705610
C       0.217405        1.861077        -0.424056
H       0.021002        1.598855        -1.468325
C       1.691516        1.574803        -0.108904
C       -0.716432       1.033910        0.471839
H       2.292205        2.220930        -0.759868
H       1.896620        1.882734        0.925006
C       2.114482        0.114381        -0.307489
O       -0.688360       1.160792        1.718933
H       1.559469        -0.535726       0.380763
H       1.856829        -0.207397       -1.325259
C       3.618504        -0.083403       -0.078392
H       4.184136        0.548184        -0.775564
H       3.882326        0.235461        0.938352
C       4.024967        -1.537113       -0.271616
H       3.523496        -2.198780       0.436972
H       3.822744        -1.885559       -1.286137
N       5.503522        -1.716197       -0.048032
H       5.768292        -1.442024       0.903715
H       5.778966        -2.693800       -0.181784
H       6.045964        -1.142867       -0.702316
N       -1.571871       0.213277        -0.156743
H       -1.603045       0.204891        -1.171406
C       -2.612997       -0.572008       0.504791
C       -3.725822       -0.909359       -0.513477
O       -3.493065       -0.712196       -1.744372
O       -4.796650       -1.385893       -0.032011
C       -2.054153       -1.857210       1.137737
H       -1.642498       -2.521328       0.370133
H       -1.260204       -1.614665       1.849447
H       -3.058326       0.044578        1.292026
H       -2.845976       -2.388836       1.672248
###
33
LysDAla4 b3lyp E=-744.007299160 au
N       0.043387        3.299447        -0.276211
H       -0.936220       3.499333        -0.474714
H       0.192503        3.553852        0.699992
C       0.288959        1.854189        -0.426767
H       0.088425        1.593459        -1.470760
C       1.758933        1.544843        -0.111355
C       -0.656390       1.041090        0.469663
H       2.369235        2.183270        -0.761384
H       1.967850        1.850764        0.922683
C       2.162446        0.078528        -0.309815
O       -0.632747       1.174866        1.716298
H       1.588683        -0.562398       0.373002
H       1.898308        -0.235995       -1.329243
C       3.659772        -0.162504       -0.077394
H       4.244948        0.469977        -0.760392
H       3.927205        0.144810        0.943906
C       4.068450        -1.625179       -0.280207
H       3.484263        -2.263754       0.392438
H       3.816459        -1.935675       -1.300927
N       5.495357        -1.921957       -0.058750
H       5.745093        -1.646079       0.890510
H       6.053067        -1.327387       -0.671194
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N -1.516968 0.224352 -0.157202
H -1.543671 0.209458 -1.171832
C -2.563375 -0.552659 0.505690
C -3.676382 -0.889268 -0.512594
O -3.442372 -0.696430 -1.743901
O -4.749336 -1.360806 -0.030632
C -2.012087 -1.837625 1.145852
H -1.601070 -2.506702 0.382242
H -1.218989 -1.595622 1.858660
H -3.007207 0.069837 1.289135
H -2.807631 -2.363573 1.680461
###
42
LysGlu1 b3lyp E=-973.290109260 au
N 1.733498 3.692917 -0.243892
H 1.846208 3.861529 0.763177
H 0.896810 4.196092 -0.558391
H 2.544698 4.087078 -0.732273
C 1.622283 2.217101 -0.512883
H 1.380389 2.110548 -1.571738
C 2.971121 1.555784 -0.192721
C 0.487657 1.692908 0.373741
H 3.727597 2.049636 -0.814322
H 3.222343 1.755749 0.855853
C 2.990833 0.047035 -0.460670
O 0.414359 2.049199 1.560637
H 2.293409 -0.462885 0.213950
H 2.648315 -0.149553 -1.484551
C 4.395899 -0.538605 -0.271031
H 5.095816 -0.053728 -0.963390
H 4.748818 -0.335893 0.748176
C 4.399791 -2.040586 -0.518390
H 3.757060 -2.569886 0.186935
H 4.086197 -2.284369 -1.534754
N 5.782240 -2.610992 -0.348644
H 6.126595 -2.460439 0.604964
H 5.788377 -3.619180 -0.531294
H 6.444784 -2.170099 -0.994741
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C -0.937211 -1.248689 0.894911
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H -2.413483 -0.449059 -1.340536
C -3.866238 -0.679590 0.258376
O -0.243995 -1.942635 0.171175
O -1.321612 -1.724597 2.092600
H -3.634470 -1.734562 0.418450
H -4.097074 -0.219069 1.225447
C -5.092794 -0.624745 -0.623079
O -5.460971 -1.540367 -1.344607
O -5.812824 0.520851 -0.621450
H -5.442187 1.178824 -0.008186
H -1.853342 -1.083000 2.595128
###
41
LysGlu2 b3lyp E=-972.843334332 au
N -1.183419 3.438313 0.678698
H -1.061234 3.739014 -0.295742
H -0.336216 3.694264 1.196900
H -1.973074 3.953053 1.082192
C -1.434487 1.955440 0.728748
H -1.413405 1.670071 1.782114
C -2.812642 1.671962 0.114326
C -0.284770 1.295969 -0.044007
H -3.544492 2.271459 0.669510
H -2.817339 2.023489 -0.924504
C -3.215629 0.194360 0.174562
O 0.075846 1.775672 -1.137806
H -2.535995 -0.405210 -0.441994
H -3.121728 -0.169330 1.205659
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C       -5.055114       -1.481894       -0.241664
H       -4.425849       -2.109459       -0.875264
H       -5.024032       -1.863754       0.780139
N       -6.467906       -1.667011       -0.725200
H       -6.567754       -1.345892       -1.693715
H       -6.746573       -2.652239       -0.689462
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N       0.256038        0.217167        0.527746
H       -0.114430       -0.123500       1.410572
C       1.292300        -0.615241       -0.084794
H       1.121277        -0.641834       -1.163729
C       2.689332        -0.010371       0.193030
C       1.163635        -2.052039       0.477379
H       2.668515        1.029955        -0.146787
H       2.868774        -0.004344       1.273575
C       3.830670        -0.764144       -0.522582
O       0.696480        -2.175222       1.649250
O       1.554889        -2.993307       -0.271221
H       3.937309        -1.773695       -0.123128
H       3.615635        -0.833539       -1.594524
C       5.146999        -0.055295       -0.317477
O       5.952082        -0.331258       0.561480
O       5.436242        0.974084        -1.149725
H       4.738445        1.098306        -1.815905
###
40
LysGlu3 b3lyp E=-972.387361404 au
N       -1.154235       3.461163        0.578152
H       -1.038397       3.737951        -0.404154
H       -0.303379       3.728905        1.084189
H       -1.941097       3.985379        0.974716
C       -1.404042       1.979758        0.664775
H       -1.369188       1.717838        1.723922
C       -2.789735       1.681012        0.075310
C       -0.262776       1.304878        -0.107305
H       -3.515411       2.290210        0.628016
H       -2.810145       2.010681        -0.970529
C       -3.185548       0.203552        0.172131
O       0.083823        1.764227        -1.215148
H       -2.514238       -0.404976       -0.444746
H       -3.070907       -0.139365       1.208250
C       -4.631900       -0.023715       -0.285112
H       -5.314427       0.576189        0.330471
H       -4.750079       0.307868        -1.324697
C       -5.018663       -1.492018       -0.177945
H       -4.398044       -2.125749       -0.813937
H       -4.959864       -1.854233       0.849810
N       -6.440065       -1.700273       -0.625158
H       -6.563145       -1.406007       -1.599526
H       -6.709074       -2.686473       -0.557188
H       -7.091225       -1.155213       -0.050686
N       0.285719        0.239427        0.479620
H       -0.073120       -0.080404       1.374547
C       1.329737        -0.595829       -0.120460
H       1.164998        -0.625451       -1.200094
C       2.726941        0.004976        0.168384
C       1.192575        -2.028445       0.446534
H       2.695848        1.055858        -0.141934
H       2.900342        -0.011016       1.249975
C       3.877444        -0.704826       -0.564306
O       0.747788        -2.143066       1.628999
O       1.555253        -2.980267       -0.304207
H       3.967974        -1.735834       -0.205960
H       3.670419        -0.736560       -1.638254
C       5.216842        0.001699        -0.325270
O       5.691016        -0.017452       0.856429
O       5.781741        0.571800        -1.313686
###
39
LysGlu4 b3lyp E=-971.925349600 au
N       -1.134347       3.340530        0.828960
H       -0.204259       3.475812        1.223164
H       -1.091219       3.693848        -0.126839
C       -1.439540       1.899890        0.785640
H       -1.420353       1.529506        1.815250
C       -2.844545       1.684227        0.205759
```

```
C       -0.387070       1.133822        -0.028241
H       -3.541848       2.268684        0.817346
H       -2.875487       2.104998        -0.807976
C       -3.297911       0.219492        0.171000
O       -0.207127       1.383893        -1.243549
H       -2.628218       -0.367131       -0.470736
H       -3.227362       -0.210471       1.178914
C       -4.734681       0.071472        -0.345458
H       -5.423424       0.625459        0.305494
H       -4.813450       0.507087        -1.350148
C       -5.159105       -1.389291       -0.399315
H       -4.525284       -1.973928       -1.068580
H       -5.153550       -1.853242       0.588468
N       -6.564474       -1.517816       -0.923849
H       -6.639832       -1.129585       -1.869398
H       -6.856340       -2.499043       -0.960736
H       -7.226799       -1.013913       -0.325385
N       0.326137        0.213319        0.639109
H       0.132873        0.050839        1.621608
C       1.371085        -0.624056       0.048964
H       1.104193        -0.814194       -0.992947
C       2.738671        0.099233        0.103042
C       1.407160        -1.971590       0.805224
H       2.597577        1.089668        -0.345548
H       3.012381        0.254767        1.151874
C       3.867121        -0.633607       -0.635965
O       1.151021        -1.947872       2.047872
O       1.713058        -3.002055       0.134789
H       4.067603        -1.598105       -0.152920
H       3.570257        -0.841999       -1.668273
C       5.185876        0.149898        -0.642127
O       5.626533        0.583939        0.470310
O       5.780135        0.308567        -1.757337
###
38
LysGlu5 b3lyp E=-971.455842077 au
N       -1.174775       3.276723        0.940786
H       -0.242094       3.398834        1.333120
H       -1.140195       3.670879        0.000768
C       -1.476845       1.838351        0.837411
H       -1.448119       1.423973        1.849995
C       -2.887016       1.644025        0.261600
C       -0.428094       1.114074        -0.018302
H       -3.577361       2.201913        0.905610
H       -2.928462       2.111673        -0.731330
C       -3.344845       0.183135        0.165534
O       -0.248215       1.431892        -1.217451
H       -2.689383       -0.369514       -0.520928
H       -3.241329       -0.295810       1.149262
C       -4.795716       0.045578        -0.314416
H       -5.464658       0.577559        0.377375
H       -4.906601       0.529781        -1.295391
C       -5.254731       -1.411872       -0.425664
H       -4.600075       -1.949388       -1.121363
H       -5.146294       -1.904340       0.547662
N       -6.645516       -1.602927       -0.876315
H       -6.760623       -1.149476       -1.782215
H       -7.266581       -1.102369       -0.241401
N       0.284760        0.154638        0.593771
H       0.095078        -0.063448       1.566107
C       1.336841        -0.636620       -0.044411
H       1.083696        -0.747035       -1.100944
C       2.701208        0.084652        0.079138
C       1.371338        -2.037846       0.605832
H       2.564740        1.101936        -0.304648
H       2.958536        0.167840        1.141840
C       3.851445        -0.594420       -0.686069
O       1.101123        -2.114295       1.843471
O       1.693344        -3.010377       -0.139447
H       4.022210        -1.600540       -0.293396
H       3.587044        -0.675756       -1.745729
C       5.142125        0.220522        -0.545749
O       5.906511        -0.045057       0.437614
O       5.366602        1.134933        -1.403125
###
48
```

PheArg1 b3lyp E=-1085.99109045 au

| | | | |
|---|---|---|---|
| N | 2.454664 | 3.647638 | -0.297387 |
| H | 1.646367 | 3.964961 | -0.843421 |
| H | 2.305233 | 3.923676 | 0.680685 |
| C | 2.631127 | 2.158156 | -0.393895 |
| H | 2.676989 | 1.914760 | -1.456110 |
| C | 3.947475 | 1.771162 | 0.311866 |
| C | 1.399776 | 1.527184 | 0.265338 |
| H | 4.747289 | 2.355087 | -0.157950 |
| H | 3.883043 | 2.073368 | 1.362113 |
| C | 4.263559 | 0.293536 | 0.212167 |
| O | 0.971369 | 1.977920 | 1.342174 |
| C | 4.113905 | -0.545420 | 1.325583 |
| C | 4.707642 | -0.262225 | -0.998510 |
| H | 3.775430 | -0.125618 | 2.269270 |
| C | 4.399284 | -1.911946 | 1.233200 |
| C | 4.990831 | -1.627193 | -1.094272 |
| H | 4.836129 | 0.377973 | -1.867902 |
| H | 4.281316 | -2.547312 | 2.106393 |
| C | 4.835733 | -2.457052 | 0.022223 |
| H | 5.335675 | -2.041595 | -2.037397 |
| H | 5.058021 | -3.517764 | -0.050996 |
| N | 0.862958 | 0.489019 | -0.389375 |
| H | 1.272956 | 0.193782 | -1.269671 |
| C | -0.265731 | -0.284204 | 0.121562 |
| H | -0.222436 | -0.282309 | 1.212586 |
| C | -1.612424 | 0.326232 | -0.344625 |
| C | -0.102031 | -1.713445 | -0.375476 |
| H | -1.596785 | 1.375049 | -0.029822 |
| H | -1.640635 | 0.311082 | -1.440171 |
| C | -2.854204 | -0.366261 | 0.226699 |
| O | 0.400519 | -2.006379 | -1.450182 |
| O | -0.592357 | -2.616300 | 0.482991 |
| H | -2.907664 | -1.403970 | -0.120214 |
| H | -2.799152 | -0.387798 | 1.321876 |
| C | -4.124622 | 0.363468 | -0.204907 |
| H | -4.117086 | 1.391985 | 0.173623 |
| H | -4.179901 | 0.402566 | -1.298807 |
| N | -5.306853 | -0.338283 | 0.312572 |
| H | -5.157833 | -1.173566 | 0.866885 |
| C | -6.569918 | 0.007963 | 0.056290 |
| N | -6.850837 | 1.105487 | -0.653329 |
| N | -7.578108 | -0.768775 | 0.489866 |
| H | -6.122179 | 1.706850 | -1.009519 |
| H | -7.812297 | 1.343903 | -0.856263 |
| H | -7.381344 | -1.532519 | 1.123630 |
| H | -8.525030 | -0.413835 | 0.461055 |
| H | 3.287339 | 4.132626 | -0.649090 |
| H | -0.514862 | -3.508653 | 0.093469 |

###

47

PheArg2 b3lyp E=-1085.54114793 au

| | | | |
|---|---|---|---|
| N | 2.468388 | 3.620712 | -0.339489 |
| H | 1.673286 | 3.935269 | -0.905922 |
| H | 2.298460 | 3.909439 | 0.631531 |
| C | 2.633788 | 2.127868 | -0.408715 |
| H | 2.687224 | 1.865744 | -1.466104 |
| C | 3.941294 | 1.745402 | 0.315454 |
| C | 1.389367 | 1.521068 | 0.250824 |
| H | 4.748596 | 2.322741 | -0.149720 |
| H | 3.865698 | 2.057745 | 1.362069 |
| C | 4.256580 | 0.266521 | 0.233418 |
| O | 0.957441 | 2.010136 | 1.314713 |
| C | 4.093092 | -0.562777 | 1.352035 |
| C | 4.714963 | -0.300260 | -0.966729 |
| H | 3.742678 | -0.134902 | 2.287701 |
| C | 4.378484 | -1.930279 | 1.274887 |
| C | 4.998108 | -1.666129 | -1.047491 |
| H | 4.853986 | 0.332162 | -1.840193 |
| H | 4.248307 | -2.558235 | 2.151676 |
| C | 4.829012 | -2.486269 | 0.074077 |
| H | 5.353100 | -2.088904 | -1.983112 |
| H | 5.050289 | -3.547898 | 0.012332 |
| N | 0.852709 | 0.474771 | -0.379492 |
| H | 1.280843 | 0.131616 | -1.234394 |
| C | -0.272878 | -0.314121 | 0.127679 |

```
H       -0.216666       -0.327743       1.218486
C       -1.613260       0.322175        -0.310322
C       -0.125647       -1.761828       -0.398865
H       -1.601182       1.367330        0.019815
H       -1.655838       0.328431        -1.406260
C       -2.854265       -0.377099       0.254145
O       0.397319        -1.908814       -1.544737
O       -0.559879       -2.689008       0.344438
H       -2.894210       -1.415447       -0.092170
H       -2.804500       -0.399554       1.349898
C       -4.129398       0.341096        -0.181902
H       -4.132044       1.370727        0.194023
H       -4.182008       0.377572        -1.276145
N       -5.309419       -0.367145       0.332969
H       -5.157080       -1.205655       0.881440
C       -6.573011       -0.026718       0.073761
N       -6.856301       1.071123        -0.634806
N       -7.579817       -0.807651       0.503722
H       -6.128117       1.671284        -0.993920
H       -7.817828       1.305122        -0.842261
H       -7.381899       -1.569613       1.139248
H       -8.527783       -0.455778       0.472688
H       3.311349        4.095454        -0.679890
###
46
PheArg3 b3lyp E=-1085.08073483 au
N       2.150509        3.449036        -0.814136
H       1.290428        3.506469        -1.358193
H       1.942675        3.867663        0.092406
C       2.505439        2.035265        -0.613152
H       2.679374        1.594089        -1.599208
C       3.806961        1.948440        0.209087
C       1.366296        1.268996        0.075271
H       4.548750        2.563976        -0.310731
H       3.630065        2.404659        1.189609
C       4.342555        0.542597        0.383503
O       0.971429        1.594197        1.218976
C       4.186459        -0.149838       1.594141
C       5.008247        -0.102031       -0.672763
H       3.679305        0.335126        2.424344
C       4.678592        -1.451005       1.746967
C       5.500505        -1.401613       -0.525157
H       5.146349        0.421729        -1.615715
H       4.549731        -1.968152       2.693830
C       5.337055        -2.081786       0.687276
H       6.015378        -1.880978       -1.353242
H       5.722367        -3.090674       0.804462
N       0.815101        0.269875        -0.630359
H       1.173751        0.055353        -1.554841
C       -0.309024       -0.552157       -0.182560
H       -0.197066       -0.734383       0.889143
C       -1.647550       0.182005        -0.438669
C       -0.256060       -1.907878       -0.922308
H       -1.563341       1.175048        0.017195
H       -1.762416       0.331908        -1.519392
C       -2.883609       -0.528315       0.122993
O       0.242887        -1.917945       -2.088644
O       -0.741109       -2.909743       -0.318427
H       -3.022619       -1.497623       -0.368052
H       -2.749572       -0.721110       1.194666
C       -4.134801       0.322458        -0.084885
H       -4.035441       1.272991        0.450954
H       -4.267391       0.544131        -1.150691
N       -5.320225       -0.388473       0.413492
H       -5.204948       -1.350264       0.712073
C       -6.563160       0.094147        0.376322
N       -6.801576       1.335595        -0.057909
N       -7.597242       -0.680776       0.754490
H       -6.056775       1.924802        -0.400881
H       -7.747365       1.692244        -0.084463
H       -7.410080       -1.541977       1.251921
H       -8.500213       -0.249622       0.904125
###
45
PheArg4 b3lyp E=-1084.60104616 au
N       2.103712        3.451074        -0.809821
```

```
H       1.254052        3.506066        -1.370275
H       1.874617        3.862779        0.094791
C       2.463489        2.038248        -0.609470
H       2.657294        1.603130        -1.594374
C       3.750868        1.955426        0.234541
C       1.317080        1.261511        0.054413
H       4.500464        2.570597        -0.274518
H       3.556917        2.414255        1.210541
C       4.285174        0.550864        0.422846
O       0.909785        1.569036        1.198816
C       4.122069        -0.131278       1.638390
C       4.957539        -0.102464       -0.623840
H       3.609463        0.360607        2.461134
C       4.614074        -1.430716       1.805497
C       5.449462        -1.400501       -0.462034
H       5.101206        0.413077        -1.570488
H       4.479695        -1.939713       2.756011
C       5.279224        -2.070209       0.755281
H       5.969336        -1.886855       -1.282888
H       5.664275        -3.077849       0.883518
N       0.773695        0.273740        -0.672932
H       1.143438        0.072691        -1.596094
C       -0.350977       -0.559627       -0.245868
H       -0.245838       -0.755322       0.824219
C       -1.692886       0.169068        -0.500962
C       -0.283111       -1.904664       -1.002981
H       -1.612138       1.161609        -0.043071
H       -1.807063       0.322019        -1.581577
C       -2.927352       -0.546145       0.058504
O       0.218718        -1.894163       -2.168334
O       -0.759005       -2.920256       -0.414750
H       -3.060067       -1.517342       -0.430067
H       -2.786701       -0.740799       1.130314
C       -4.188728       0.293724        -0.139981
H       -4.068472       1.270420        0.351307
H       -4.336410       0.483267        -1.209322
N       -5.362261       -0.406764       0.383902
H       -5.173693       -1.031985       1.160103
C       -6.605819       0.184393        0.386316
N       -6.953270       1.242904        -0.285646
N       -7.567605       -0.505140       1.113511
H       -6.161090       1.607845        -0.810312
H       -7.230809       -1.026413       1.915098
H       -8.384999       0.054487        1.323085
###
22
SerGly1 b3lyp E=-607.510897419 au
N       -3.253676       -0.837736       0.081998
H       -3.105907       -1.809053       -0.220189
H       -4.119389       -0.478199       -0.333024
H       -3.368213       -0.852567       1.102644
C       -2.083082       -0.004497       -0.328906
H       -2.182932       0.165103        -1.405677
C       -2.138899       1.343051        0.398199
C       -0.819832       -0.850111       -0.103288
H       -3.150371       1.754721        0.300304
H       -1.909623       1.212229        1.462067
O       -1.183473       2.200949        -0.229896
O       -0.914121       -2.084781       0.025469
H       -1.054959       2.978361        0.333718
N       0.338557        -0.184274       -0.106227
H       0.323673        0.831795        -0.191552
C       1.613630        -0.860573       0.034149
C       2.738551        0.150098        0.018045
H       1.663958        -1.422193       0.974618
H       1.770604        -1.577614       -0.780048
O       2.572919        1.355685        -0.060895
O       3.984857        -0.346521       0.098803
H       3.995319        -1.318978       0.149703
###
21
SerGly2 b3lyp E=-607.062341666 au
N       -3.207235       -0.816923       0.073012
H       -3.037538       -1.794468       -0.198925
H       -4.064219       -0.476293       -0.373604
H       -3.348568       -0.806618       1.090263
```

C -2.027336 0.009886 -0.328258
H -2.121339 0.184808 -1.404606
C -2.076964 1.354266 0.403709
C -0.774582 -0.853187 -0.100689
H -3.089681 1.766109 0.316601
H -1.839254 1.219522 1.465335
O -1.128428 2.215840 -0.228648
O -0.897889 -2.092130 0.005173
H -1.000292 2.993002 0.335175
N 0.391879 -0.212737 -0.076995
H 0.410616 0.803299 -0.153614
C 1.670204 -0.897250 0.059107
C 2.844410 0.091192 0.022114
H 1.709062 -1.451559 1.002829
H 1.798139 -1.624754 -0.749023
O 2.589496 1.325628 -0.095959
O 3.996342 -0.428697 0.114629
###
20
SerGly3 b3lyp E=-606.601199303 au
N -3.332978 -0.746450 0.045631
H -3.333163 -1.647115 -0.428407
H -3.300265 -0.967113 1.041303
C -2.109970 -0.031125 -0.320888
H -2.149919 0.168848 -1.399541
C -2.102367 1.324677 0.393383
C -0.832115 -0.872971 -0.096898
H -3.097758 1.769597 0.294633
H -1.880335 1.196687 1.460349
O -1.122401 2.182696 -0.218069
O -0.903517 -2.117593 0.026385
H -1.013200 2.965710 0.340899
N 0.338615 -0.222017 -0.090878
H 0.341714 0.792975 -0.170677
C 1.621842 -0.892194 0.052243
C 2.794616 0.097249 0.021182
H 1.664581 -1.447288 0.996100
H 1.763923 -1.622188 -0.752116
O 2.544163 1.332759 -0.098867
O 3.948370 -0.420944 0.120559
###
34
SerLeu1 b3lyp E=-764.777605153 au
N 3.709835 -1.740437 -0.375257
H 3.193819 -2.627548 -0.409904
H 4.602127 -1.885922 0.107703
H 3.907047 -1.470950 -1.346413
C 2.891566 -0.702288 0.321729
H 2.853266 -0.988957 1.376961
C 3.588599 0.657109 0.193876
C 1.467308 -0.785821 -0.250995
H 4.651816 0.534389 0.433253
H 3.496566 1.034759 -0.830892
O 2.963163 1.543303 1.124418
O 1.134454 -1.767406 -0.939518
H 3.203575 2.451920 0.889317
N 0.650483 0.222463 0.077806
H 1.027626 0.993140 0.627136
C -0.753576 0.264809 -0.325898
H -0.839260 -0.244757 -1.287461
C -1.654717 -0.428468 0.730851
C -1.139424 1.732206 -0.487773
H -1.233348 -1.429761 0.882012
H -1.539211 0.118368 1.674041
C -3.151115 -0.557932 0.386708
O -0.689919 2.619074 0.220583
O -2.040093 2.042243 -1.435599
H -3.555957 0.446305 0.200359
C -3.394658 -1.416480 -0.863560
C -3.898265 -1.140577 1.596029
H -2.979000 -2.423388 -0.730166
H -4.468436 -1.520307 -1.055614
H -2.941845 -0.985574 -1.763752
H -3.765479 -0.515312 2.486281
H -4.972368 -1.214132 1.392536
H -3.531998 -2.147391 1.833717

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H       -2.306317       1.267869        -1.961833
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33
SerLeu2 b3lyp E=-764.327487412 au
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H       3.064502        -2.565170       -0.544447
H       4.467520        -2.041070       0.220697
H       4.027804        -1.423614       -1.257792
C       2.856449        -0.701437       0.330658
H       2.806281        -0.981676       1.387181
C       3.567591        0.648432        0.198179
C       1.431019        -0.790492       -0.246103
H       4.626318        0.518083        0.452910
H       3.493862        1.012764        -0.833190
O       2.941278        1.554752        1.108069
O       1.093037        -1.820725       -0.867086
H       3.210694        2.455476        0.874427
N       0.630029        0.244872        0.001565
H       1.006215        1.046544        0.504700
C       -0.782592       0.298200        -0.392161
H       -0.882328       -0.218128       -1.347465
C       -1.658219       -0.393051       0.682927
C       -1.185481       1.777218        -0.582305
H       -1.242583       -1.395934       0.847088
H       -1.533800       0.161871        1.621268
C       -3.160419       -0.524790       0.366556
O       -0.653240       2.629462        0.191802
O       -2.041427       2.027697        -1.481666
H       -3.559457       0.477320        0.160579
C       -3.426853       -1.408703       -0.861154
C       -3.897488       -1.076462       1.596739
H       -3.014459       -2.415168       -0.712585
H       -4.503902       -1.512495       -1.036603
H       -2.984026       -0.996245       -1.773653
H       -3.752036       -0.431988       2.471499
H       -4.974725       -1.149879       1.408280
H       -3.534121       -2.079660       1.854722
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32
SerLeu3 b3lyp E=-763.866098394 au
N       3.806338        -1.772587       -0.285347
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H       3.871340        -1.593759       -1.287498
C       2.916150        -0.777742       0.313172
H       2.826205        -1.008563       1.382474
C       3.576863        0.600413        0.196951
C       1.477550        -0.841538       -0.254809
H       4.633285        0.496583        0.465255
H       3.511396        0.971131        -0.833697
O       2.932824        1.520680        1.096200
O       1.095133        -1.847284       -0.895279
H       3.217674        2.417645        0.868310
N       0.673924        0.198992        0.011250
H       1.062227        0.991122        0.518432
C       -0.735159       0.273949        -0.385521
H       -0.842155       -0.245121       -1.338547
C       -1.631482       -0.397417       0.685322
C       -1.121020       1.755640        -0.585802
H       -1.239259       -1.409340       0.852117
H       -1.499042       0.154670        1.624401
C       -3.135034       -0.494233       0.361749
O       -0.625216       2.602285        0.219081
O       -1.929823       2.020704        -1.525566
H       -3.507400       0.515726        0.142950
C       -3.416211       -1.382093       -0.859918
C       -3.896449       -1.014063       1.590846
H       -3.035930       -2.398919       -0.697037
H       -4.494127       -1.454780       -1.045826
H       -2.951245       -0.992607       -1.771450
H       -3.740019       -0.365621       2.460815
H       -4.974031       -1.059539       1.394964
H       -3.563331       -2.024505       1.861218
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49
TyrArg1 b3lyp E=-1161.22471569 au
N       1.904438        3.949424        -0.280765
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H 2.325303 2.266915 -1.460241
C 3.537077 2.206317 0.354706
C 1.027007 1.731998 0.206822
H 4.299479 2.852933 -0.094178
H 3.411071 2.512810 1.398387
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C 4.610030 0.249571 -0.855482
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C 5.018705 -1.083893 -0.922748
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H 4.016047 -2.102225 2.169264
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C -0.218297 -1.592458 -0.557501
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H -1.917613 0.311975 -1.559852
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H -2.973628 -0.451537 1.226048
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N -7.724291 -0.941851 0.824555
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H -8.696073 -0.836988 0.562730
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H 2.705995 4.515408 -0.578757
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48
TyrArg2 b3lyp E=-1160.77470918 au
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C 2.218339 2.447943 -0.405796
H 2.344829 2.213753 -1.463519
C 3.523096 2.183915 0.374236
C 1.012806 1.710524 0.187496
H 4.291622 2.834277 -0.059014
H 3.372973 2.491721 1.414324
C 3.978133 0.741466 0.320990
O 0.512227 2.117665 1.255816
C 3.761513 -0.123272 1.404265
C 4.628278 0.232383 -0.813124
H 3.264340 0.249508 2.295866
C 4.175678 -1.455853 1.363140
C 5.047995 -1.098019 -0.871491
H 4.816700 0.882975 -1.663407
H 4.006843 -2.117427 2.207243
C 4.819295 -1.941205 0.221287
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O 5.215130 -3.265724 0.224253
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C -0.493216 -0.237700 -0.036687
H -0.436246 -0.301173 1.052570

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C       -1.876053       0.326516        -0.441351
C       -0.253568       -1.644978       -0.632157
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H       -1.946449       0.337384        -1.535882
C       -3.058145       -0.444460       0.154178
O       0.285977        -1.703633       -1.778205
O       -0.635997       -2.632687       0.060224
H       -3.048926       -1.482878       -0.193354
H       -2.972052       -0.465451       1.247935
C       -4.388430       0.197064        -0.234512
H       -4.432204       1.232953        0.121978
H       -4.495393       0.207234        -1.325239
N       -5.499010       -0.565193       0.353221
H       -5.268942       -1.337723       0.967974
C       -6.790569       -0.273743       0.197237
N       -7.174684       0.730341        -0.598279
N       -7.721991       -0.985158       0.858311
H       -6.497251       1.344690        -1.026923
H       -8.152046       0.984389        -0.652976
H       -7.448459       -1.843220       1.319595
H       -8.693397       -0.892585       0.590350
H       5.664907        -3.476188       -0.608985
H       2.710566        4.479015        -0.608299
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47
TyrArg3 b3lyp E=-1160.31406952 au
N       -1.710106       3.784913        0.622298
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H       -1.457045       4.115706        -0.308751
C       -2.127223       2.376913        0.524904
H       -2.346712       2.025026        1.537421
C       -3.411184       2.283166        -0.323504
C       -1.011401       1.505467        -0.069401
H       -4.134887       2.970851        0.127252
H       -3.189850       2.655947        -1.330041
C       -4.008736       0.894552        -0.411207
O       -0.573889       1.720828        -1.223762
C       -3.870009       0.109325        -1.566037
C       -4.723818       0.350776        0.667643
H       -3.325951       0.505502        -2.419432
C       -4.422332       -1.171520       -1.650267
C       -5.280554       -0.928277       0.602912
H       -4.855290       0.936472        1.574156
H       -4.313422       -1.766154       -2.552310
C       -5.129572       -1.688355       -0.561741
H       -5.836086       -1.333530       1.444902
O       -5.669341       -2.956934       -0.688116
N       -0.525943       0.537976        0.723848
H       -0.927625       0.396250        1.644720
C       0.541377        -0.388891       0.346223
H       0.418369        -0.639751       -0.710464
C       1.930177        0.265230        0.551239
C       0.395189        -1.682003       1.180055
H       1.898612        1.249250        0.069899
H       2.085729        0.435505        1.623811
C       3.096966        -0.540920       -0.027632
O       -0.119453       -1.576844       2.334832
O       0.826311        -2.752916       0.658928
H       3.182221        -1.507764       0.479787
H       2.914801        -0.744849       -1.090441
C       4.415825        0.214973        0.116927
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H       4.619193        0.424135        1.173688
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H       5.288308        -1.506321       -0.807618
C       6.788149        -0.204908       -0.499533
N       7.169719        0.984714        -0.022548
N       7.703136        -1.012653       -1.064831
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H       8.134123        1.276677        -0.108510
H       7.460766        -1.974702       -1.263394
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H       -6.149695       -3.190761       0.121548
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46
TyrArg4 b3lyp E=-1159.83696185 au
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H -3.236322 2.616411 -1.342224
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C -5.328651 -0.986199 0.572554
H -4.953935 0.895383 1.532232
H -4.258494 -1.840561 -2.544708
C -5.160299 -1.817955 -0.575497
H -5.902648 -1.375487 1.411495
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H 2.050138 0.448496 1.628289
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H 7.422470 -1.952345 -1.276561
H 8.646763 -0.763341 -0.991060
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45
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H -4.331380 -1.792536 -2.459499
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32
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31
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H -2.853582 1.004962 2.210062
C -3.224078 0.918188 0.087213

H -3.414226 0.595227 -2.033871
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C 2.295695 2.565392 -0.260557
H 1.923105 1.397474 1.512663
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30
TyrGly3 b3lyp E=-837.679598987 au
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H -1.262008 3.895645 0.242513
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H -0.549835 1.700376 -1.556622
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C 2.902362 -0.753833 -1.186521
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H 2.958836 -1.231804 2.186717
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29
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H -0.461125 1.694610 -1.559966
C 1.025713 2.282221 -0.107202
C -1.244127 1.274754 0.397476
H 1.511709 2.967152 -0.811703
H 1.033937 2.771285 0.874679
C 1.788021 0.975202 -0.039628
O -1.416425 1.616141 1.592157
C 2.035927 0.322138 1.179588
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H 1.684140 0.776180 2.104687
C 2.725526 -0.891004 1.242001
C 2.961153 -0.860543 -1.160679
H 2.109888 0.830255 -2.169482
H 2.901194 -1.364887 2.206028
C 3.214176 -1.538534 0.069642
H 3.323850 -1.311561 -2.082515
O 3.862519 -2.687590 0.117341
N -1.772116 0.151620 -0.107978
H -1.630686 -0.086043 -1.084532
C -2.597818 -0.772208 0.653055
C -3.131548 -1.909202 -0.229648
H -2.027968 -1.209809 1.479950
H -3.451610 -0.246434 1.093948
O -2.826151 -1.912914 -1.458858
O -3.854162 -2.768188 0.360098

```
###
46
TyrHisOMe3 b3lyp E=-1142.71351150 au
N       1.797400        4.035051        -0.485274
H       1.601162        4.361875        0.468575
H       1.042770        4.370307        -1.093912
H       2.675465        4.460722        -0.801325
C       1.896182        2.535288        -0.507577
H       1.995015        2.241746        -1.553538
C       3.142280        2.111329        0.298153
C       0.588662        2.006003        0.091527
H       3.997173        2.637942        -0.141691
H       3.027475        2.463236        1.328614
C       3.388830        0.618180        0.281924
O       0.100691        2.546246        1.098639
C       3.145663        -0.164471       1.418427
C       3.867193        -0.020696       -0.873748
H       2.781249        0.307130        2.327193
C       3.366033        -1.544828       1.409289
C       4.089096        -1.397212       -0.900967
H       4.074316        0.565218        -1.765694
H       3.176896        -2.140328       2.298571
C       3.833522        -2.159304       0.244594
H       4.460623        -1.883880       -1.797565
O       4.063519        -3.519919       0.172225
H       3.852286        -3.932951       1.024186
N       0.047655        0.952371        -0.538271
H       0.511545        0.568462        -1.355821
C       -1.163556       0.288624        -0.083157
H       -1.221912       0.363269        1.004169
C       -2.419152       0.976091        -0.708194
C       -1.070518       -1.178702       -0.481576
H       -2.313405       2.045507        -0.510990
H       -2.402920       0.832386        -1.792563
C       -3.729634       0.522184        -0.154196
O       -0.410292       -1.581648       -1.428565
O       -1.816566       -1.953590       0.302922
N       -4.552422       -0.398623       -0.789528
C       -4.388134       0.877226        0.991135
H       -4.347336       -0.862804       -1.669474
C       -5.656972       -0.604070       -0.070412
N       -5.571658       0.165482        1.015581
H       -4.119068       1.567962        1.773777
H       -6.470688       -1.265123       -0.323721
H       -6.281463       0.216747        1.739601
C       -1.872322       -3.368637       -0.030653
H       -2.258369       -3.496449       -1.043329
H       -0.877206       -3.807317       0.059140
H       -2.552293       -3.804362       0.699055
###
45
TyrHisOMe4 b3lyp E=-1142.25671457 au
N       1.844502        4.024719        -0.445593
H       1.687054        4.347100        0.516813
H       1.076873        4.379167        -1.026560
H       2.719669        4.436209        -0.787743
C       1.912630        2.522997        -0.483278
H       1.977286        2.238272        -1.534157
C       3.171267        2.067407        0.283949
C       0.613168        2.011771        0.149765
H       4.024777        2.579670        -0.175159
H       3.091784        2.413529        1.319689
C       3.383646        0.569426        0.249373
O       0.184450        2.532238        1.194780
C       3.152732        -0.218136       1.385133
C       3.814887        -0.069676       -0.924566
H       2.824790        0.253431        2.307703
C       3.337754        -1.603497       1.357244
C       4.001566        -1.450874       -0.970552
H       4.011615        0.519443        -1.816747
H       3.158102        -2.203358       2.245615
C       3.757779        -2.217662       0.174364
H       4.335803        -1.938015       -1.881485
O       3.950010        -3.583004       0.082582
H       3.745165        -3.999432       0.934400
N       0.017862        0.996295        -0.490918
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H 0.427782 0.649806 -1.352652
C -1.213206 0.364576 -0.026293
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H -2.391442 1.094756 -1.693669
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O -0.726984 -1.466476 -1.537701
O -1.729198 -1.902763 0.441589
N -4.514617 -0.318600 -0.979625
C -4.448892 0.746724 1.012522
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H -6.330344 -0.068550 1.627473
C -1.828302 -3.309878 0.089871
H -2.417313 -3.423979 -0.821604
H -0.829528 -3.728967 -0.044204
H -2.331084 -3.778608 0.933933
###
44
TyrHisOMe5 b3lyp E=-1141.79718066 au
N 1.752779 4.014846 -0.621861
H 0.900993 4.269342 -1.119886
H 1.651504 4.380510 0.324733
C 1.863628 2.550619 -0.557459
H 1.915697 2.177490 -1.584225
C 3.165249 2.165887 0.177958
C 0.646973 1.922925 0.138484
H 3.980687 2.681064 -0.340718
H 3.118919 2.569141 1.195818
C 3.445138 0.678593 0.226946
O 0.339110 2.237117 1.306719
C 3.243107 -0.064642 1.398528
C 3.910400 -0.003655 -0.910168
H 2.889240 0.435834 2.296088
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C 4.161671 -1.375861 -0.885782
H 4.084539 0.547044 -1.831344
H 3.334439 -2.001748 2.360329
C 3.949649 -2.093808 0.296035
H 4.524046 -1.891912 -1.769870
O 4.213824 -3.452296 0.277304
H 4.039534 -3.830580 1.153202
N -0.065064 1.038000 -0.589277
H 0.215251 0.851228 -1.545771
C -1.263124 0.365994 -0.098977
H -1.206846 0.316404 0.988368
C -2.549317 1.144858 -0.509978
C -1.276255 -1.048909 -0.660560
H -2.437258 2.150822 -0.094790
H -2.563001 1.234169 -1.600917
C -3.836044 0.539729 -0.037965
O -0.961674 -1.325444 -1.810783
O -1.687970 -1.945491 0.238406
N -4.577543 -0.330405 -0.826206
C -4.467280 0.719321 1.172199
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H -0.833751 -3.698718 -0.522679
H -2.174399 -3.871512 0.654947
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43
TyrHisOMe6 b3lyp E=-1141.31980301 au
N 1.879578 4.082947 -0.052001
H 1.010640 4.476171 -0.411206
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C 1.883048 2.627566 -0.260972
H 1.823791 2.447162 -1.338171

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C       3.203043        2.029284        0.270548
C       0.676984        1.965575        0.419611
H       4.009877        2.586250        -0.219767
H       3.267456        2.246096        1.343810
C       3.371873        0.543357        0.032535
O       0.477840        2.092762        1.643983
C       3.161680        -0.399979       1.052435
C       3.740687        0.043859        -1.229984
H       2.881557        -0.052801       2.045799
C       3.306082        -1.771721       0.831692
C       3.888487        -1.322495       -1.468291
H       3.922074        0.743344        -2.045242
H       3.141467        -2.471825       1.648599
C       3.675715        -2.292718       -0.443055
H       4.181141        -1.672169       -2.456622
O       3.820344        -3.586046       -0.660931
N       -0.162172       1.282483        -0.391074
H       0.074584        1.204586        -1.374175
C       -1.386177       0.620319        0.053994
H       -1.589952       0.963997        1.067927
C       -2.549465       0.969769        -0.888251
C       -1.138685       -0.892220       0.089236
H       -2.646038       2.062129        -0.894457
H       -2.285935       0.668088        -1.907388
C       -3.855941       0.329690        -0.515369
O       -1.011142       -1.584697       -0.911249
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N       -4.799676       0.017345        -1.484411
C       -4.343294       -0.003391       0.728786
C       -5.831210       -0.490741       -0.826635
N       -5.602194       -0.524491       0.509725
H       -3.928819       0.083341        1.721371
H       -6.750866       -0.846751       -1.267550
H       -6.235989       -0.881265       1.214155
C       -0.767748       -2.782520       1.482512
H       -1.557303       -3.367141       1.006931
H       0.202295        -3.015739       1.039662
H       -0.751761       -2.960452       2.556522
###
27
ValGly1 b3lyp E=-610.922015572 au
N       -2.680925       -1.351426       -0.932773
H       -2.881357       -1.814742       -0.039457
H       -2.304090       -2.063438       -1.567046
H       -3.558853       -1.001603       -1.330563
C       -1.704488       -0.223330       -0.747097
H       -1.448731       0.121145        -1.750926
C       -2.374360       0.940048        0.034523
C       -0.472289       -0.838951       -0.074327
H       -3.347919       1.081670        -0.454677
C       -2.617323       0.626298        1.517128
C       -1.585617       2.245527        -0.138425
O       -0.582179       -1.856208       0.634169
H       -1.672365       0.519290        2.061398
H       -3.174425       1.449490        1.975258
H       -3.202621       -0.287522       1.664793
H       -1.397137       2.464633        -1.194923
H       -2.161847       3.075559        0.281882
H       -0.624805       2.214482        0.385336
N       0.696878        -0.226773       -0.303015
H       0.737213        0.608210        -0.879368
C       1.929503        -0.680846       0.311193
C       3.070343        0.235411        -0.068482
H       1.844355        -0.695074       1.404413
H       2.174750        -1.700738       -0.007495
O       2.941580        1.241780        -0.745317
O       4.285972        -0.111521       0.386060
H       4.268555        -0.941326       0.895524
###
26
ValGly2 b3lyp E=-610.473720427 au
N       -2.541032       -1.350081       -1.055283
H       -2.761621       -1.863056       -0.194246
H       -2.116236       -2.017486       -1.706905
H       -3.412307       -1.007042       -1.472590
C       -1.606786       -0.205742       -0.767702
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H       -1.292462       0.176117        -1.740700
C       -2.359651       0.916982        -0.003741
C       -0.409007       -0.810269       -0.022770
H       -3.289728       1.066028        -0.569301
C       -2.726892       0.553511        1.442279
C       -1.576063       2.235515        -0.063806
O       -0.566989       -1.816271       0.700534
H       -1.833694       0.454856        2.068616
H       -3.345996       1.349574        1.867751
H       -3.298659       -0.377995       1.513647
H       -1.327906       2.508301        -1.095120
H       -2.184489       3.039656        0.361671
H       -0.646744       2.183849        0.512705
N       0.764898        -0.202548       -0.200743
H       0.845199        0.601882        -0.816801
C       1.994101        -0.622679       0.456371
C       3.196845        0.195172        -0.036028
H       1.909737        -0.503774       1.542133
H       2.183114        -1.682392       0.258452
O       2.991450        1.116744        -0.879814
O       4.316721        -0.129855       0.458686
###
25
ValGly3 b3lyp E=-610.009245808 au
N       2.321919        -1.387563       1.326466
H       2.665760        -1.924215       0.531713
H       3.147455        -1.050018       1.819558
C       1.577336        -0.219587       0.825977
H       1.157545        0.293422        1.696969
C       2.453495        0.832606        0.078436
C       0.411314        -0.742754       -0.012941
H       3.252057        1.061932        0.799003
C       3.119385        0.314782        -1.203833
C       1.685651        2.134741        -0.189710
O       0.578391        -1.631297       -0.880620
H       2.384335        0.142597        -1.997885
H       3.838978        1.054100        -1.573343
H       3.665644        -0.620491       -1.039642
H       1.194918        2.506445        0.717324
H       2.369948        2.913608        -0.544021
H       0.917274        1.998728        -0.959704
N       -0.794558       -0.214018       0.240366
H       -0.899278       0.505889        0.947689
C       -2.005810       -0.590237       -0.470684
C       -3.223412       0.200493        0.027601
H       -1.893179       -0.412469       -1.545909
H       -2.208736       -1.659116       -0.342365
O       -3.054948       1.053566        0.948705
O       -4.322443       -0.069720       -0.543869
###
28
AlaGlyGly1 b3lyp E=-740.332930605 au
N       5.053939        0.515759        -0.633882
H       5.171392        1.218629        0.105182
H       4.888065        1.016924        -1.512958
H       5.925362        -0.016384       -0.725478
C       3.913255        -0.399780       -0.299719
H       3.739474        -1.017506       -1.182751
C       4.287138        -1.263585       0.904080
C       2.695593        0.486028        -0.017753
H       4.471291        -0.643210       1.786811
H       3.472394        -1.957050       1.124323
H       5.184918        -1.847529       0.680926
O       2.842753        1.667064        0.349356
N       1.505618        -0.104221       -0.169292
H       1.449664        -1.085272       -0.429044
C       0.259114        0.553077        0.178501
C       -0.900576       -0.402656       -0.062135
H       0.256776        0.847203        1.234735
H       0.123196        1.462580        -0.414756
O       -0.713488       -1.606452       -0.320170
N       -2.122475       0.141325        0.044696
H       -2.221920       1.131007        0.247451
C       -3.330180       -0.650076       -0.087306
C       -4.548224       0.231662        0.014296
H       -3.359390       -1.169391       -1.051408
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H       -3.391726       -1.417750       0.692417
O       -4.522540       1.446368        0.139302
O       -5.679398       -0.486506       -0.048257
H       -6.444403       0.115901        0.012259
###
27
AlaGlyGly2 b3lyp E=-739.881611110 au
N       5.040619        0.423910        -0.450538
H       5.096399        1.206932        0.211108
H       4.969112        0.821512        -1.392806
H       5.909459        -0.117437       -0.394652
C       3.858092        -0.442077       -0.129188
H       3.771638        -1.167523       -0.940612
C       4.088958        -1.148805       1.205960
C       2.631844        0.475420        -0.093823
H       4.186261        -0.424965       2.021034
H       3.246594        -1.810349       1.420131
H       4.997645        -1.755996       1.155132
O       2.760698        1.692675        0.140311
N       1.453874        -0.122231       -0.293534
H       1.404707        -1.119310       -0.484475
C       0.191347        0.585795        -0.183023
C       -0.959799       -0.410438       -0.269929
H       0.143642        1.131538        0.764418
H       0.088627        1.320867        -0.989468
O       -0.756069       -1.616224       -0.525875
N       -2.176114       0.104787        -0.069621
H       -2.287949       1.090199        0.151556
C       -3.406362       -0.669349       -0.139869
C       -4.629567       0.206665        0.167369
H       -3.531307       -1.104335       -1.137425
H       -3.380211       -1.498529       0.574828
O       -4.441031       1.432768        0.422893
O       -5.749891       -0.384361       0.136684
###
26
AlaGlyGly3 b3lyp E=-739.419533340 au
N       4.963137        -0.178851       -0.916539
H       5.230897        0.801605        -0.834278
H       4.580863        -0.291237       -1.854517
C       3.918345        -0.467004       0.074245
H       3.614742        -1.509779       -0.058559
C       4.468967        -0.287331       1.492093
C       2.682228        0.424253        -0.104703
H       4.829103        0.737002        1.639139
H       3.698768        -0.492134       2.242499
H       5.303181        -0.975566       1.657093
O       2.784853        1.666169        -0.218279
N       1.491093        -0.196424       -0.117292
H       1.440913        -1.209072       -0.075661
C       0.233553        0.514932        -0.250897
C       -0.926689       -0.471122       -0.190906
H       0.129568        1.266819        0.537521
H       0.189961        1.044690        -1.210451
O       -0.739375       -1.702817       -0.289373
N       -2.138206       0.077132        -0.049951
H       -2.241388       1.083013        0.047781
C       -3.374828       -0.688530       -0.030157
C       -4.594519       0.231585        0.127555
H       -3.485879       -1.265244       -0.954442
H       -3.370766       -1.404547       0.798917
O       -4.394379       1.476566        0.247842
O       -5.722907       -0.344823       0.128317
###
46
AlaLysAla1 b3lyp E=-992.738508576 au
N       3.917962        -3.074073       -0.882574
H       3.965593        -2.580362       -1.782244
H       3.253292        -3.847645       -0.988097
C       3.488957        -2.125777       0.199703
H       3.273212        -2.733169       1.080436
C       4.614706        -1.134158       0.488073
C       2.216861        -1.431977       -0.303023
H       4.846261        -0.534625       -0.397598
H       4.315178        -0.465750       1.298361
H       5.513287        -1.673644       0.802107
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O       2.039068        -1.262432       -1.522557
N       1.372941        -1.016413       0.652515
H       1.567530        -1.256344       1.619856
C       0.109138        -0.331634       0.370434
H       0.211088        0.129421        -0.610973
C       -1.064040       -1.335312       0.350466
C       -0.073403       0.718197        1.474503
H       -0.794046       -2.122059       -0.362632
H       -1.138932       -1.802049       1.339594
C       -2.411683       -0.723716       -0.049308
O       0.012411        0.368269        2.664498
H       -2.693610       0.069248        0.654471
C       -3.520203       -1.784005       -0.075644
H       -3.248114       -2.589298       -0.770091
H       -3.623221       -2.233493       0.920517
C       -4.856187       -1.189825       -0.498196
H       -5.187572       -0.402131       0.180701
H       -4.822889       -0.792429       -1.514069
N       -5.931778       -2.242949       -0.485070
H       -6.046582       -2.635382       0.454788
H       -6.832923       -1.853942       -0.778917
H       -5.698814       -3.015066       -1.118104
N       -0.308536       2.013127        1.150212
H       -0.445738       2.624873        1.951975
C       -0.525180       2.611798        -0.167723
H       -1.008028       1.888827        -0.827446
C       -1.439480       3.838754        -0.030414
C       0.776064        3.021973        -0.872996
H       -0.995762       4.581054        0.640751
H       -1.595347       4.297139        -1.008794
H       -2.408045       3.529859        0.370241
O       1.918076        3.009893        -0.167228
O       0.789344        3.370757        -2.042658
H       1.759656        2.688417        0.740040
H       4.840259        -3.468934       -0.672946
H       -2.324345       -0.258172       -1.039215
###
45
AlaLysAla2 b3lyp E=-992.289026439 au
N       3.414252        -3.669057       -0.867700
H       3.662536        -3.131139       -1.706726
H       2.651121        -4.305535       -1.121107
C       3.006282        -2.736937       0.236753
H       2.612670        -3.360173       1.041820
C       4.220378        -1.940199       0.710700
C       1.910304        -1.829745       -0.335014
H       4.638940        -1.342045       -0.104279
H       3.923517        -1.270803       1.521410
H       4.988196        -2.620655       1.090211
O       1.927829        -1.517672       -1.539135
N       0.996676        -1.407448       0.551204
H       1.043602        -1.757955       1.503037
C       -0.112584       -0.504271       0.223953
H       0.066612        -0.136354       -0.784262
C       -1.454477       -1.257265       0.263254
C       -0.076499       0.641174        1.248585
H       -1.377066       -2.092094       -0.442606
H       -1.589680       -1.684567       1.263558
C       -2.662128       -0.385065       -0.099504
O       -0.354821       0.391878        2.444779
H       -2.732523       0.464559        0.591625
C       -3.972529       -1.180886       -0.048722
H       -3.927898       -2.017955       -0.757471
H       -4.106347       -1.607769       0.953829
C       -5.171173       -0.303693       -0.380202
H       -5.274467       0.525817        0.321466
H       -5.120829       0.093806        -1.395377
N       -6.448032       -1.097041       -0.294856
H       -6.564832       -1.502446       0.639149
H       -7.263775       -0.508601       -0.489304
H       -6.447067       -1.867469       -0.970818
N       0.269387        1.874139        0.853469
H       0.337401        2.574120        1.590099
C       0.753591        2.340814        -0.451959
H       1.348812        1.551988        -0.917076
C       -0.395412       2.737448        -1.392940
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C       1.701347        3.546737        -0.231900
H       -0.979294       3.560512        -0.967478
H       0.004593        3.055503        -2.359535
H       -1.063569       1.887005        -1.556916
O       1.695439        4.116697        0.899442
O       2.402038        3.886375        -1.230753
H       4.223062        -4.232357       -0.586162
H       -2.526163       0.033558        -1.104593
###
44
AlaLysAla3 b3lyp E=-991.827485708 au
N       2.941244        -4.213162       -0.434105
H       3.087585        -4.063297       -1.432027
H       2.025710        -4.651260       -0.342818
C       2.931054        -2.910184       0.241734
H       2.720534        -3.088160       1.300753
C       4.300870        -2.237120       0.114228
C       1.851870        -1.970919       -0.318839
H       4.551206        -2.067112       -0.938705
H       4.316283        -1.273058       0.632163
H       5.069789        -2.878292       0.555266
O       1.731425        -1.787060       -1.548192
N       1.069839        -1.356948       0.592552
H       1.175486        -1.610790       1.568592
C       -0.033180       -0.452455       0.253298
H       0.150780        -0.092204       -0.757368
C       -1.385372       -1.189444       0.290819
C       0.009253        0.699678        1.266611
H       -1.308362       -2.037706       -0.399138
H       -1.534639       -1.598685       1.296647
C       -2.581411       -0.312706       -0.098374
O       -0.270026       0.463707        2.465964
H       -2.651420       0.547410        0.580029
C       -3.899770       -1.095489       -0.051421
H       -3.858737       -1.937167       -0.754932
H       -4.044062       -1.515415       0.952658
C       -5.088641       -0.209700       -0.395005
H       -5.189586       0.623816        0.302256
H       -5.028962       0.182654        -1.411704
N       -6.372456       -0.992367       -0.313665
H       -6.497396       -1.392673       0.621444
H       -7.182753       -0.398795       -0.515161
H       -6.373513       -1.765888       -0.986071
N       0.361189        1.928666        0.862990
H       0.434364        2.632425        1.595375
C       0.849706        2.383631        -0.444604
H       1.442269        1.588850        -0.903147
C       -0.295542       2.778780        -1.390826
C       1.801700        3.587544        -0.231611
H       -0.876383       3.607703        -0.972559
H       0.107892        3.088109        -2.358835
H       -0.967325       1.930459        -1.550204
O       1.798268        4.163908        0.896609
O       2.502848        3.920100        -1.232556
H       -2.430819       0.090814        -1.107584
###
43
AlaLysAla4 b3lyp E=-991.358859786 au
N       2.941529        -4.183107       -0.450489
H       3.074609        -4.025853       -1.449179
H       2.036032        -4.640205       -0.352504
C       2.910546        -2.883316       0.230795
H       2.713270        -3.069510       1.290970
C       4.265125        -2.181748       0.093311
C       1.808204        -1.962949       -0.315877
H       4.502669        -2.004240       -0.961382
H       4.264912        -1.218583       0.613142
H       5.050979        -2.807924       0.525933
O       1.667392        -1.784490       -1.544100
N       1.030032        -1.358262       0.604670
H       1.155648        -1.604003       1.580399
C       -0.084803       -0.462965       0.277011
H       0.083700        -0.107373       -0.738072
C       -1.434588       -1.202611       0.336439
C       -0.033384       0.695620        1.282670
H       -1.351852       -2.076421       -0.320348
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H       -1.586467       -1.575588       1.356109
C       -2.631389       -0.346864       -0.096725
O       -0.303714       0.468715        2.485938
H       -2.682567       0.563547        0.515959
C       -3.963111       -1.100584       0.014668
H       -3.902829       -2.042091       -0.550126
H       -4.143912       -1.372845       1.064368
C       -5.156485       -0.290179       -0.501325
H       -5.215486       0.659904        0.042255
H       -4.996740       -0.038083       -1.555997
N       -6.466431       -0.956409       -0.388463
H       -6.628286       -1.193153       0.590065
H       -6.422656       -1.848568       -0.880412
N       0.319742        1.921331        0.869818
H       0.399770        2.628722        1.597896
C       0.799244        2.368327        -0.443693
H       1.386782        1.569963        -0.902605
C       -0.352270       2.761000        -1.383397
C       1.754879        3.571668        -0.243905
H       -0.929275       3.592113        -0.964173
H       0.044586        3.066244        -2.355440
H       -1.026137       1.912913        -1.534755
O       1.759421        4.155015        0.880759
O       2.450705        3.897094        -1.250957
H       -2.483103       -0.016907       -1.133803
###
29
CysGlyGly1 b3lyp E=-1138.51618407 au
N       4.068630        -1.780156       0.922016
H       3.498529        -2.377304       1.531987
H       4.962897        -1.608687       1.394739
H       4.254479        -2.297464       0.053798
C       3.364101        -0.482423       0.620670
H       3.103491        -0.036778       1.581750
C       4.335992        0.418569        -0.153849
C       2.117611        -0.841200       -0.199960
H       5.231893        0.571248        0.453446
H       4.632958        -0.057254       -1.091366
S       3.685388        2.100585        -0.489664
O       2.233207        -1.549328       -1.217478
H       2.856038        1.761094        -1.499494
N       0.957933        -0.353027       0.245964
H       0.925496        0.219865        1.085037
C       -0.298379       -0.547814       -0.453428
C       -1.420269       0.096080        0.350888
H       -0.262035       -0.093885       -1.450277
H       -0.502448       -1.615082       -0.586266
O       -1.186811       0.768662        1.372518
N       -2.657385       -0.105502       -0.125864
H       -2.797957       -0.682537       -0.949061
C       -3.830813       0.441976        0.527269
C       -5.081309       -0.003912       -0.187161
H       -3.892961       0.111874        1.570186
H       -3.808015       1.537304        0.537076
O       -5.103129       -0.742372       -1.159821
O       -6.181366       0.515333        0.378134
H       -6.969643       0.203021        -0.105129
###
28
CysGlyGly2 b3lyp E=-1138.06514973 au
N       4.233455        -1.630257       0.797280
H       3.819436        -2.256480       1.496386
H       5.164956        -1.355109       1.127726
H       4.337702        -2.158722       -0.078209
C       3.365840        -0.422768       0.567963
H       3.156889        0.009627        1.547313
C       4.156725        0.562576        -0.307797
C       2.088752        -0.935221       -0.111478
H       5.104495        0.783963        0.191027
H       4.377276        0.117174        -1.280821
S       3.343475        2.190332        -0.540088
O       2.174783        -1.783123       -1.020502
H       2.441498        1.798411        -1.464016
N       0.938504        -0.419929       0.325143
H       0.929762        0.283532        1.059246
C       -0.343438       -0.751923       -0.269816
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C       -1.438511       0.057409        0.417551
H       -0.338968       -0.522734       -1.341110
H       -0.551065       -1.821756       -0.163272
O       -1.165400       0.885884        1.311823
N       -2.681519       -0.185280       -0.007086
H       -2.850945       -0.864365       -0.743907
C       -3.857318       0.503759        0.501771
C       -5.133348       0.023545        -0.203745
H       -3.967708       0.332003        1.577570
H       -3.761894       1.584780        0.353721
O       -5.024668       -0.849404       -1.115366
O       -6.212507       0.552688        0.197257
###
27
CysGlyGly3 b3lyp E=-1137.59662584 au
N       -4.562178       -1.472108       0.050364
H       -4.282679       -2.372571       -0.356352
H       -5.484024       -1.201604       -0.302841
H       -4.634528       -1.605430       1.064978
C       -3.536676       -0.416343       -0.282581
H       -3.691784       -0.172352       -1.337659
C       -3.781031       0.827211        0.581568
C       -2.167395       -1.099865       -0.143528
H       -4.858450       1.023339        0.564538
H       -3.510261       0.592471        1.618239
S       -2.873848       2.321681        -0.013995
O       -2.102785       -2.348585       -0.086317
N       -1.096563       -0.304962       -0.126145
H       -1.248437       0.718508        -0.136205
C       0.241057        -0.861669       -0.023859
C       1.299466        0.230608        -0.108055
H       0.363486        -1.404990       0.920320
H       0.410033        -1.583509       -0.830256
O       1.003151        1.431951        -0.271619
N       2.561273        -0.202647       0.004057
H       2.758115        -1.190763       0.132192
C       3.724247        0.667624        -0.067415
C       5.027331        -0.130692       0.086881
H       3.750482        1.197223        -1.025884
H       3.686403        1.427852        0.720236
O       4.948443        -1.383057       0.259163
O       6.096624        0.547404        0.028350
###
26
CysGlyGly4 b3lyp E=-1137.12827618 au
N       -4.691939       -1.436704       -0.008034
H       -4.492978       -2.308816       -0.495885
H       -4.668365       -1.676211       0.983753
C       -3.606390       -0.483772       -0.283386
H       -3.687223       -0.188556       -1.337083
C       -3.800790       0.779968        0.579199
C       -2.214955       -1.136097       -0.130746
H       -4.875060       0.985476        0.585644
H       -3.516816       0.546908        1.614011
S       -2.909075       2.300003        0.003679
O       -2.094134       -2.380520       -0.025822
N       -1.144442       -0.326331       -0.156261
H       -1.307495       0.693968        -0.172748
C       0.198032        -0.864641       -0.037935
C       1.253868        0.229547        -0.122806
H       0.322517        -1.398559       0.912056
H       0.384609        -1.594997       -0.833457
O       0.960932        1.431597        -0.290154
N       2.517485        -0.200719       -0.005525
H       2.715948        -1.187858       0.125879
C       3.677458        0.673791        -0.067785
C       4.983487        -0.118576       0.091508
H       3.707291        1.206778        -1.024333
H       3.632595        1.431757        0.721828
O       4.910628        -1.371965       0.259018
O       6.049849        0.565266        0.042199
###
31
GlyAlaAla1 b3lyp E=-779.646012226 au
N       3.370910        -2.429780       0.127648
H       3.583093        -2.240693       1.114522
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C       3.240981        -1.150062       -0.625090
H       4.115850        -3.010682       -0.268398
H       2.496638        -2.965462       0.098369
C       2.343508        -0.204306       0.162499
H       4.237152        -0.711576       -0.718674
H       2.850163        -1.368354       -1.619183
O       2.186543        -0.357387       1.384555
N       1.782180        0.791264        -0.546091
H       1.965371        0.840555        -1.543312
C       1.023818        1.875527        0.074942
H       1.524537        2.151224        1.007335
C       0.991233        3.085705        -0.865591
C       -0.406350       1.482723        0.479596
H       0.515162        2.829154        -1.817648
H       0.430719        3.900701        -0.402758
H       2.010006        3.431996        -1.060464
O       -1.018372       2.192349        1.301078
N       -0.949335       0.405182        -0.109789
H       -0.382540       -0.163081       -0.730086
C       -2.302118       -0.055675       0.173991
H       -2.502522       0.091296        1.240707
C       -3.365597       0.702310        -0.645700
C       -2.364501       -1.551015       -0.112551
H       -3.228599       0.522870        -1.716039
H       -4.373009       0.388707        -0.357381
H       -3.269617       1.772553        -0.448593
O       -1.506372       -2.160153       -0.731315
O       -3.450137       -2.212604       0.325184
H       -4.057826       -1.644752       0.830645
###
30
GlyAlaAla2 b3lyp E=-779.196703317 au
N       3.316502        -2.377325       0.174540
H       3.517154        -2.179788       1.162176
C       3.203910        -1.103735       -0.591703
H       4.062391        -2.967138       -0.206039
H       2.438868        -2.907200       0.138669
C       2.296578        -0.148344       0.172685
H       4.203030        -0.669396       -0.671724
H       2.828844        -1.329532       -1.589951
O       2.144990        -0.272084       1.399341
N       1.722763        0.821064        -0.559815
H       1.896822        0.841569        -1.559515
C       0.935454        1.901351        0.032610
H       1.433330        2.217544        0.953557
C       0.865759        3.082035        -0.942227
C       -0.480525       1.477067        0.459172
H       0.393284        2.784643        -1.884210
H       0.283227        3.893556        -0.500748
H       1.872801        3.453080        -1.152572
O       -1.094775       2.191855        1.281436
N       -1.001635       0.380463        -0.100892
H       -0.427317       -0.205635       -0.698942
C       -2.313624       -0.172289       0.237573
H       -2.453891       -0.081050       1.319167
C       -3.455975       0.569191        -0.476537
C       -2.337707       -1.676746       -0.116402
H       -3.383516       0.445711        -1.562275
H       -4.421510       0.177636        -0.145276
H       -3.419628       1.637092        -0.243786
O       -1.404098       -2.135829       -0.841886
O       -3.317433       -2.340403       0.335312
###
29
GlyAlaAla3 b3lyp E=-778.735441227 au
N       3.831398        -2.275296       0.108319
H       4.494891        -1.797738       0.715772
C       3.089573        -1.286235       -0.660711
H       3.189734        -2.764735       0.729378
C       2.308933        -0.259110       0.163741
H       3.775557        -0.746352       -1.321152
H       2.370888        -1.796983       -1.310747
O       2.203597        -0.339988       1.401709
N       1.728800        0.733995        -0.548279
H       1.880437        0.753440        -1.551074
C       0.971460        1.827676        0.050898
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H       1.470405        2.121019        0.979141
C       0.944780        3.022572        -0.910047
C       -0.463359       1.451903        0.459735
H       0.473381        2.748598        -1.859985
H       0.382286        3.847732        -0.467702
H       1.964331        3.365303        -1.108167
O       -1.080008       2.204392        1.247393
N       -0.998771       0.351104        -0.078466
H       -0.422477       -0.263698       -0.644478
C       -2.339072       -0.148357       0.226971
H       -2.521148       -0.009677       1.297107
C       -3.424654       0.600655        -0.563973
C       -2.400463       -1.663997       -0.068720
H       -3.302462       0.439638        -1.640369
H       -4.416459       0.248203        -0.268111
H       -3.366670       1.674333        -0.363911
O       -1.459891       -2.182767       -0.742410
O       -3.416931       -2.276429       0.375299
###
40
GlyGlyAspAla1 b3lyp E=-1175.82472565 au
N       -7.826261       -0.518237       -0.465652
H       -8.039042       -0.388861       0.529102
C       -6.535399       0.130300        -0.826153
H       -7.794585       -1.527595       -0.643803
H       -8.592004       -0.116918       -1.015869
C       -5.417798       -0.475779       0.013144
H       -6.359498       -0.031066       -1.891135
H       -6.630256       1.201358        -0.638895
O       -5.661561       -1.361472       0.853483
N       -4.195375       0.011049        -0.223144
H       -4.051272       0.729458        -0.927560
C       -3.020185       -0.470680       0.477448
C       -1.782875       0.245385        -0.048619
H       -3.112032       -0.291184       1.554221
H       -2.903903       -1.550216       0.334271
O       -1.860425       1.119817        -0.931692
N       -0.626877       -0.144698       0.511772
H       -0.626464       -0.871347       1.221715
C       0.672681        0.393272        0.133645
H       0.683318        0.548284        -0.947450
C       0.942978        1.741916        0.837649
C       1.724427        -0.662698       0.516300
H       0.020728        2.334536        0.831136
H       1.214691        1.596075        1.887969
C       1.989722        2.592603        0.164851
O       1.494432        -1.467222       1.443971
O       2.317978        3.664972        0.912671
O       2.479518        2.386495        -0.936664
N       2.863606        -0.639863       -0.182046
H       3.006704        0.078105        -0.887359
C       4.011621        -1.502435       0.107237
H       4.099948        -1.597249       1.193050
C       3.840202        -2.902531       -0.505174
C       5.303641        -0.840526       -0.420781
H       3.790398        -2.844743       -1.597636
H       4.684608        -3.539508       -0.227641
H       2.921217        -3.368170       -0.138275
O       5.194162        0.086368        -1.278278
O       6.391678        -1.306633       0.031367
H       2.961456        4.209731        0.421511
###
39
GlyGlyAspAla2 b3lyp E=-1175.36882226 au
N       -7.781224       -0.580309       -0.604582
H       -7.966584       -0.824570       0.375090
C       -6.549172       0.251575        -0.704323
H       -7.681422       -1.457815       -1.125934
H       -8.589139       -0.074315       -0.979808
C       -5.426218       -0.426362       0.068749
H       -6.305255       0.386161        -1.758192
H       -6.766608       1.225004        -0.258887
O       -5.681385       -1.297977       0.921310
N       -4.193007       0.000302        -0.216948
H       -4.042851       0.710668        -0.928400
C       -3.017845       -0.483435       0.483068
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C       -1.782411       0.240491        -0.040120
H       -3.113398       -0.308485       1.560125
H       -2.899342       -1.562084       0.335129
O       -1.871517       1.126369        -0.913191
N       -0.623973       -0.151584       0.507398
H       -0.615407       -0.898728       1.195760
C       0.674501        0.399767        0.132502
H       0.673995        0.577315        -0.944817
C       0.958365        1.736164        0.854343
C       1.728345        -0.666814       0.469380
H       0.031641        2.320788        0.862118
H       1.222457        1.556500        1.902175
C       2.030824        2.632011        0.215245
O       1.472809        -1.569033       1.298117
O       2.355361        3.668788        0.873985
O       2.504500        2.313777        -0.918503
N       2.902247        -0.549271       -0.159344
H       3.057389        0.272179        -0.744097
C       4.043879        -1.430626       0.094934
H       4.112220        -1.602483       1.173097
C       3.884140        -2.784926       -0.618188
C       5.352200        -0.749817       -0.361696
H       3.852992        -2.647077       -1.704239
H       4.723800        -3.441026       -0.372172
H       2.959046        -3.275035       -0.302642
O       5.275805        0.205728        -1.189799
O       6.424242        -1.235043       0.111413
###
43
GlyGlyGluAla1 b3lyp E=-1215.14177103 au
N       -7.854069       -0.678173       -0.342648
H       -7.980677       -0.668918       0.675896
C       -6.585063       0.004923        -0.718082
H       -7.849075       -1.659166       -0.641468
H       -8.656368       -0.214601       -0.780276
C       -5.446846       -0.560270       0.120887
H       -6.419120       -0.135857       -1.786492
H       -6.704095       1.070669        -0.510956
O       -5.685612       -1.199910       1.162298
N       -4.215276       -0.288905       -0.322357
H       -4.077589       0.200896        -1.201707
C       -3.025190       -0.711893       0.391721
C       -1.787047       -0.154907       -0.300365
H       -3.059972       -0.365819       1.428935
H       -2.954858       -1.805885       0.412782
O       -1.850417       0.374216        -1.425289
N       -0.647498       -0.308944       0.394358
H       -0.697797       -0.674976       1.340030
C       0.653545        0.199219        -0.037104
H       0.708933        0.115819        -1.124749
C       0.814705        1.678869        0.377013
C       1.716450        -0.693621       0.615755
H       -0.011558       2.232668        -0.079143
H       0.712163        1.757183        1.464233
C       2.162007        2.287193        -0.065851
O       1.639954        -0.959545       1.834771
H       2.991613        1.821394        0.469349
H       2.307930        2.135980        -1.141256
C       2.205917        3.763558        0.245712
O       2.706295        4.240752        1.254788
O       1.628234        4.607175        -0.642578
N       2.687116        -1.146124       -0.184712
H       2.735668        -0.829015       -1.148685
C       3.837138        -1.923075       0.280793
H       4.132513        -1.537732       1.261340
C       3.500243        -3.417583       0.412736
C       5.024875        -1.711442       -0.685560
H       3.238524        -3.844774       -0.561054
H       4.359457        -3.961200       0.814257
H       2.655155        -3.557083       1.092844
O       4.800686        -1.142340       -1.795837
O       6.146059        -2.147727       -0.289592
H       1.271239        4.128637        -1.410770
###
42
GlyGlyGluAla2 b3lyp E=-1214.68620591 au
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N       7.816769        -0.666621       0.396329
H       7.951370        -0.667817       -0.621308
C       6.541669        0.015188        0.752760
H       7.813228        -1.644269       0.705797
H       8.613600        -0.195120       0.835385
C       5.415196        -0.555407       -0.098694
H       6.362313        -0.119931       1.819679
H       6.660748        1.080147        0.541569
O       5.668407        -1.188718       -1.140707
N       4.178286        -0.293033       0.334197
H       4.030601        0.184337        1.218764
C       2.994206        -0.715980       -0.390865
C       1.752568        -0.157768       0.294232
H       3.039845        -0.372019       -1.428036
H       2.921837        -1.810105       -0.409217
O       1.804496        0.315657        1.445022
N       0.624915        -0.251383       -0.429128
H       0.693654        -0.550573       -1.396610
C       -0.669661       0.281216        0.005006
H       -0.729438       0.165065        1.089275
C       -0.799119       1.774254        -0.364929
C       -1.749799       -0.568329       -0.673797
H       0.042082        2.293307        0.103309
H       -0.681200       1.875651        -1.449589
C       -2.118017       2.403399        0.086612
O       -1.743550       -0.706680       -1.916958
H       -2.967087       1.950437        -0.437321
H       -2.282836       2.209128        1.155416
C       -2.222599       3.924199        -0.104752
O       -3.378725       4.435561        0.056329
O       -1.179708       4.590753        -0.388756
N       -2.659751       -1.131576       0.128894
H       -2.646611       -0.934658       1.125201
C       -3.817930       -1.890086       -0.345892
H       -4.209988       -1.391400       -1.237417
C       -3.447328       -3.338705       -0.706719
C       -4.920870       -1.866789       0.736443
H       -3.096024       -3.882133       0.176766
H       -4.319017       -3.858598       -1.113008
H       -2.655488       -3.350499       -1.460794
O       -4.604209       -1.490059       1.904704
O       -6.068337       -2.258241       0.369574
###
25
GlyGlyGly1 b3lyp E=-701.013039402 au
N       5.475501        0.023108        0.118305
H       5.533704        0.957369        -0.302132
C       4.214235        -0.653229       -0.296436
H       5.517446        0.141870        1.135888
C       3.042375        0.289065        -0.060914
H       4.290965        -0.881432       -1.361860
H       4.119245        -1.583399       0.263879
O       3.228462        1.516028        0.042357
N       1.838948        -0.290696       -0.015853
H       1.749556        -1.301762       -0.065398
C       0.612223        0.474045        0.116360
C       -0.581207       -0.469254       0.075766
H       0.598219        1.019792        1.066766
H       0.531165        1.214023        -0.686174
O       -0.439132       -1.706236       0.090026
N       -1.782440       0.127771        0.037728
H       -1.848240       1.140743        0.030118
C       -3.015457       -0.633670       0.053212
C       -4.203679       0.288935        -0.038355
H       -3.057161       -1.335081       -0.787230
H       -3.107300       -1.225891       0.970950
O       -4.139166       1.506488        -0.110790
O       -5.356447       -0.397203       -0.031444
H       6.290827        -0.523537       -0.174547
H       -6.103151       0.228047        -0.090504
###
24
GlyGlyGly2 b3lyp E=-700.561938314 au
N       -5.403568       0.062486        -0.133796
H       -5.397244       1.034533        0.198811
C       -4.158732       -0.630275       0.303552
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H       -5.477257       0.088001        -1.156141
C       -2.970959       0.290401        0.059284
H       -4.245888       -0.832214       1.373475
H       -4.075735       -1.574365       -0.234560
O       -3.140755       1.519777        -0.051091
N       -1.776544       -0.305608       0.019211
H       -1.701424       -1.317957       0.067180
C       -0.538314       0.440580        -0.116722
C       0.645487        -0.517478       -0.064613
H       -0.515271       0.974443        -1.073837
H       -0.453092       1.189309        0.676753
O       0.482686        -1.754888       -0.118837
N       1.845213        0.065090        0.020840
H       1.924903        1.077467        0.056400
C       3.102768        -0.665659       -0.012236
C       4.302115        0.292941        0.030427
H       3.174188        -1.350937       0.838983
H       3.169929        -1.271067       -0.922540
O       4.073929        1.537430        0.089475
O       5.444181        -0.255247       0.005126
H       -6.233325       -0.410627       0.236160
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23
GlyGlyGly3 b3lyp E=-700.100566177 au
N       -5.542927       -0.003343       -0.172009
H       -5.677402       0.673547        0.576637
C       -4.245729       -0.646541       -0.009201
H       -5.544975       0.536083        -1.036149
C       -3.042165       0.296552        0.039629
H       -4.244670       -1.219826       0.924649
H       -4.093623       -1.368978       -0.816624
O       -3.170722       1.531695        0.172666
N       -1.836403       -0.291991       -0.049969
H       -1.766582       -1.302818       -0.113686
C       -0.593258       0.443493        0.083702
C       0.589300        -0.515753       0.035196
H       -0.496398       1.192206        -0.709131
H       -0.564742       0.980856        1.039425
O       0.429819        -1.753855       0.090939
N       1.790995        0.065569        -0.048780
H       1.871245        1.077799        -0.081688
C       3.047590        -0.665754       -0.002484
C       4.248553        0.291156        -0.033488
H       3.105335        -1.270641       0.908944
H       3.127887        -1.352191       -0.852010
O       4.023124        1.536126        -0.093267
O       5.389846        -0.258541       0.001515
###
45
GlyGlyHisAla1 b3lyp E=-1212.74315099 au
N       8.017977        0.032058        0.302857
H       8.140211        -0.900337       -0.108709
C       6.694882        0.124608        0.980630
H       8.779355        0.206381        0.966118
H       8.093378        0.714591        -0.458518
C       5.621371        -0.421173       0.049251
H       6.738518        -0.488184       1.884028
H       6.519091        1.163363        1.259820
O       5.927154        -1.182188       -0.887820
N       4.369027        -0.052017       0.336075
H       4.181224        0.565613        1.121093
C       3.219323        -0.552862       -0.393566
C       1.957390        0.123342        0.125592
H       3.335246        -0.368353       -1.465614
H       3.113764        -1.635699       -0.255375
O       1.961492        0.782383        1.180317
N       0.857464        -0.082571       -0.621635
H       0.945419        -0.579931       -1.502109
C       -0.468771       0.404414        -0.253594
H       -0.516861       0.457173        0.835253
C       -0.710181       1.822927        -0.837773
C       -1.481119       -0.617556       -0.789148
H       0.132268        2.447187        -0.530315
H       -0.707571       1.767952        -1.930433
C       -1.970857       2.466872        -0.361260
O       -1.498323       -0.888305       -2.008989
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N       -3.184585       2.369004        -1.030790
C       -2.224213       3.221430        0.751387
H       -3.337369       1.866334        -1.900458
C       -4.134767       3.027276        -0.363821
N       -3.565929       3.550148        0.722950
H       -1.571698       3.546517        1.545642
H       -5.169738       3.120812        -0.652585
N       -2.295757       -1.175587       0.111041
H       -2.267735       -0.873193       1.080223
C       -3.342793       -2.145284       -0.214471
H       -3.824070       -1.827135       -1.144218
C       -2.769309       -3.559162       -0.405344
C       -4.412314       -2.134543       0.901709
H       -2.310557       -3.920126       0.521112
H       -3.565267       -4.250243       -0.694724
H       -2.010379       -3.557613       -1.192621
O       -4.144184       -1.526938       1.981568
O       -5.483695       -2.761329       0.650571
H       -4.056012       4.106927        1.416183
###
44
GlyGlyHisAla2 b3lyp E=-1212.28440956 au
N       -8.094555       0.076916        -0.368563
H       -8.252884       -0.895365       -0.080441
C       -6.746282       0.218929        -0.984433
H       -8.825299       0.349642        -1.033146
H       -8.184122       0.664745        0.467061
C       -5.706686       -0.400332       -0.059800
H       -6.754080       -0.316265       -1.936404
H       -6.560220       1.276887        -1.170337
O       -6.046715       -1.216088       0.817753
N       -4.444126       -0.028266       -0.289097
H       -4.228638       0.647245        -1.017712
C       -3.314135       -0.574807       0.438527
C       -2.032965       0.074279        -0.073595
H       -3.420559       -0.390710       1.512479
H       -3.247902       -1.659013       0.294435
O       -2.047296       0.850001        -1.047954
N       -0.914641       -0.277300       0.580866
H       -0.985250       -0.869210       1.402488
C       0.411060        0.230514        0.236377
H       0.456028        0.344869        -0.848527
C       0.672819        1.611793        0.901713
C       1.431440        -0.814531       0.697246
H       -0.183156       2.244922        0.647656
H       0.676102        1.483068        1.988142
C       1.948375        2.271192        0.468882
O       1.321094        -1.343203       1.825101
N       3.047201        2.390266        1.309414
C       2.241208        2.831655        -0.754813
C       3.976121        3.011196        0.596959
N       3.534667        3.296469        -0.654721
H       1.661629        2.940042        -1.659007
H       4.966287        3.276671        0.937497
N       2.417587        -1.093091       -0.161333
H       2.472285        -0.589008       -1.041578
C       3.545919        -1.977295       0.133978
H       3.863055        -1.795650       1.164984
C       3.166706        -3.459983       -0.021422
C       4.725591        -1.628449       -0.800653
H       2.883960        -3.680537       -1.056178
H       4.013712        -4.094681       0.253061
H       2.325092        -3.708129       0.631142
O       4.480850        -0.945218       -1.840011
O       5.857789        -2.085172       -0.462977
H       4.060218        3.767999        -1.380665
###
48
GlyGlyLysAla1 b3lyp E=-1160.55392908 au
N       8.128801        0.294836        0.408177
H       8.382964        -0.656403       0.147948
C       6.764932        0.298438        0.921168
H       8.164092        0.836901        -0.453575
C       5.703184        -0.260965       -0.027534
H       6.725841        -0.300288       1.838271
H       6.482812        1.317098        1.203842
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O       6.001026        -0.926287       -1.041319
N       4.427631        -0.002683       0.311719
H       4.224483        0.510736        1.163356
C       3.294785        -0.531195       -0.424037
C       1.995208        -0.072894       0.225931
H       3.325298        -0.202441       -1.467359
H       3.311390        -1.628197       -0.429047
O       1.980589        0.442541        1.360397
N       0.890198        -0.290743       -0.506690
H       0.988665        -0.656551       -1.448220
C       -0.459208       0.075631        -0.070641
H       -0.489264       -0.009216       1.017840
C       -0.803465       1.523130        -0.480449
C       -1.422724       -0.934273       -0.704572
H       -0.012293       2.165696        -0.077551
H       -0.758524       1.598103        -1.573543
C       -2.165986       2.009065        0.026156
O       -1.387442       -1.138581       -1.938044
H       -2.970002       1.409098        -0.418091
H       -2.225698       1.867080        1.113227
C       -2.397305       3.488216        -0.308885
H       -1.599709       4.096361        0.136947
H       -2.350384       3.633519        -1.395987
C       -3.745085       3.974303        0.204067
H       -4.575226       3.427947        -0.246873
H       -3.820333       3.899735        1.290303
N       -3.949920       5.425160        -0.139936
H       -3.934884       5.568083        -1.155040
H       -4.848115       5.769417        0.213289
H       -3.208723       6.005082        0.266574
N       -2.267166       -1.557169       0.125089
H       -2.294011       -1.297898       1.106707
C       -3.317650       -2.479463       -0.308022
H       -3.755272       -2.087494       -1.231788
C       -2.767146       -3.889251       -0.578514
C       -4.435112       -2.519379       0.760350
H       -2.365776       -4.333825       0.338283
H       -3.561853       -4.535237       -0.960614
H       -1.968730       -3.848202       -1.324577
O       -4.223166       -1.946909       1.871497
O       -5.488521       -3.146149       0.440850
###
47
GlyGlyLysAla2 b3lyp E=-1160.08522925 au
N       8.115297        0.225831        0.375786
H       8.353071        -0.729892       0.116534
C       6.755885        0.252001        0.899717
H       8.152045        0.765087        -0.487663
C       5.677328        -0.288851       -0.040876
H       6.713904        -0.346806       1.816636
H       6.493461        1.275071        1.185323
O       5.956239        -0.959797       -1.056445
N       4.408493        -0.008660       0.306611
H       4.219537        0.506016        1.160794
C       3.263970        -0.524584       -0.419819
C       1.973708        -0.058167       0.242769
H       3.287835        -0.193661       -1.462607
H       3.271750        -1.621685       -0.427532
O       1.971717        0.444527        1.383094
N       0.862622        -0.256578       -0.486004
H       0.954925        -0.603655       -1.435165
C       -0.481786       0.124343        -0.044544
H       -0.514287       0.024704        1.042592
C       -0.805112       1.581517        -0.438187
C       -1.458473       -0.862535       -0.693698
H       -0.012267       2.209356        -0.015280
H       -0.739673       1.668686        -1.529573
C       -2.170449       2.080080        0.048374
O       -1.441377       -1.030208       -1.933184
H       -2.970541       1.481706        -0.407180
H       -2.247400       1.932870        1.134540
C       -2.401488       3.560311        -0.283818
H       -1.610544       4.168506        0.177933
H       -2.321517       3.709386        -1.370183
C       -3.764724       4.074468        0.189168
H       -4.559989       3.473618        -0.266745
```

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H       -3.851251       3.936096        1.273119
N       -4.042855       5.491095        -0.108438
H       -3.969190       5.635690        -1.114968
H       -3.306143       6.063123        0.303369
N       -2.295706       -1.506863       0.127195
H       -2.292399       -1.296620       1.120620
C       -3.359412       -2.404347       -0.325431
H       -3.800143       -1.978833       -1.231558
C       -2.827948       -3.812430       -0.642363
C       -4.462597       -2.476142       0.754221
H       -2.417814       -4.285400       0.256095
H       -3.636389       -4.439131       -1.028936
H       -2.040699       -3.760104       -1.399508
O       -4.175171       -2.090895       1.927221
O       -5.576990       -2.948863       0.380590
###
47
GlyGlyTyrAla1 b3lyp E=-1293.07414211 au
N       8.534634        -0.661475       -0.579504
H       8.850724        0.275648        -0.336617
C       7.153405        -0.590562       -1.041106
H       8.571117        -1.198895       0.285274
C       6.166680        0.052732        -0.065747
H       7.115393        -0.002108       -1.965142
H       6.801354        -1.594257       -1.295995
O       6.541460        0.819791        0.846344
N       4.871058        -0.238789       -0.272408
H       4.602997        -0.865334       -1.024841
C       3.793469        0.346667        0.500174
C       2.452223        -0.105969       -0.064155
H       3.857841        0.046620        1.552308
H       3.845810        1.440813        0.472665
O       2.381174        -0.844947       -1.064025
N       1.376686        0.358587        0.594971
H       1.515692        0.904955        1.439156
C       0.002487        -0.016218       0.266277
H       -0.058439       -0.154294       -0.814774
C       -0.395653       -1.339835       0.977360
C       -0.898533       1.143136        0.702029
H       0.362189        -2.080251       0.701309
H       -0.327586       -1.181586       2.058367
C       -1.773683       -1.843919       0.609867
O       -0.773149       1.634155        1.845286
C       -2.861780       -1.682239       1.479198
C       -2.005514       -2.474000       -0.624373
H       -2.710696       -1.203233       2.443185
C       -4.142087       -2.124746       1.133803
C       -3.276806       -2.920240       -0.986411
H       -1.178621       -2.621201       -1.314708
H       -4.976670       -1.994388       1.818075
C       -4.347634       -2.737521       -0.105023
H       -3.445318       -3.406122       -1.942782
O       -5.592650       -3.189068       -0.505209
H       -6.250821       -2.973501       0.173983
N       -1.792970       1.572141        -0.194892
H       -1.899427       1.077854        -1.075965
C       -2.806949       2.591245        0.081203
H       -3.162630       2.446467        1.106032
C       -2.241132       4.014378        -0.052355
C       -4.011242       2.387992        -0.867000
H       -1.911404       4.207794        -1.078568
H       -3.007296       4.747724        0.212477
H       -1.388467       4.148692        0.619061
O       -3.881879       1.581958        -1.836614
O       -5.046844       3.068104        -0.602297
###
46
GlyGlyTyrAla2 b3lyp E=-1292.59691816 au
N       8.451159        -0.504569       -0.664403
H       8.567512        0.442057        -1.021647
C       7.048757        -0.887148       -0.766778
H       8.713660        -0.464386       0.318653
C       6.064651        0.006120        -0.008648
H       6.755538        -0.924283       -1.819984
H       6.925531        -1.902576       -0.373289
O       6.438216        0.798412        0.881768
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N       4.771158        -0.143269       -0.342384
H       4.508758        -0.783080       -1.085557
C       3.691066        0.555262        0.327115
C       2.354100        -0.010589       -0.135600
H       3.784520        0.456255        1.412910
H       3.711545        1.627402        0.094506
O       2.277478        -0.763519       -1.125302
N       1.285873        0.394155        0.572386
H       1.434113        0.939406        1.415258
C       -0.083372       -0.035827       0.277580
H       -0.167212       -0.149699       -0.804902
C       -0.411697       -1.390665       0.961995
C       -1.016189       1.076293        0.766009
H       0.386212        -2.082921       0.671382
H       -0.343070       -1.248426       2.045845
C       -1.763370       -1.959838       0.590652
O       -0.976972       1.443867        1.960936
C       -2.878003       -1.834629       1.437452
C       -1.962440       -2.627731       -0.631498
H       -2.761768       -1.329385       2.395145
C       -4.130180       -2.344746       1.088669
C       -3.206134       -3.142661       -0.995341
H       -1.120683       -2.752154       -1.311509
H       -4.969997       -2.232493       1.771807
C       -4.349295       -3.019296       -0.148790
H       -3.322011       -3.658613       -1.946632
O       -5.527766       -3.505372       -0.488246
N       -1.836992       1.611060        -0.144730
H       -1.855314       1.241147        -1.090069
C       -2.846247       2.629230        0.150519
H       -3.333262       2.363947        1.093887
C       -2.230068       4.032035        0.285615
C       -3.922508       2.617059        -0.958925
H       -1.772565       4.349315        -0.657451
H       -3.003557       4.754457        0.559381
H       -1.462336       4.036948        1.063985
O       -3.671165       1.987482        -2.029999
O       -4.980844       3.268907        -0.713901
###
35
GlyHisGly2 b3lyp E=-965.386584605 au
N       -5.565476       -0.937643       -0.721980
H       -5.527197       -0.191352       -1.427147
C       -4.595286       -0.651481       0.372570
H       -6.519763       -0.999779       -0.354694
H       -5.346499       -1.820405       -1.195563
C       -3.276599       -0.196216       -0.240121
H       -5.005667       0.160229        0.977690
H       -4.488139       -1.542662       0.990376
O       -3.256906       0.328236        -1.367058
N       -2.195043       -0.380852       0.531770
H       -2.303291       -0.805834       1.447937
C       -0.865770       0.103412        0.176814
H       -0.769383       0.062989        -0.909546
C       -0.683025       1.573624        0.648847
C       0.154274        -0.829936       0.838478
H       -1.522560       2.148017        0.248058
H       -0.742800       1.611724        1.740420
C       0.597487        2.194441        0.191920
O       0.007344        -1.172964       2.031090
N       1.649644        2.484033        1.050470
C       1.021096        2.575852        -1.052184
H       1.654711        2.312045        2.051838
C       2.667519        3.016708        0.371573
N       2.299544        3.079147        -0.908428
H       0.527195        2.535074        -2.009418
H       3.610359        3.339561        0.783779
N       1.176978        -1.223927       0.076502
H       1.253987        -0.910286       -0.886876
C       2.263179        -2.065979       0.556056
C       3.279791        -2.349606       -0.559364
H       2.784781        -1.583305       1.389658
H       1.870872        -3.018217       0.926905
O       3.094412        -1.811644       -1.690755
O       4.243419        -3.107916       -0.241365
H       2.881710        3.446287        -1.654588
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###
34
GlyHisGly3 b3lyp E=-964.928180528 au
N       -5.569652       -0.908654       -0.738570
H       -5.521617       -0.165781       -1.446867
C       -4.604061       -0.621896       0.360231
H       -6.526715       -0.963337       -0.377484
H       -5.352717       -1.795046       -1.206129
C       -3.281022       -0.171222       -0.247661
H       -5.015754       0.192866        0.960246
H       -4.503057       -1.511521       0.981363
O       -3.261103       0.370144        -1.368194
N       -2.202666       -0.379304       0.518724
H       -2.316709       -0.824679       1.424357
C       -0.864396       0.103352        0.184492
H       -0.770210       0.107803        -0.902831
C       -0.655213       1.548035        0.720387
C       0.134498        -0.883305       0.795337
H       -1.498329       2.138425        0.347606
H       -0.721421       1.530076        1.812436
C       0.639793        2.178464        0.304772
O       -0.043179       -1.324261       1.952151
N       1.701731        2.345918        1.183396
C       0.987744        2.660585        -0.937369
C       2.664387        2.917066        0.474213
N       2.278814        3.125179        -0.810692
H       0.446776        2.716914        -1.869788
H       3.640335        3.200551        0.840410
N       1.175657        -1.225017       0.032102
H       1.287570        -0.824890       -0.894882
C       2.248613        -2.102089       0.476868
C       3.358014        -2.206418       -0.579742
H       2.682669        -1.733212       1.411672
H       1.862865        -3.108397       0.673983
O       3.200384        -1.596205       -1.678242
O       4.355259        -2.918779       -0.257992
H       2.838092        3.550755        -1.539758
###
50
GlyHisLys3 b3lyp E=-1178.48098999 au
N       -4.368682       4.663838        0.597338
H       -5.275289       4.188066        0.541078
C       -3.346787       3.974802        -0.237095
H       -4.490250       5.631541        0.282961
H       -4.091910       4.675171        1.584713
C       -3.160102       2.549987        0.268734
H       -3.691397       3.980702        -1.272419
H       -2.415309       4.539178        -0.167930
O       -3.800925       2.134018        1.247856
N       -2.259741       1.823357        -0.413550
H       -1.824260       2.221251        -1.240775
C       -1.972483       0.422068        -0.119955
H       -2.066335       0.273680        0.957028
C       -2.988436       -0.499995       -0.853360
C       -0.533971       0.149692        -0.576073
H       -3.990442       -0.167543       -0.571809
H       -2.879764       -0.360386       -1.933207
C       -2.857873       -1.948675       -0.514931
O       -0.180662       0.467145        -1.731576
N       -2.095517       -2.840782       -1.259616
C       -3.390740       -2.684602       0.507950
C       -2.154312       -4.060228       -0.721549
N       -2.938690       -3.981293       0.353739
H       -4.046331       -2.399324       1.314840
H       -1.661136       -4.945840       -1.090110
H       -3.169774       -4.767647       0.952841
N       0.267401        -0.438072       0.317695
H       -0.092298       -0.672908       1.237748
C       1.650892        -0.839664       0.048466
H       1.711135        -1.168777       -0.991616
C       2.615872        0.351017        0.262098
C       1.999874        -2.032481       0.967946
H       2.230110        1.191341        -0.326894
H       2.575761        0.650736        1.316815
C       4.065995        0.072633        -0.148020
O       1.462791        -2.056098       2.116880
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O       2.815192        -2.887606       0.513375
H       4.484277        -0.731587       0.467955
H       4.091819        -0.278448       -1.188007
C       4.947953        1.320914        -0.010010
H       4.560537        2.126561        -0.647155
H       4.919388        1.681737        1.026574
C       6.389655        1.022430        -0.395799
H       6.825874        0.246246        0.235406
H       6.479384        0.720430        -1.440780
N       7.254753        2.243660        -0.229545
H       7.240982        2.573161        0.741018
H       8.227772        2.044998        -0.481352
H       6.923748        3.010452        -0.823470
H       -1.557356       -2.604811       -2.088590
###
49
GlyHisLys4 b3lyp E=-1178.02301374 au
N       4.563794        -4.472684       0.711060
H       5.264860        -3.885406       1.177461
C       3.872287        -3.695618       -0.355738
H       5.028653        -5.295830       0.316194
H       3.902929        -4.789275       1.428057
C       3.458262        -2.341403       0.207036
H       4.578487        -3.548349       -1.175747
H       3.023286        -4.277048       -0.715098
O       4.019361        -1.887621       1.220716
N       2.495887        -1.707873       -0.476449
H       2.097599        -2.147032       -1.301140
C       2.042142        -0.356170       -0.156866
H       2.100657        -0.229413       0.925823
C       2.945870        0.710324        -0.839208
C       0.586636        -0.241641       -0.621509
H       3.976259        0.466825        -0.560636
H       2.863993        0.601550        -1.924707
C       2.622046        2.122753        -0.454736
O       0.240483        -0.719564       -1.723545
N       2.049427        3.019950        -1.345951
C       2.804089        2.735940        0.764882
C       1.896420        4.148028        -0.667580
N       2.335818        4.022773        0.610435
H       3.215685        2.384626        1.698881
H       1.481072        5.068455        -1.051085
H       2.325911        4.747454        1.317858
N       -0.243370       0.401941        0.206740
H       0.120469        0.791914        1.071091
C       -1.639158       0.726041        -0.100150
H       -1.713766       0.934672        -1.170224
C       -2.568789       -0.460151       0.251926
C       -2.024816       2.001790        0.684844
H       -2.166231       -1.349163       -0.247481
H       -2.511146       -0.642430       1.332415
C       -4.028588       -0.259624       -0.169803
O       -1.490108       2.163123        1.824030
O       -2.865149       2.779464        0.145085
H       -4.456001       0.600001        0.358637
H       -4.070287       -0.025406       -1.241702
C       -4.891641       -1.496810       0.112243
H       -4.504833       -2.360880       -0.443446
H       -4.846761       -1.746476       1.180426
C       -6.339853       -1.248071       -0.283539
H       -6.776415       -0.421890       0.280158
H       -6.440656       -1.040526       -1.350400
N       -7.193140       -2.455403       -0.001653
H       -7.163849       -2.700337       0.993437
H       -8.170699       -2.284748       -0.256221
H       -6.864281       -3.267760       -0.532932
###
48
GlyHisLys5 b3lyp E=-1177.56233145 au
N       -4.604378       4.658289        0.588857
H       -5.429041       4.138797        0.884094
C       -3.805766       3.817498        -0.293596
H       -4.076717       4.846827        1.439411
C       -3.417450       2.449472        0.273578
H       -4.367300       3.630399        -1.216112
H       -2.898158       4.353420        -0.586191
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O       -3.976295       1.971565        1.280898
N       -2.448089       1.798468        -0.401621
H       -2.065469       2.224291        -1.239625
C       -2.044932       0.424469        -0.117184
H       -2.117526       0.268318        0.960868
C       -2.978325       -0.592164       -0.836642
C       -0.592447       0.262123        -0.572119
H       -4.000821       -0.331899       -0.545611
H       -2.894185       -0.441439       -1.917276
C       -2.698159       -2.028494       -0.511012
O       -0.228050       0.701169        -1.684976
N       -2.053501       -2.878634       -1.399790
C       -2.995368       -2.711722       0.647167
C       -1.969252       -4.046069       -0.779352
N       -2.524333       -3.993400       0.458285
H       -3.489013       -2.410132       1.558612
H       -1.526571       -4.947068       -1.178337
H       -2.579745       -4.758995       1.118961
N       0.220188        -0.379043       0.276177
H       -0.155521       -0.736150       1.149205
C       1.606130        -0.748282       -0.022267
H       1.671648        -0.991341       -1.085812
C       2.568384        0.423258        0.289080
C       1.962892        -2.008633       0.799547
H       2.167082        1.314685        -0.206836
H       2.547888        0.617997        1.368830
C       4.010623        0.194295        -0.176850
O       1.416666        -2.132857       1.937910
O       2.795946        -2.812816       0.287467
H       4.438958        -0.673568       0.337211
H       4.014480        -0.039015       -1.249801
C       4.900718        1.417497        0.080259
H       4.505638        2.289644        -0.456710
H       4.895278        1.661845        1.150625
C       6.332659        1.156411        -0.365376
H       6.777426        0.318402        0.173957
H       6.397975        0.962232        -1.437498
N       7.207595        2.351094        -0.093924
H       7.204365        2.587842        0.903574
H       8.176807        2.171300        -0.372700
H       6.875776        3.171738        -0.610500
###
47
GlyHisLys6 b3lyp E=-1177.09339992 au
N       -4.605052       4.635593        0.343388
H       -5.378590       4.113472        -0.065268
C       -3.346506       4.017583        -0.058127
H       -4.712101       4.546406        1.352093
C       -3.173023       2.557071        0.363683
H       -3.229586       4.099173        -1.142463
H       -2.515372       4.574523        0.389689
O       -3.785266       2.080848        1.341097
N       -2.287423       1.845147        -0.361071
H       -1.874112       2.269329        -1.184925
C       -1.964574       0.443738        -0.105104
H       -2.037967       0.272883        0.970660
C       -2.962425       -0.499740       -0.834746
C       -0.525881       0.212239        -0.576164
H       -3.965488       -0.175250       -0.540427
H       -2.869197       -0.341879       -1.913521
C       -2.778246       -1.954579       -0.522273
O       -0.160599       0.623084        -1.699634
N       -2.210714       -2.843700       -1.425444
C       -3.103579       -2.621375       0.638026
C       -2.199679       -4.017601       -0.811438
N       -2.727505       -3.931960       0.436254
H       -3.559410       -2.290990       1.559117
H       -1.830641       -4.945870       -1.222617
H       -2.826455       -4.695339       1.094361
N       0.274915        -0.443690       0.271694
H       -0.097566       -0.767169       1.158869
C       1.661957        -0.816938       -0.018783
H       1.730845        -1.069355       -1.079767
C       2.619850        0.360488        0.286904
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H       2.207529        1.248372        -0.206783
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H       2.599570        0.556028        1.366819
C       4.064299        0.152682        -0.183407
O       1.473297        -2.177898       1.957194
O       2.847333        -2.880566       0.311933
H       4.504369        -0.713689       0.325137
H       4.064765        -0.080615       -1.257329
C       4.944542        1.384187        0.069944
H       4.511915        2.259424        -0.435895
H       4.954023        1.614104        1.145253
C       6.388181        1.197707        -0.408499
H       6.825341        0.321948        0.084761
H       6.393463        0.986447        -1.484083
N       7.282802        2.344872        -0.169647
H       7.277201        2.560136        0.827039
H       6.888140        3.166089        -0.627324
###
29
GlySerGly1 b3lyp E=-815.544822020 au
N       4.972002        -1.364923       -0.096226
H       5.116384        -1.192442       0.904403
C       4.040437        -0.360862       -0.679223
H       5.880341        -1.323569       -0.569224
H       4.600933        -2.315823       -0.192934
C       2.729041        -0.377390       0.095986
H       4.510735        0.621252        -0.599135
H       3.892504        -0.600142       -1.733031
O       2.628935        -1.008151       1.161127
N       1.738640        0.338182        -0.460821
H       1.911081        0.847395        -1.322593
C       0.440416        0.538209        0.174231
H       0.213592        -0.349418       0.765335
C       0.503936        1.766369        1.101307
C       -0.588655       0.757648        -0.940028
H       1.293658        1.594835        1.841410
H       0.756969        2.654562        0.510480
O       -0.766282       1.924781        1.737951
O       -0.282759       1.468574        -1.918523
H       -0.744949       2.744343        2.253150
N       -1.803088       0.192782        -0.833765
H       -2.442602       0.394357        -1.596192
C       -2.273273       -0.692399       0.226563
C       -3.745837       -1.015514       0.134056
H       -1.742480       -1.650430       0.212563
H       -2.120957       -0.241640       1.211048
O       -4.386399       -0.413248       -0.876840
O       -4.291875       -1.768021       0.926452
H       -5.327431       -0.673421       -0.868274
###
28
GlySerGly2 b3lyp E=-815.096986031 au
N       -4.779371       -1.576527       0.013591
H       -4.823183       -1.477528       -1.007003
C       -3.964525       -0.479438       0.605024
H       -5.732512       -1.562099       0.389316
H       -4.367982       -2.493813       0.214820
C       -2.644674       -0.377907       -0.148615
H       -4.522046       0.452777        0.489751
H       -3.824017       -0.684453       1.666613
O       -2.520291       -0.898587       -1.269911
N       -1.685540       0.320561        0.478415
H       -1.878212       0.729262        1.388083
C       -0.402970       0.652243        -0.135481
H       -0.166012       -0.124864       -0.861663
C       -0.515823       2.005711        -0.859253
C       0.643896        0.715971        0.982551
H       -1.323097       1.933624        -1.597018
H       -0.765682       2.788320        -0.133104
O       0.733116        2.285499        -1.497134
O       0.355993        1.312629        2.045457
H       0.669638        3.156927        -1.914385
N       1.835836        0.142035        0.789694
H       2.511759        0.217361        1.547923
C       2.325950        -0.591617       -0.374948
C       3.764463        -1.082440       -0.141854
H       1.702638        -1.468399       -0.577134
H       2.322463        0.037572        -1.268485
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O       4.312664        -0.835429       0.972041
O       4.288751        -1.709400       -1.109722
###
27
GlySerGly3 b3lyp E=-814.636270894 au
N       -4.786034       -1.757530       0.157923
H       -4.244029       -2.594996       0.364657
C       -4.004733       -0.580528       0.519387
H       -4.935248       -1.762067       -0.849466
C       -2.671143       -0.425017       -0.213149
H       -4.588200       0.319816        0.293012
H       -3.829662       -0.576642       1.598833
O       -2.477907       -0.924178       -1.338741
N       -1.741505       0.309836        0.434369
H       -1.969552       0.699822        1.342663
C       -0.457235       0.692086        -0.141491
H       -0.200425       -0.042578       -0.903902
C       -0.575184       2.078176        -0.797442
C       0.579239        0.713644        0.987625
H       -1.369826       2.034539        -1.551089
H       -0.845397       2.821332        -0.037834
O       0.680542        2.406312        -1.401637
O       0.293395        1.290988        2.062235
H       0.614439        3.300596        -1.766970
N       1.763847        0.122874        0.795217
H       2.432634        0.168256        1.561870
C       2.254041        -0.586908       -0.383774
C       3.687430        -1.095358       -0.155980
H       1.624400        -1.453187       -0.610583
H       2.260331        0.064022        -1.261831
O       4.230697        -0.884118       0.967852
O       4.213509        -1.699221       -1.137581
###
58
PheAlaArg1 b3lyp E=-1333.34766525 au
N       -6.448371       -0.324326       0.091578
H       -6.632820       -0.116192       -0.897673
H       -6.722152       0.496231        0.642841
H       -7.040874       -1.111445       0.376067
C       -4.994914       -0.656637       0.285476
H       -4.831358       -0.734717       1.360991
C       -4.705715       -2.002210       -0.410939
C       -4.198912       0.507349        -0.317516
H       -5.426689       -2.726841       -0.014788
H       -4.900005       -1.891003       -1.482677
C       -3.297295       -2.511058       -0.184654
O       -4.543317       0.983107        -1.415628
C       -2.357134       -2.503708       -1.224824
C       -2.913073       -3.012893       1.069289
H       -2.643490       -2.123275       -2.201878
C       -1.059926       -2.986402       -1.018904
C       -1.618166       -3.493849       1.278212
H       -3.633979       -3.034432       1.882872
H       -0.345859       -2.977228       -1.837564
C       -0.686338       -3.481555       0.233798
H       -1.338375       -3.882727       2.253206
H       0.318942        -3.860144       0.394689
N       -3.150261       0.936945        0.393863
H       -2.938492       0.508026        1.289783
C       -2.260376       2.001733        -0.066367
H       -2.177883       1.922641        -1.152916
C       -2.791593       3.398821        0.301250
C       -0.886919       1.771018        0.570832
H       -2.842669       3.523150        1.387055
H       -2.138112       4.171794        -0.112879
H       -3.792295       3.532721        -0.117923
O       -0.782861       1.253782        1.697656
N       0.162098        2.205255        -0.152107
H       -0.004178       2.543124        -1.093812
C       1.545029        2.112733        0.311764
H       1.527879        2.065285        1.400971
C       2.240627        0.848797        -0.247096
C       2.310995        3.376229        -0.056573
H       1.635820        -0.003303       0.082018
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C       3.688086        0.673113        0.224701
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O 2.073784 3.786916 -1.313319
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H 3.736652 0.741906 1.317999
C 4.238875 -0.678429 -0.224887
H 3.673426 -1.486550 0.252048
H 4.135657 -0.785154 -1.311208
N 5.656097 -0.796681 0.142571
H 6.113341 0.014348 0.543164
C 6.408333 -1.878536 -0.070507
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N 7.699380 -1.880200 0.304111
H 4.914289 -3.032170 -0.883553
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H 8.301032 -2.639325 0.013232
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57
PheAlaArg2 b3lyp E=-1332.89814642 au
N 6.367552 -0.175193 -0.610672
H 6.692674 0.101505 0.323933
H 6.503668 0.621984 -1.241872
H 6.952028 -0.949827 -0.942278
C 4.921908 -0.589288 -0.549940
H 4.597228 -0.746206 -1.579121
C 4.824379 -1.894975 0.264129
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H 5.175776 -1.698718 1.282275
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O 4.618526 1.095924 1.138850
C 2.633674 -2.371919 1.447640
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H 3.027920 -1.863512 2.323661
C 1.344633 -2.914886 1.478467
C 1.620172 -3.688061 -0.796430
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O -3.326549 3.956210 -0.174369
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H -3.817103 0.887363 -1.357074
C -4.257665 -0.678757 0.057079
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H       -8.283450       -2.694129       -0.275242
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56
PheAlaArg3 b3lyp E=-1332.43812070 au
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H       -6.102541       -1.127151       -1.750745
H       -6.744681       -0.514849       -0.382301
C       -4.941161       0.310156        -0.870555
H       -4.400853       0.520319        -1.798101
C       -5.154574       1.634229        -0.108380
C       -4.115759       -0.676896       -0.032840
H       -5.792935       2.259915        -0.741026
H       -5.710431       1.420746        0.811434
C       -3.877039       2.376833        0.223543
O       -4.537233       -1.099842       1.066213
C       -3.349411       2.366396        1.523843
C       -3.186461       3.089720        -0.771261
H       -3.873804       1.825537        2.307516
C       -2.162811       3.044742        1.824223
C       -2.000425       3.767606        -0.476315
H       -3.584374       3.116853        -1.782948
H       -1.773510       3.026188        2.838467
C       -1.483240       3.746751        0.824287
H       -1.483193       4.315309        -1.259368
H       -0.563314       4.276235        1.055666
N       -2.945525       -1.071551       -0.563103
H       -2.644249       -0.686452       -1.452155
C       -2.038391       -2.019307       0.073738
H       -2.035819       -1.821445       1.149416
C       -2.461878       -3.480266       -0.165170
C       -0.632356       -1.768617       -0.485857
H       -2.416905       -3.729755       -1.229849
H       -1.806872       -4.161404       0.385651
H       -3.485940       -3.627786       0.187957
O       -0.472118       -1.225987       -1.600224
N       0.376758        -2.205676       0.277730
H       0.173821        -2.649140       1.168294
C       1.786829        -2.176603       -0.115369
H       1.844167        -2.347312       -1.193075
C       2.413498        -0.801428       0.215409
C       2.523337        -3.328073       0.607126
H       1.777277        -0.036906       -0.245076
H       2.369731        -0.647432       1.300511
C       3.853466        -0.628167       -0.278897
O       2.113116        -3.646554       1.764349
O       3.501682        -3.853966       -0.000899
H       4.518507        -1.335454       0.228694
H       3.908185        -0.841979       -1.353681
C       4.349418        0.792882        -0.021181
H       3.737103        1.514770        -0.574131
H       4.272605        1.028873        1.046589
N       5.751456        0.922541        -0.441257
H       6.204665        0.112684        -0.848705
C       6.486439        2.026554        -0.298558
N       5.960379        3.134606        0.234105
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H       4.981982        3.185989        0.478399
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H       8.222569        1.163408        -0.933607
H       8.356462        2.821756        -0.465708
###
55
PheAlaArg4 b3lyp E=-1331.95634503 au
C       -6.545660       3.782168        -0.570562
C       -5.299318       3.482072        -1.133094
C       -4.559354       2.395290        -0.660108
C       -5.048340       1.584142        0.378067
C       -6.296393       1.898363        0.935878
C       -7.040790       2.987358        0.467295
C       -4.234374       0.410376        0.880761
C       -4.159054       -0.770565       -0.115298
C       -3.089070       -1.757479       0.372223
N       -1.947256       -1.789114       -0.336886
C       -0.811605       -2.651611       -0.022652
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C       2.909347        -1.772185       -0.322745
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C       -0.973034       -4.060136       -0.621383
O       0.396393        -1.261037       -1.594981
C       3.193139        -0.367358       0.259188
C       4.488857        0.273959        -0.248838
C       4.683155        1.676461        0.326782
N       5.918413        2.273934        -0.202487
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N       7.018268        4.226252        -0.791209
O       3.762866        -3.377645       1.254563
N       5.852505        4.086449        1.278996
H       -5.402422       -2.149640       -0.968024
H       -5.724553       -1.858768       0.605866
H       -3.854786       -0.386677       -1.093180
H       -3.210634       0.744133        1.088042
H       -4.650548       0.041936        1.824950
H       -3.589172       2.174574        -1.099097
H       -6.688299       1.286662        1.744639
H       -4.901368       4.096759        -1.935910
H       -8.005361       3.213124        0.913802
H       -7.120794       4.628396        -0.935540
H       -1.851037       -1.197417       -1.155386
H       -0.737135       -2.731553       1.064812
H       -1.008454       -4.016305       -1.714384
H       -0.138234       -4.700674       -0.321938
H       -1.900729       -4.509714       -0.257088
H       1.553548        -2.821887       0.920795
H       2.923586        -1.720552       -1.413566
H       2.342258        0.271422        -0.005072
H       3.213073        -0.440614       1.353841
H       5.350829        -0.346564       0.019267
H       4.464070        0.333471        -1.345573
H       3.810896        2.301746        0.087901
H       4.748709        1.608331        1.417499
H       6.087298        2.048658        -1.177317
H       5.660118        3.427028        2.023553
H       6.344868        4.913950        1.592371
H       7.298578        5.124880        -0.397591
###
# AMINO ACIDS optimized with m052x
# opt(tight) freq m052x/6-31+G(d,p) scf=(xqc,tight) integral=ultrafine scrf(smd,solvent=water)
###
14
Ala1 m052x E=-324.199808644 au
N       -1.451112       -1.003945       -0.145290
H       -1.441582       -1.248449       0.849031
H       -1.121613       -1.817746       -0.669630
H       -2.417009       -0.808735       -0.418408
C       -0.601467       0.191335        -0.402930
H       -0.637968       0.390765        -1.473321
C       -1.120885       1.381080        0.392934
C       0.817328        -0.175053       -0.032878
H       -1.056097       1.183864        1.463937
H       -0.529628       2.262161        0.151843
H       -2.159345       1.570084        0.120808
O       1.138494        -1.253070       0.425642
O       1.660217        0.822728        -0.267193
H       2.561483        0.554240        -0.017579
###
12
Ala3 m052x E=-323.285616990 au
N       -1.444089       -1.052775       -0.364942
H       -1.016052       -1.776640       -0.932845
H       -1.418831       -1.405170       0.587313
C       -0.611421       0.145721        -0.421715
H       -0.620371       0.524426        -1.444753
C       -1.186568       1.212143        0.509541
C       0.861098        -0.070693       -0.039661
H       -1.191493       0.843511        1.539414
H       -0.592375       2.125981        0.471552
H       -2.212384       1.448710        0.222660
O       1.161551        -1.060047       0.686457
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O       1.686134        0.795744        -0.458674
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13
AlaZW m052x E=-323.753611696 au
N       -1.339952       -1.059916       -0.170636
H       -0.950525       -1.841694       -0.699300
H       -1.302491       -1.314746       0.818722
C       -0.554636       0.188862        -0.408963
H       -0.619192       0.400800        -1.474850
C       -1.155275       1.322119        0.408005
C       0.913120        -0.066472       -0.043849
H       -1.087285       1.102448        1.475556
H       -0.608546       2.240335        0.201048
H       -2.202155       1.472085        0.140195
O       1.204693        -1.181216       0.462562
O       1.701241        0.884142        -0.282452
H       -2.316862       -0.930277       -0.438961
###
28
Arg1 m052x E=-607.477477593 au
N       3.498225        -1.519619       -0.293183
H       3.599971        -1.690415       0.711471
H       4.415208        -1.256629       -0.663017
H       3.208973        -2.391231       -0.743903
C       2.482811        -0.459383       -0.541749
H       2.456485        -0.266681       -1.612299
C       1.124389        -0.952427       -0.034037
C       2.949468        0.779874        0.192429
H       0.923432        -1.900013       -0.541170
H       1.200074        -1.150861       1.038651
C       -0.010965       0.027466        -0.317747
O       3.664836        0.739844        1.173270
H       0.122218        0.944962        0.258559
H       -0.018173       0.290509        -1.378794
C       -1.342858       -0.606506       0.057486
H       -1.503406       -1.511385       -0.532890
H       -1.346064       -0.873162       1.117027
N       -2.418663       0.347286        -0.208720
H       -2.174271       1.274643        -0.528222
C       -3.701097       0.106625        0.042360
N       -4.089729       -1.081641       0.499854
N       -4.610747       1.059594        -0.171947
H       -3.435034       -1.838745       0.611543
H       -5.068938       -1.260022       0.662070
H       -4.319538       1.989201        -0.431739
H       -5.578839       0.897102        0.057224
O       2.472418        1.893722        -0.345917
H       2.755779        2.660955        0.182171
###
27
Arg2 m052x E=-607.033115272 au
N       3.559064        -1.432336       -0.292683
H       3.697758        -1.508861       0.718682
H       4.453901        -1.169629       -0.709599
H       3.282098        -2.341950       -0.667008
C       2.516391        -0.397135       -0.562148
H       2.499420        -0.221419       -1.635199
C       1.173247        -0.933119       -0.068632
C       2.922006        0.884430        0.181198
H       0.973469        -1.873657       -0.590643
H       1.251791        -1.151991       1.000714
C       0.027692        0.042684        -0.322288
O       3.537458        0.728159        1.269440
H       0.163144        0.948358        0.272586
H       0.012866        0.331536        -1.376881
C       -1.300936       -0.601976       0.044893
H       -1.460423       -1.497751       -0.559689
H       -1.301497       -0.886565       1.099793
N       -2.381743       0.351559        -0.203963
H       -2.140280       1.284346        -0.509571
C       -3.663142       0.102326        0.041467
N       -4.047533       -1.093992       0.481776
N       -4.576978       1.054060        -0.162766
H       -3.388706       -1.848461       0.586631
H       -5.026002       -1.279307       0.640293
H       -5.543573       0.886484        0.068841
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O 2.574108 1.972010 -0.341709
H -4.287710 1.989223 -0.404284
###
26
Arg3 m052x E=-606.567048457 au
N 3.693575 -1.410026 -0.306629
H 3.743663 -1.563421 0.696012
H 3.435122 -2.300272 -0.720368
C 2.609435 -0.454956 -0.555641
H 2.583433 -0.227647 -1.621719
C 1.237296 -0.988765 -0.121223
C 2.901748 0.844009 0.197992
H 1.047384 -1.913082 -0.676656
H 1.289470 -1.247889 0.941672
C 0.096257 -0.002836 -0.362005
O 3.217462 0.740620 1.418449
H 0.244422 0.899986 0.237759
H 0.080249 0.296851 -1.414360
C -1.241820 -0.625070 0.007144
H -1.417370 -1.518285 -0.596904
H -1.242245 -0.910728 1.061757
N -2.312809 0.343002 -0.234576
H -2.061006 1.270587 -0.547844
C -3.592788 0.116325 0.036210
N -3.987774 -1.069609 0.495298
N -4.497290 1.078285 -0.165935
H -3.338070 -1.832272 0.597485
H -4.965934 -1.238237 0.672836
H -4.196574 2.009782 -0.407589
H -5.457707 0.933039 0.103245
O 2.773098 1.936602 -0.425610
###
25
Arg4 m052x E=-606.087404570 au
N -3.605641 1.493903 0.044068
H -3.623871 1.443424 1.058433
H -3.336703 2.444488 -0.190163
C -2.552488 0.588061 -0.426686
H -2.553493 0.592427 -1.517023
C -1.157151 0.982130 0.075865
C -2.874181 -0.834648 0.035219
H -0.938970 1.986526 -0.302871
H -1.189559 1.043105 1.169071
C -0.053675 0.018212 -0.357185
O -3.143116 -0.995276 1.260886
H -0.202367 -0.956215 0.120369
H -0.095862 -0.137363 -1.439691
C 1.318732 0.554030 0.022436
H 1.497771 1.480617 -0.524898
H 1.343064 0.784675 1.093471
N 2.350283 -0.428905 -0.322473
H 2.070179 -1.381505 -0.128421
C 3.666188 -0.230868 0.032358
N 4.069018 1.082356 0.100802
N 4.421292 -1.251315 0.288453
H 3.566948 1.748775 -0.466522
H 5.068298 1.221725 0.107672
H 5.375545 -0.940103 0.443808
O -2.820658 -1.762768 -0.822289
###
18
Asn1 m052x E=-492.909320264 au
N -1.805836 -1.577391 -0.013482
H -2.650527 -1.371773 0.526712
H -1.503960 -2.530217 0.204972
H -2.054718 -1.536512 -1.006150
C -0.726043 -0.609352 0.307599
H -0.501121 -0.704597 1.369662
C 0.516875 -0.907646 -0.526915
C -1.272545 0.778414 0.047985
H 0.717221 -1.981670 -0.481181
H 0.359546 -0.630905 -1.570042
C 1.741878 -0.227480 0.053439
O -2.410613 0.995824 -0.311683
O 1.940190 -0.205249 1.277524
N 2.596487 0.289181 -0.830561

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H       3.454474        0.707612        -0.501507
H       2.401886        0.269751        -1.819241
O       -0.353243       1.709629        0.259880
H       -0.729020       2.590537        0.086653
###
16
Asn3 m052x E=-492.000080506 au
N       1.941106        -1.543665       0.021184
H       2.737217        -1.321143       -0.567607
H       2.219180        -1.294539       0.965994
C       0.827219        -0.682317       -0.361269
H       0.580463        -0.869461       -1.405753
C       -0.388078       -1.041062       0.508854
C       1.097918        0.823406        -0.200484
H       -0.594388       -2.105854       0.388397
H       -0.152958       -0.843125       1.557057
C       -1.624949       -0.290997       0.077472
O       1.831817        1.192553        0.758690
O       -2.147820       -0.501454       -1.032605
N       -2.128381       0.594840        0.943263
H       -2.938754       1.138608        0.685316
H       -1.675664       0.771093        1.825816
O       0.523899        1.597903        -1.019559
###
17
AsnZW m052x E=-492.465404847 au
N       1.816144        1.524599        -0.097855
H       2.689411        1.236447        0.348937
H       1.581700        2.476270        0.190239
H       1.979480        1.522066        -1.107622
C       0.733561        0.567441        0.269690
H       0.533452        0.714584        1.330441
C       -0.517299       0.865683        -0.545599
C       1.245325        -0.868151       0.069205
H       -0.713542       1.942070        -0.529115
H       -0.384303       0.555983        -1.583010
C       -1.735874       0.214126        0.070615
O       2.481027        -1.019863       -0.109167
O       -1.945714       0.273365        1.293806
N       -2.592993       -0.358981       -0.777866
H       -3.440437       -0.774380       -0.420045
H       -2.389600       -0.419053       -1.762710
O       0.368126        -1.764489       0.125294
###
17
Asp1 m052x E=-512.767868177 au
N       -1.816265       -1.560968       0.056506
H       -2.643074       -1.326315       0.612584
H       -1.528515       -2.514808       0.290534
H       -2.088137       -1.537264       -0.930874
C       -0.712195       -0.607315       0.331572
H       -0.469622       -0.681512       1.391040
C       0.497403        -0.952041       -0.538106
C       -1.234837       0.785972        0.045447
H       0.729989        -2.013452       -0.409027
H       0.287624        -0.762845       -1.589917
C       1.745783        -0.199175       -0.159408
O       -2.376060       1.020456        -0.289571
O       1.951952        -0.149787       1.158136
O       2.520707        0.270214        -0.969758
O       -0.284182       1.695650        0.203634
H       -0.633975       2.582965        0.009908
H       2.783304        0.323097        1.333649
###
16
Asp2 m052x E=-512.325493693 au
N       1.844624        1.497966        -0.027230
H       2.695223        1.171689        0.437465
H       1.634300        2.451501        0.273233
H       2.035098        1.507883        -1.032490
C       0.724420        0.569660        0.292996
H       0.520457        0.684426        1.356810
C       -0.497917       0.937027        -0.538391
C       1.182879        -0.876032       0.041540
H       -0.730098       1.998299        -0.403699
H       -0.320573       0.745631        -1.596001
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C       -1.727609       0.178815        -0.125832
O       2.418866        -1.076518       -0.062771
O       -1.916592       0.163265        1.199185
O       -2.524943       -0.309519       -0.905643
O       0.260862        -1.726414       -0.013637
H       -2.742958       -0.308523       1.396335
###
15
Asp3 m052x E=-511.870517948 au
N       1.707018        1.573479        -0.026789
H       2.589342        1.298895        0.410087
H       1.431706        2.499328        0.304349
H       1.872436        1.626544        -1.034461
C       0.657441        0.556968        0.284599
H       0.439249        0.651116        1.347727
C       -0.591417       0.837612        -0.536325
C       1.242533        -0.841717       0.034471
H       -0.812548       1.909090        -0.493169
H       -0.432260       0.564549        -1.579813
C       -1.833640       0.125578        0.003056
O       2.490912        -0.926339       -0.112508
O       -1.991176       0.081874        1.255380
O       -2.651488       -0.323417       -0.848828
O       0.415933        -1.786435       0.020707
###
14
Asp4 m052x E=-511.402400271 au
N       1.863306        1.578223        0.066688
H       2.658322        1.330984        0.647233
H       2.148734        1.384088        -0.888773
C       0.752370        0.684781        0.390341
H       0.487101        0.821995        1.438333
C       -0.454980       1.057828        -0.482693
C       1.060019        -0.805652       0.175755
H       -0.705873       2.101298        -0.283381
H       -0.178465       0.948875        -1.533460
C       -1.668343       0.188033        -0.171401
O       1.774562        -1.124311       -0.817295
O       -2.261250       0.391561        0.929332
O       -2.006116       -0.690348       -1.017603
O       0.544384        -1.624995       0.990719
###
15
Cys1 m052x E=-722.358799385 au
N       -1.464851       1.647236        -0.240527
H       -2.308700       1.469199        -0.792483
H       -1.104327       2.570071        -0.499412
H       -1.727131       1.669134        0.750331
C       -0.428865       0.601339        -0.482295
H       -0.267973       0.532280        -1.555188
C       0.843342        1.012591        0.256776
C       -0.978561       -0.705019       0.064643
H       1.186659        1.970642        -0.130813
H       0.630702        1.117556        1.321694
S       2.166683        -0.227930       0.125713
O       -1.496769       -0.777350       1.160068
H       2.311777        -0.148088       -1.208366
O       -0.826981       -1.720160       -0.771138
H       -1.159478       -2.537949       -0.359669
###
14
Cys2 m052x E=-721.913177172 au
N       -1.538338       1.539093        -0.251529
H       -1.862503       1.457477        0.716544
H       -2.340068       1.360406        -0.859789
H       -1.207770       2.491464        -0.420796
C       -0.462019       0.532918        -0.490115
H       -0.253075       0.518297        -1.556899
C       0.760135        0.976135        0.309472
C       -0.982893       -0.838198       -0.022500
H       1.065045        1.965193        -0.030306
H       0.508021        1.016757        1.369517
S       2.152986        -0.183449       0.042920
O       -1.819169       -0.824727       0.918553
H       3.084004        0.653803        0.527766
O       -0.501383       -1.841147       -0.600202
```

```
###
13
Cys3 m052x E=-721.444000078 au
N       -1.423864       1.599362        -0.233242
H       -1.686301       1.567953        0.755588
H       -2.267014       1.449945        -0.790699
H       -1.053011       2.527023        -0.447080
C       -0.389186       0.537545        -0.493281
H       -0.227220       0.499952        -1.567264
C       0.880328        0.934643        0.252415
C       -0.989845       -0.783586       0.013189
H       1.175934        1.921631        -0.113439
H       0.626037        1.036698        1.311138
S       2.249258        -0.259525       0.030705
O       -1.466163       -0.750373       1.182353
O       -0.983497       -1.771871       -0.762450
###
12
Cys4 m052x E=-720.974591182 au
N       -1.434267       1.680535        -0.250869
H       -1.603407       1.750497        0.748424
H       -1.030997       2.568761        -0.532490
C       -0.424150       0.628154        -0.463678
H       -0.239291       0.543322        -1.534665
C       0.895066        0.918736        0.252254
C       -1.038620       -0.688470       0.014851
H       1.247865        1.891267        -0.104370
H       0.679584        1.024228        1.319897
S       2.192938        -0.356789       -0.015503
O       -1.332415       -0.770586       1.245015
O       -1.254418       -1.602379       -0.834168
###
21
Gln1 m052x E=-532.221491855 au
N       2.114356        -1.672026       -0.476457
H       2.243028        -1.912591       0.510811
H       3.039748        -1.530469       -0.888967
H       1.670636        -2.464271       -0.947796
C       1.265416        -0.455472       -0.610291
H       1.216003        -0.197205       -1.666391
C       -0.126240       -0.767636       -0.050095
C       1.958149        0.651385        0.155375
H       -0.490644       -1.649196       -0.582373
H       -0.035546       -1.021891       1.007414
C       -1.109099       0.383148        -0.242463
O       2.759864        0.445430        1.044316
H       -0.845358       1.233442        0.391164
H       -1.106611       0.731280        -1.276785
C       -2.507422       -0.028311       0.156498
O       -2.713415       -0.887529       1.030907
N       -3.506551       0.608412        -0.464329
H       -4.460551       0.416922        -0.196766
H       -3.321718       1.298787        -1.174642
O       1.573322        1.855438        -0.244707
H       1.993388        2.535103        0.311563
###
19
Gln3 m052x E=-531.309918296 au
N       -2.304420       1.590633        -0.557821
H       -2.386146       1.845932        0.421927
H       -1.885128       2.387112        -1.027309
C       -1.374082       0.460746        -0.644790
H       -1.319427       0.133615        -1.683447
C       0.035706        0.818350        -0.155347
C       -1.924458       -0.701139       0.186200
H       0.410844        1.633289        -0.781158
H       -0.035769       1.192597        0.869114
C       0.997894        -0.364690       -0.216539
O       -2.274590       -0.439401       1.372897
H       0.707512        -1.131650       0.509585
H       0.975249        -0.834399       -1.202682
C       2.418789        0.022267        0.118275
O       2.688611        0.991282        0.850664
N       3.378368        -0.755536       -0.399890
H       4.343221        -0.580637       -0.162380
H       3.148619        -1.538635       -0.990623
```

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O       -1.963985       -1.847643       -0.345542
###
20
GlnZW m052x E=-531.776476928 au
N       2.188770        -1.576847       -0.501441
H       2.388763        -1.723040       0.492213
H       3.080533        -1.431120       -0.978063
H       1.747421        -2.413897       -0.887480
C       1.302857        -0.381767       -0.640973
H       1.268345        -0.119145       -1.695725
C       -0.083935       -0.758976       -0.119689
C       1.927637        0.764517        0.169836
H       -0.443951       -1.610991       -0.702261
H       0.001627        -1.074509       0.922437
C       -1.075643       0.394333        -0.240180
O       2.609031        0.434503        1.176760
H       -0.798530       1.212610        0.429883
H       -1.086611       0.794641        -1.255535
C       -2.468255       -0.034594       0.157116
O       -2.665438       -0.893513       1.035007
N       -3.476994       0.584337        -0.467114
H       -4.428577       0.374042        -0.205098
H       -3.302240       1.269527        -1.184843
O       1.678260        1.930056        -0.225805
###
20
Glu1 m052x E=-552.078458968 au
N       -2.003495       1.801665        -0.015306
H       -2.940707       1.808591        -0.425946
H       -1.527010       2.665468        -0.286072
H       -2.106244       1.791162        1.003620
C       -1.220980       0.623106        -0.476846
H       -1.204057       0.638446        -1.564756
C       0.195775        0.722156        0.096139
C       -1.947113       -0.613090       0.010170
H       0.596046        1.690405        -0.212835
H       0.143356        0.701451        1.187551
C       1.105843        -0.399977       -0.426381
O       -2.687573       -0.612495       0.972431
H       0.814737        -1.363764       -0.005452
H       1.063547        -0.452088       -1.512934
C       2.532180        -0.112281       -0.039376
O       2.861300        -0.276615       1.252883
O       3.384577        0.278678        -0.814148
O       -1.661206       -1.680628       -0.721703
H       -2.108658       -2.462559       -0.352415
H       2.122448        -0.619771       1.778441
###
19
Glu2 m052x E=-551.634222774 au
N       -2.076445       1.723479        0.008069
H       -2.230971       1.599194        1.012594
H       -2.992251       1.749629        -0.444479
H       -1.607233       2.616240        -0.155491
C       -1.261225       0.581148        -0.501602
H       -1.254526       0.638979        -1.587346
C       0.150923        0.720182        0.065712
C       -1.925372       -0.725254       -0.038915
H       0.549168        1.688472        -0.247778
H       0.099675        0.707307        1.158107
C       1.071988        -0.400846       -0.440021
O       -2.520716       -0.687494       1.070181
H       0.777424        -1.361357       -0.013105
H       1.037595        -0.463955       -1.526380
C       2.493197        -0.106139       -0.045512
O       2.811845        -0.254120       1.252198
O       3.353169        0.279805        -0.815546
O       -1.780392       -1.720742       -0.789807
H       2.067920        -0.592989       1.773217
###
18
Glu3 m052x E=-551.179941012 au
N       -2.026302       1.729060        0.126873
H       -2.169065       1.543896        1.123628
H       -2.946218       1.791827        -0.313068
H       -1.550101       2.626047        0.014751
```

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C       -1.221930       0.613331        -0.458889
H       -1.229838       0.735736        -1.539284
C       0.197544        0.707628        0.098313
C       -1.893632       -0.711627       -0.068541
H       0.609409        1.677828        -0.194042
H       0.151500        0.671592        1.190708
C       1.105095        -0.412349       -0.423334
O       -2.434573       -0.751466       1.068651
H       0.769621        -1.375954       -0.038999
H       1.079978        -0.430739       -1.513936
C       2.530296        -0.147448       0.050679
O       2.851527        -0.561383       1.203102
O       3.296303        0.504352        -0.718680
O       -1.817682       -1.646611       -0.903977
###
17
Glu4 m052x E=-550.712175271 au
N       -2.150981       1.745926        -0.208296
H       -2.212521       1.795812        0.804284
H       -1.685393       2.596745        -0.508138
C       -1.287100       0.607681        -0.542197
H       -1.262601       0.495942        -1.626436
C       0.145647        0.776781        -0.021718
C       -1.898961       -0.664758       0.048157
H       0.553367        1.693582        -0.460307
H       0.108619        0.916490        1.062328
C       1.055396        -0.407571       -0.367303
O       -2.203295       -0.637264       1.275905
H       0.709033        -1.304041       0.155525
H       1.028712        -0.602301       -1.440643
C       2.490985        -0.137653       0.066532
O       2.702477        0.028171        1.305251
O       3.389094        -0.081374       -0.824835
O       -2.040545       -1.667105       -0.709992
###
11
Gly1 m052x E=-284.886342170 au
N       1.831396        0.081847        -0.000011
H       1.851854        0.684614        -0.826012
C       0.626605        -0.775847       0.000012
H       2.675387        -0.494944       -0.000078
H       1.851920        0.684502        0.826063
C       -0.597503       0.096616        0.000004
H       0.636891        -1.403807       -0.888211
H       0.636889        -1.403779       0.888255
O       -0.559694       1.310009        0.000007
O       -1.710841       -0.626211       -0.000007
H       -2.483047       -0.034516       -0.000031
###
Gly3 m052x E=-283.973615682 au
###
10
GlyZW m052x E=-284.440304020 au
N       -1.768683       0.079782        0.010191
C       -0.562750       -0.787777       -0.014515
C       0.707155        0.058437        -0.000782
O       1.785531        -0.589684       0.010904
O       0.572728        1.308810        -0.006911
H       -1.790854       0.636274        0.866127
H       -0.597432       -1.391962       -0.917903
H       -0.590709       -1.437805       0.856400
H       -1.749350       0.734395        -0.773435
H       -2.623376       -0.476334       -0.042689
###
22
His1 m052x E=-549.684742592 au
N       2.573888        -1.450858       0.029583
H       3.343296        -1.221332       -0.605114
H       2.350718        -2.444126       -0.072893
H       2.903193        -1.291441       0.986508
C       1.374199        -0.625770       -0.266590
H       1.047772        -0.870628       -1.276972
C       0.268340        -0.953861       0.751709
C       1.801952        0.825669        -0.232598
H       0.246634        -2.037415       0.875388
H       0.509015        -0.508248       1.718611
```

```
C       -1.084447       -0.507403       0.306982
O       2.937692        1.182653        0.000938
N       -1.749696       0.564055        0.866744
C       -1.920161       -1.014021       -0.642655
H       -1.382532       1.168921        1.592461
C       -2.935638       0.715250        0.290483
N       -3.053828       -0.233789       -0.630198
H       -1.803874       -1.851037       -1.308782
H       -3.666738       1.468519        0.527872
O       0.788594        1.640851        -0.485466
H       1.093224        2.564867        -0.450237
H       -3.869017       -0.361144       -1.217501
###
21
His2 m052x E=-549.245717074 au
N       -2.394688       1.565099        -0.270645
H       -3.211462       1.199806        -0.766999
H       -2.096521       2.446816        -0.691200
H       -2.683328       1.744887        0.694471
C       -1.302538       0.550544        -0.315093
H       -0.936831       0.535069        -1.342360
C       -0.188075       0.975381        0.650431
C       -1.922087       -0.829009       -0.014280
H       -0.119650       2.064240        0.655281
H       -0.438840       0.651569        1.663032
C       1.160815        0.466866        0.264711
O       -3.166435       -0.927470       -0.128358
N       1.437600        -0.868923       0.059956
C       2.333511        1.132200        0.067582
H       0.700592        -1.579844       0.112956
C       2.716685        -1.022843       -0.254576
N       3.279171        0.181191        -0.249630
H       2.569313        2.180185        0.127780
H       3.211419        -1.952376       -0.478677
O       -1.120265       -1.751016       0.292365
H       4.254462        0.357128        -0.456760
###
20
His3 m052x E=-548.787547914 au
N       -2.724637       -1.170635       0.000270
H       -3.032630       -0.727846       -0.871129
H       -3.435898       -0.987016       0.710436
H       -2.655339       -2.180765       -0.138022
C       -1.408322       -0.581656       0.389903
H       -1.207848       -0.866240       1.419673
C       -0.342388       -1.148563       -0.558449
C       -1.520791       0.945224        0.266344
H       -0.331927       -2.233965       -0.435466
H       -0.633083       -0.923835       -1.587105
C       1.019213        -0.586583       -0.298980
O       -2.274433       1.376534        -0.647044
N       1.581867        0.381695        -1.105711
C       1.874010        -0.891322       0.729131
C       2.754676        0.651355        -0.564510
N       2.972304        -0.090414       0.543163
H       1.797067        -1.585501       1.549200
H       3.475513        1.361123        -0.936343
O       -0.831002       1.627872        1.062935
H       3.802491        -0.066458       1.116928
###
19
His4 m052x E=-548.320829851 au
N       2.712058        -1.194824       -0.558092
H       2.578463        -2.048672       -1.090792
H       2.887611        -1.483484       0.400245
C       1.451102        -0.439491       -0.571018
H       1.257131        -0.120312       -1.594982
C       0.274117        -1.268695       -0.051672
C       1.673586        0.813698        0.286008
H       0.204449        -2.174471       -0.663748
H       0.499290        -1.589172       0.969356
C       -1.037273       -0.546071       -0.062356
O       1.855088        0.628383        1.524095
N       -2.127429       -1.022776       0.641685
C       -1.384915       0.604887        -0.723945
C       -3.105269       -0.169645       0.404567
```

```
N       -2.705977       0.827312        -0.412851
H       -0.831427       1.266995        -1.367459
H       -4.106912       -0.228630       0.798469
O       1.695806        1.939463        -0.287458
H       -3.274405       1.598886        -0.728873
###
23
Ile1 m052x E=-442.128463321 au
N       1.351220        -1.696789       -0.613525
H       1.560850        -1.952176       0.355078
H       2.242827        -1.622936       -1.110083
H       0.806788        -2.450703       -1.038642
C       0.588927        -0.416664       -0.684033
H       0.470017        -0.174979       -1.739275
C       -0.793989       -0.575558       -0.014770
C       1.451495        0.637088        -0.025413
H       -1.170255       -1.542591       -0.366678
C       -0.696232       -0.600785       1.512357
C       -1.766772       0.500374        -0.515907
O       2.409128        0.374651        0.675587
H       -0.431244       0.388493        1.897624
H       -1.656246       -0.883868       1.942848
H       0.042841        -1.319238       1.874653
H       -1.703318       0.547978        -1.606676
H       -1.464928       1.476374        -0.129579
C       -3.210607       0.212043        -0.107076
H       -3.343863       0.268979        0.974381
H       -3.884821       0.939471        -0.562661
H       -3.516470       -0.784576       -0.436016
O       1.035183        1.867620        -0.291419
H       1.597874        2.510136        0.175413
###
22
Ile2 m052x E=-441.682200100 au
N       1.434725        -1.541492       -0.739892
H       1.825111        -1.698808       0.192950
H       2.223644        -1.452594       -1.382243
H       0.875355        -2.348195       -1.022198
C       0.621494        -0.284265       -0.730043
H       0.507886        0.026851        -1.766539
C       -0.761303       -0.568689       -0.115405
C       1.418334        0.779946        0.041234
H       -1.141946       -1.454417       -0.638683
C       -0.673555       -0.878670       1.380591
C       -1.732785       0.582091        -0.406986
O       2.307702        0.366848        0.833226
H       -0.389035       0.015503        1.942228
H       -1.639602       -1.219762       1.753315
H       0.052511        -1.665664       1.597574
H       -1.656957       0.846418        -1.465882
H       -1.434405       1.462733        0.166512
C       -3.182595       0.223815        -0.082051
H       -3.329065       0.057492        0.986430
H       -3.851148       1.032006        -0.384742
H       -3.487382       -0.682929       -0.611476
O       1.100350        1.976458        -0.172231
###
21
Ile3 m052x E=-441.213570643 au
N       1.482778        -1.524230       -0.924914
H       1.804970        -1.806367       -0.005472
H       0.887122        -2.269907       -1.270449
C       0.676691        -0.309944       -0.775777
H       0.536259        0.133634        -1.763233
C       -0.735031       -0.571086       -0.189872
C       1.438599        0.714090        0.070697
H       -1.146120       -1.382099       -0.805956
C       -0.691110       -1.050379       1.261941
C       -1.660233       0.639943        -0.355405
O       2.204119        0.285080        0.981092
H       -0.428188       -0.227569       1.933619
H       -1.662787       -1.438934       1.571122
H       0.040004        -1.850365       1.399891
H       -1.593134       0.994648        -1.389111
H       -1.308567       1.455646        0.282726
C       -3.120228       0.329478        -0.024256
```

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H       -3.254022       0.111087        1.036920
H       -3.761851       1.178569        -0.269582
H       -3.472603       -0.534982       -0.594139
O       1.236798        1.939125        -0.178081
###
23
Leu1 m052x E=-442.129262256 au
N       1.695352        1.679091        0.472734
H       1.948280        1.886694        -0.497846
H       2.557371        1.503293        0.994862
H       1.239021        2.502972        0.872201
C       0.771920        0.510176        0.525820
H       0.605483        0.270558        1.573202
C       -0.528005       0.891748        -0.194331
C       1.474243        -0.636741       -0.166517
H       -0.926727       1.772441        0.319738
H       -0.272001       1.185305        -1.217220
C       -1.609433       -0.193723       -0.222888
O       2.307882        -0.475510       -1.036188
H       -1.222728       -1.065597       -0.758286
C       -2.030803       -0.617977       1.184214
C       -2.813244       0.346536        -0.995984
H       -2.370398       0.252544        1.753911
H       -2.856569       -1.330948       1.131066
H       -1.217534       -1.093085       1.735927
H       -2.532969       0.643990        -2.009203
H       -3.595938       -0.411767       -1.065153
H       -3.230635       1.219847        -0.485958
O       1.058812        -1.820102       0.263176
H       1.486256        -2.525099       -0.254158
###
21
Leu3 m052x E=-441.216222935 au
N       1.747520        -1.650719       -0.689769
H       2.640788        -1.350030       -1.066162
H       1.934851        -1.972165       0.255300
C       0.851830        -0.492087       -0.601311
H       0.702439        -0.104611       -1.608861
C       -0.484268       -0.944787       -0.009358
C       1.432429        0.641977        0.257391
H       -0.910317       -1.704203       -0.674568
H       -0.275298       -1.432301       0.950161
C       -1.519661       0.163709        0.206289
O       1.828357        0.342512        1.422418
H       -1.088588       0.921527        0.871318
C       -1.914409       0.835794        -1.109588
C       -2.756998       -0.418947       0.890063
H       -2.301188       0.089188        -1.811140
H       -2.699059       1.577968        -0.941777
H       -1.070740       1.341847        -1.582319
H       -2.497434       -0.890882       1.841018
H       -3.499304       0.358743        1.085703
H       -3.221050       -1.176502       0.250574
O       1.471484        1.805300        -0.240139
###
22
LeuZW m052x E=-441.683365716 au
N       1.769754        -1.569307       -0.523669
H       2.084738        -1.693963       0.442690
H       2.592396        -1.375892       -1.097363
H       1.336618        -2.433274       -0.855364
C       0.801598        -0.430216       -0.563188
H       0.640784        -0.178829       -1.608108
C       -0.486237       -0.889707       0.124411
C       1.443788        0.748577        0.182790
H       -0.877193       -1.749389       -0.431653
H       -0.226098       -1.234655       1.130873
C       -1.582966       0.175660        0.220447
O       2.181792        0.451734        1.161044
H       -1.193068       1.029512        0.783070
C       -2.031859       0.656219        -1.160014
C       -2.769579       -0.405869       0.989811
H       -2.375656       -0.191949       -1.760542
H       -2.860837       1.361543        -1.065475
H       -1.228636       1.157207        -1.703298
H       -2.469022       -0.745446       1.983983
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H       -3.558303       0.340728        1.106477
H       -3.189168       -1.260334       0.450019
O       1.154045        1.902253        -0.220440
###
26
Lys1 m052x E=-497.947839886 au
N       2.717246        -1.593613       -0.112769
H       2.817938        -1.631755       0.905777
H       3.637457        -1.398326       -0.514599
H       2.412848        -2.513237       -0.442168
C       1.720314        -0.554822       -0.497356
H       1.711635        -0.482989       -1.582318
C       0.347921        -0.959135       0.048749
C       2.188349        0.751323        0.106930
H       0.108294        -1.934734       -0.382758
H       0.425352        -1.076328       1.133769
C       -0.752322       0.041566        -0.297983
O       2.790590        0.813955        1.160352
H       -0.565533       0.995631        0.201581
H       -0.753689       0.228941        -1.375660
C       -2.117107       -0.491585       0.134509
H       -2.331467       -1.430136       -0.384958
H       -2.108214       -0.697093       1.209135
C       -3.205158       0.519481        -0.176055
H       -3.048495       1.455364        0.355666
H       -3.278476       0.718297        -1.243002
N       -4.536567       -0.006740       0.258104
H       -4.538067       -0.204980       1.260593
H       -5.280364       0.665842        0.065403
H       -4.758475       -0.874502       -0.233504
O       1.844194        1.801184        -0.626405
H       2.114232        2.620399        -0.174646
###
25
Lys2 m052x E=-497.503258680 au
N       2.761917        -1.520837       -0.097155
H       2.932591        -1.418073       0.907558
H       3.650910        -1.380699       -0.580431
H       2.434075        -2.469596       -0.288252
C       1.751184        -0.501791       -0.515035
H       1.748249        -0.466257       -1.601706
C       0.389218        -0.929938       0.030382
C       2.185115        0.853830        0.061417
H       0.150474        -1.909538       -0.394782
H       0.467091        -1.045624       1.116278
C       -0.724985       0.057923        -0.307908
O       2.752769        0.826609        1.186388
H       -0.542807       1.012401        0.192316
H       -0.732532       0.250119        -1.385087
C       -2.084700       -0.486865       0.126165
H       -2.295292       -1.423639       -0.398409
H       -2.070436       -0.699948       1.199421
C       -3.181612       0.517826        -0.172466
H       -3.031987       1.449572        0.368453
H       -3.258566       0.726864        -1.237217
N       -4.508609       -0.022882       0.258815
H       -4.505770       -0.231780       1.259084
H       -5.257573       0.646526        0.075589
H       -4.725670       -0.886894       -0.241341
O       1.904577        1.871727        -0.618692
###
23
Lys3 m052x E=-496.568387349 au
N       2.752735        -1.605406       -0.106079
H       3.676838        -1.312619       -0.406417
H       2.786686        -1.645648       0.908215
C       1.776338        -0.580209       -0.484315
H       1.769081        -0.496334       -1.571841
C       0.388885        -1.007620       -0.003663
C       2.102705        0.809225        0.082168
H       0.150077        -1.963619       -0.479107
H       0.437899        -1.183633       1.077356
C       -0.714837       0.003807        -0.308214
O       2.368170        0.890462        1.317393
H       -0.518961       0.940776        0.224203
H       -0.708921       0.238628        -1.378702
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C       -2.093372       -0.518836       0.091318
H       -2.301258       -1.455005       -0.436955
H       -2.097309       -0.746591       1.163867
C       -3.201496       0.479425        -0.207054
H       -2.958083       1.434835        0.273829
H       -3.245158       0.662193        -1.282737
N       -4.505693       -0.044735       0.221449
H       -4.496436       -0.147275       1.231045
H       -5.224919       0.638935        0.014410
O       2.063309        1.793487        -0.713166
###
24
LysZW m052x E=-497.036624312 au
N       -2.886419       1.521134        -0.120217
H       -2.939064       1.545233        0.893832
H       -2.598504       2.450144        -0.411621
C       -1.826535       0.574626        -0.485899
H       -1.789497       0.499702        -1.572960
C       -0.444567       0.988856        0.035425
C       -2.183633       -0.807382       0.064858
H       -0.202149       1.964543        -0.399368
H       -0.509727       1.120255        1.121199
C       0.659870        -0.011576       -0.301797
O       -2.476144       -0.879143       1.293811
H       0.463712        -0.963996       0.201258
H       0.657906        -0.210614       -1.378716
C       2.037349        0.498508        0.118040
H       2.266686        1.427968        -0.411999
H       2.039527        0.716178        1.190596
C       3.105973        -0.534366       -0.187266
H       2.941582        -1.457795       0.363687
H       3.161892        -0.754432       -1.251140
N       4.453223        -0.024225       0.219677
H       4.469680        0.195095        1.217515
H       5.182192        -0.714563       0.033865
H       4.685709        0.828708        -0.292407
O       -2.134896       -1.792955       -0.726327
###
21
Met1 m052x E=-800.982462537 au
N       2.433000        -1.586145       -0.245051
H       2.562171        -1.698049       0.764735
H       3.344877        -1.376084       -0.658774
H       2.103674        -2.475119       -0.630670
C       1.443753        -0.511407       -0.533049
H       1.377486        -0.397882       -1.612959
C       0.092460        -0.916918       0.067337
C       1.973202        0.760927        0.091316
H       -0.164715       -1.888510       -0.362714
H       0.208262        -1.038661       1.147386
C       -1.009200       0.090567        -0.242738
O       2.703896        0.768739        1.061517
H       -0.840342       1.033760        0.276972
H       -1.062043       0.281402        -1.316165
S       -2.602302       -0.594862       0.315914
C       -3.662431       0.806795        -0.134179
H       -3.623981       0.984383        -1.208613
H       -4.682577       0.550021        0.148254
H       -3.357586       1.704276        0.403379
O       1.529206        1.846380        -0.526425
H       1.849077        2.640534        -0.062957
###
19
Met3 m052x E=-800.071388304 au
N       2.597184        -1.513095       -0.290374
H       2.732040        -1.562005       0.714880
H       2.259964        -2.425025       -0.582125
C       1.547902        -0.524750       -0.548677
H       1.450895        -0.388600       -1.626051
C       0.184830        -0.946765       0.025538
C       1.952234        0.818356        0.062184
H       -0.077496       -1.909644       -0.423900
H       0.293873        -1.100047       1.103878
C       -0.917785       0.068931        -0.252856
O       2.431284        0.800185        1.232300
H       -0.733548       1.003242        0.280291
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H       -0.977557       0.284407        -1.322157
S       -2.525662       -0.590609       0.296664
C       -3.564443       0.833457        -0.136198
H       -3.518294       1.027140        -1.207802
H       -4.590643       0.591069        0.137361
H       -3.247373       1.719141        0.414065
O       1.746468        1.863110        -0.620098
###
20
MetZW m052x E=-800.537668348 au
N       2.509805        -1.489944       -0.183950
H       2.705630        -1.415413       0.818827
H       3.385212        -1.326844       -0.685005
H       2.186817        -2.436044       -0.396338
C       1.483394        -0.467106       -0.546550
H       1.446712        -0.403766       -1.631176
C       0.139791        -0.919370       0.027319
C       1.925286        0.876492        0.053525
H       -0.108429       -1.884566       -0.423550
H       0.245618        -1.064101       1.106246
C       -0.968448       0.087466        -0.258617
O       2.530424        0.822025        1.156991
H       -0.811826       1.009550        0.302028
H       -1.008138       0.324813        -1.323425
S       -2.567358       -0.624621       0.248537
C       -3.610411       0.828685        -0.053095
H       -3.557277       1.126102        -1.100085
H       -4.636757       0.554211        0.187266
H       -3.304546       1.657574        0.584773
O       1.613128        1.908604        -0.589992
###
24
Phe1 m052x E=-555.246280096 au
N       -3.022769       -1.085994       -0.125473
H       -3.311950       -0.594575       -0.976962
H       -3.713332       -0.891537       0.604312
H       -3.028169       -2.091636       -0.315336
C       -1.660566       -0.646422       0.285629
H       -1.442229       -1.080653       1.258154
C       -0.648966       -1.108490       -0.775955
C       -1.688028       0.865351        0.376435
H       -0.680358       -2.199710       -0.796274
H       -0.973079       -0.730225       -1.748096
C       0.745222        -0.621655       -0.466358
O       -2.352582       1.556370        -0.369893
C       1.260346        0.500330        -1.119641
C       1.517296        -1.259740       0.508532
H       0.662398        0.997799        -1.876151
C       2.530284        0.981182        -0.802203
C       2.786360        -0.780802       0.826994
H       1.121750        -2.133005       1.016339
H       2.920397        1.851446        -1.315898
C       3.294618        0.342251        0.172865
H       3.378431        -1.283338       1.582230
H       4.281451        0.714447        0.419689
O       -0.894714       1.331834        1.329611
H       -0.896950       2.305289        1.310773
###
Phe3 m052x E=-554.335926984 au
###
23
PheZW m052x E=-554.801181852 au
N       -3.009409       -1.081185       -0.171366
H       -3.313488       -0.481530       -0.944093
H       -3.697304       -0.993715       0.578882
H       -2.992819       -2.054392       -0.482868
C       -1.657960       -0.632312       0.278488
H       -1.431825       -1.140620       1.212517
C       -0.650243       -1.006274       -0.817231
C       -1.709336       0.888790        0.491658
H       -0.674467       -2.091911       -0.939977
H       -0.972786       -0.547134       -1.755154
C       0.747341        -0.552299       -0.478263
O       -2.459073       1.534194        -0.288995
C       1.281322        0.595221        -1.069102
C       1.513932        -1.255185       0.456222
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H       0.689694        1.145776        -1.792866
C       2.561213        1.035493        -0.732797
C       2.792187        -0.816572       0.795720
H       1.106162        -2.148562       0.917446
H       2.964236        1.925897        -1.200085
C       3.318990        0.330987        0.201328
H       3.377501        -1.370147       1.520070
H       4.313594        0.671244        0.462797
O       -0.976842       1.356593        1.397339
###
18
Pro1 m052x E=-401.613638604 au
N       0.758597        -1.041061       0.548145
H       0.211452        -1.849831       0.237604
H       1.138567        -1.242442       1.473822
C       1.886184        -0.730721       -0.403381
C       -0.113025       0.180779        0.622854
H       1.523949        -0.951308       -1.405559
H       2.734982        -1.361180       -0.156798
C       2.087800        0.759023        -0.193165
C       0.650674        1.283724        -0.143864
H       -0.259029       0.436267        1.670353
C       -1.450217       -0.134979       0.002794
H       2.664367        1.203792        -1.001864
H       2.601113        0.938384        0.753473
H       0.252534        1.376939        -1.155293
H       0.551799        2.239066        0.364971
O       -1.738004       -1.207982       -0.489679
O       -2.260812       0.914730        0.046122
H       -3.107882       0.696802        -0.380704
###
16
Pro3 m052x E=-400.694491669 au
N       0.748000        -0.959325       0.817518
H       1.275494        -0.800481       1.670084
C       1.711518        -0.837918       -0.291294
C       -0.150144       0.200957        0.671627
H       1.241206        -1.201259       -1.208248
H       2.595586        -1.443560       -0.095486
C       1.996785        0.659572        -0.402456
C       0.605992        1.271488        -0.183626
H       -0.390001       0.592768        1.659430
C       -1.479364       -0.110158       -0.015404
H       2.436439        0.946771        -1.358802
H       2.679364        0.957026        0.398055
H       0.101780        1.413815        -1.142322
H       0.640323        2.236092        0.321517
O       -1.628654       -1.184405       -0.659997
O       -2.361960       0.798211        0.080005
###
17
ProZW m052x E=-401.168154853 au
N       0.663679        -1.036692       0.528450
H       0.074670        -1.770459       0.117957
H       0.941205        -1.317322       1.468291
C       1.878711        -0.758894       -0.317371
C       -0.165520       0.222670        0.585616
H       1.619457        -1.019916       -1.341552
H       2.701023        -1.376762       0.031030
C       2.071665        0.739924        -0.156660
C       0.634897        1.262127        -0.218653
H       -0.261065       0.510948        1.629795
C       -1.552106       -0.039395       -0.006337
H       2.704820        1.147504        -0.943083
H       2.522304        0.960179        0.813365
H       0.287669        1.276205        -1.254101
H       0.514684        2.256374        0.205544
O       -1.759785       -1.167476       -0.528478
O       -2.359765       0.921413        0.060232
###
15
Ser1 m052x E=-399.411830661 au
N       -0.256541       1.919355        -0.265685
H       -0.495053       2.079983        0.718159
H       -1.083049       2.137525        -0.828230
H       0.489936        2.567553        -0.531137
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C       0.180145        0.515134        -0.476546
H       0.355169        0.362270        -1.538764
C       1.463516        0.292339        0.325319
C       -0.932914       -0.386622       0.016013
H       2.212662        1.003110        -0.030550
H       1.263474        0.472671        1.385233
O       1.872102        -1.045289       0.098811
O       -1.697738       -0.058816       0.900654
H       2.688609        -1.198619       0.589819
O       -0.955045       -1.554535       -0.607548
H       -1.654986       -2.115958       -0.228787
###
13
Ser3 m052x E=-398.503862773 au
N       -0.209433       1.949134        -0.300242
H       -0.388379       2.088243        0.689706
H       0.585537        2.533157        -0.539685
C       0.156990        0.545776        -0.500276
H       0.303963        0.362247        -1.564186
C       1.435008        0.189602        0.249317
C       -0.981611       -0.352156       -0.007684
H       2.254266        0.808156        -0.128060
H       1.294675        0.392912        1.315267
O       1.720605        -1.197390       0.040563
O       -1.417275       -0.130562       1.158404
H       2.522321        -1.421273       0.527277
O       -1.399416       -1.260388       -0.779812
###
14
SerZW m052x E=-398.967034385 au
N       -0.571050       1.802301        -0.272385
H       -0.941081       1.835249        0.682253
H       -1.359379       1.922452        -0.911216
H       0.079587        2.577953        -0.414946
C       0.085124        0.482942        -0.490508
H       0.305740        0.383733        -1.550211
C       1.370955        0.467445        0.330685
C       -0.884121       -0.616358       -0.023446
H       2.000556        1.305833        0.021138
H       1.127227        0.573484        1.391994
O       2.018027        -0.771585       0.078406
O       -1.639692       -0.312056       0.937765
H       2.842736        -0.789179       0.578203
O       -0.814558       -1.720084       -0.615036
###
18
Thr1 m052x E=-438.732449011 au
N       0.235419        1.715342        -0.019452
H       -0.574992       2.322928        -0.164523
H       1.049126        2.151599        -0.459010
H       0.404727        1.651322        0.989505
C       -0.008621       0.363699        -0.587741
H       0.010023        0.438061        -1.674301
C       1.057298        -0.618062       -0.105365
C       -1.388793       -0.071408       -0.139683
H       0.831754        -1.579747       -0.569107
C       2.466360        -0.185938       -0.468311
O       0.869248        -0.694153       1.308632
O       -2.114734       0.612585        0.551660
H       2.740970        0.744321        0.033050
H       3.167354        -0.960303       -0.153824
H       2.555419        -0.055134       -1.548104
H       1.551250        -1.265415       1.685151
O       -1.698741       -1.275880       -0.598606
H       -2.587213       -1.525189       -0.289561
###
16
Thr3 m052x E=-437.820076498 au
N       0.109376        1.797324        -0.110597
H       1.051338        2.109141        -0.316594
H       -0.002265       1.814899        0.897180
C       -0.060188       0.426612        -0.577572
H       -0.020930       0.418885        -1.668347
C       1.009098        -0.567843       -0.099568
C       -1.430077       -0.134678       -0.172828
H       0.786562        -1.534632       -0.559358
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C       2.423384        -0.151287       -0.463637
O       0.866155        -0.683868       1.326718
O       -2.071042       0.432996        0.752677
H       2.703699        0.776605        0.039224
H       3.127761        -0.928669       -0.159005
H       2.511716        -0.011773       -1.543336
H       1.555820        -1.275328       1.652115
O       -1.811693       -1.172531       -0.790153
###
17
ThrZW m052x E=-438.287673603 au
N       0.099403        1.681010        0.022327
H       -0.791617       2.180738        -0.021896
H       0.823434        2.219983        -0.454520
H       0.351950        1.595524        1.010957
C       -0.068752       0.325274        -0.576731
H       -0.038793       0.435067        -1.659860
C       1.061809        -0.583259       -0.116553
C       -1.448215       -0.227242       -0.172175
H       0.884297        -1.559292       -0.570604
C       2.439965        -0.072807       -0.502473
O       0.919223        -0.673542       1.306274
O       -2.205303       0.539415        0.477145
H       2.659533        0.883685        -0.022955
H       3.195642        -0.792614       -0.183106
H       2.509478        0.044743        -1.585329
H       1.669883        -1.165852       1.661514
O       -1.697480       -1.398478       -0.548782
###
28
Trp1 m052x E=-686.825663397 au
N       3.336960        1.434054        -0.511071
H       3.937192        0.729308        -0.949689
H       3.848373        1.842869        0.275222
H       3.153045        2.173744        -1.193882
C       2.055230        0.818852        -0.066415
H       1.482729        1.576069        0.463580
C       1.297509        0.302736        -1.302891
C       2.402076        -0.323541       0.862964
H       1.114535        1.167303        -1.946834
H       1.947360        -0.394251       -1.837606
C       0.016101        -0.373354       -0.934499
O       3.405306        -0.997254       0.733335
C       -0.229806       -1.721713       -0.966508
C       -1.173277       0.246013        -0.410338
H       0.412446        -2.527091       -1.288832
N       -1.496364       -1.979705       -0.502932
C       -2.098431       -0.795195       -0.152666
C       -1.541978       1.575410        -0.137866
H       -1.916204       -2.893505       -0.434811
C       -3.375167       -0.548698       0.365174
C       -2.805006       1.824383        0.376058
H       -0.851110       2.389166        -0.327558
H       -4.068956       -1.358659       0.554479
C       -3.711446       0.770555        0.626110
H       -3.105709       2.842380        0.591887
H       -4.690669       0.998648        1.029240
O       1.484516        -0.513760       1.800451
H       1.719374        -1.290995       2.337806
###
26
Trp3 m052x E=-685.914221885 au
N       -3.342720       -1.548077       -0.549624
H       -3.865173       -1.903668       0.244357
H       -3.931626       -0.840393       -0.979281
C       -2.128953       -0.888317       -0.064402
H       -1.522844       -1.622215       0.467202
C       -1.340060       -0.350425       -1.267858
C       -2.411594       0.275292        0.895746
H       -1.107157       -1.197566       -1.918865
H       -1.992913       0.327839        -1.825058
C       -0.085885       0.368310        -0.875618
O       -3.254268       1.142859        0.521776
C       0.112038        1.724479        -0.834432
C       1.136144        -0.228570       -0.399269
H       -0.562709       2.522989        -1.103276
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N       1.377476        2.007831        -0.370506
C       2.028855        0.830393        -0.098456
C       1.559165        -1.555980       -0.207567
H       1.767724        2.930799        -0.265940
C       3.323593        0.602258        0.382607
C       2.840124        -1.787290       0.269757
H       0.893526        -2.382717       -0.429157
H       3.991676        1.425406        0.605394
C       3.713519        -0.716246       0.561430
H       3.181515        -2.803960       0.422724
H       4.708427        -0.929814       0.933194
O       -1.781408       0.308591        1.992972
###
27
TrpZW m052x E=-686.379966236 au
N       -3.341554       -1.426289       -0.497739
H       -3.974723       -0.675947       -0.790721
H       -3.799400       -1.948041       0.251975
H       -3.181207       -2.059814       -1.283483
C       -2.064203       -0.810929       -0.025372
H       -1.494898       -1.579974       0.490181
C       -1.309065       -0.282617       -1.254362
C       -2.416588       0.335263        0.933438
H       -1.117598       -1.130486       -1.919144
H       -1.958755       0.421606        -1.780886
C       -0.027788       0.393961        -0.883722
O       -3.456208       0.991943        0.655005
C       0.212509        1.743365        -0.884347
C       1.172780        -0.231150       -0.392164
H       -0.438531       2.554026        -1.174238
N       1.485495        1.997165        -0.431564
C       2.097558        0.807451        -0.120696
C       1.552198        -1.565151       -0.160095
H       1.901228        2.911000        -0.344196
C       3.382991        0.553368        0.371592
C       2.824009        -1.821967       0.328027
H       0.861680        -2.376836       -0.359761
H       4.075812        1.361470        0.572345
C       3.729555        -0.770726       0.592028
H       3.132451        -2.843843       0.512525
H       4.715783        -1.004527       0.974403
O       -1.625437       0.541810        1.886264
###
25
Tyr1 m052x E=-630.473143405 au
N       3.481458        -0.927428       0.039816
H       4.141067        -0.656254       -0.693994
H       3.560150        -1.937097       0.186731
H       3.754436        -0.451794       0.905372
C       2.082567        -0.570691       -0.326917
H       1.870848        -0.992227       -1.306509
C       1.132034        -1.131969       0.743657
C       2.000468        0.940557        -0.375223
H       1.238978        -2.218522       0.728010
H       1.459187        -0.763986       1.718843
C       -0.299891       -0.732116       0.491385
O       2.633668        1.658990        0.372490
C       -0.880648       0.316847        1.205838
C       -1.056831       -1.372672       -0.494523
H       -0.305600       0.825370        1.972378
C       -2.188349       0.723740        0.949108
C       -2.362568       -0.978447       -0.764089
H       -0.620116       -2.190396       -1.057701
H       -2.636954       1.537602        1.507579
C       -2.923048       0.072672        -0.038840
H       -2.951924       -1.474859       -1.525054
O       -4.217200       0.430913        -0.335263
H       -4.491177       1.162556        0.233459
O       1.147795        1.372818        -1.293067
H       1.074402        2.342301        -1.243471
###
23
Tyr3 m052x E=-629.562414113 au
N       -3.529372       -0.971242       -0.093508
H       -4.162699       -0.681960       0.644789
H       -3.786019       -0.425347       -0.911059
```

```
C       -2.165538       -0.598469       0.282399
H       -1.910270       -1.101978       1.215344
C       -1.200648       -1.063163       -0.819868
C       -1.983014       0.910907        0.498802
H       -1.294333       -2.148108       -0.906936
H       -1.524324       -0.618864       -1.765608
C       0.232150        -0.682417       -0.542265
O       -2.456097       1.685132        -0.383265
C       0.826022        0.410332        -1.177153
C       0.986963        -1.386665       0.402959
H       0.260409        0.972260        -1.912572
C       2.134303        0.795741        -0.885542
C       2.292950        -1.016899       0.707758
H       0.545670        -2.238907       0.909087
H       2.588063        1.643961        -1.386121
C       2.861818        0.078593        0.059767
H       2.874601        -1.565747       1.438388
O       4.158170        0.413036        0.388413
H       4.432143        1.187034        -0.120888
O       -1.355531       1.287907        1.530975
###
22
Tyr4 m052x E=-629.085111078 au
N       -3.481738       -1.006129       -0.101784
H       -4.124966       -0.713461       0.626546
H       -3.737120       -0.474340       -0.928952
C       -2.124131       -0.612149       0.280034
H       -1.869059       -1.106423       1.218118
C       -1.142740       -1.066393       -0.811173
C       -1.970216       0.900177        0.490355
H       -1.230463       -2.152869       -0.897501
H       -1.469630       -0.630112       -1.760533
C       0.286677        -0.670355       -0.533159
O       -2.436624       1.661880        -0.407004
C       0.883353        0.424186        -1.168230
C       1.056346        -1.356104       0.415489
H       0.313543        0.979465        -1.908264
C       2.187959        0.819591        -0.880286
C       2.359501        -0.974251       0.716064
H       0.623793        -2.210909       0.928903
H       2.624501        1.669525        -1.395279
C       2.979510        0.133475        0.077037
H       2.933307        -1.528339       1.452258
O       4.214801        0.493772        0.354060
O       -1.376840       1.297011        1.535494
###
24
TyrZW m052x E=-630.027914555 au
N       3.456771        -0.969801       0.034370
H       3.766396        -0.401159       0.827763
H       4.101838        -0.801868       -0.740243
H       3.502364        -1.958876       0.287528
C       2.065649        -0.566865       -0.330607
H       1.819755        -1.041853       -1.277192
C       1.125416        -1.036047       0.787625
C       2.041782        0.962439        -0.471786
H       1.218549        -2.121836       0.871273
H       1.458142        -0.589854       1.728450
C       -0.307875       -0.655914       0.514046
O       2.779199        1.605090        0.323281
C       -0.876179       0.471457        1.109788
C       -1.086294       -1.404759       -0.373871
H       -0.286476       1.067173        1.798352
C       -2.188803       0.848601        0.832979
C       -2.397866       -1.042583       -0.662559
H       -0.661932       -2.284848       -0.845148
H       -2.625653       1.723685        1.300961
C       -2.944124       0.087336        -0.055618
H       -3.001997       -1.625397       -1.346909
O       -4.246019       0.410110        -0.365683
H       -4.507033       1.207650        0.113336
O       1.270372        1.439024        -1.339942
###
20
Val1 m052x E=-402.819653058 au
N       -0.699439       1.784376        -0.621493
```

```
H       -0.842457       2.069586        0.350628
H       -1.603506       1.846542        -1.096038
H       -0.056020       2.445405        -1.063010
C       -0.144897       0.402427        -0.702956
H       -0.115689       0.129827        -1.756764
C       1.278599        0.359069        -0.106574
C       -1.119721       -0.498870       0.021873
H       1.794312        1.217017        -0.548443
C       1.288300        0.499372        1.416459
C       2.014975        -0.908107       -0.540030
O       -1.969601       -0.084852       0.785751
H       0.812067        -0.363594       1.890516
H       2.321934        0.541012        1.763256
H       0.787117        1.406056        1.763688
H       1.968405        -1.045688       -1.622155
H       3.063042        -0.826469       -0.247771
H       1.598204        -1.792923       -0.057235
O       -0.928623       -1.779616       -0.262191
H       -1.549076       -2.325006       0.252666
###
18
Val3 m052x E=-401.904874333 au
N       -0.645083       1.712041        -0.916910
H       -0.883227       2.056413        0.007026
H       0.126818        2.279019        -1.252929
C       -0.185762       0.327748        -0.778712
H       -0.176281       -0.136238       -1.766749
C       1.249921        0.212262        -0.208141
C       -1.181378       -0.460964       0.077523
H       1.853436        0.872535        -0.842563
C       1.362859        0.703093        1.235352
C       1.816722        -1.201663       -0.334187
O       -1.788748       0.152403        1.001478
H       0.838885        0.027109        1.916641
H       2.412207        0.734664        1.537867
H       0.946749        1.705430        1.361758
H       1.706448        -1.585568       -1.351651
H       2.879966        -1.202793       -0.082303
H       1.310064        -1.889602       0.346519
O       -1.320459       -1.693417       -0.177260
###
19
ValZW m052x E=-402.373494597 au
N       0.822733        -1.667651       -0.673994
H       1.703254        -1.670031       -1.191889
H       1.046827        -1.911110       0.293474
C       0.185431        -0.314451       -0.721675
H       0.133197        -0.028966       -1.770598
C       -1.233218       -0.396904       -0.130013
C       1.098278        0.661827        0.034157
H       -1.702501       -1.265079       -0.604431
C       -1.229435       -0.603699       1.385806
C       -2.057062       0.835880        -0.500388
O       1.929495        0.160750        0.837569
H       -0.802412       0.266433        1.891973
H       -2.255656       -0.725826       1.737343
H       -0.668346       -1.489825       1.692090
H       -2.028485       1.024246        -1.575864
H       -3.096427       0.676252        -0.207257
H       -1.690347       1.723645        0.016748
O       0.921806        1.883921        -0.200010
H       0.207390        -2.379463       -1.071431
###
# PEPTIDES optimized with m052x
# opt(tight) freq m052x/6-31+G(d,p) scf=(xqc,tight) integral=ultrafine scrf(smd,solvent=water)
###
24
AlaAla1 m052x E=-571.524649666 au
N       3.500310        -0.480573       0.113132
H       3.560934        -0.681119       -0.888572
H       3.446370        -1.376105       0.603813
H       4.352903        0.001941        0.404285
C       2.311685        0.369890        0.399299
H       2.267185        0.507296        1.478295
C       2.460600        1.703950        -0.320385
C       1.089878        -0.402609       -0.079445
```

```
H       2.473536        1.553735        -1.401296
H       1.628912        2.357582        -0.060724
H       3.387881        2.186424        -0.009680
O       1.216098        -1.409800       -0.788807
N       -0.087074       0.098150        0.296930
H       -0.125331       0.939994        0.858853
C       -1.337907       -0.494804       -0.137571
H       -1.234794       -0.805992       -1.179132
C       -1.734908       -1.700407       0.724114
C       -2.405424       0.578248        -0.068755
H       -1.904505       -1.389663       1.755518
H       -2.638539       -2.172347       0.337155
H       -0.924615       -2.428214       0.697437
O       -2.252169       1.643249        0.495330
O       -3.577681       0.294156        -0.640918
H       -3.576123       -0.563027       -1.094769
###
23
AlaAla2 m052x E=-571.077103265 au
N       3.415131        0.482777        -0.366461
H       3.502965        0.903703        0.562677
H       3.313900        1.241784        -1.043544
H       4.270894        -0.033182       -0.580124
C       2.238363        -0.430164       -0.394492
H       2.098811        -0.747541       -1.425498
C       2.500510        -1.616487       0.523421
C       1.042255        0.375780        0.094195
H       2.630840        -1.277515       1.552729
H       1.657117        -2.304269       0.478847
H       3.397593        -2.144681       0.198287
O       1.218382        1.366749        0.823749
N       -0.147227       -0.084761       -0.272249
H       -0.219089       -0.931942       -0.824026
C       -1.399122       0.473850        0.218581
H       -1.288446       0.689011        1.282580
C       -1.772895       1.754518        -0.530269
C       -2.511194       -0.573094       0.060854
H       -1.951340       1.535925        -1.585100
H       -2.675674       2.187704        -0.100083
H       -0.964586       2.482043        -0.452801
O       -2.260392       -1.613180       -0.606784
O       -3.612467       -0.290265       0.604695
###
22
AlaAla3 m052x E=-570.615832498 au
N       -3.289283       0.401717        0.942448
H       -2.866432       0.936976        1.693892
H       -3.578301       1.071161        0.235485
C       -2.288458       -0.484824       0.353894
H       -1.950969       -1.180290       1.122982
C       -2.902883       -1.263476       -0.804359
C       -1.083216       0.282810        -0.176880
H       -3.282905       -0.570500       -1.558814
H       -2.163555       -1.916674       -1.271389
H       -3.730673       -1.872576       -0.439673
O       -1.236973       1.257839        -0.941117
N       0.117779        -0.158675       0.196387
H       0.197489        -0.964792       0.802124
C       1.367157        0.419830        -0.271872
H       1.294329        0.588629        -1.347133
C       1.678706        1.740934        0.437374
C       2.510997        -0.569839       -0.017378
H       1.826180        1.566959        1.505475
H       2.584427        2.183846        0.022660
H       0.853474        2.440726        0.304136
O       2.300880        -1.534031       0.768645
O       3.601550        -0.315978       -0.598311
###
21
AlaGly1 m052x E=-532.215171050 au
N       -3.296355       -0.406638       -0.597421
H       -3.458737       -1.033324       0.195546
H       -3.138776       -0.984560       -1.425967
H       -4.134571       0.158745        -0.748419
C       -2.127417       0.474202        -0.319712
H       -1.935246       1.050163        -1.222531
```

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C       -2.446511       1.383830        0.859247
C       -0.954126       -0.442594       -0.009060
H       -2.630945       0.791927        1.757407
H       -1.605773       2.053021        1.038195
H       -3.327727       1.984909        0.632483
O       -1.144735       -1.600672       0.388814
N       0.255128        0.091119        -0.164165
H       0.357189        1.046024        -0.485389
C       1.443102        -0.662858       0.168128
C       2.660909        0.182369        -0.071436
H       1.437967        -0.967882       1.216764
H       1.520796        -1.564884       -0.441911
O       2.638857        1.333125        -0.462039
O       3.781055        -0.485567       0.200341
H       4.547264        0.089712        0.034996
###
20
AlaGly2 m052x E=-531.765338545 au
N       -3.303511       -0.401355       -0.359176
H       -3.425429       -0.858156       0.548005
H       -3.248948       -1.134935       -1.068887
H       -4.123135       0.179067        -0.548697
C       -2.072326       0.438494        -0.354752
H       -1.963222       0.845860        -1.358377
C       -2.221502       1.550727        0.674491
C       -0.905877       -0.491763       -0.043583
H       -2.312198       1.132494        1.678503
H       -1.351717       2.205471        0.639290
H       -3.107467       2.145209        0.448026
O       -1.113185       -1.664312       0.312987
N       0.305418        0.035070        -0.167964
H       0.430685        1.002540        -0.440874
C       1.506881        -0.717306       0.137110
C       2.750880        0.151417        -0.040261
H       1.481094        -1.075368       1.168060
H       1.591366        -1.586664       -0.516791
O       2.595687        1.358774        -0.364982
O       3.850909        -0.429581       0.164957
###
19
AlaGly3 m052x E=-531.304165568 au
N       -3.214160       -0.160330       -0.961431
H       -2.878294       -0.554023       -1.834464
H       -3.513607       -0.945956       -0.391481
C       -2.113421       0.507260        -0.275500
H       -1.756828       1.323995        -0.904168
C       -2.597290       1.067289        1.059987
C       -0.946041       -0.432823       0.003305
H       -2.967356       0.256211        1.692086
H       -1.789871       1.579382        1.585744
H       -3.408957       1.774971        0.887517
O       -1.139647       -1.603052       0.391643
N       0.277490        0.069219        -0.158674
H       0.404085        1.025686        -0.462658
C       1.477885        -0.677502       0.157169
C       2.727680        0.175524        -0.051192
H       1.461362        -1.007767       1.198075
H       1.555995        -1.567202       -0.470102
O       2.583550        1.376283        -0.405054
O       3.825758        -0.408982       0.160609
###
32
AlaHis1 m052x E=-797.013129557 au
N       -4.380930       -1.468612       -0.466107
H       -4.320934       -1.951144       0.435062
H       -3.962297       -2.074955       -1.174711
H       -5.366585       -1.329315       -0.699117
C       -3.682264       -0.155348       -0.386143
H       -3.686285       0.276480        -1.384469
C       -4.406057       0.740347        0.610033
C       -2.259806       -0.438394       0.072662
H       -4.389224       0.293322        1.605446
H       -3.915296       1.712027        0.646326
H       -5.439667       0.882316        0.293026
O       -1.999418       -1.448553       0.737284
N       -1.358241       0.491445        -0.253576
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H       -1.626764       1.281247        -0.828354
C       0.019762        0.396072        0.178448
H       0.048659        -0.007040       1.191504
C       0.823665        -0.529553       -0.769201
C       0.605895        1.797174        0.160745
H       0.310820        -1.491038       -0.782925
H       0.805089        -0.113048       -1.776854
C       2.237354        -0.723647       -0.334264
O       0.206215        2.661545        -0.591656
O       1.627860        2.044016        0.980227
N       3.313473        -0.232627       -1.048158
C       2.765504        -1.332888       0.765434
H       3.255247        0.274917        -1.923991
C       4.447854        -0.526361       -0.423458
N       4.132186        -1.192183       0.680316
H       2.290087        -1.847965       1.581896
H       5.440902        -0.274330       -0.753881
H       1.814016        1.308445        1.585330
H       4.808111        -1.546552       1.346019
###
31
AlaHis2 m052x E=-796.568995228 au
N       4.304085        -1.470674       0.568770
H       4.164025        -2.086118       -0.237527
H       3.906344        -1.933909       1.389219
H       5.307358        -1.346162       0.720027
C       3.649878        -0.154979       0.316441
H       3.726726        0.427346        1.231542
C       4.344546        0.540437        -0.846816
C       2.195043        -0.442527       -0.026022
H       4.249494        -0.055992       -1.755928
H       3.887601        1.515856        -1.009454
H       5.400553        0.684419        -0.615611
O       1.881664        -1.516777       -0.563413
N       1.338316        0.537897        0.242897
H       1.661287        1.400513        0.665645
C       -0.055383       0.492893        -0.158301
H       -0.126956       0.042495        -1.148451
C       -0.869819       -0.359061       0.844027
C       -0.611799       1.923526        -0.212643
H       -0.339294       -1.299790       0.990222
H       -0.917662       0.158851        1.803916
C       -2.248314       -0.666340       0.366465
O       0.011391        2.816177        0.422402
O       -1.676528       2.077633        -0.864812
N       -3.369340       0.032093        0.770644
C       -2.695979       -1.613638       -0.505686
H       -3.367285       0.825061        1.401390
C       -4.451617       -0.451461       0.172643
N       -4.060458       -1.453115       -0.605764
H       -2.165216       -2.375712       -1.049078
H       -5.460813       -0.098507       0.298019
H       -4.685943       -2.011126       -1.173814
###
30
AlaHis3 m052x E=-796.112004787 au
N       -4.361790       -1.413426       -0.478770
H       -4.312609       -1.900102       0.420603
H       -3.953391       -2.026434       -1.187294
H       -5.343139       -1.251294       -0.713960
C       -3.631554       -0.117141       -0.389450
H       -3.616765       0.315783        -1.387227
C       -4.347124       0.792942        0.599210
C       -2.218495       -0.437281       0.081391
H       -4.347266       0.346859        1.595337
H       -3.838024       1.754895        0.639700
H       -5.375519       0.955173        0.274415
O       -1.997059       -1.475472       0.726498
N       -1.299975       0.478836        -0.205592
H       -1.545828       1.286868        -0.764878
C       0.088912        0.370525        0.217046
H       0.120173        -0.053897       1.219351
C       0.870383        -0.539704       -0.756502
C       0.701952        1.776862        0.240350
H       0.376048        -1.512725       -0.760428
H       0.796652        -0.115923       -1.759876
```

```
C       2.310545        -0.692499       -0.386050
O       0.324123        2.575723        -0.661257
O       1.554959        2.016647        1.134936
N       3.310123        0.042604        -0.992583
C       2.851124        -1.497938       0.583795
C       4.427972        -0.317095       -0.390793
N       4.200107        -1.242909       0.566297
H       2.405577        -2.205997       1.262360
H       5.415345        0.054060        -0.612514
H       4.901015        -1.670214       1.153554
###
29
AlaHis4 m052x E=-795.651031568 au
N       -4.298419       -1.266091       -0.975872
H       -3.723803       -1.572020       -1.754291
H       -4.299747       -2.024955       -0.300957
C       -3.688719       -0.097443       -0.348603
H       -3.653370       0.709572        -1.081304
C       -4.523849       0.338194        0.850875
C       -2.271096       -0.380566       0.136994
H       -4.587084       -0.477613       1.575085
H       -4.081667       1.207001        1.341544
H       -5.531823       0.593709        0.522226
O       -2.018587       -1.400077       0.809713
N       -1.343481       0.530314        -0.167838
H       -1.584946       1.313974        -0.759751
C       0.049810        0.414876        0.233026
H       0.094362        0.016676        1.245562
C       0.806304        -0.531859       -0.725589
C       0.687680        1.809077        0.209383
H       0.295279        -1.495875       -0.701452
H       0.730128        -0.130837       -1.738235
C       2.246927        -0.703055       -0.365255
O       0.340739        2.577987        -0.730309
O       1.530064        2.073146        1.108418
N       3.252552        0.019075        -0.977761
C       2.783783        -1.519493       0.597562
C       4.369959        -0.359904       -0.387100
N       4.136453        -1.285309       0.569047
H       2.333329        -2.223875       1.276697
H       5.360965        -0.003400       -0.616516
H       4.836120        -1.725694       1.148029
###
34
AlaLys3 m052x E=-744.366584575 au
N       3.913465        -2.167653       0.737835
H       3.846587        -2.695671       -0.127209
H       3.183375        -2.520104       1.348246
C       3.659398        -0.762049       0.435233
H       3.689148        -0.196460       1.367388
C       4.731797        -0.236014       -0.513458
C       2.298773        -0.553310       -0.221640
H       4.726207        -0.814730       -1.440355
H       4.559312        0.813975        -0.755681
H       5.712501        -0.333488       -0.046385
O       1.934998        -1.271344       -1.175241
N       1.553515        0.444830        0.256027
H       1.877108        0.976631        1.052868
C       0.249481        0.803176        -0.283193
H       0.278742        0.693770        -1.366991
C       -0.842276       -0.108242       0.301994
C       -0.037076       2.270062        0.062778
H       -0.548412       -1.141553       0.097588
H       -0.855638       0.023345        1.388531
C       -2.232208       0.148254        -0.274676
O       0.389558        2.691711        1.173995
O       -0.706329       2.937797        -0.771240
H       -2.565503       1.157049        -0.018176
H       -2.191512       0.088168        -1.367278
C       -3.247080       -0.863486       0.255897
H       -2.926630       -1.879776       0.007558
H       -3.306551       -0.788327       1.346193
C       -4.617654       -0.608822       -0.341850
H       -4.977812       0.392402        -0.115663
H       -4.621586       -0.759033       -1.419136
N       -5.615382       -1.565661       0.231877
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H       -5.707980       -1.427106       1.239742
H       -6.535430       -1.440833       -0.191871
H       -5.321866       -2.531602       0.073842
###
33
AlaLys4 m052x E=-743.897746425 au
N       -3.853932       -2.149907       -0.757921
H       -3.776701       -2.695293       0.095410
H       -3.123771       -2.482137       -1.379621
C       -3.611463       -0.748434       -0.427025
H       -3.649864       -0.164414       -1.347392
C       -4.684276       -0.251938       0.536629
C       -2.249347       -0.542843       0.227682
H       -4.670688       -0.850515       1.450743
H       -4.518214       0.793760        0.801176
H       -5.666116       -0.346529       0.071352
O       -1.881235       -1.270495       1.172518
N       -1.507419       0.461097        -0.242465
H       -1.832885       0.996436        -1.036120
C       -0.193744       0.805206        0.284171
H       -0.210847       0.685042        1.367059
C       0.884538        -0.107773       -0.323541
C       0.098164        2.273220        -0.050338
H       0.586591        -1.140544       -0.120815
H       0.878929        0.029264        -1.409623
C       2.287504        0.132255        0.229074
O       -0.332097       2.706482        -1.155987
O       0.774338        2.931583        0.785744
H       2.631298        1.134198        -0.043950
H       2.258585        0.090848        1.323568
C       3.283967        -0.900331       -0.295595
H       2.948507        -1.905798       -0.015902
H       3.314330        -0.862787       -1.389532
C       4.685465        -0.675310       0.249694
H       5.044931        0.306084        -0.066678
H       4.643336        -0.666362       1.345867
N       5.615396        -1.689964       -0.264275
H       6.539633        -1.517056       0.114370
H       5.331744        -2.597650       0.090004
###
25
AsnGly1 m052x E=-700.923199763 au
N       -2.700132       -1.926409       -0.340681
H       -2.378060       -2.719570       -0.899874
H       -3.630260       -1.654297       -0.667955
H       -2.771377       -2.244613       0.629426
C       -1.755196       -0.783510       -0.452373
H       -1.703006       -0.506028       -1.503139
C       -2.285725       0.381255        0.382017
C       -0.398909       -1.295624       0.025802
H       -3.352185       0.508908        0.170130
H       -2.178065       0.175734        1.448991
C       -1.613164       1.690166        0.020043
O       -0.311475       -2.382616       0.613365
O       -0.991332       1.829639        -1.047133
N       -1.757686       2.676258        0.904246
H       -1.370196       3.585767        0.699838
H       -2.259871       2.534558        1.767172
N       0.645025        -0.507836       -0.220093
H       0.516453        0.372086        -0.710149
C       1.967221        -0.887551       0.220145
C       2.931612        0.233941        -0.060719
H       1.978453        -1.091242       1.293761
H       2.315339        -1.786234       -0.295494
O       2.606686        1.302819        -0.535746
O       4.208648        -0.000739       0.250714
H       4.347085        -0.894042       0.603907
###
24
AsnGly2 m052x E=-700.475930713 au
N       -2.794539       -1.731726       -0.449681
H       -2.527245       -2.529343       -1.031206
H       -3.695721       -1.377292       -0.778964
H       -2.897449       -2.071875       0.510422
C       -1.760696       -0.663991       -0.509547
H       -1.627407       -0.394746       -1.554465
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C       -2.244073       0.539363        0.297625
C       -0.479691       -1.256360       0.070602
H       -3.248154       0.812487        -0.041447
H       -2.296935       0.294266        1.359735
C       -1.364246       1.750006        0.060965
O       -0.538576       -2.234987       0.833632
O       -0.792907       1.928323        -1.027757
N       -1.273801       2.611108        1.074130
H       -0.757555       3.469729        0.949204
H       -1.749485       2.441689        1.946702
N       0.644255        -0.644936       -0.275316
H       0.616624        0.184324        -0.859992
C       1.928540        -0.999657       0.297257
C       2.988443        0.033420        -0.084884
H       1.858770        -1.041499       1.385411
H       2.252036        -1.979948       -0.056976
O       2.640563        1.005043        -0.807669
O       4.144851        -0.181579       0.368736
###
23
AsnGly3 m052x E=-700.018169977 au
N       -2.442569       -2.062876       -0.798919
H       -1.869025       -2.787757       -1.217634
H       -2.693328       -2.392976       0.128386
C       -1.649933       -0.848958       -0.658227
H       -1.326375       -0.523920       -1.646804
C       -2.521753       0.247772        -0.033178
C       -0.424524       -1.054155       0.230857
H       -3.386568       0.405766        -0.679404
H       -2.866785       -0.074448       0.951017
C       -1.766862       1.553354        0.051688
O       -0.524550       -1.644534       1.325416
O       -1.326040       2.103051        -0.973988
N       -1.585302       2.068161        1.270985
H       -1.086606       2.939985        1.373505
H       -1.952963       1.608962        2.089237
N       0.726203        -0.554038       -0.212087
H       0.762020        -0.050601       -1.089570
C       1.954123        -0.614093       0.554704
C       3.082227        0.125404        -0.161896
H       1.813344        -0.156829       1.536610
H       2.260933        -1.649816       0.710369
O       2.823465        0.705169        -1.250279
O       4.204296        0.094684        0.413945
###
24
AspGly1 m052x E=-720.785176119 au
N       -2.644479       -1.964583       -0.400918
H       -2.303420       -2.738356       -0.976271
H       -3.574465       -1.698401       -0.733716
H       -2.722447       -2.309270       0.559799
C       -1.714130       -0.806529       -0.470263
H       -1.651450       -0.502362       -1.513528
C       -2.279094       0.323855        0.389989
C       -0.358695       -1.312829       0.021680
H       -3.356153       0.412402        0.218026
H       -2.132291       0.126918        1.454398
C       -1.686074       1.662603        0.052750
O       -0.280057       -2.384228       0.637956
O       -2.149892       2.622170        0.852384
O       -0.889751       1.873313        -0.844436
N       0.686641        -0.535631       -0.243151
H       0.554779        0.339175        -0.739875
C       2.005449        -0.879308       0.239966
C       2.949431        0.252419        -0.049736
H       1.994781        -1.055372       1.317470
H       2.386532        -1.781271       -0.243408
O       2.631664        1.294331        -0.589353
O       4.187632        -0.022868       0.356877
H       -1.756756       3.473696        0.595868
H       4.767658        0.731335        0.155972
###
23
AspGly2 m052x E=-720.335411393 au
N       -2.572311       -1.976592       -0.443843
H       -2.217805       -2.737561       -1.027899
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H       -3.499319       -1.710415       -0.784150
H       -2.658546       -2.339246       0.509382
C       -1.647219       -0.812517       -0.478665
H       -1.562735       -0.497113       -1.516796
C       -2.236102       0.306892        0.378929
C       -0.299715       -1.313746       0.041464
H       -3.311422       0.388751        0.191960
H       -2.103019       0.107389        1.444466
C       -1.650206       1.651814        0.052819
O       -0.238363       -2.388036       0.662468
O       -2.108301       2.600625        0.869962
O       -0.867491       1.877309        -0.852098
N       0.745105        -0.537288       -0.202535
H       0.631679        0.340070        -0.698897
C       2.073029        -0.853643       0.287904
C       3.047402        0.278597        -0.034100
H       2.054789        -1.000072       1.369411
H       2.442451        -1.773599       -0.167874
O       2.594023        1.315471        -0.587668
O       4.246899        0.071874        0.294617
H       -1.722908       3.456629        0.616689
###
22
AspGly3 m052x E=-719.884255513 au
N       -2.691669       -1.842797       -0.372216
H       -2.390927       -2.625648       -0.956438
H       -3.611110       -1.529812       -0.690890
H       -2.775676       -2.192091       0.585413
C       -1.712786       -0.720637       -0.438547
H       -1.656158       -0.407220       -1.478699
C       -2.206502       0.427599        0.438596
C       -0.369570       -1.288439       0.013231
H       -3.286824       0.535678        0.309642
H       -2.024906       0.211500        1.493825
C       -1.593997       1.789779        0.099323
O       -0.310542       -2.421449       0.525401
O       -1.936775       2.745427        0.845967
O       -0.816705       1.876212        -0.892434
N       0.682114        -0.503975       -0.169266
H       0.548931        0.425757        -0.560681
C       2.014127        -0.896709       0.244443
C       3.019405        0.222740        -0.019948
H       2.030840        -1.129272       1.311123
H       2.336216        -1.788690       -0.295833
O       2.594545        1.311666        -0.488796
O       4.218532        -0.046705       0.266153
###
21
AspGly4 m052x E=-719.419059198 au
N       -2.759978       -1.871589       -0.273989
H       -2.430333       -2.705754       -0.746567
H       -3.600205       -1.569183       -0.754191
C       -1.760901       -0.811936       -0.414590
H       -1.648944       -0.477868       -1.450859
C       -2.198172       0.385626        0.436017
C       -0.399712       -1.348302       0.018792
H       -3.280688       0.497225        0.322018
H       -2.016932       0.185371        1.495113
C       -1.602608       1.750447        0.092757
O       -0.255842       -2.501706       0.470907
O       -1.931699       2.704204        0.855000
O       -0.851244       1.867294        -0.918721
N       0.630307        -0.515409       -0.129170
H       0.467361        0.417010        -0.499481
C       1.979163        -0.888150       0.239742
C       2.962046        0.250143        -0.023889
H       2.033565        -1.146348       1.299634
H       2.307125        -1.762065       -0.327147
O       2.518913        1.336743        -0.481693
O       4.169604        -0.001081       0.248334
###
35
AspHis0 m052x E=-985.586057049 au
N       -3.191178       -2.671116       -0.510803
H       -2.603745       -3.184563       -1.172761
H       -4.169684       -2.796741       -0.781659
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34
AspHis2 m052x E=-985.132445620 au
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H 1.984686 -3.340406 -0.594583
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C 3.824005 0.665601 0.481764
O 0.280533 -1.974783 -0.612779
O 4.650533 0.271534 1.450204
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H 1.391549 0.963099 -0.107315
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33
AspHis3 m052x E=-984.688766432 au
N -3.302750 2.630949 0.284355
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C       -3.745746       -1.149588       -0.100796
O       -0.873863       2.158282        -0.542770
O       -4.400698       -1.906793       -0.865599
O       -3.113535       -1.515658       0.929809
N       -0.767059       0.023479        0.230703
H       -1.283973       -0.752365       0.641003
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C       1.572646        0.481374        0.825628
C       0.890379        -1.704778       -0.236042
H       1.239606        1.509480        0.967880
H       1.516187        -0.032062       1.787275
C       2.983606        0.498354        0.344743
O       0.131154        -2.467714       0.418103
O       1.893280        -2.052583       -0.914418
N       3.968606        -0.328162       0.848199
C       3.583402        1.239655        -0.629435
H       3.838316        -1.016595       1.580237
C       5.115929        -0.113614       0.213998
N       4.898783        0.835323        -0.687821
H       3.187896        2.004914        -1.274161
H       6.050380        -0.614709       0.400019
H       5.606558        1.203115        -1.311151
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32
AspHis4 m052x E=-984.230867400 au
N       -3.323334       2.599999        0.268548
H       -2.731450       3.241020        0.801005
H       -4.283905       2.680294        0.607729
H       -3.293793       2.897005        -0.709938
C       -2.848605       1.193561        0.401983
H       -2.899624       0.937452        1.457996
C       -3.762081       0.282014        -0.413779
C       -1.397413       1.176180        -0.074219
H       -4.799140       0.595771        -0.264772
H       -3.544812       0.372427        -1.480126
C       -3.702100       -1.195838       -0.016627
O       -0.916472       2.172902        -0.641580
O       -4.367931       -1.984269       -0.739900
O       -3.026480       -1.524805       0.998718
N       -0.735642       0.047424        0.147990
H       -1.214303       -0.717756       0.618447
C       0.652798        -0.137657       -0.244538
H       0.806508        0.302028        -1.229428
C       1.589465        0.546339        0.777095
C       0.951804        -1.641191       -0.308415
H       1.266132        1.584895        0.869330
H       1.457594        0.063819        1.747502
C       3.031625        0.484229        0.386431
O       0.338103        -2.381897       0.508448
O       1.812493        -2.019130       -1.147655
N       3.942022        -0.316678       1.046418
C       3.655162        1.141455        -0.644052
C       5.089871        -0.138676       0.419738
N       4.964186        0.728699        -0.607686
H       3.292201        1.843790        -1.375672
H       6.027644        -0.607241       0.670235
H       5.705460        1.025482        -1.225151
###
31
AspHis5 m052x E=-983.766923232 au
N       -4.893617       0.641872        0.804022
C       -3.600514       1.104754        0.808588
C       -3.012978       0.571960        -0.310832
N       -3.929995       -0.202438       -0.994223
C       -5.044609       -0.134275       -0.290877
C       -1.595292       0.715363        -0.764431
C       -0.594667       -0.078833       0.105768
C       -0.908463       -1.578393       0.034119
O       -1.682806       -2.045524       0.912671
```

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N       0.763325        0.144175        -0.361472
C       1.502117        1.189149        0.018090
O       1.071858        2.082941        0.772796
C       2.937768        1.204957        -0.488400
C       3.798324        0.304030        0.411003
C       3.576789        -1.200117       0.246163
O       3.131435        -1.626593       -0.858656
N       3.396717        2.590546        -0.538676
O       3.898730        -1.935335       1.223482
O       -0.394878       -2.227946       -0.918610
H       4.382958        2.586643        -0.775550
H       3.321655        2.987449        0.392692
H       2.953815        0.797340        -1.498121
H       4.847780        0.483775        0.154132
H       3.670980        0.577489        1.460900
H       1.201398        -0.582473       -0.917164
H       -0.674752       0.253255        1.140382
H       -1.287658       1.762489        -0.736123
H       -1.510929       0.365503        -1.795045
H       -3.220646       1.748760        1.584013
H       -5.977420       -0.616530       -0.534023
H       -5.607744       0.845314        1.487747
###
34
AspHis m052x E=-985.137255542 au
N       -3.405345       2.604742        0.154855
H       -2.821490       3.284401        0.647145
H       -4.364941       2.687370        0.496884
H       -3.389293       2.850448        -0.838346
C       -2.907039       1.216448        0.363544
H       -2.948741       1.019909        1.433197
C       -3.810975       0.244536        -0.392815
C       -1.454343       1.200707        -0.104706
H       -4.850441       0.553260        -0.252820
H       -3.602569       0.277412        -1.464364
C       -3.728390       -1.208497       0.084313
O       -0.960852       2.189751        -0.664421
O       -4.437408       -2.034005       -0.548070
O       -2.986310       -1.483262       1.070631
N       -0.793510       0.067314        0.130385
H       -1.286642       -0.693154       0.599374
C       0.591332        -0.095667       -0.249242
H       0.769231        0.379728        -1.214230
C       1.524569        0.543721        0.812517
C       0.869359        -1.576683       -0.376472
H       1.197599        1.575741        0.936016
H       1.394418        0.025408        1.763671
C       2.962065        0.537649        0.421013
O       0.170806        -2.444483       0.108500
O       1.989178        -1.819824       -1.053036
N       3.864689        -0.405106       0.872926
C       3.659696        1.347692        -0.423480
H       3.645786        -1.174314       1.495818
C       5.055627        -0.195593       0.325711
N       4.950005        0.868031        -0.461761
H       3.348290        2.209331        -0.987883
H       5.945859        -0.776474       0.496040
H       5.714746        1.262112        -0.995863
H       2.162602        -2.777340       -1.060607
###
29
CysAsn1 m052x E=-1138.40213768 au
N       -3.291826       -2.185427       -0.018375
H       -2.801361       -3.023188       -0.341770
H       -4.247247       -2.210780       -0.383592
H       -3.328432       -2.213975       1.005348
C       -2.592963       -0.947797       -0.470966
H       -2.468991       -1.012812       -1.549538
C       -3.456155       0.253122        -0.080401
C       -1.253839       -0.920796       0.255894
H       -4.441136       0.133603        -0.532428
H       -3.572483       0.295737        1.002634
S       -2.811855       1.836513        -0.704778
O       -1.198362       -1.260455       1.441678
H       -1.774535       1.937260        0.144009
N       -0.211595       -0.496848       -0.465487
```

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H       -0.363225       -0.217261       -1.427112
C       1.105512        -0.287257       0.109241
H       1.180111        -0.909525       1.001974
C       2.190243        -0.663120       -0.888390
C       1.261103        1.157436        0.569946
H       2.031679        -1.698245       -1.199469
H       2.139364        -0.027008       -1.773163
C       3.564759        -0.602236       -0.259435
O       0.238346        1.561705        1.322259
O       2.213931        1.859287        0.299222
O       3.739688        -0.881503       0.938451
N       4.571517        -0.283925       -1.077036
H       5.516343        -0.282753       -0.722466
H       4.404247        -0.046158       -2.042003
H       0.377896        2.485928        1.592106
###
28
CysAsn2 m052x E=-1137.95338118 au
N       -3.084314       -2.202742       -0.687260
H       -2.596814       -2.713139       -1.428416
H       -4.085621       -2.215057       -0.895838
H       -2.920784       -2.696141       0.196115
C       -2.580271       -0.803541       -0.583657
H       -2.645952       -0.350027       -1.569915
C       -3.447845       -0.057987       0.433725
C       -1.142314       -0.893878       -0.090886
H       -4.484563       -0.085557       0.097834
H       -3.381896       -0.543135       1.407480
S       -3.030061       1.707683        0.580679
O       -0.843019       -1.743488       0.761982
H       -1.832347       1.549917        1.171950
N       -0.299184       0.003006        -0.589228
H       -0.637736       0.725168        -1.215152
C       1.018171        0.220065        -0.016000
H       0.952176        0.086979        1.065812
C       2.042898        -0.773210       -0.580588
C       1.462032        1.664724        -0.295904
H       1.597845        -1.771525       -0.571194
H       2.290873        -0.516305       -1.611240
C       3.281604        -0.859662       0.279160
O       0.675136        2.416750        -0.929149
O       2.605728        1.969837        0.132373
O       3.199140        -1.009210       1.511443
N       4.456110        -0.836032       -0.358669
H       5.310886        -0.920409       0.171222
H       4.505088        -0.673498       -1.351718
###
27
CysAsn3 m052x E=-1137.48756443 au
N       3.168766        -2.241457       -0.200859
H       2.576758        -3.031376       0.065473
H       4.101795        -2.363044       0.195038
H       3.248519        -2.246528       -1.220549
C       2.573695        -0.952915       0.275769
H       2.648695        -0.963478       1.363518
C       3.372231        0.219130        -0.293837
C       1.096822        -1.002796       -0.111241
H       4.429096        -0.045979       -0.223169
H       3.127750        0.323445        -1.354348
S       3.074594        1.784601        0.615433
O       0.589508        -2.086638       -0.458287
N       0.415089        0.133982        -0.027653
H       0.921879        0.994063        0.210233
C       -1.002955       0.180513        -0.341801
H       -1.178204       -0.380231       -1.261551
C       -1.837866       -0.448708       0.786153
C       -1.462554       1.625997        -0.577423
H       -1.361669       -1.385346       1.086339
H       -1.866844       0.215479        1.651066
C       -3.229456       -0.814955       0.329389
O       -0.625596       2.556185        -0.448823
O       -2.682099       1.758771        -0.871269
O       -3.416182       -1.463069       -0.716540
N       -4.236775       -0.464128       1.135430
H       -5.182138       -0.714004       0.886011
H       -4.073245       0.085013        1.963891
```

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###
26
CysAsn4 m052x E=-1137.02072955 au
N       3.267205        -2.284566       -0.174258
H       2.659842        -3.069342       0.037874
H       3.337943        -2.265461       -1.188111
C       2.603370        -1.054860       0.258148
H       2.628026        -1.019539       1.351187
C       3.374424        0.158830        -0.277174
C       1.119124        -1.054477       -0.131359
H       4.431250        -0.106203       -0.229751
H       3.122753        0.292330        -1.334270
S       3.112176        1.727896        0.647332
O       0.554221        -2.112782       -0.480275
N       0.453117        0.100671        -0.044948
H       0.974125        0.947178        0.204336
C       -0.964573       0.173812        -0.347363
H       -1.160914       -0.398439       -1.255781
C       -1.807334       -0.421283       0.794972
C       -1.409132       1.619877        -0.602781
H       -1.337571       -1.353755       1.117067
H       -1.831044       0.263566        1.644039
C       -3.202446       -0.787123       0.350328
O       -0.565997       2.546886        -0.488695
O       -2.628895       1.762370        -0.896536
O       -3.398625       -1.456843       -0.680453
N       -4.205559       -0.410394       1.150613
H       -5.153545       -0.657941       0.909060
H       -4.035261       0.155592        1.966240
###
42
DLeuTyr3 m052x E=-994.814829758 au
C       -2.735302       -0.843422       -1.408659
C       -3.407314       -1.744739       -0.355539
C       -1.348971       -0.467197       -0.903268
H       -4.432534       -1.938799       -0.691976
H       -2.880588       -2.701876       -0.369968
C       -3.436278       -1.239740       1.093693
O       -0.476176       -1.350511       -0.753156
H       -2.407363       -1.023825       1.405358
C       -4.276941       0.024688        1.283762
C       -3.974050       -2.356950       1.990779
H       -5.295442       -0.138705       0.916126
H       -4.338670       0.279080        2.344976
H       -3.858362       0.880108        0.752572
H       -3.370996       -3.263726       1.901068
H       -3.974159       -2.047736       3.038627
H       -5.003368       -2.604729       1.712427
N       -1.137199       0.813667        -0.624562
H       -1.922417       1.447818        -0.711185
C       0.092258        1.307142        -0.034306
H       0.323290        0.701933        0.847559
C       1.295326        1.237722        -1.017085
C       -0.137235       2.742526        0.469594
H       0.939978        0.830812        -1.964065
H       1.648702        2.252662        -1.212688
C       2.450033        0.394228        -0.527353
O       -1.269865       3.268273        0.293924
O       0.846983        3.290372        1.035526
C       2.903390        -0.697456       -1.270621
C       3.101870        0.685404        0.677145
H       2.411448        -0.948565       -2.204042
C       3.974498        -1.478576       -0.836971
C       4.169585        -0.084745       1.127807
H       2.769512        1.528352        1.272338
H       4.318559        -2.324964       -1.421230
C       4.603269        -1.167518       0.365155
H       4.669972        0.146317        2.060405
O       5.664247        -1.904885       0.846901
H       5.876252        -2.614121       0.226003
N       -3.535817       0.334636        -1.750960
H       -3.462392       0.521485        -2.743362
H       -4.511541       0.152680        -1.551054
H       -2.555127       -1.466498       -2.289588
###
41
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DLeuTyr4 m052x E=-994.337533995 au
C -2.660282 -0.855844 -1.393895
C -3.385757 -1.735091 -0.358361
C -1.292872 -0.481363 -0.836192
H -4.397632 -1.924422 -0.735199
H -2.868999 -2.697406 -0.335751
C -3.469597 -1.207494 1.080262
O -0.443929 -1.372762 -0.613381
H -2.451609 -1.001297 1.431516
C -4.296807 0.072851 1.214201
C -4.061377 -2.302705 1.970327
H -5.301809 -0.079972 0.806826
H -4.398480 0.346958 2.267365
H -3.840624 0.911691 0.687391
H -3.468789 -3.219394 1.919470
H -4.100448 -1.977658 3.012641
H -5.081678 -2.539917 1.652442
N -1.073174 0.805462 -0.597416
H -1.837659 1.448523 -0.764918
C 0.149865 1.317762 -0.007448
H 0.376670 0.735833 0.890011
C 1.366284 1.236112 -0.978013
C -0.087860 2.766161 0.449632
H 1.005586 0.854309 -1.934480
H 1.734235 2.249671 -1.156245
C 2.503878 0.361356 -0.501431
O -1.186918 3.317471 0.168537
O 0.862808 3.305911 1.078887
C 2.893536 -0.775138 -1.217483
C 3.222070 0.655850 0.665349
H 2.356121 -1.036904 -2.124718
C 3.948354 -1.583504 -0.799820
C 4.275618 -0.143284 1.098995
H 2.951177 1.531777 1.247386
H 4.224658 -2.458039 -1.380266
C 4.683119 -1.298735 0.379701
H 4.812350 0.113172 2.007028
O 5.682004 -2.056293 0.782980
N -3.434412 0.321274 -1.797276
H -3.338177 0.468414 -2.794192
H -4.416927 0.165953 -1.609045
H -2.445605 -1.494666 -2.255531
###
41
GluHisOMe2 m052x E=-1064.19079892 au
N -3.163131 -3.147823 -0.076793
H -3.205606 -3.172270 0.946685
H -2.621356 -3.955509 -0.393592
H -4.114248 -3.234410 -0.443240
C -2.549043 -1.868345 -0.532717
H -2.418430 -1.932117 -1.611190
C -3.486157 -0.720854 -0.150900
C -1.212682 -1.736140 0.183989
H -4.421933 -0.859624 -0.694366
H -3.697561 -0.778589 0.919359
C -2.881013 0.634716 -0.488539
O -1.124918 -2.006483 1.385436
H -1.988565 0.839527 0.109293
H -2.583196 0.691562 -1.540650
C -3.844447 1.759534 -0.231166
O -5.001403 1.622194 0.114822
O -3.360403 3.000558 -0.408897
N -0.192773 -1.286624 -0.559063
H -0.374718 -1.000293 -1.513819
C 1.069936 -0.892111 0.043821
H 1.335225 -1.619778 0.808625
C 2.136626 -0.831045 -1.049309
C 0.901301 0.454527 0.745537
H 2.239555 -1.828354 -1.481484
H 1.814020 -0.149085 -1.838695
C 3.451843 -0.371297 -0.513627
O 1.024411 0.614055 1.944702
N 4.392702 0.247311 -1.313593
C 4.010965 -0.452331 0.726767
C 5.479103 0.531755 -0.604165
N 5.263697 0.114729 0.636115

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H       3.635030        -0.860690       1.648620
H       6.367377        1.018722        -0.968296
H       5.928276        0.207456        1.394752
O       0.581554        1.420158        -0.106131
C       0.324941        2.723485        0.470622
H       -0.505051       2.653334        1.171187
H       1.221028        3.079113        0.974562
H       0.074347        3.363290        -0.369365
H       4.276665        0.464145        -2.296846
H       -2.426488       2.985213        -0.669526
###
40
GluHisOMe3 m052x E=-1063.73790076 au
N       -3.219744       -3.096778       -0.087992
H       -3.252366       -3.123246       0.935519
H       -2.697010       -3.913622       -0.412453
H       -4.175741       -3.162304       -0.445296
C       -2.586921       -1.825250       -0.543406
H       -2.460894       -1.890070       -1.622481
C       -3.498298       -0.657739       -0.157870
C       -1.245188       -1.721069       0.165462
H       -4.446573       -0.794305       -0.681318
H       -3.693185       -0.705976       0.916273
C       -2.878384       0.684242        -0.524386
O       -1.147319       -2.025807       1.358389
H       -1.975117       0.866985        0.063292
H       -2.576836       0.699865        -1.575617
C       -3.784422       1.889539        -0.284665
O       -4.909992       1.717171        0.259824
O       -3.321072       3.011398        -0.648481
N       -0.226157       -1.262181       -0.574344
H       -0.420274       -0.932542       -1.512652
C       1.042763        -0.889383       0.029597
H       1.315361        -1.643906       0.765298
C       2.097849        -0.790567       -1.071438
C       0.880302        0.430793        0.781380
H       2.193170        -1.770582       -1.543037
H       1.769762        -0.077912       -1.830845
C       3.420320        -0.355473       -0.533396
O       0.998205        0.543340        1.986640
N       4.362582        0.271469        -1.325304
C       3.985123        -0.467133       0.702081
C       5.455159        0.531432        -0.615904
N       5.242329        0.090918        0.616652
H       3.610394        -0.891702       1.617095
H       6.345815        1.018027        -0.974687
H       5.911713        0.162096        1.373379
O       0.567700        1.429700        -0.032954
C       0.285668        2.704254        0.595198
H       -0.550620       2.591716        1.282294
H       1.171668        3.052286        1.121657
H       0.030037        3.372959        -0.219619
H       4.243628        0.509948        -2.303148
###
39
GluHisOMe4 m052x E=-1063.28411294 au
N       -3.179238       -3.099928       -0.064233
H       -3.193541       -3.122359       0.959836
H       -2.661240       -3.917325       -0.394712
H       -4.141215       -3.167586       -0.404702
C       -2.554443       -1.829186       -0.533939
H       -2.437817       -1.900483       -1.613694
C       -3.465688       -0.662240       -0.146671
C       -1.207682       -1.715877       0.164232
H       -4.419003       -0.804220       -0.659427
H       -3.649504       -0.704610       0.929704
C       -2.853776       0.679497        -0.527058
O       -1.105689       -2.006581       1.361660
H       -1.940872       0.865883        0.044335
H       -2.569697       0.691947        -1.583212
C       -3.758781       1.883724        -0.277687
O       -4.881576       1.709103        0.272056
O       -3.298404       3.007035        -0.640684
N       -0.194093       -1.265066       -0.584280
H       -0.389263       -0.958311       -1.529802
C       1.083976        -0.887814       0.002765
```

```
H       1.363237        -1.639254       0.739153
C       2.132401        -0.782199       -1.103153
C       0.917951        0.430762        0.754000
H       2.217014        -1.763829       -1.575919
H       1.784968        -0.077046       -1.861282
C       3.462208        -0.327744       -0.587075
O       1.023497        0.547038        1.960948
N       4.376156        0.289611        -1.416473
C       3.987057        -0.449413       0.675037
C       5.430789        0.530549        -0.661600
N       5.241736        0.104447        0.605349
H       3.597844        -0.870282       1.586777
H       6.341018        1.011276        -0.980973
H       5.902576        0.185923        1.364209
O       0.606457        1.431274        -0.061089
C       0.321488        2.704093        0.566825
H       -0.514894       2.591193        1.253911
H       1.206240        3.054838        1.093811
H       0.064928        3.372938        -0.247751
###
21
GlyAla1 m052x E=-532.213551948 au
N       -3.775775       -0.184568       0.005916
H       -3.847192       0.176724        -0.947838
C       -2.481987       -0.877656       0.202392
H       -3.865613       0.610130        0.642740
H       -4.553584       -0.824959       0.175504
C       -1.361940       0.082272        -0.147607
H       -2.416151       -1.206915       1.236237
H       -2.453149       -1.741779       -0.458732
O       -1.602682       1.151214        -0.724258
N       -0.139003       -0.326658       0.188553
H       -0.015109       -1.214266       0.659561
C       1.041936        0.457047        -0.123387
H       0.936557        0.866680        -1.129469
C       1.268102        1.596029        0.876707
C       2.228250        -0.477744       -0.130805
H       1.443622        1.193226        1.875114
H       2.123825        2.198465        0.574484
H       0.381268        2.228505        0.897088
O       2.194845        -1.639528       0.227522
O       3.335818        0.127321        -0.556785
H       4.078956        -0.498973       -0.521592
###
20
GlyAla2 m052x E=-531.763595883 au
N       -3.694548       -0.328975       -0.232469
H       -3.832249       0.678583        -0.121990
C       -2.437838       -0.747897       0.431709
H       -4.494392       -0.820349       0.169996
H       -3.662947       -0.528515       -1.234528
C       -1.315247       0.149970        -0.053087
H       -2.564872       -0.620159       1.505254
H       -2.254233       -1.794853       0.205555
O       -1.578263       1.244383        -0.579393
N       -0.087031       -0.307315       0.156105
H       0.059588        -1.233521       0.539367
C       1.109312        0.459152        -0.163650
H       0.987992        0.895345        -1.155872
C       1.356687        1.567516        0.862767
C       2.316028        -0.487855       -0.203235
H       1.533077        1.133277        1.848982
H       2.227250        2.155633        0.572790
H       0.490857        2.227946        0.917086
O       2.177107        -1.649350       0.268038
O       3.377073        -0.005616       -0.683534
###
19
GlyAla3 m052x E=-531.302803682 au
N       -3.832851       -0.327613       0.061945
H       -3.913076       0.450423        0.707505
C       -2.492891       -0.878408       0.152544
H       -3.961013       0.066109        -0.863600
C       -1.375317       0.110345        -0.156473
H       -2.327466       -1.285988       1.150264
H       -2.392883       -1.707640       -0.550510
```

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O       -1.606177       1.220716        -0.671632
N       -0.141957       -0.306348       0.139638
H       -0.002233       -1.231348       0.525298
C       1.055909        0.465682        -0.147373
H       0.953505        0.914222        -1.136504
C       1.279963        1.565933        0.894200
C       2.273765        -0.466672       -0.172893
H       1.440234        1.122291        1.879257
H       2.151519        2.164410        0.628061
H       0.407406        2.218285        0.939899
O       2.150467        -1.625370       0.310427
O       3.333095        0.022863        -0.652642
###
24
GlyAsp1 m052x E=-720.786087354 au
N       4.309998        -0.630934       -0.295027
H       4.055206        -1.621748       -0.292155
C       3.313062        0.158309        0.464975
H       4.352672        -0.326459       -1.270055
C       1.933943        -0.174750       -0.065982
H       3.376748        -0.129204       1.512954
H       3.547099        1.214486        0.360222
O       1.741233        -1.203761       -0.724455
N       0.970817        0.692735        0.253100
H       1.191841        1.544627        0.753904
C       -0.403092       0.463619        -0.137765
H       -0.426971       0.142492        -1.182253
C       -1.049363       -0.624443       0.744949
C       -1.138546       1.794829        -0.048454
H       -0.306261       -1.389259       0.965999
H       -1.388782       -0.208353       1.698265
C       -2.223902       -1.291762       0.095392
O       -0.612635       2.811885        0.361554
O       -2.402053       1.788917        -0.444189
O       -2.907706       -0.786494       -0.788262
O       -2.474214       -2.498439       0.580642
H       5.238351        -0.527886       0.117869
H       -3.269261       -2.863287       0.154206
H       -2.685975       0.880305        -0.726470
###
23
GlyAsp2 m052x E=-720.338374764 au
N       4.372895        -0.575150       -0.166339
H       4.133065        -1.570122       -0.167982
C       3.330480        0.192522        0.555133
H       4.442268        -0.272960       -1.140399
C       1.975968        -0.223031       0.015147
H       3.390394        -0.064475       1.611247
H       3.520139        1.254595        0.423952
O       1.841606        -1.319278       -0.550042
N       0.981745        0.634517        0.224932
H       1.167867        1.556195        0.601590
C       -0.375986       0.365350        -0.205904
H       -0.349881       -0.038842       -1.220133
C       -1.068824       -0.644735       0.719113
C       -1.184771       1.672528        -0.239985
H       -0.410702       -1.504801       0.866726
H       -1.289420       -0.196634       1.686716
C       -2.323316       -1.176200       0.090233
O       -0.586754       2.753818        -0.005291
O       -2.409516       1.532036        -0.497620
O       -2.388900       -1.624410       -1.042229
O       -3.375641       -1.176687       0.918728
H       5.284408        -0.452409       0.276861
H       -4.138299       -1.568550       0.460481
###
22
GlyAsp3 m052x E=-719.880964089 au
N       4.322269        -0.531080       -0.178038
H       4.084387        -1.526562       -0.187519
C       3.272402        0.226864        0.543552
H       5.231527        -0.408098       0.269458
H       4.393916        -0.222656       -1.149887
C       1.922361        -0.202047       0.000999
H       3.334203        -0.031280       1.599243
H       3.453051        1.290462        0.413384
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O       1.803988        -1.304461       -0.559820
N       0.921959        0.647202        0.198502
H       1.089047        1.558477        0.607859
C       -0.442547       0.354565        -0.209917
H       -0.423572       -0.088175       -1.205964
C       -1.118988       -0.621060       0.765322
C       -1.243242       1.662147        -0.270238
H       -0.416113       -1.432192       0.974440
H       -1.348391       -0.112741       1.702634
C       -2.379602       -1.266562       0.193479
O       -0.716535       2.706689        0.200422
O       -2.397481       1.572758        -0.766964
O       -2.295631       -1.788391       -0.955782
O       -3.415586       -1.282037       0.918885
###
21
GlyAsp4 m052x E=-719.419525669 au
N       4.462525        -0.596759       0.040511
H       4.304071        -1.487158       0.499037
C       3.362683        0.296806        0.354038
H       4.455072        -0.791932       -0.954704
C       1.988022        -0.206150       -0.070103
H       3.335298        0.477526        1.429666
H       3.527212        1.263140        -0.125267
O       1.829095        -1.319969       -0.603138
N       0.973737        0.631376        0.164231
H       1.152891        1.549115        0.550970
C       -0.397282       0.348217        -0.220092
H       -0.404183       -0.080657       -1.222885
C       -1.061837       -0.640715       0.751789
C       -1.199929       1.656098        -0.247132
H       -0.361042       -1.461887       0.924412
H       -1.260318       -0.150155       1.705628
C       -2.343577       -1.261242       0.201453
O       -0.671112       2.694319        0.236368
O       -2.360580       1.577447        -0.733167
O       -2.292427       -1.775408       -0.953758
O       -3.366390       -1.266188       0.946224
###
18
GlyGly1 m052x E=-492.901515254 au
N       3.624084        0.191129        -0.192939
H       3.643703        -0.053374       -1.185442
C       2.335678        0.824248        0.173366
H       3.757475        -0.672481       0.339340
C       1.243040        -0.221365       0.075330
H       2.409950        1.177083        1.200430
H       2.156086        1.665513        -0.490350
O       1.521969        -1.428021       0.052892
N       -0.001233       0.249306        0.042170
H       -0.174587       1.246730        0.047258
C       -1.136290       -0.645092       0.017362
C       -2.402192       0.161996        -0.026385
H       -1.110219       -1.292228       -0.861780
H       -1.160042       -1.282186       0.903687
O       -2.445494       1.376648        -0.047210
H       4.402805        0.823520        0.000230
O       -3.482133       -0.617415       -0.039390
H       -4.281282       -0.064034       -0.066365
###
17
GlyGly2 m052x E=-492.451781378 au
N       -3.557006       0.217036        0.199830
H       -3.577497       -0.016436       1.194840
C       -2.260298       0.828382        -0.176072
H       -3.699390       -0.651123       -0.322317
C       -1.182078       -0.233999       -0.078241
H       -2.336009       1.176048        -1.204738
H       -2.066499       1.671008        0.481639
O       -1.488976       -1.438303       -0.070981
N       0.064479        0.214768        -0.030655
H       0.261701        1.208408        -0.028214
C       1.209368        -0.674308       -0.007276
C       2.510389        0.125992        0.028846
H       1.175158        -1.318729       0.872776
H       1.217431        -1.313101       -0.892080
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O       2.437535        1.383614        0.029175
O       3.568545        -0.559239       0.055506
H       -4.328325       0.856322        0.000722
###
16
GlyGly3 m052x E=-491.991110176 au
N       -3.652070       -0.367243       -0.244116
H       -3.590413       -0.121117       -1.226393
C       -2.343583       -0.799905       0.217233
H       -3.901956       0.486102        0.243497
C       -1.251588       0.250548        0.088482
H       -2.402706       -1.057277       1.277188
H       -2.041162       -1.701487       -0.314758
O       -1.516674       1.468734        0.082519
N       -0.001068       -0.206138       0.017891
H       0.184410        -1.200555       0.020068
C       1.151134        0.670698        -0.011436
C       2.450334        -0.131809       -0.031211
H       1.129513        1.307583        -0.897951
H       1.162148        1.322240        0.864595
O       2.379599        -1.389823       -0.019638
O       3.511368        0.551212        -0.058015
###
27
GlyHis2 m052x E=-756.798533443 au
N       -4.870479       -0.941720       0.059080
H       -4.537537       -1.906033       -0.016005
C       -3.879911       -0.011965       -0.531725
H       -5.012264       -0.742547       1.051514
C       -2.516146       -0.325669       0.054810
H       -3.858518       -0.178257       -1.607264
H       -4.188921       1.009190        -0.325248
O       -2.320558       -1.405037       0.636429
N       -1.589330       0.609396        -0.125789
H       -1.816959       1.463888        -0.619662
C       -0.199735       0.428126        0.268479
H       -0.170029       -0.090021       1.225611
C       0.547678        -0.404233       -0.797090
C       0.452100        1.808298        0.418518
H       0.004083        -1.343463       -0.915575
H       0.507517        0.134299        -1.746062
C       1.975812        -0.670156       -0.444020
O       0.055514        2.715076        -0.365110
O       1.355419        1.922751        1.288373
N       3.019848        0.006932        -1.042675
C       2.466897        -1.543738       0.492783
C       4.115197        -0.456167       -0.470837
N       3.831077        -1.390611       0.461751
H       1.979317        -2.237128       1.157458
H       5.124971        -0.155554       -0.698309
H       4.505644        -1.890002       1.022697
H       -5.769458       -0.861640       -0.418773
###
28
GlyHis3 m052x E=-757.255463687 au
N       4.762740        -1.197721       0.198295
H       4.599534        -1.744696       -0.650352
C       3.958129        0.045318        0.166625
H       4.504604        -1.782408       0.995823
H       5.757820        -0.977259       0.266285
C       2.518385        -0.315677       -0.143842
H       4.052837        0.550413        1.124000
H       4.351581        0.682631        -0.623349
O       2.238328        -1.427768       -0.617042
N       1.628856        0.643503        0.096311
H       1.924525        1.537723        0.470528
C       0.226278        0.519550        -0.255465
H       0.142027        0.019539        -1.220323
C       -0.517915       -0.315057       0.814053
C       -0.393410       1.921414        -0.357247
H       0.047191        -1.233171       0.973416
H       -0.537609       0.239971        1.754005
C       -1.906100       -0.680561       0.412531
O       0.207383        2.867862        0.218606
O       -1.482613       2.000288        -0.982314
N       -3.028055       0.003691        0.838069
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C       -2.363510       -1.671964       -0.403749
H       -3.021336       0.822245        1.435154
C       -4.120493       -0.529125       0.303501
N       -3.734716       -1.549133       -0.453263
H       -1.835392       -2.440437       -0.940613
H       -5.132785       -0.197125       0.457786
H       -4.367754       -2.146260       -0.970667
###
26
GlyHis4 m052x E=-756.337995699 au
N       -5.012870       -0.914666       -0.020077
H       -4.767984       -1.887418       -0.168104
C       -3.937144       -0.078772       -0.521420
H       -5.083402       -0.792979       0.984204
C       -2.566862       -0.379195       0.070838
H       -3.847550       -0.212368       -1.601672
H       -4.173540       0.971321        -0.348918
O       -2.328368       -1.449013       0.661128
N       -1.643442       0.571183        -0.106579
H       -1.884248       1.415010        -0.610149
C       -0.249846       0.412759        0.275182
H       -0.201496       -0.101335       1.233913
C       0.505441        -0.412527       -0.791182
C       0.388779        1.799529        0.414224
H       -0.028528       -1.357673       -0.906483
H       0.456102        0.123993        -1.741011
C       1.937654        -0.662485       -0.442820
O       -0.008698       2.695379        -0.382270
O       1.286501        1.935248        1.288365
N       2.973219        0.023780        -1.046169
C       2.440881        -1.528252       0.494917
C       4.075167        -0.426388       -0.476426
N       3.803456        -1.361300       0.459349
H       1.962353        -2.224821       1.162844
H       5.081027        -0.115494       -0.707437
H       4.484828        -1.852147       1.019487
###
33
GlyLys1 m052x E=-705.960285014 au
N       -4.607588       -1.924467       -0.034538
C       -3.936072       -0.712027       -0.557286
H       -5.521472       -2.040387       -0.475875
H       -4.738988       -1.857409       0.977107
C       -2.611811       -0.542342       0.158649
H       -3.793743       -0.828213       -1.629092
H       -4.577446       0.145748        -0.364715
O       -2.321280       -1.251332       1.130354
N       -1.830508       0.426538        -0.322593
H       -2.103656       0.924566        -1.160993
C       -0.531739       0.717250        0.260784
H       -0.595393       0.555594        1.336753
C       0.565638        -0.178342       -0.342052
C       -0.220259       2.174893        -0.027043
H       0.261520        -1.210961       -0.154379
H       0.578776        -0.020938       -1.424073
C       1.951437        0.071002        0.248548
O       -0.507791       2.706771        -1.081191
O       0.429182        2.865732        0.910740
H       2.285035        1.086501        0.016108
H       1.906418        -0.015986       1.339132
C       2.970220        -0.923011       -0.306253
H       2.657779        -1.945478       -0.074775
H       3.022599        -0.825855       -1.394915
C       4.341670        -0.667350       0.289405
H       4.694036        0.339220        0.074967
H       4.351236        -0.832158       1.364500
N       5.342161        -1.609652       -0.302066
H       5.428863        -1.457312       -1.308565
H       6.263508        -1.483275       0.118489
H       5.056835        -2.579813       -0.155014
H       0.569176        2.350161        1.720520
H       -4.048927       -2.760749       -0.218526
###
32
GlyLys2 m052x E=-705.513736140 au
N       4.711315        -1.719195       -0.095159
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C       3.810926        -0.847107       0.695880
H       5.505351        -2.025632       0.469094
H       5.069118        -1.227331       -0.916602
C       2.539141        -0.622319       -0.100949
H       3.567463        -1.364345       1.622495
H       4.327789        0.082172        0.919579
O       2.225702        -1.410570       -1.008562
N       1.819445        0.432169        0.263104
H       2.139075        1.030943        1.014599
C       0.520869        0.750169        -0.318708
H       0.564903        0.563932        -1.391210
C       -0.577638       -0.116077       0.318955
C       0.239639        2.240437        -0.082159
H       -0.291558       -1.162494       0.179901
H       -0.592996       0.083032        1.394966
C       -1.964655       0.115031        -0.275246
O       0.675997        2.742504        0.990993
O       -0.432139       2.842223        -0.961460
H       -2.293970       1.137501        -0.074545
H       -1.922535       -0.004829       -1.362717
C       -2.985007       -0.861793       0.307782
H       -2.678863       -1.891160       0.098355
H       -3.032210       -0.740466       1.394462
C       -4.358321       -0.614476       -0.286692
H       -4.710907       0.394355        -0.083635
H       -4.370519       -0.791909       -1.359833
N       -5.357929       -1.550392       0.317527
H       -5.441267       -1.387490       1.322604
H       -6.280531       -1.428407       -0.101451
H       -5.072740       -2.521896       0.179890
H       4.198381        -2.540504       -0.425193
###
31
GlyLys3 m052x E=-705.050511354 au
N       -4.870163       -1.592681       0.152503
C       -3.809221       -1.037354       -0.679062
H       -5.616754       -1.912052       -0.452520
H       -5.259983       -0.858550       0.733093
C       -2.551725       -0.760377       0.124768
H       -3.527915       -1.781114       -1.427794
H       -4.097938       -0.127707       -1.213545
O       -2.178015       -1.502358       1.052186
N       -1.859070       0.316885        -0.256746
H       -2.197511       0.888953        -1.018489
C       -0.570845       0.684678        0.312582
H       -0.599023       0.504201        1.386575
C       0.557062        -0.144569       -0.323387
C       -0.338110       2.181052        0.067613
H       0.306417        -1.199584       -0.180774
H       0.564922        0.051150        -1.400266
C       1.936217        0.135066        0.268645
O       -0.768443       2.659238        -1.019267
O       0.293908        2.817325        0.953627
H       2.231786        1.167408        0.064098
H       1.898338        0.018046        1.356667
C       2.986934        -0.810919       -0.310690
H       2.707176        -1.848564       -0.104898
H       3.036312        -0.686666       -1.396933
C       4.350659        -0.530714       0.291010
H       4.683143        0.484451        0.085548
H       4.359833        -0.703152       1.365004
N       5.373315        -1.448769       -0.302701
H       5.456233        -1.292185       -1.308804
H       6.291377        -1.302230       0.118184
H       5.109592        -2.425261       -0.157782
###
30
GlyLys4 m052x E=-704.581585604 au
N       -4.832700       -1.566647       0.172110
C       -3.779582       -1.007435       -0.667254
H       -5.591454       -1.869871       -0.426033
H       -5.207195       -0.838081       0.769569
C       -2.507629       -0.753917       0.121834
H       -3.516854       -1.741191       -1.432348
H       -4.068598       -0.086987       -1.182675
O       -2.128532       -1.512652       1.033471
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N       -1.810233       0.322218        -0.253748
H       -2.154352       0.908717        -1.001782
C       -0.511388       0.671049        0.304349
H       -0.527003       0.469396        1.374829
C       0.605071        -0.151414       -0.360241
C       -0.274189       2.170550        0.086978
H       0.352414        -1.207645       -0.228266
H       0.596221        0.058006        -1.434654
C       1.994628        0.114702        0.214428
O       -0.710478       2.671681        -0.987535
O       0.365827        2.787898        0.980714
H       2.298041        1.143388        -0.001928
H       1.961667        0.013766        1.304921
C       3.036749        -0.846355       -0.355022
H       2.747726        -1.877573       -0.121098
H       3.065678        -0.758661       -1.446144
C       4.426188        -0.581509       0.203307
H       4.745455        0.423433        -0.080289
H       4.380083        -0.608439       1.299071
N       5.399294        -1.540042       -0.337482
H       6.314881        -1.337455       0.047046
H       5.155139        -2.468943       -0.009843
###
31
GlyPhe1 m052x E=-763.261790921 au
N       -5.097717       -1.036530       0.034049
H       -4.745220       -1.992036       -0.062235
C       -4.135314       -0.072960       -0.547259
H       -6.002165       -0.968014       -0.435743
H       -5.236729       -0.858174       1.030964
C       -2.762868       -0.358514       0.029017
H       -4.111944       -0.222800       -1.625273
H       -4.469057       0.937036        -0.324687
O       -2.524743       -1.437842       0.585041
N       -1.865076       0.616108        -0.130815
H       -2.123093       1.458426        -0.630577
C       -0.473127       0.432922        0.237347
H       -0.420125       -0.147889       1.156437
C       0.303782        -0.285002       -0.893075
C       0.129315        1.799071        0.470199
H       -0.214222       -1.229406       -1.069987
H       0.229461        0.325898        -1.794893
C       1.749090        -0.535854       -0.546044
O       -0.186611       2.787239        -0.165579
C       2.756914        0.284111        -1.059942
C       2.096170        -1.575590       0.322463
H       2.493544        1.093521        -1.732817
C       4.091145        0.068284        -0.715416
C       3.428011        -1.793106       0.669033
H       1.318341        -2.217781       0.722542
H       4.863391        0.709157        -1.123670
C       4.429214        -0.970511       0.150690
H       3.684959        -2.604953       1.338762
H       5.465198        -1.141508       0.416886
O       1.068686        1.796258        1.411015
H       1.474581        2.679138        1.465764
###
30
GlyPhe2 m052x E=-762.814096813 au
N       1.095731        3.675063        -0.388271
C       0.235670        2.827030        0.469105
H       1.903205        3.141512        -0.718443
H       1.425016        4.489584        0.132472
C       -0.118296       1.564587        -0.294162
H       0.800324        2.563858        1.362355
H       -0.648373       3.394509        0.748904
O       0.521570        1.253158        -1.310415
N       -1.121198       0.862112        0.226587
H       -1.621581       1.230441        1.026103
C       -1.538543       -0.444672       -0.250535
H       -1.300620       -0.517441       -1.310984
C       -0.826401       -1.581287       0.519164
C       -3.054802       -0.613182       -0.067567
H       -1.109218       -1.512849       1.572736
H       -1.196012       -2.528239       0.122863
C       0.670479        -1.500991       0.374164
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O -3.648391 0.173379 0.718077
C 1.449216 -0.840128 1.328177
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H 0.976589 -0.440267 2.218872
C 2.823893 -0.688104 1.142830
C 2.669345 -1.881028 -0.947567
H 0.700422 -2.545859 -1.504222
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C 3.436668 -1.203077 0.001549
H 3.140203 -2.292720 -1.832324
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O -3.580361 -1.570894 -0.696467
H 0.583132 4.000337 -1.210471
###
29
GlyPhe3 m052x E=-762.350079214 au
C 3.610129 -0.801644 -0.020716
C 2.953729 -0.354591 1.124953
C 1.604394 -0.652303 1.319621
C 0.893796 -1.393409 0.371529
C 1.564111 -1.845553 -0.770327
C 2.911878 -1.554239 -0.966803
C -0.582487 -1.644742 0.531449
C -1.428101 -0.599047 -0.232660
C -2.910375 -0.956112 -0.050463
O -3.325250 -1.948081 -0.710417
N -1.175116 0.747822 0.239699
C -0.300516 1.595264 -0.318762
O 0.341000 1.328288 -1.349131
C -0.137080 2.907445 0.426950
N 0.414197 3.953310 -0.423758
O -3.589030 -0.274934 0.765199
H -0.270862 4.205148 -1.127888
H 0.562398 4.778602 0.144679
H 0.562424 2.710445 1.243152
H -1.097814 3.166820 0.882592
H -1.718432 1.055218 1.034872
H -1.184734 -0.644111 -1.293433
H -0.860794 -1.607866 1.587835
H -0.840745 -2.630191 0.140155
H 1.098820 -0.307499 2.215126
H 1.020202 -2.422768 -1.511044
H 3.490308 0.223205 1.868233
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H 4.657821 -0.572260 -0.173367
###
32
GlyTyr1 m052x E=-838.490018376 au
N 5.586560 -0.251868 -0.476612
H 5.500089 -0.793185 -1.339685
C 4.515156 -0.604507 0.483161
H 6.503515 -0.436812 -0.066500
H 5.535481 0.737892 -0.728466
C 3.176881 -0.278798 -0.142866
H 4.594055 -1.662809 0.719555
H 4.657847 -0.016696 1.387889
O 3.101454 0.345628 -1.208423
N 2.101202 -0.692286 0.530683
H 2.209644 -1.166444 1.417928
C 0.767818 -0.396375 0.041734
H 0.600930 -0.889438 -0.916641
C -0.265653 -0.885560 1.073362
C 0.576925 1.089101 -0.204864
H -0.099618 -1.956629 1.206479
H -0.072881 -0.385427 2.024891
C -1.681259 -0.626387 0.624011
O 1.096636 1.856583 0.754626
O -0.046848 1.532838 -1.149392
C -2.402009 0.462701 1.116631
C -2.287519 -1.452418 -0.328125
H -1.947321 1.115648 1.854069
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H       -4.050876       -1.846057       -1.510911
O       -5.557987       0.096104        -0.742141
H       -5.946098       0.873691        -0.319488
H       0.904006        2.788854        0.556928
###
31
GlyTyr2 m052x E=-838.034724932 au
N       3.391954        -3.147847       -0.520831
H       2.540324        -3.614127       -0.198360
C       3.499854        -1.807335       0.101091
H       4.200181        -3.723752       -0.280245
H       3.337084        -3.074556       -1.538713
C       2.182877        -1.080459       -0.094966
H       3.685407        -1.942051       1.165294
H       4.331736        -1.274209       -0.350910
O       1.149406        -1.719009       -0.353272
N       2.231075        0.236209        0.058166
H       3.116789        0.708175        0.198529
C       1.063434        1.094364        -0.077467
H       0.580964        0.871661        -1.032454
C       0.034673        0.897945        1.070568
C       1.541817        2.555611        -0.154076
H       0.462456        0.211947        1.802854
H       -0.113524       1.856476        1.572265
C       -1.305832       0.365632        0.617840
O       2.773868        2.788019        -0.023531
O       0.642725        3.416306        -0.344197
C       -1.813021       -0.830753       1.128078
C       -2.079862       1.062224        -0.317929
H       -1.230640       -1.391805       1.850738
C       -3.052259       -1.327065       0.724041
C       -3.317072       0.581481        -0.735333
H       -1.711069       1.995772        -0.728467
H       -3.434614       -2.258898       1.125974
C       -3.799441       -0.616051       -0.210481
H       -3.911441       1.123977        -1.460468
O       -5.028542       -1.058454       -0.650945
H       -5.245515       -1.895600       -0.220010
###
30
GlyTyr3 m052x E=-837.574069583 au
N       3.635436        -3.174255       -0.513699
H       2.885543        -3.740400       -0.132697
C       3.565873        -1.849150       0.077332
H       3.453236        -3.101441       -1.508840
C       2.237132        -1.133625       -0.120727
H       3.724891        -1.926349       1.155033
H       4.366105        -1.223965       -0.319243
O       1.191085        -1.754984       -0.387628
N       2.264472        0.190358        0.042581
H       3.144712        0.667411        0.189567
C       1.089583        1.036107        -0.079518
H       0.599296        0.816908        -1.031689
C       0.069253        0.817734        1.073876
C       1.543051        2.505149        -0.145941
H       0.494280        0.097946        1.774540
H       -0.058161       1.758881        1.613359
C       -1.283992       0.320885        0.619591
O       2.771155        2.760114        -0.017203
O       0.629863        3.355114        -0.324919
C       -1.797290       -0.890786       1.086190
C       -2.063766       1.063816        -0.274969
H       -1.210679       -1.488590       1.775120
C       -3.048022       -1.355991       0.680643
C       -3.312489       0.614613        -0.693516
H       -1.689255       2.009377        -0.650993
H       -3.434860       -2.300096       1.048181
C       -3.800751       -0.598560       -0.211786
H       -3.911085       1.193878        -1.386001
O       -5.041512       -1.009629       -0.650697
H       -5.259597       -1.862343       -0.251992
###
29
GlyTyr4 m052x E=-837.101569160 au
N       -5.502998       -1.195961       0.017151
H       -5.197152       -2.151495       -0.130271
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C       -4.493780       -0.294650       -0.512176
H       -5.559796       -1.071146       1.022012
C       -3.092252       -0.518457       0.036995
H       -4.426155       -0.423417       -1.594850
H       -4.789039       0.738279        -0.329864
O       -2.741629       -1.620333       0.500291
N       -2.268850       0.531594        -0.035208
H       -2.596567       1.392345        -0.453728
C       -0.852168       0.462613        0.294900
H       -0.728801       -0.132293       1.198780
C       -0.059113       -0.180850       -0.865475
C       -0.339415       1.884517        0.548941
H       -0.523108       -1.148888       -1.070561
H       -0.192022       0.449131        -1.749178
C       1.407812        -0.354790       -0.567928
O       -0.787925       2.792939        -0.206549
O       0.514621        2.042288        1.462083
C       2.361212        0.560711        -1.026874
C       1.867597        -1.424342       0.210430
H       2.034850        1.404420        -1.629254
C       3.714629        0.417787        -0.733728
C       3.216097        -1.581013       0.514500
H       1.151741        -2.152679       0.582555
H       4.432157        1.139873        -1.110273
C       4.197171        -0.664692       0.048280
H       3.545008        -2.424456       1.113239
O       5.475567        -0.816156       0.318001
###
27
GlyVal1 m052x E=-610.832666439 au
N       4.164095        -0.014280       -0.084313
H       4.131536        -1.025690       -0.232641
C       2.935448        0.447715        0.601686
H       4.989769        0.213380        0.472283
H       4.259323        0.426612        -1.001399
C       1.733104        -0.055201       -0.172935
H       2.929608        0.031857        1.607472
H       2.952871        1.533231        0.655917
O       1.868702        -0.903482       -1.063671
N       0.562424        0.477301        0.185959
H       0.533124        1.125690        0.961794
C       -0.684232       0.013641        -0.402695
H       -0.488868       -0.244924       -1.442859
C       -1.231221       -1.242107       0.325937
C       -1.715812       1.117642        -0.416126
H       -0.365185       -1.906492       0.394685
C       -1.723275       -0.918256       1.735424
C       -2.313528       -1.943632       -0.491135
O       -2.678070       1.114413        -1.159790
H       -2.628092       -0.303944       1.701609
H       -1.970892       -1.842717       2.260282
H       -0.967953       -0.389001       2.320891
H       -1.976158       -2.135875       -1.512150
H       -2.558465       -2.899453       -0.023820
H       -3.226995       -1.347387       -0.534782
O       -1.501322       2.073284        0.490520
H       -2.216644       2.731038        0.443796
###
26
GlyVal2 m052x E=-610.383698889 au
N       -4.129525       -0.007687       -0.119473
H       -4.073811       0.995991        -0.311840
C       -2.906905       -0.455117       0.589224
H       -4.961979       -0.197643       0.440614
H       -4.227081       -0.486069       -1.017372
C       -1.698189       0.086513        -0.151443
H       -2.929654       -0.043828       1.596668
H       -2.905997       -1.540666       0.637068
O       -1.828473       1.040441        -0.937261
N       -0.546007       -0.510724       0.125038
H       -0.518468       -1.302504       0.756008
C       0.727668        -0.069669       -0.428611
H       0.576466        0.180554        -1.479431
C       1.244903        1.185916        0.316198
C       1.725493        -1.234689       -0.348346
H       0.372630        1.840184        0.407412
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C       1.748845        0.850135        1.719254
C       2.310205        1.932227        -0.484291
O       2.743066        -1.154681       -1.087343
H       2.663383        0.251653        1.670151
H       1.980741        1.768684        2.262593
H       1.005588        0.294270        2.295788
H       1.968592        2.135622        -1.502201
H       2.533240        2.886247        -0.001266
H       3.236515        1.357996        -0.540884
O       1.472462        -2.171200       0.459082
###
25
GlyVal3 m052x E=-609.922979627 au
N       -4.252121       -0.066441       -0.024515
H       -4.303755       0.944557        -0.081477
C       -2.977608       -0.435335       0.565543
H       -4.281881       -0.401841       -0.981217
C       -1.758005       0.096959        -0.175286
H       -2.926394       -0.045378       1.584297
H       -2.901666       -1.520636       0.635980
O       -1.847773       1.041047        -0.983646
N       -0.599650       -0.500815       0.114057
H       -0.581019       -1.273121       0.767030
C       0.680021        -0.069788       -0.427535
H       0.540901        0.182595        -1.479559
C       1.202114        1.183937        0.318569
C       1.676019        -1.235151       -0.343907
H       0.331267        1.840411        0.407741
C       1.700108        0.846217        1.723359
C       2.272606        1.928373        -0.476765
O       2.691464        -1.163489       -1.088847
H       2.614264        0.246728        1.677478
H       1.930523        1.763324        2.269947
H       0.953676        0.289727        2.295256
H       1.933811        2.137574        -1.494526
H       2.500547        2.879548        0.009877
H       3.196263        1.349737        -0.534591
O       1.429349        -2.166772       0.471630
###
29
HisGly1 m052x E=-757.701293816 au
N       -3.446321       -1.172610       -0.391779
H       -3.466050       -2.036843       -0.940092
H       -4.220483       -0.578704       -0.699893
H       -3.591629       -1.418896       0.592726
C       -2.147119       -0.466428       -0.551159
H       -1.980869       -0.302486       -1.613427
C       -2.221867       0.871297        0.205671
C       -1.069411       -1.347953       0.060946
H       -2.986232       1.489370        -0.265190
H       -2.514599       0.681036        1.240786
C       -0.920515       1.599158        0.180113
O       -1.295215       -1.958954       1.112011
N       0.052506        1.429005        1.149141
C       -0.407485       2.489195        -0.713628
H       -0.016625       0.814069        1.953094
C       1.113162        2.173468        0.861351
N       0.846198        2.831665        -0.259127
H       -0.829369       2.905890        -1.611503
H       2.019695        2.238635        1.438395
H       1.484564        3.479092        -0.705149
N       0.100643        -1.345475       -0.578482
H       0.206763        -0.760088       -1.398747
C       1.300950        -1.875159       0.026835
C       2.472852        -0.983405       -0.303729
H       1.182045        -1.909197       1.111343
H       1.523708        -2.886817       -0.320791
O       2.384961        0.037658        -0.952983
O       3.659257        -1.385073       0.158209
H       3.602483        -2.223255       0.643874
###
28
HisGly2 m052x E=-757.255774018 au
N       -3.460092       -1.032466       -0.444453
H       -3.512851       -1.879793       -1.016065
H       -4.205027       -0.397293       -0.741343
```

```
H       -3.620685       -1.300223       0.532017
C       -2.128477       -0.384196       -0.572002
H       -1.931383       -0.221391       -1.629283
C       -2.162938       0.952356        0.192279
C       -1.105377       -1.317718       0.059185
H       -2.891323       1.605754        -0.287872
H       -2.481897       0.768532        1.220994
C       -0.831643       1.624475        0.191722
O       -1.414482       -1.976872       1.064555
N       0.131735        1.384801        1.155148
C       -0.272799       2.503586        -0.685275
H       0.034977        0.754081        1.943970
C       1.231118        2.075725        0.879100
N       0.998718        2.768875        -0.228586
H       -0.671742       2.957560        -1.575564
H       2.140662        2.080588        1.455331
H       1.670389        3.390521        -0.662313
N       0.102967        -1.303591       -0.490090
H       0.298008        -0.663446       -1.253421
C       1.267726        -1.839440       0.190932
C       2.538986        -1.141226       -0.295015
H       1.169731        -1.682203       1.266395
H       1.370392        -2.911501       0.015918
O       2.430739        -0.260326       -1.189213
O       3.608479        -1.521038       0.252352
###
27
HisGly3 m052x E=-756.802154648 au
N       -3.342987       -1.282380       -0.465975
H       -3.294493       -2.148931       -1.007415
H       -4.128349       -0.726875       -0.812226
H       -3.519079       -1.532286       0.511953
C       -2.072295       -0.509592       -0.562282
H       -1.866431       -0.339501       -1.616962
C       -2.244052       0.823480        0.183290
C       -0.986405       -1.352469       0.087639
H       -3.027189       1.390403        -0.322892
H       -2.569066       0.615382        1.205292
C       -0.966370       1.599333        0.217575
O       -1.259104       -2.050148       1.079234
N       -0.091566       1.508569        1.280803
C       -0.441015       2.414151        -0.752495
C       0.942806        2.256241        0.948350
N       0.772551        2.827231        -0.264458
H       -0.817112       2.727644        -1.711959
H       1.822496        2.423509        1.548463
N       0.223497        -1.252824       -0.448356
H       0.386611        -0.573341       -1.183608
C       1.408951        -1.742800       0.228989
C       2.656081        -1.010545       -0.266889
H       1.315711        -1.584905       1.304492
H       1.544621        -2.812143       0.057905
O       2.521430        -0.141541       -1.169105
O       3.738734        -1.352459       0.281344
H       1.427134        3.443260        -0.724001
###
26
HisGly4 m052x E=-756.342306460 au
N       -3.376575       -1.333294       -0.580924
H       -3.248737       -2.222162       -1.053658
H       -3.618970       -1.553158       0.380754
C       -2.115325       -0.604532       -0.578469
H       -1.820694       -0.405637       -1.609956
C       -2.304226       0.741828        0.144482
C       -0.992312       -1.369316       0.112455
H       -3.084601       1.287803        -0.387655
H       -2.659144       0.543743        1.159563
C       -1.047090       1.550179        0.204806
O       -1.206436       -2.021100       1.153576
N       -0.189622       1.498075        1.286265
C       -0.516813       2.360206        -0.767598
C       0.837284        2.259896        0.960402
N       0.679789        2.807484        -0.264280
H       -0.879061       2.649310        -1.740079
H       1.701288        2.455887        1.574710
N       0.216875        -1.280175       -0.445453
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H       0.354829        -0.622055       -1.202976
C       1.421107        -1.705845       0.238809
C       2.643496        -0.943848       -0.272267
H       1.326432        -1.526103       1.310814
H       1.599921        -2.773859       0.097486
O       2.488739        -0.115046       -1.208706
O       3.733623        -1.218543       0.301130
H       1.331347        3.427698        -0.721976
###
44
HisLys0 m052x E=-970.762246017 au
N       2.560666        3.444575        -0.328916
H       1.892605        3.935335        -0.928804
H       2.353769        3.687765        0.645576
C       2.458663        1.972453        -0.510054
H       2.519554        1.755723        -1.574331
C       3.615043        1.300714        0.252619
C       1.126529        1.534298        0.081784
H       4.554310        1.598418        -0.213097
H       3.610605        1.645704        1.288848
C       3.498183        -0.185637       0.221487
O       0.715855        2.055693        1.126097
N       2.829638        -0.901171       1.198295
C       3.911107        -1.101691       -0.697906
C       2.825641        -2.192881       0.891344
N       3.483781        -2.332567       -0.252611
H       4.465487        -0.979944       -1.612072
H       2.380056        -2.983655       1.470654
H       3.636319        -3.219368       -0.717722
N       0.519230        0.534863        -0.555909
H       0.931730        0.156346        -1.401056
C       -0.611824       -0.169502       0.025170
H       -0.535705       -0.103529       1.112106
C       -1.947837       0.435830        -0.440835
C       -0.496409       -1.621218       -0.406976
H       -1.933461       1.481971        -0.125240
H       -1.976420       0.413415        -1.533157
C       -3.177066       -0.264881       0.134427
O       -0.040550       -1.947240       -1.485085
O       -0.945609       -2.552565       0.434119
H       -3.269225       -1.271133       -0.284763
H       -3.069585       -0.370459       1.219068
C       -4.445764       0.527360        -0.176206
H       -4.386051       1.513969        0.292487
H       -4.535672       0.674619        -1.256767
C       -5.673516       -0.202994       0.334118
H       -5.808346       -1.161681       -0.161941
H       -5.634751       -0.355915       1.410538
N       -6.902637       0.603303        0.055948
H       -7.001120       0.778932        -0.945831
H       -7.741617       0.119100        0.378374
H       -6.856476       1.507948        0.529006
H       3.501689        3.775247        -0.557665
H       2.383655        -0.503727       2.018768
H       -1.250178       -2.176314       1.274491
###
43
HisLys1 m052x E=-970.317736597 au
N       -2.650708       3.405153        0.324239
H       -1.997807       3.920996        0.919552
H       -2.454512       3.652974        -0.651213
C       -2.490052       1.938092        0.505620
H       -2.536452       1.721445        1.570459
C       -3.626944       1.224374        -0.247454
C       -1.143761       1.554323        -0.095095
H       -4.575323       1.506425        0.209773
H       -3.628388       1.550036        -1.289979
C       -3.475529       -0.257789       -0.187085
O       -0.750618       2.129791        -1.122441
N       -2.796093       -0.979215       -1.151531
C       -3.865061       -1.163269       0.752911
C       -2.760700       -2.263445       -0.816886
N       -3.412397       -2.393668       0.331878
H       -4.418427       -1.034525       1.666748
H       -2.299218       -3.056119       -1.380780
H       -3.544855       -3.274001       0.815007
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N       -0.511274       0.553042        0.505238
H       -0.924444       0.119781        1.323907
C       0.625835        -0.133963       -0.098762
H       0.548385        -0.029789       -1.180717
C       1.949427        0.470796        0.390243
C       0.530314        -1.623505       0.265372
H       1.944402        1.530856        0.120349
H       1.981235        0.405779        1.481824
C       3.179123        -0.209654       -0.205875
O       0.125026        -1.901923       1.427755
O       0.888948        -2.451094       -0.613544
H       3.223849        -1.251791       0.122235
H       3.103862        -0.216628       -1.298044
C       4.464562        0.501752        0.213825
H       4.447788        1.538108        -0.136569
H       4.537884        0.518099        1.305660
C       5.677257        -0.205917       -0.360996
H       5.750722        -1.231592       -0.006363
H       5.670458        -0.199717       -1.448771
N       6.931662        0.489952        0.066427
H       7.011834        0.497649        1.084922
H       7.758724        0.028238        -0.314601
H       6.933467        1.459582        -0.255977
H       -3.602216       3.700846        0.556331
H       -2.352979       -0.588445       -1.976581
###
42
HisLys2 m052x E=-969.864709639 au
N       -2.673373       3.383710        0.319111
H       -2.021833       3.895842        0.918264
H       -2.476396       3.637384        -0.654161
C       -2.517178       1.911792        0.486031
H       -2.562718       1.689538        1.549914
C       -3.652291       1.200720        -0.268559
C       -1.167655       1.537471        -0.108884
H       -4.595547       1.495238        0.194485
H       -3.651119       1.539698        -1.306966
C       -3.486965       -0.284475       -0.227509
O       -0.760829       2.132551        -1.121145
N       -2.833193       -0.971175       -1.230170
C       -3.854919       -1.150649       0.769913
C       -2.807373       -2.228874       -0.834242
N       -3.417317       -2.385120       0.361491
H       -4.375229       -0.999604       1.700925
H       -2.376250       -3.055076       -1.375948
H       -3.528118       -3.256755       0.858826
N       -0.527014       0.541494        0.492324
H       -0.970048       0.073058        1.274554
C       0.614549        -0.133910       -0.114791
H       0.550020        -0.007087       -1.194886
C       1.934570        0.459146        0.397843
C       0.520277        -1.630773       0.215851
H       1.931958        1.524928        0.151008
H       1.958795        0.370666        1.488013
C       3.168415        -0.208401       -0.204310
O       0.117206        -1.936100       1.372569
O       0.884177        -2.439292       -0.678976
H       3.215584        -1.255079       0.108944
H       3.095795        -0.200419       -1.296684
C       4.450627        0.501463        0.227733
H       4.431893        1.541585        -0.111229
H       4.520539        0.506049        1.319933
C       5.667110        -0.196237       -0.351058
H       5.744212        -1.224607       -0.005144
H       5.661896        -0.180699       -1.438757
N       6.918249        0.500992        0.084048
H       6.997135        0.500245        1.102652
H       7.747576        0.045741        -0.299871
H       6.916574        1.473361        -0.229970
H       -3.625630       3.675774        0.550773
###
41
HisLys3 m052x E=-969.405481029 au
N       -2.768569       3.417167        0.427860
H       -2.016480       3.901343        0.907130
H       -2.714379       3.698788        -0.546506
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C       -2.537688       1.981097        0.500488
H       -2.541053       1.675962        1.547759
C       -3.676163       1.242010        -0.227929
C       -1.214663       1.561569        -0.131980
H       -4.608942       1.517920        0.266080
H       -3.718671       1.600551        -1.259942
C       -3.500887       -0.243460       -0.223122
O       -0.823336       2.083748        -1.194398
N       -2.885352       -0.916179       -1.260736
C       -3.816328       -1.126768       0.778238
C       -2.830105       -2.178516       -0.880799
N       -3.385471       -2.354321       0.338003
H       -4.295897       -0.991137       1.733276
H       -2.416043       -2.994610       -1.450525
H       -3.467093       -3.232595       0.828851
N       -0.538250       0.597478        0.498070
H       -0.960365       0.160273        1.307863
C       0.589468        -0.101490       -0.104333
H       0.515590        -0.001157       -1.186457
C       1.920189        0.492345        0.379328
C       0.493515        -1.589640       0.259751
H       1.923642        1.551379        0.104454
H       1.952452        0.433890        1.471513
C       3.145167        -0.200320       -0.212208
O       0.130387        -1.868905       1.436741
O       0.816704        -2.422966       -0.629339
H       3.179191        -1.242705       0.117443
H       3.072702        -0.208577       -1.304643
C       4.436290        0.499390        0.209712
H       4.427642        1.536668        -0.138415
H       4.508618        0.513237        1.301686
C       5.644961        -0.214948       -0.365130
H       5.713396        -1.241158       -0.011030
H       5.638454        -0.207972       -1.452891
N       6.902730        0.474660        0.062991
H       6.983010        0.480363        1.081488
H       7.727877        0.010397        -0.318955
H       6.908154        1.444862        -0.257611
###
40
HisLys4 m052x E=-968.936555620 au
N       -2.737850       3.411049        0.426748
H       -1.988590       3.897398        0.908257
H       -2.681715       3.693479        -0.547299
C       -2.501773       1.975706        0.498861
H       -2.505965       1.669935        1.545945
C       -3.636208       1.232928        -0.232016
C       -1.175987       1.561640        -0.131607
H       -4.570978       1.504994        0.260355
H       -3.678174       1.591850        -1.263918
C       -3.455059       -0.251847       -0.228075
O       -0.786252       2.085200        -1.194142
N       -2.836877       -0.921200       -1.266260
C       -3.766840       -1.137245       0.772602
C       -2.776502       -2.183621       -0.887416
N       -3.331114       -2.362711       0.331245
H       -4.246639       -1.004309       1.727897
H       -2.359089       -2.997536       -1.457804
H       -3.408527       -3.241603       0.821672
N       -0.496012       0.601444        0.499930
H       -0.916864       0.163664        1.310043
C       0.637984        -0.091768       -0.098329
H       0.569777        0.013465        -1.180354
C       1.964923        0.501666        0.396366
C       0.542047        -1.581567       0.257983
H       1.968059        1.561969        0.125225
H       1.987277        0.441085        1.488927
C       3.197761        -0.185519       -0.185875
O       0.177992        -1.866834       1.433496
O       0.864913        -2.411135       -0.634831
H       3.228457        -1.229601       0.141597
H       3.128825        -0.195674       -1.279230
C       4.490169        0.508404        0.240744
H       4.479641        1.547868        -0.107134
H       4.551208        0.534117        1.333740
C       5.723580        -0.189042       -0.311678
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H       5.762544        -1.211317       0.069990
H       5.635117        -0.254217       -1.403079
N       6.948667        0.504874        0.108505
H       7.752871        0.028892        -0.284207
H       6.947283        1.435090        -0.297339
###
44
LeuTyr1 m052x E=-995.733601243 au
N       -4.145654       -2.484441       -0.184421
H       -4.102315       -2.703334       0.815753
H       -3.685846       -3.239790       -0.698620
H       -5.128714       -2.454801       -0.465521
C       -3.495221       -1.165885       -0.443350
H       -3.456739       -1.030112       -1.521458
C       -4.317001       -0.077664       0.251172
C       -2.103076       -1.236357       0.165545
H       -5.306828       -0.055106       -0.215930
H       -4.442557       -0.373065       1.297301
C       -3.690434       1.320144        0.191151
O       -1.961171       -1.658159       1.319245
H       -2.688958       1.274677        0.635535
C       -3.576081       1.839466        -1.242460
C       -4.538207       2.276990        1.029587
H       -4.566750       1.876726        -1.705827
H       -3.162661       2.850527        -1.245744
H       -2.933818       1.216688        -1.868465
H       -4.605116       1.940783        2.066727
H       -4.108400       3.280896        1.019790
H       -5.552403       2.338753        0.623696
N       -1.100483       -0.804432       -0.607973
H       -1.321098       -0.417168       -1.517422
C       0.242416        -0.604070       -0.094513
H       0.414240        -1.305131       0.718533
C       1.274834        -0.819697       -1.213660
C       0.390494        0.795174        0.483115
H       1.195388        -1.862055       -1.526838
H       1.015602        -0.182206       -2.061713
C       2.672615        -0.506937       -0.739800
O       -0.022274       1.742313        -0.360791
O       0.859930        1.033756        1.578565
C       3.298088        0.689753        -1.093063
C       3.349849        -1.388355       0.110193
H       2.788689        1.385748        -1.750647
C       4.570314        1.005990        -0.618418
C       4.618163        -1.088343       0.593777
H       2.878740        -2.322911       0.395878
H       5.053000        1.934863        -0.901038
C       5.224444        0.113091        0.226735
H       5.144113        -1.772228       1.248490
O       6.480486        0.367576        0.728442
H       6.801258        1.219074        0.402754
H       0.111193        2.617597        0.041780
###
43
LeuTyr2 m052x E=-995.279434251 au
N       -2.395212       -2.360753       -1.880173
H       -1.756435       -3.004867       -1.404243
H       -1.977950       -2.102886       -2.777269
H       -3.275904       -2.848086       -2.059625
C       -2.627193       -1.162772       -1.018066
H       -3.196330       -0.447756       -1.606990
C       -3.379569       -1.612514       0.234356
C       -1.251970       -0.620859       -0.654081
H       -4.329919       -2.052219       -0.086109
H       -2.790010       -2.398655       0.716692
C       -3.660729       -0.492045       1.241690
O       -0.367249       -1.408515       -0.276805
H       -2.707860       -0.050518       1.553582
C       -4.545905       0.605107        0.648055
C       -4.329780       -1.099894       2.474810
H       -5.480058       0.173687        0.275334
H       -4.795390       1.342685        1.414071
H       -4.063841       1.136168        -0.175732
H       -3.703679       -1.875216       2.922404
H       -4.518051       -0.332667       3.228817
H       -5.288907       -1.549753       2.200997
```

```
N       -1.095078       0.692168        -0.743296
H       -1.872103       1.284695        -1.013217
C       0.097606        1.382213        -0.277361
H       0.325848        1.030804        0.732378
C       1.328490        1.138778        -1.194186
C       -0.226323       2.882798        -0.163729
H       0.996800        0.591763        -2.077802
H       1.703839        2.106450        -1.533636
C       2.454591        0.376647        -0.534495
O       -1.361359       3.277256        -0.544528
O       0.689399        3.605715        0.309245
C       2.922659        -0.822273       -1.074948
C       3.067187        0.858061        0.628532
H       2.461845        -1.218097       -1.973403
C       3.968261        -1.528902       -0.481336
C       4.108352        0.164601        1.237714
H       2.725778        1.789742        1.066716
H       4.321978        -2.459766       -0.910647
C       4.555262        -1.031369       0.678454
H       4.578665        0.540449        2.138182
O       5.588181        -1.686653       1.314427
H       5.796313        -2.503745       0.842614
###
42
LeuTyr3 m052x E=-994.818838109 au
N       -2.597267       -1.933636       -2.258003
H       -2.052026       -2.723132       -1.924509
H       -2.069357       -1.518027       -3.018751
C       -2.721783       -0.968274       -1.165353
H       -3.279016       -0.107768       -1.535952
C       -3.470606       -1.617923       -0.001231
C       -1.353345       -0.499779       -0.683523
H       -4.452770       -1.929328       -0.371985
H       -2.925102       -2.525176       0.282136
C       -3.658041       -0.732521       1.235213
O       -0.492914       -1.324748       -0.312461
H       -2.671876       -0.410849       1.591322
C       -4.495807       0.509523        0.925458
C       -4.320563       -1.547140       2.346826
H       -5.472012       0.213924        0.527720
H       -4.663020       1.093737        1.833549
H       -4.015792       1.163286        0.193926
H       -3.724576       -2.426728       2.602294
H       -4.445956       -0.944906       3.249664
H       -5.310176       -1.888779       2.027489
N       -1.125293       0.813155        -0.695309
H       -1.868732       1.456873        -0.935626
C       0.103870        1.408400        -0.201331
H       0.321772        0.989606        0.784743
C       1.313330        1.144372        -1.142561
C       -0.120533       2.916707        -0.002140
H       0.948314        0.621380        -2.027547
H       1.714221        2.104195        -1.476406
C       2.426931        0.334521        -0.519224
O       -1.215322       3.414880        -0.380047
O       0.832083        3.546613        0.531063
C       2.852061        -0.861783       -1.099954
C       3.073506        0.766626        0.644834
H       2.362275        -1.221342       -1.998419
C       3.892430        -1.609209       -0.548558
C       4.110723        0.032305        1.211864
H       2.763687        1.692568        1.116605
H       4.214539        -2.535896       -1.010471
C       4.518811        -1.156093       0.608896
H       4.608922        0.371765        2.111867
O       5.553803        -1.849715       1.199857
H       5.747511        -2.646664       0.688954
###
41
LeuTyr4 m052x E=-994.341611147 au
N       -2.644739       -1.909561       -2.229377
H       -2.130283       -2.714046       -1.883080
H       -2.095491       -1.519806       -2.988626
C       -2.746191       -0.928368       -1.147920
H       -3.264178       -0.051391       -1.536497
C       -3.536228       -1.534491       0.012064
```

```
C       -1.365606       -0.510079       -0.653247
H       -4.525169       -1.810599       -0.368467
H       -3.031185       -2.459138       0.313601
C       -3.704097       -0.626946       1.235199
O       -0.549020       -1.365264       -0.252361
H       -2.710154       -0.344793       1.602797
C       -4.482415       0.646401        0.897644
C       -4.417270       -1.398579       2.345965
H       -5.465478       0.387879        0.491028
H       -4.635641       1.249912        1.795508
H       -3.964753       1.267977        0.163733
H       -3.862122       -2.298305       2.622508
H       -4.532420       -0.779699       3.238881
H       -5.414787       -1.703970       2.014743
N       -1.078777       0.790509        -0.689227
H       -1.790709       1.458950        -0.955281
C       0.175268        1.342709        -0.205545
H       0.388793        0.915580        0.777397
C       1.370950        1.037450        -1.159149
C       0.003495        2.857936        -0.013822
H       0.979791        0.473996        -2.008385
H       1.752921        1.983689        -1.550535
C       2.500211        0.252520        -0.530781
O       -1.061693       3.397848        -0.420534
O       0.967385        3.456334        0.535511
C       2.755912        -1.071997       -0.901812
C       3.336894        0.812746        0.444036
H       2.126865        -1.538752       -1.654572
C       3.791720        -1.810095       -0.334124
C       4.374498        0.088454        1.023279
H       3.174014        1.839656        0.756535
H       3.963634        -2.835001       -0.647534
C       4.645028        -1.256941       0.655267
H       5.006830        0.551814        1.774120
O       5.628468        -1.944532       1.196139
###
36
LysAla1 m052x E=-745.274003806 au
N       -0.364700       3.642032        -0.220433
H       -0.443416       3.770359        0.792919
H       -1.240944       3.949913        -0.648874
H       0.389464        4.238305        -0.568743
C       -0.081864       2.210042        -0.524540
H       -0.152836       2.081518        -1.602760
C       1.317496        1.859412        -0.014516
C       -1.133599       1.388259        0.204218
H       2.030837        2.492403        -0.548804
H       1.374315        2.106358        1.049839
C       1.668013        0.387909        -0.232289
O       -1.506878       1.727528        1.335339
H       1.026856        -0.247557       0.385628
H       1.486905        0.116113        -1.277331
C       3.128464        0.117704        0.124936
H       3.784524        0.726051        -0.504399
H       3.308973        0.396202        1.167389
C       3.457262        -1.350081       -0.072129
H       2.844443        -1.989426       0.559723
H       3.341638        -1.652132       -1.110699
N       4.882094        -1.615025       0.300692
H       5.044619        -1.394300       1.285020
H       5.125380        -2.595218       0.151442
H       5.517451        -1.042073       -0.258281
N       -1.560355       0.299553        -0.437286
H       -1.156270       0.073150        -1.338015
C       -2.349473       -0.720983       0.224261
H       -2.232517       -0.594099       1.301657
C       -3.833933       -0.636940       -0.147670
C       -1.782164       -2.075974       -0.156089
H       -3.964310       -0.772988       -1.221782
H       -4.406494       -1.399017       0.382414
H       -4.208311       0.345434        0.139162
O       -1.019107       -2.252896       -1.084219
O       -2.192250       -3.115290       0.575812
H       -2.764912       -2.845733       1.311125
###
35
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LysAla2 m052x E=-744.827618237 au
N 0.166345 3.510507 0.455435
H 0.229960 3.740506 -0.540930
H 1.038594 3.795820 0.906423
H -0.599973 4.048142 0.866937
C -0.078893 2.047215 0.614444
H 0.010786 1.811692 1.673010
C -1.478527 1.721622 0.094084
C 0.985123 1.332436 -0.207502
H -2.193934 2.299102 0.685857
H -1.554350 2.050415 -0.946577
C -1.801658 0.232957 0.202872
O 1.272024 1.763875 -1.337712
H -1.161774 -0.340057 -0.473880
H -1.596259 -0.113580 1.220891
C -3.263608 -0.037724 -0.147339
H -3.917737 0.533864 0.517657
H -3.462028 0.284596 -1.173788
C -3.575095 -1.515947 -0.009873
H -2.961196 -2.122827 -0.671865
H -3.448055 -1.858528 1.014672
N -5.000551 -1.779707 -0.381688
H -5.171756 -1.523739 -1.355953
H -5.235033 -2.766775 -0.267299
H -5.635745 -1.233216 0.203222
N 1.520498 0.250374 0.343036
H 1.176764 -0.083390 1.236283
C 2.386906 -0.658194 -0.395341
H 2.005176 -0.743027 -1.414589
C 3.832051 -0.157438 -0.428395
C 2.320781 -2.050201 0.249594
H 4.246719 -0.136084 0.581460
H 4.439789 -0.816306 -1.047973
H 3.867886 0.849152 -0.846153
O 1.710627 -2.170789 1.346764
O 2.911805 -2.972127 -0.374073
###
34
LysAla3 m052x E=-744.368143438 au
N 0.021953 3.404356 0.624010
H 0.988433 3.607481 0.858871
H -0.114670 3.716961 -0.332708
C -0.196785 1.958543 0.668033
H -0.031619 1.615982 1.690718
C -1.634135 1.643281 0.258488
C 0.763655 1.223317 -0.260237
H -2.297959 2.145547 0.966920
H -1.817644 2.076933 -0.730322
C -1.944006 0.147764 0.230950
O 0.802751 1.498472 -1.477904
H -1.353037 -0.342985 -0.549448
H -1.659459 -0.305782 1.186200
C -3.426995 -0.106098 -0.032826
H -4.025224 0.341835 0.766434
H -3.720002 0.367865 -0.974709
C -3.718747 -1.593035 -0.106538
H -3.185992 -2.069141 -0.926625
H -3.474491 -2.099087 0.824988
N -5.179096 -1.817382 -0.351335
H -5.468339 -1.379196 -1.227886
H -5.399727 -2.812853 -0.403590
H -5.736229 -1.407859 0.400924
N 1.545243 0.297193 0.295233
H 1.438147 0.066075 1.274521
C 2.478840 -0.520378 -0.463308
H 2.001432 -0.816836 -1.398723
C 3.771568 0.239939 -0.771027
C 2.803135 -1.795373 0.326749
H 4.291475 0.492308 0.155519
H 4.426767 -0.371943 -1.390952
H 3.542367 1.161216 -1.307534
O 2.436828 -1.862965 1.531799
O 3.447908 -2.680938 -0.298852
###
33
LysAla4 m052x E=-743.900110816 au

```
N       -0.085338       3.397516        0.625734
H       0.877360        3.619183        0.859450
H       -0.228096       3.707027        -0.331072
C       -0.276408       1.947640        0.668776
H       -0.107977       1.607735        1.691908
C       -1.705938       1.603041        0.253903
C       0.701276        1.232016        -0.256189
H       -2.381425       2.095795        0.958444
H       -1.893074       2.033015        -0.736177
C       -1.991359       0.102524        0.226890
O       0.748542        1.518052        -1.471170
H       -1.381224       -0.378494       -0.546012
H       -1.700626       -0.342519       1.185353
C       -3.464229       -0.196450       -0.047491
H       -4.082958       0.245471        0.741896
H       -3.763734       0.271749        -0.992284
C       -3.747791       -1.693149       -0.123361
H       -3.137309       -2.137847       -0.912499
H       -3.447891       -2.167275       0.813976
N       -5.151051       -2.037131       -0.382330
H       -5.436382       -1.591994       -1.248837
H       -5.723840       -1.618242       0.343385
N       1.488725        0.309778        0.297999
H       1.373864        0.067230        1.273625
C       2.433690        -0.494506       -0.460604
H       1.963125        -0.791592       -1.399349
C       3.720337        0.279712        -0.759273
C       2.768229        -1.769545       0.325010
H       4.234320        0.532209        0.170537
H       4.383636        -0.323055       -1.379532
H       3.484693        1.201397        -1.292185
O       2.397622        -1.846448       1.528175
O       3.425628        -2.645182       -0.301555
###
34
LysDAla3 m052x E=-744.368325023 au
N       -0.008826       3.454765        -0.242455
H       -0.978193       3.692485        -0.425924
H       0.154758        3.645715        0.741741
C       0.191651        2.024438        -0.472139
H       -0.031222       1.807927        -1.518066
C       1.644368        1.655340        -0.176097
C       -0.722549       1.185823        0.413432
H       2.279334        2.249410        -0.838333
H       1.872745        1.951377        0.853438
C       1.945949        0.169678        -0.363416
O       -0.690052       1.316392        1.655015
H       1.330563        -0.428623       0.317466
H       1.685615        -0.132356       -1.383291
C       3.418589        -0.138003       -0.097308
H       4.050079        0.443302        -0.775954
H       3.672444        0.152568        0.926747
C       3.702915        -1.615714       -0.287013
H       3.095373        -2.232235       0.372107
H       3.547955        -1.928086       -1.317357
N       5.132560        -1.911829       0.045019
H       5.328572        -1.690286       1.022885
H       5.350420        -2.897548       -0.106381
H       5.762806        -1.355140       -0.535633
N       -1.542091       0.332548        -0.200345
H       -1.559197       0.281786        -1.210404
C       -2.438519       -0.564872       0.510981
C       -3.525694       -1.068664       -0.447115
O       -3.368485       -0.875916       -1.683781
O       -4.493891       -1.674513       0.088601
C       -1.682629       -1.758020       1.104596
H       -1.236956       -2.358033       0.308475
H       -0.890849       -1.406478       1.766915
H       -2.925926       -0.007693       1.312068
H       -2.364888       -2.384208       1.679755
###
33
LysDAla4 m052x E=-743.900516513 au
N       0.101865        3.444068        -0.286939
H       -0.861859       3.697966        -0.478493
H       0.266299        3.652979        0.693420
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C       0.273184        2.004903        -0.484672
H       0.057140        1.772391        -1.528691
C       1.713561        1.605727        -0.166007
C       -0.669256       1.203097        0.405085
H       2.368985        2.169619        -0.835110
H       1.940575        1.920269        0.858577
C       1.984020        0.109695        -0.318750
O       -0.658574       1.364197        1.643608
H       1.367617        -0.456912       0.389005
H       1.690528        -0.212580       -1.324396
C       3.453781        -0.234674       -0.083366
H       4.079571        0.314786        -0.795995
H       3.749854        0.087493        0.921640
C       3.730238        -1.727509       -0.228875
H       3.109670        -2.282628       0.478255
H       3.438810        -2.053930       -1.229868
N       5.128994        -2.115237       -0.010652
H       5.403869        -1.821090       0.921154
H       5.713635        -1.587487       -0.650833
N       -1.489003       0.345791        -0.202933
H       -1.480256       0.263998        -1.211007
C       -2.403903       -0.530488       0.510956
C       -3.476676       -1.047507       -0.456479
O       -3.294662       -0.883468       -1.693914
O       -4.460132       -1.633512       0.073622
C       -1.666595       -1.715779       1.142445
H       -1.204952       -2.330949       0.367254
H       -0.888752       -1.355770       1.816579
H       -2.902169       0.046213        1.291293
H       -2.364721       -2.329236       1.712337
###
42
LysGlu1 m052x E=-973.154998345 au
N       1.784620        3.735181        -0.234830
H       1.898791        3.865055        0.775011
H       0.964887        4.267588        -0.535754
H       2.607310        4.118496        -0.706785
C       1.640527        2.283561        -0.544809
H       1.406515        2.196717        -1.603796
C       2.950545        1.574328        -0.203337
C       0.513827        1.749084        0.325816
H       3.727811        1.983447        -0.853963
H       3.214591        1.808564        0.832059
C       2.855208        0.061130        -0.387501
O       0.452158        2.073278        1.517257
H       2.154650        -0.361001       0.339450
H       2.467667        -0.167794       -1.385465
C       4.221922        -0.595128       -0.203152
H       4.928387        -0.190222       -0.933598
H       4.606554        -0.371775       0.796417
C       4.116467        -2.097812       -0.382016
H       3.451955        -2.547196       0.352806
H       3.777553        -2.359275       -1.381879
N       5.458662        -2.733734       -0.197616
H       5.810953        -2.565473       0.746506
H       5.411171        -3.743015       -0.344596
H       6.135749        -2.348804       -0.858864
N       -0.340183       0.918449        -0.282439
H       -0.166550       0.665971        -1.248081
C       -1.333291       0.148747        0.437976
H       -1.483771       0.614174        1.411337
C       -2.645888       0.136539        -0.356895
C       -0.820401       -1.280147       0.608436
H       -2.978642       1.172490        -0.438200
H       -2.446546       -0.244094       -1.361638
C       -3.729600       -0.716663       0.319694
O       -0.217164       -1.864076       -0.268490
O       -1.092579       -1.903052       1.756917
H       -3.454665       -1.770370       0.329862
H       -3.890186       -0.374878       1.345391
C       -5.016717       -0.599854       -0.450020
O       -5.436151       -1.447314       -1.215860
O       -5.721008       0.532956        -0.289302
H       -5.303221       1.128127        0.351990
H       -1.560303       -1.333040       2.386670
###
```

41
LysGlu2 m052x E=-972.709424145 au
N -1.193689 3.486466 0.602297
H -1.069976 3.742074 -0.381953
H -0.353893 3.768867 1.112696
H -1.990423 4.004856 0.978997
C -1.430103 2.017070 0.709173
H -1.413358 1.757759 1.766150
C -2.785297 1.692250 0.083018
C -0.289910 1.344147 -0.043552
H -3.542884 2.259494 0.630977
H -2.787699 2.037079 -0.955138
C -3.113762 0.202247 0.146159
O 0.091602 1.819573 -1.126444
H -2.435236 -0.359011 -0.501660
H -2.970502 -0.162739 1.168095
C -4.553765 -0.056593 -0.293117
H -5.242000 0.495846 0.353490
H -4.697978 0.297276 -1.318297
C -4.873862 -1.537562 -0.219702
H -4.246802 -2.121295 -0.890035
H -4.773182 -1.919964 0.793596
N -6.291369 -1.777504 -0.635050
H -6.444593 -1.452295 -1.591510
H -6.526685 -2.770373 -0.595126
H -6.937658 -1.273483 -0.025040
N 0.212609 0.252219 0.519388
H -0.163725 -0.083763 1.397986
C 1.232750 -0.572567 -0.112067
H 1.060264 -0.583744 -1.188104
C 2.626297 0.005621 0.183759
C 1.109907 -2.004235 0.432384
H 2.643419 1.030728 -0.193625
H 2.774390 0.036884 1.265637
C 3.749678 -0.813429 -0.471995
O 0.698559 -2.132183 1.617887
O 1.459358 -2.935536 -0.338820
H 3.830726 -1.798838 -0.019094
H 3.556332 -0.922592 -1.542160
C 5.063967 -0.112937 -0.275269
O 5.891814 -0.421262 0.562918
O 5.312163 0.946521 -1.065858
H 4.595244 1.087997 -1.702532
###
40
LysGlu3 m052x E=-972.254622453 au
N -1.129899 3.470159 0.557801
H -0.999315 3.708167 -0.430069
H -0.286879 3.746711 1.066177
H -1.918723 4.007731 0.923897
C -1.390664 2.006086 0.686013
H -1.376724 1.761519 1.746533
C -2.751244 1.696543 0.064351
C -0.262896 1.305048 -0.060183
H -3.500170 2.280368 0.606582
H -2.748592 2.031312 -0.977098
C -3.102208 0.212450 0.140622
O 0.102844 1.747448 -1.163108
H -2.426428 -0.365770 -0.495146
H -2.973247 -0.143339 1.167675
C -4.541602 -0.030215 -0.309633
H -5.227960 0.541237 0.322261
H -4.669921 0.311955 -1.340899
C -4.885377 -1.504888 -0.220052
H -4.256756 -2.107737 -0.871804
H -4.806981 -1.874143 0.800050
N -6.299428 -1.729352 -0.655158
H -6.431539 -1.419503 -1.619873
H -6.551301 -2.717451 -0.601435
H -6.947878 -1.203865 -0.065752
N 0.246257 0.230397 0.527390
H -0.110316 -0.073473 1.425205
C 1.272832 -0.600998 -0.088454
H 1.085046 -0.648100 -1.160922
C 2.663834 0.001439 0.171510
C 1.174214 -2.014594 0.501993

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H       2.639969        1.035379        -0.183477
H       2.840513        0.020292        1.249618
C       3.790285        -0.756657       -0.537639
O       0.785005        -2.111026       1.698910
O       1.519160        -2.969000       -0.243664
H       3.908729        -1.748564       -0.097057
H       3.556825        -0.869807       -1.597226
C       5.105906        -0.002799       -0.381442
O       5.592667        0.079546        0.785827
O       5.630907        0.510554        -1.412964
###
39
LysGlu4 m052x E=-971.794760084 au
N       -1.176427       3.448601        0.700828
H       -0.255846       3.637534        1.083986
H       -1.147372       3.727809        -0.275477
C       -1.441450       2.011999        0.760424
H       -1.421224       1.699622        1.805800
C       -2.820596       1.718255        0.172013
C       -0.390320       1.220226        -0.008654
H       -3.557436       2.258851        0.771852
H       -2.858401       2.125724        -0.843833
C       -3.163563       0.230078        0.141493
O       -0.180839       1.451844        -1.217408
H       -2.469083       -0.299127       -0.519297
H       -3.046280       -0.196448       1.143155
C       -4.590663       -0.006660       -0.349179
H       -5.301419       0.467874        0.333879
H       -4.721686       0.446904        -1.336585
C       -4.887926       -1.491253       -0.438311
H       -4.230635       -1.989927       -1.147282
H       -4.810971       -1.980236       0.530217
N       -6.287816       -1.705659       -0.922975
H       -6.419156       -1.277822       -1.841072
H       -6.505801       -2.700059       -1.001636
H       -6.961121       -1.283467       -0.281025
N       0.268960        0.283909        0.674275
H       0.071673        0.149384        1.656893
C       1.280243        -0.582274       0.086423
H       0.989260        -0.810304       -0.938452
C       2.652419        0.111524        0.097141
C       1.333581        -1.886502       0.893006
H       2.544437        1.057304        -0.440927
H       2.915615        0.344056        1.131344
C       3.751876        -0.730081       -0.553130
O       1.149868        -1.797527       2.139167
O       1.587797        -2.945585       0.258665
H       3.958989        -1.611710       0.060118
H       3.436580        -1.071608       -1.540124
C       5.055439        0.050281        -0.683217
O       5.517928        0.596440        0.362016
O       5.610573        0.100346        -1.820499
###
38
LysGlu5 m052x E=-971.325874101 au
N       -1.208356       3.403988        0.813813
H       -0.283930       3.576647        1.195584
H       -1.188235       3.727508        -0.148949
C       -1.468719       1.965110        0.806922
H       -1.434745       1.603897        1.836022
C       -2.854344       1.691331        0.223844
C       -0.423027       1.217049        -0.011803
H       -3.582386       2.213861        0.850343
H       -2.903970       2.133732        -0.777123
C       -3.201735       0.205456        0.150866
O       -0.204527       1.532911        -1.199656
H       -2.519623       -0.301585       -0.540893
H       -3.054499       -0.251882       1.136011
C       -4.639072       -0.031894       -0.309195
H       -5.334135       0.445689        0.390682
H       -4.793610       0.435577        -1.288563
C       -4.973030       -1.516735       -0.409843
H       -4.279705       -1.995858       -1.104739
H       -4.823485       -1.989793       0.563342
N       -6.340800       -1.810019       -0.854703
H       -6.489092       -1.362213       -1.753271
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H       -6.991175       -1.365725       -0.214527
N       0.224859        0.227008        0.604184
H       0.016913        0.017933        1.571569
C       1.240520        -0.592333       -0.039729
H       0.976698        -0.712019       -1.089823
C       2.616996        0.084138        0.075190
C       1.260068        -1.972854       0.629445
H       2.524579        1.086109        -0.352080
H       2.863484        0.191910        1.135489
C       3.733684        -0.679451       -0.646082
O       1.023546        -2.015794       1.869259
O       1.544575        -2.959889       -0.100974
H       3.873214        -1.661232       -0.193769
H       3.472560        -0.802777       -1.699164
C       5.030611        0.112409        -0.532269
O       5.799915        -0.152620       0.438825
O       5.247679        1.016645        -1.392862
###
48
PheArg1 m052x E=-1085.85685737 au
N       3.080737        3.619939        -0.174449
H       2.423083        4.136585        -0.763600
H       2.870816        3.837748        0.804990
C       2.963859        2.151731        -0.392681
H       3.027887        1.963504        -1.462712
C       4.098222        1.441557        0.364309
C       1.622620        1.718598        0.176549
H       5.044238        1.781320        -0.061894
H       4.055891        1.743950        1.413293
C       3.969168        -0.057951       0.248995
O       1.202283        2.228930        1.223459
C       3.381715        -0.797702       1.279195
C       4.375765        -0.714854       -0.915661
H       3.058745        -0.289754       2.182107
C       3.205820        -2.175085       1.149688
C       4.201891        -2.091802       -1.046557
H       4.830622        -0.144789       -1.718884
H       2.748717        -2.737547       1.954883
C       3.616612        -2.824692       -0.013801
H       4.523223        -2.591613       -1.952414
H       3.479580        -3.894300       -0.116932
N       1.004746        0.743896        -0.490338
H       1.455868        0.348452        -1.307055
C       -0.095530       -0.003077       0.095888
H       -0.037723       0.080632        1.180835
C       -1.452213       0.524317        -0.400881
C       0.092738        -1.453402       -0.295722
H       -1.489421       1.580945        -0.124340
H       -1.470698       0.460211        -1.491892
C       -2.649928       -0.214029       0.191231
O       0.576887        -1.805119       -1.354761
O       -0.358935       -2.299474       0.626010
H       -2.668161       -1.250540       -0.153728
H       -2.582972       -0.223555       1.282699
C       -3.939835       0.469770        -0.235990
H       -3.963755       1.494186        0.142949
H       -3.999470       0.498272        -1.326721
N       -5.084937       -0.273104       0.290463
H       -4.910423       -1.095953       0.850719
C       -6.348632       0.042600        0.029580
N       -6.637603       1.121276        -0.694684
N       -7.339340       -0.735084       0.475653
H       -5.912873       1.728442        -1.041240
H       -7.598793       1.348157        -0.897587
H       -7.131528       -1.511219       1.084816
H       -8.294760       -0.422308       0.399345
H       4.027891        3.942100        -0.387072
H       -0.266726       -3.211957       0.300400
###
47
PheArg2 m052x E=-1085.40815021 au
N       3.001044        3.610454        -0.223128
H       2.332970        4.095011        -0.827037
H       2.778880        3.843465        0.750025
C       2.923818        2.134155        -0.406954
H       2.997723        1.923970        -1.472131
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C       4.076384        1.473877        0.366926
C       1.588742        1.680214        0.164683
H       5.013765        1.829666        -0.065380
H       4.024350        1.797757        1.409116
C       3.987792        -0.030370       0.284076
O       1.155710        2.208976        1.202491
C       3.413972        -0.761727       1.327517
C       4.414316        -0.702021       -0.864966
H       3.075556        -0.242477       2.218220
C       3.266907        -2.144526       1.225249
C       4.268796        -2.084411       -0.969065
H       4.859489        -0.138650       -1.678285
H       2.817042        -2.699991       2.039270
C       3.693355        -2.808350       0.075514
H       4.602801        -2.595540       -1.863952
H       3.576422        -3.882040       -0.007292
N       0.998699        0.682428        -0.481365
H       1.460589        0.270664        -1.284219
C       -0.101325       -0.087292       0.086386
H       -0.030188       -0.041306       1.173343
C       -1.449932       0.487412        -0.372699
C       0.060336        -1.549359       -0.360867
H       -1.473452       1.539021        -0.072984
H       -1.489506       0.452300        -1.465308
C       -2.653641       -0.243956       0.214927
O       0.571793        -1.747345       -1.497154
O       -0.357577       -2.436738       0.429165
H       -2.673335       -1.279206       -0.132407
H       -2.586342       -0.258719       1.306650
C       -3.942241       0.444813        -0.207619
H       -3.963777       1.469152        0.172008
H       -4.005004       0.474560        -1.298225
N       -5.089174       -0.295249       0.320434
H       -4.914706       -1.119282       0.878979
C       -6.352310       0.020373        0.059061
N       -6.640912       1.098996        -0.665811
N       -7.343983       -0.756695       0.505129
H       -5.915298       1.703358        -1.015351
H       -7.601760       1.324789        -0.871260
H       -7.136510       -1.530377       1.117534
H       -8.298719       -0.441370       0.431164
H       3.940066        3.953564        -0.438336
###
46
PheArg3 m052x E=-1084.94947109 au
N       3.074029        3.652449        -0.316211
H       2.306976        4.096287        -0.810627
H       2.976849        3.914677        0.660201
C       2.937315        2.205831        -0.416038
H       2.982936        1.918635        -1.467780
C       4.099497        1.528424        0.335114
C       1.632135        1.690400        0.181322
H       5.026858        1.867552        -0.129980
H       4.085239        1.876865        1.371589
C       4.005939        0.023464        0.291693
O       1.211390        2.131968        1.268719
C       3.453170        -0.690904       1.358976
C       4.400428        -0.674671       -0.854439
H       3.140277        -0.157270       2.250520
C       3.289970        -2.074020       1.281232
C       4.241646        -2.057143       -0.934665
H       4.830146        -0.128335       -1.687730
H       2.853858        -2.612703       2.114111
C       3.683070        -2.760747       0.133036
H       4.551363        -2.584620       -1.829042
H       3.553985        -3.834465       0.069890
N       1.011104        0.727526        -0.503488
H       1.457570        0.354511        -1.331747
C       -0.073089       -0.070635       0.052165
H       0.009835        -0.057508       1.139040
C       -1.432851       0.506201        -0.370445
C       0.085994        -1.519010       -0.435916
H       -1.456361       1.549878        -0.043775
H       -1.488744       0.500261        -1.463070
C       -2.627048       -0.243242       0.213627
O       0.559943        -1.687323       -1.593753
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O       -0.297336       -2.431643       0.344484
H       -2.642439       -1.273568       -0.148839
H       -2.553155       -0.273039       1.304656
C       -3.921303       0.444838        -0.192459
H       -3.940956       1.466778        0.193865
H       -3.993027       0.482020        -1.282299
N       -5.064307       -0.299054       0.338997
H       -4.886346       -1.121410       0.898877
C       -6.328569       0.016683        0.083883
N       -6.620005       1.095909        -0.639008
N       -7.318693       -0.760785       0.532947
H       -5.895692       1.702240        -0.987828
H       -7.581611       1.322790        -0.839588
H       -7.108906       -1.534785       1.144106
H       -8.273349       -0.443932       0.464672
###
45
PheArg4 m052x E=-1084.47157081 au
N       2.908812        3.688541        -0.314885
H       2.153468        4.095652        -0.856435
H       2.746280        3.955511        0.651557
C       2.837978        2.236650        -0.406448
H       2.951069        1.942530        -1.451189
C       3.984774        1.615766        0.414278
C       1.526163        1.669888        0.125236
H       4.922644        1.974009        -0.013999
H       3.909219        1.987345        1.440009
C       3.936047        0.108292        0.405226
O       1.033403        2.095159        1.188786
C       3.365458        -0.594537       1.470701
C       4.381992        -0.605582       -0.711879
H       3.012915        -0.048411       2.339516
C       3.233257        -1.982230       1.418309
C       4.253110        -1.992326       -0.767062
H       4.826017        -0.068359       -1.543584
H       2.782648        -2.512265       2.249043
C       3.674046        -2.684525       0.297266
H       4.600410        -2.531980       -1.640076
H       3.567334        -3.761642       0.252993
N       0.980977        0.681008        -0.585721
H       1.480263        0.326967        -1.391629
C       -0.100743       -0.154482       -0.082130
H       -0.053742       -0.159948       1.007252
C       -1.460451       0.398326        -0.536204
C       0.110177        -1.589069       -0.589350
H       -1.508305       1.440193        -0.205801
H       -1.488322       0.397672        -1.630122
C       -2.656963       -0.369798       0.018370
O       0.636667        -1.726288       -1.728705
O       -0.284830       -2.524131       0.158019
H       -2.668805       -1.389627       -0.373044
H       -2.581701       -0.434709       1.108978
C       -3.956349       0.329208        -0.354840
H       -3.952129       1.350213        0.043401
H       -4.036699       0.395389        -1.442910
N       -5.095221       -0.417037       0.167816
H       -4.894162       -1.010390       0.961022
C       -6.352589       0.127142        0.132395
N       -6.713927       1.142977        -0.583625
N       -7.294877       -0.556698       0.875725
H       -5.923955       1.501265        -1.108692
H       -6.950414       -1.035705       1.695292
H       -8.131743       -0.019515       1.045239
###
22
SerGly1 m052x E=-607.427348658 au
N       -3.227263       -0.842647       0.065932
H       -3.149281       -1.772182       -0.355039
H       -4.103994       -0.409768       -0.233067
H       -3.257985       -0.970694       1.081590
C       -2.070349       -0.003466       -0.336333
H       -2.168848       0.190992        -1.405301
C       -2.119503       1.319229        0.422990
C       -0.811139       -0.835979       -0.110987
H       -3.131897       1.723721        0.355298
H       -1.859891       1.164597        1.472423
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O       -1.189609       2.189736        -0.212485
O       -0.894955       -2.063025       0.042558
H       -1.050135       2.958239        0.354380
N       0.338925        -0.169725       -0.126570
H       0.329760        0.840695        -0.228750
C       1.598960        -0.858276       0.030607
C       2.718685        0.149519        0.012919
H       1.638391        -1.403099       0.977120
H       1.759956        -1.576016       -0.777338
O       2.549924        1.347411        -0.089527
O       3.953692        -0.345725       0.118926
H       3.959953        -1.313215       0.192178
###
21
SerGly2 m052x E=-606.979971589 au
N       -3.187977       -0.810336       0.055654
H       -3.101478       -1.750804       -0.338873
H       -4.054522       -0.381375       -0.276222
H       -3.245137       -0.912443       1.072888
C       -2.014486       0.011179        -0.338123
H       -2.102962       0.205392        -1.407944
C       -2.053961       1.334568        0.419450
C       -0.769395       -0.841994       -0.103776
H       -3.063459       1.746957        0.351294
H       -1.796922       1.178324        1.469374
O       -1.117667       2.199049        -0.214265
O       -0.883926       -2.073498       0.027697
H       -0.975704       2.967018        0.352539
N       0.388645        -0.200014       -0.090055
H       0.410408        0.810388        -0.185293
C       1.651924        -0.895762       0.060355
C       2.820514        0.087711        0.019306
H       1.684547        -1.433445       1.009638
H       1.782763        -1.624820       -0.741041
O       2.566422        1.315111        -0.108930
O       3.966449        -0.429032       0.119394
###
20
SerGly3 m052x E=-606.520972954 au
N       -3.304443       -0.751916       0.044528
H       -3.304172       -1.645324       -0.434609
H       -3.258659       -0.973749       1.035226
C       -2.095356       -0.030775       -0.327306
H       -2.133792       0.178001        -1.400411
C       -2.083873       1.309885        0.400123
C       -0.824498       -0.861315       -0.099886
H       -3.079011       1.747944        0.315643
H       -1.844901       1.167853        1.457691
O       -1.119584       2.170925        -0.216366
O       -0.888594       -2.100873       0.025883
H       -1.019224       2.959044        0.330426
N       0.336748        -0.209444       -0.087287
H       0.344797        0.800776        -0.172726
C       1.606154        -0.891588       0.057092
C       2.770947        0.095728        0.020720
H       1.649085        -1.436523       1.002503
H       1.746064        -1.617054       -0.746703
O       2.516995        1.324304        -0.099937
O       3.920364        -0.417237       0.116397
###
34
SerLeu1 m052x E=-764.669651821 au
N       3.642916        -1.749695       -0.386267
H       3.129140        -2.635132       -0.381781
H       4.548891        -1.881995       0.068094
H       3.802838        -1.496968       -1.365720
C       2.855379        -0.703039       0.313081
H       2.817444        -0.976426       1.368345
C       3.563331        0.639977        0.161084
C       1.437622        -0.761359       -0.250983
H       4.624164        0.504990        0.384815
H       3.452671        1.009339        -0.860784
O       2.963150        1.531228        1.094354
O       1.073291        -1.750866       -0.902145
H       3.218659        2.433678        0.866421
N       0.656141        0.278517        0.031322
```

```
H       1.033632        1.045784        0.578636
C       -0.746303       0.296848        -0.350779
H       -0.843766       -0.189810       -1.320204
C       -1.602132       -0.422142       0.712613
C       -1.166413       1.750443        -0.454050
H       -1.162734       -1.416559       0.839544
H       -1.479561       0.119284        1.655217
C       -3.090879       -0.575802       0.387249
O       -0.699456       2.616514        0.259892
O       -2.113413       2.064884        -1.339735
H       -3.531416       0.416678        0.243413
C       -3.314756       -1.409716       -0.875575
C       -3.785181       -1.235315       1.579603
H       -2.833238       -2.386875       -0.768385
H       -4.382458       -1.574832       -1.037134
H       -2.914826       -0.933843       -1.773889
H       -3.653768       -0.645822       2.489958
H       -4.855734       -1.343428       1.392138
H       -3.368697       -2.231899       1.755310
H       -2.387236       1.308636        -1.881768
###
33
SerLeu2 m052x E=-764.221270462 au
N       3.628528        -1.748548       -0.361680
H       3.110155        -2.631498       -0.355515
H       4.531158        -1.879659       0.099112
H       3.794989        -1.502307       -1.341618
C       2.834866        -0.696691       0.324479
H       2.806164        -0.954268       1.383985
C       3.534112        0.647186        0.146530
C       1.413037        -0.779328       -0.231013
H       4.597626        0.521543        0.363729
H       3.414369        0.999652        -0.880355
O       2.938470        1.552038        1.069488
O       1.053908        -1.806150       -0.833607
H       3.197393        2.450272        0.829454
N       0.633939        0.268275        -0.000319
H       1.009176        1.066575        0.501232
C       -0.771581       0.302577        -0.389277
H       -0.872190       -0.198004       -1.349972
C       -1.624743       -0.399316       0.682539
C       -1.202242       1.766534        -0.537481
H       -1.215718       -1.406733       0.818384
H       -1.486186       0.141221        1.624454
C       -3.120362       -0.515509       0.373168
O       -0.670921       2.605002        0.242749
O       -2.081985       2.017833        -1.404185
H       -3.536716       0.489609        0.251554
C       -3.373764       -1.313094       -0.906960
C       -3.820449       -1.184896       1.556755
H       -2.896701       -2.296200       -0.837402
H       -4.445339       -1.468415       -1.055012
H       -2.985079       -0.806800       -1.792451
H       -3.660109       -0.623567       2.480631
H       -4.896635       -1.256205       1.382433
H       -3.432640       -2.197874       1.703347
###
32
SerLeu3 m052x E=-763.762124832 au
N       3.748780        -1.779340       -0.307505
H       3.308510        -2.686060       -0.200530
H       3.784740        -1.610862       -1.308823
C       2.888605        -0.774109       0.299784
H       2.814044        -0.984091       1.370726
C       3.551298        0.591105        0.143211
C       1.453682        -0.825322       -0.245977
H       4.610124        0.480198        0.380524
H       3.450865        0.946222        -0.886071
O       2.942047        1.518551        1.049001
O       1.041539        -1.837797       -0.846227
H       3.231124        2.408789        0.816050
N       0.681068        0.236946        -0.015213
H       1.071753        1.027839        0.484113
C       -0.725204       0.291690        -0.392877
H       -0.841173       -0.196113       -1.358479
C       -1.585696       -0.410847       0.673289
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C       -1.146986       1.759356        -0.522707
H       -1.195023       -1.427602       0.791777
H       -1.431077       0.112681        1.622442
C       -3.085573       -0.492694       0.373248
O       -0.631213       2.582677        0.284475
O       -2.007741       2.033685        -1.402985
H       -3.482133       0.522529        0.268455
C       -3.365435       -1.266073       -0.916179
C       -3.793196       -1.163907       1.551327
H       -2.916173       -2.263124       -0.861176
H       -4.441507       -1.389410       -1.062252
H       -2.965675       -0.759692       -1.796569
H       -3.614428       -0.620430       2.482529
H       -4.871905       -1.208944       1.383322
H       -3.427025       -2.187302       1.680171
###
49
TyrArg1 m052x E=-1161.08407952 au
N       2.713839        3.970669        -0.162613
H       2.052418        4.441450        -0.784617
H       2.443756        4.174098        0.804899
C       2.709222        2.497942        -0.383296
H       2.847948        2.318886        -1.447649
C       3.844507        1.859803        0.438547
C       1.371424        1.966196        0.102275
H       4.791409        2.220672        0.032776
H       3.753642        2.199355        1.473197
C       3.765676        0.354320        0.380864
O       0.852527        2.432300        1.125376
C       3.138498        -0.359787       1.406126
C       4.221915        -0.345172       -0.738624
H       2.776293        0.169498        2.281187
C       2.955688        -1.736459       1.316705
C       4.048312        -1.723004       -0.843507
H       4.711724        0.191765        -1.543849
H       2.462301        -2.287848       2.107605
C       3.403222        -2.411749       0.183116
H       4.397426        -2.262005       -1.717262
O       3.175975        -3.766539       0.121088
N       0.869229        0.952384        -0.604008
H       1.402188        0.595808        -1.388569
C       -0.184003       0.105008        -0.067780
H       -0.138350       0.135648        1.021323
C       -1.572833       0.565971        -0.542338
C       0.106665        -1.308268       -0.528579
H       -1.654264       1.619761        -0.264819
H       -1.611316       0.500795        -1.632743
C       -2.720313       -0.223090       0.081827
O       0.650562        -1.571820       -1.584567
O       -0.322556       -2.230547       0.327542
H       -2.704530       -1.259992       -0.260778
H       -2.618632       -0.226886       1.170910
C       -4.052340       0.404428        -0.300562
H       -4.097657       1.437120        0.053739
H       -4.166232       0.401836        -1.387226
N       -5.140299       -0.365720       0.302618
H       -4.903435       -1.129951       0.920439
C       -6.426637       -0.075564       0.144985
N       -6.799200       0.928269        -0.646503
N       -7.356044       -0.787314       0.789767
H       -6.116551       1.525093        -1.084984
H       -7.774738       1.171831        -0.722941
H       -7.087553       -1.617288       1.295355
H       -8.330544       -0.652171       0.568489
H       3.541878        -4.127023       -0.697797
H       3.645933        4.356739        -0.330446
H       -0.141863       -3.115826       -0.035116
###
48
TyrArg2 m052x E=-1160.63513488 au
N       2.637553        3.962402        -0.190811
H       1.968304        4.409874        -0.821277
H       2.358508        4.173675        0.772430
C       2.660591        2.485887        -0.387175
H       2.803479        2.292062        -1.448290
C       3.809645        1.886363        0.442713
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C 1.329617 1.941254 0.106949
H 4.748001 2.274852 0.042136
H 3.702981 2.225395 1.476124
C 3.779261 0.379285 0.387053
O 0.807998 2.427023 1.124795
C 3.171216 -0.354697 1.409738
C 4.266592 -0.305525 -0.728211
H 2.782530 0.163436 2.280136
C 3.040333 -1.737205 1.323340
C 4.145860 -1.689232 -0.829666
H 4.740936 0.246997 -1.532181
H 2.560681 -2.304363 2.111485
C 3.522148 -2.398915 0.195793
H 4.520965 -2.217121 -1.699355
O 3.357713 -3.763574 0.142439
N 0.842491 0.911571 -0.575855
H 1.377458 0.534428 -1.349768
C -0.209561 0.050366 -0.048704
H -0.157010 0.071298 1.040568
C -1.591475 0.539360 -0.507895
C 0.058690 -1.385486 -0.529161
H -1.675465 1.590377 -0.217441
H -1.636251 0.491339 -1.599898
C -2.743805 -0.253445 0.101750
O 0.620210 -1.521117 -1.651106
O -0.332011 -2.318248 0.221236
H -2.717946 -1.288884 -0.243851
H -2.650693 -0.262504 1.191891
C -4.076958 0.367783 -0.286373
H -4.130846 1.400070 0.068180
H -4.185879 0.365547 -1.373636
N -5.164861 -0.408068 0.310998
H -4.926275 -1.176196 0.923313
C -6.451578 -0.123918 0.149989
N -6.826834 0.880529 -0.639675
N -7.380109 -0.840848 0.791513
H -6.145543 1.480725 -1.075645
H -7.803134 1.120420 -0.717286
H -7.108287 -1.674441 1.289404
H -8.353470 -0.716549 0.559221
H 3.712806 -4.108615 -0.687660
H 3.561719 4.365147 -0.361531
###
47
TyrArg3 m052x E=-1160.17636762 au
N 2.715924 4.006143 -0.261112
H 1.954523 4.413893 -0.793513
H 2.549456 4.247523 0.711344
C 2.671249 2.556193 -0.387498
H 2.795002 2.288499 -1.438172
C 3.825281 1.935242 0.424716
C 1.368812 1.950704 0.123161
H 4.759207 2.312228 0.003808
H 3.744507 2.292356 1.455383
C 3.792476 0.427673 0.397614
O 0.854183 2.349291 1.186360
C 3.209765 -0.296120 1.442496
C 4.246481 -0.275531 -0.721484
H 2.847558 0.231593 2.318552
C 3.067069 -1.679543 1.373191
C 4.115085 -1.659561 -0.807202
H 4.701882 0.265744 -1.544140
H 2.605479 -2.235882 2.179873
C 3.514023 -2.355673 0.240500
H 4.464525 -2.198017 -1.681321
O 3.340911 -3.721860 0.203599
N 0.856289 0.953705 -0.602760
H 1.379342 0.615169 -1.400459
C -0.180883 0.066358 -0.093691
H -0.111579 0.045060 0.994666
C -1.573746 0.566909 -0.506911
C 0.076718 -1.351533 -0.626901
H -1.652305 1.606863 -0.177448
H -1.641025 0.559123 -1.598931
C -2.715557 -0.246404 0.095310
O 0.611567 -1.453518 -1.765742

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O       -0.294293       -2.310893       0.101756
H       -2.686425       -1.274294       -0.272077
H       -2.613647       -0.277212       1.184360
C       -4.054710       0.375287        -0.269975
H       -4.106011       1.403976        0.095467
H       -4.175990       0.383871        -1.355843
N       -5.135824       -0.407624       0.330617
H       -4.891163       -1.175982       0.940220
C       -6.424015       -0.124681       0.180110
N       -6.806086       0.882385        -0.603144
N       -7.347560       -0.845825       0.824319
H       -6.128392       1.490133        -1.034258
H       -7.782891       1.123577        -0.669527
H       -7.071308       -1.682966       1.313762
H       -8.322237       -0.723223       0.596630
H       3.675070        -4.073588       -0.632220
###
46
TyrArg4 m052x E=-1159.69959042 au
N       2.726341        3.972713        -0.266249
H       1.953852        4.373723        -0.787687
H       2.572619        4.215029        0.708023
C       2.692003        2.520930        -0.387736
H       2.808700        2.251774        -1.438925
C       3.854734        1.905887        0.415732
C       1.396174        1.911277        0.132675
H       4.781447        2.299595        -0.008228
H       3.776109        2.264590        1.446940
C       3.839921        0.397854        0.390190
O       0.889575        2.307055        1.201654
C       3.281390        -0.343089       1.437732
C       4.271776        -0.310887       -0.737911
H       2.930622        0.178304        2.324467
C       3.147709        -1.727341       1.366831
C       4.146784        -1.693452       -0.824523
H       4.707743        0.235183        -1.570419
H       2.704672        -2.274250       2.193131
C       3.565503        -2.458418       0.223334
H       4.487439        -2.216687       -1.712372
O       3.424596        -3.762709       0.136448
N       0.872624        0.920538        -0.593972
H       1.390782        0.579845        -1.393777
C       -0.172897       0.042804        -0.084958
H       -0.096660       0.010350        1.002570
C       -1.561623       0.565318        -0.485359
C       0.058004        -1.373245       -0.634508
H       -1.627588       1.602112        -0.143429
H       -1.633427       0.571091        -1.577115
C       -2.709475       -0.243880       0.110721
O       0.566584        -1.469748       -1.785797
O       -0.308682       -2.334972       0.093133
H       -2.683960       -1.270571       -0.260320
H       -2.610902       -0.279386       1.199932
C       -4.045140       0.383986        -0.256749
H       -4.094501       1.411973        0.110960
H       -4.162940       0.395424        -1.342950
N       -5.130351       -0.397466       0.338511
H       -4.889170       -1.164932       0.950651
C       -6.417555       -0.114317       0.181079
N       -6.795589       0.892346        -0.604561
N       -7.344321       -0.834492       0.822093
H       -6.115804       1.498404        -1.034753
H       -7.772333       1.131278        -0.679211
H       -7.070374       -1.672925       1.310665
H       -8.317684       -0.712975       0.588290
###
45
TyrArg5 m052x E=-1159.21914519 au
N       -2.589358       3.987736        0.360989
H       -1.814433       4.355695        0.902784
H       -2.412867       4.246466        -0.605198
C       -2.595908       2.532959        0.450921
H       -2.735371       2.244236        1.494077
C       -3.762437       1.967532        -0.383331
C       -1.310425       1.899159        -0.066057
H       -4.685926       2.366964        0.042176
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H       -3.664101       2.356518       -1.401784
C       -3.779310       0.459438       -0.405512
O       -0.786466       2.296705       -1.126077
C       -3.203608       -0.258719      -1.459861
C       -4.258481       -0.276327      0.685330
H       -2.816707       0.283468       -2.318608
C       -3.097317       -1.646447      -1.429386
C       -4.162910       -1.663540      0.730636
H       -4.709257       0.251301       1.521812
H       -2.639949       -2.175530      -2.259495
C       -3.565508       -2.405739      -0.324318
H       -4.541705       -2.207863      1.589842
O       -3.454481       -3.715314      -0.279599
N       -0.817442       0.885321       0.649617
H       -1.346996       0.548490       1.443554
C       0.205471        -0.015028      0.132799
H       0.117646        -0.048536      -0.954094
C       1.609227        0.480908       0.513635
C       -0.051562       -1.424971      0.685567
H       1.693710        1.508188       0.147067
H       1.688025        0.512655       1.604356
C       2.741114        -0.360922      -0.070507
O       -0.570217       -1.511265      1.833526
O       0.303776        -2.394516      -0.037222
H       2.764463        -1.346961      0.400978
H       2.579008        -0.511015      -1.142099
C       4.080897        0.328275       0.144254
H       4.070206        1.290034       -0.372187
H       4.226790        0.518076       1.214459
N       5.157975        -0.499520      -0.396316
H       4.999234        -1.495025      -0.324763
C       6.482820        -0.182258      -0.229086
N       6.758634        1.151158       -0.030186
N       7.382915        -1.107676      -0.354983
H       6.046567        1.727043       0.392135
H       7.692525        1.345159       0.298020
H       8.306790        -0.699297      -0.252423
###
32
TyrGly1 m052x E=-838.489783511 au
N       3.969423        -0.493089      -0.388518
H       4.395611        0.208246       -0.998769
H       4.354830        -1.408792      -0.630939
H       4.227044        -0.272781      0.578683
C       2.486169        -0.497337      -0.520919
H       2.242928        -0.580141      -1.578392
C       1.918174        -1.686819      0.272762
C       1.976750        0.806329       0.070357
H       2.305504        -2.601245      -0.180925
H       2.286019        -1.622446      1.299825
C       0.409856        -1.679037      0.260534
O       2.518129        1.287904       1.074419
C       -0.306945       -1.141200      1.331758
C       -0.297178       -2.138046      -0.854766
H       0.226892        -0.775514      2.202697
C       -1.697182       -1.057874      1.297864
C       -1.685434       -2.064291      -0.904259
H       0.244355        -2.557797      -1.695678
H       -2.250109       -0.637640      2.130664
C       -2.380304       -1.518157      0.173844
H       -2.234666       -2.419748      -1.767320
O       -3.750732       -1.453542      0.079106
H       -4.116457       -1.048076      0.876414
N       0.906543        1.331080       -0.525733
H       0.464064        0.814502       -1.277411
C       0.109756        2.342659       0.131487
C       -1.300957       2.281089       -0.396582
H       0.086882        2.168546       1.210190
H       0.500179        3.348639       -0.040899
O       -1.665038       1.517866       -1.266990
O       -2.165816       3.139937       0.147541
H       -1.753418       3.697092       0.826535
###
31
TyrGly2 m052x E=-838.042455589 au
N       3.926605        -0.569091      -0.423733
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H       4.360006        0.124057        -1.037984
H       4.285382        -1.493196       -0.674310
H       4.202857        -0.356639       0.540001
C       2.441287        -0.533597       -0.531634
H       2.179736        -0.593136       -1.586073
C       1.856489        -1.722714       0.250431
C       1.975459        0.774243        0.088540
H       2.219183        -2.639063       -0.219667
H       2.234947        -1.681458       1.274850
C       0.348870        -1.681704       0.250178
O       2.562513        1.225432        1.086894
C       -0.346970       -1.116264       1.320950
C       -0.376971       -2.129559       -0.857355
H       0.201778        -0.756267       2.185056
C       -1.734113       -0.992525       1.293183
C       -1.762910       -2.016324       -0.900628
H       0.147856        -2.570210       -1.698191
H       -2.270184       -0.547789       2.124235
C       -2.435941       -1.440893       0.175860
H       -2.326435       -2.362292       -1.758320
O       -3.804552       -1.336832       0.087347
H       -4.152746       -0.902498       0.877314
N       0.904308        1.329231        -0.463701
H       0.418802        0.840768        -1.208811
C       0.134402        2.354765        0.214564
C       -1.280603       2.429234        -0.360310
H       0.065582        2.125429        1.279851
H       0.604508        3.334012        0.110589
O       -1.574400       1.671496        -1.322129
O       -2.046268       3.266070        0.190491
###
30
TyrGly3 m052x E=-837.582919203 au
N       3.979896        -0.567112       -0.522397
H       4.366979        0.232161        -1.013099
H       4.286479        -0.488554       0.442718
C       2.525764        -0.488443       -0.547630
H       2.188975        -0.502771       -1.585299
C       1.932259        -1.708083       0.184910
C       1.984405        0.764176        0.130198
H       2.287930        -2.600914       -0.332628
H       2.331229        -1.720103       1.203278
C       0.424440        -1.677432       0.217546
O       2.467928        1.168220        1.205883
C       -0.263076       -1.155689       1.316163
C       -0.318733       -2.083773       -0.895829
H       0.293301        -0.830253       2.189045
C       -1.651327       -1.028290       1.307690
C       -1.705345       -1.969785       -0.920532
H       0.196078        -2.490676       -1.759870
H       -2.177848       -0.615386       2.161208
C       -2.366094       -1.432675       0.182713
H       -2.277923       -2.283490       -1.784813
O       -3.737365       -1.321759       0.113044
H       -4.073766       -0.916879       0.923381
N       0.949719        1.363867        -0.463795
H       0.514007        0.904350        -1.254821
C       0.113565        2.322948        0.231503
C       -1.292137       2.358999        -0.368298
H       0.031002        2.051168        1.285607
H       0.534160        3.329194        0.179808
O       -1.532383       1.649355        -1.380634
O       -2.111960       3.122078        0.213985
###
29
TyrGly4 m052x E=-837.105666776 au
N       3.952045        -0.457939       -0.555657
H       4.303794        0.378883        -1.009261
H       4.264106        -0.413277       0.409867
C       2.494524        -0.434143       -0.565454
H       2.149518        -0.426838       -1.600608
C       1.948342        -1.695785       0.130726
C       1.917806        0.778863        0.152477
H       2.334925        -2.557424       -0.418484
H       2.362832        -1.727226       1.143414
C       0.440939        -1.720060       0.184737
```

```
O       2.393287        1.165517        1.239101
C       -0.256773       -1.275892       1.313546
C       -0.316825       -2.081151       -0.936385
H       0.301869        -0.982118       2.198350
C       -1.646015       -1.183085       1.326261
C       -1.705614       -1.999427       -0.938841
H       0.195287        -2.427397       -1.830386
H       -2.159586       -0.831050       2.215405
C       -2.427445       -1.535155       0.193969
H       -2.266144       -2.286749       -1.822750
O       -3.739109       -1.437083       0.193703
N       0.869656        1.373131        -0.422899
H       0.436510        0.923347        -1.220755
C       0.030155        2.312311        0.294314
C       -1.354563       2.410444        -0.344859
H       -0.093709       1.990069        1.330504
H       0.473062        3.309970        0.307597
O       -1.592428       1.724631        -1.374046
O       -2.161944       3.194677        0.226748
###
46
TyrHisOMe3 m052x E=-1142.58709202 au
N       -3.074247       -3.644541       -0.239171
H       -2.855447       -3.952434       0.713270
H       -2.590709       -4.264765       -0.893248
H       -4.081440       -3.740355       -0.390917
C       -2.654884       -2.228063       -0.420911
H       -2.795629       -1.969805       -1.468584
C       -3.513042       -1.332755       0.490031
C       -1.197408       -2.123299       -0.006420
H       -4.552358       -1.441795       0.173430
H       -3.420472       -1.696667       1.516159
C       -3.081216       0.110944        0.410721
O       -0.773988       -2.782060       0.950781
C       -2.228878       0.654119        1.374986
C       -3.474116       0.914958        -0.663433
H       -1.908214       0.042192        2.211708
C       -1.778510       1.969362        1.278821
C       -3.033745       2.229961        -0.774716
H       -4.134512       0.508626        -1.422023
H       -1.117558       2.388322        2.029969
C       -2.184964       2.752285        0.200120
H       -3.340286       2.854037        -1.605053
O       -1.773925       4.055688        0.053774
H       -1.169320       4.289628        0.771023
N       -0.466149       -1.239980       -0.693252
H       -0.916205       -0.694653       -1.420182
C       0.795248        -0.751476       -0.174098
H       0.816010        -0.895818       0.905487
C       1.989945        -1.498787       -0.812682
C       0.882489        0.730964        -0.478329
H       1.860168        -2.558200       -0.593365
H       1.963949        -1.360168       -1.894745
C       3.299161        -1.037538       -0.269469
O       0.391139        1.244242        -1.466705
O       1.597687        1.379602        0.426856
N       4.064120        -0.060559       -0.878471
C       3.960354        -1.370258       0.874118
H       3.832219        0.416206        -1.742959
C       5.138412        0.201821        -0.143573
N       5.092168        -0.587028       0.922982
H       3.720539        -2.084651       1.641973
H       5.910561        0.914631        -0.376649
H       5.798038        -0.607387       1.648875
C       1.827206        2.787002        0.169447
H       2.398820        2.896922        -0.750008
H       0.872985        3.303668        0.092616
H       2.394000        3.142016        1.023292
###
45
TyrHisOMe4 m052x E=-1142.13372001 au
N       -3.231418       -3.523694       -0.243155
H       -3.074613       -3.828650       0.722255
H       -2.755705       -4.180881       -0.865994
H       -4.234513       -3.562074       -0.440162
C       -2.721010       -2.136679       -0.423475
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H       -2.801223       -1.886140       -1.479727
C       -3.564976       -1.181146       0.436650
C       -1.279610       -2.110545       0.058573
H       -4.596035       -1.241272       0.082150
H       -3.530789       -1.529646       1.471668
C       -3.054488       0.235949        0.347863
O       -0.950419       -2.760561       1.059743
C       -2.207371       0.753410        1.330513
C       -3.371130       1.039016        -0.751737
H       -1.943163       0.140948        2.186374
C       -1.692470       2.044441        1.230063
C       -2.866124       2.330067        -0.867673
H       -4.024262       0.651609        -1.526360
H       -1.036370       2.442413        1.996692
C       -2.027844       2.829290        0.128222
H       -3.115823       2.954267        -1.716749
O       -1.556940       4.112131        -0.022726
H       -0.975349       4.339386        0.715503
N       -0.460799       -1.306166       -0.621443
H       -0.833992       -0.774270       -1.399183
C       0.820246        -0.882143       -0.085005
H       0.813022        -1.016362       0.995524
C       1.992731        -1.683077       -0.697534
C       0.978397        0.593433        -0.395849
H       1.883502        -2.714378       -0.359780
H       1.898299        -1.659620       -1.784291
C       3.317054        -1.119997       -0.297015
O       0.573039        1.108386        -1.423297
O       1.630682        1.241025        0.556712
N       3.960345        -0.175851       -1.072230
C       4.013402        -1.321252       0.866737
C       5.022937        0.183506        -0.378819
N       5.096476        -0.481059       0.795749
H       3.833399        -1.963872       1.712192
H       5.766162        0.902279        -0.683735
H       5.829290        -0.386101       1.483642
C       1.931539        2.632366        0.294326
H       2.560905        2.706767        -0.590332
H       1.005809        3.186292        0.153697
H       2.460619        2.979018        1.175662
###
44
TyrHisOMe5 m052x E=-1141.67590677 au
N       -3.227905       -3.611239       -0.272013
H       -2.628661       -4.267405       -0.761515
H       -3.199595       -3.869106       0.709994
C       -2.689080       -2.265858       -0.412954
H       -2.678411       -1.998950       -1.470974
C       -3.587459       -1.271213       0.345038
C       -1.281573       -2.128442       0.153904
H       -4.587870       -1.348689       -0.084533
H       -3.639230       -1.590383       1.389770
C       -3.090085       0.151443        0.264287
O       -0.992665       -2.605687       1.263536
C       -2.320760       0.709519        1.288871
C       -3.348510       0.931471        -0.868019
H       -2.101884       0.121090        2.173817
C       -1.828557       2.011146        1.198324
C       -2.867817       2.232881        -0.975154
H       -3.941265       0.516725        -1.676551
H       -1.231291       2.436132        1.998040
C       -2.110363       2.769698        0.064490
H       -3.076207       2.836819        -1.849824
O       -1.661390       4.063508        -0.077950
H       -1.145992       4.318247        0.699022
N       -0.406180       -1.440934       -0.596479
H       -0.737234       -1.027341       -1.458815
C       0.860891        -0.963029       -0.080082
H       0.897302        -1.163077       0.988343
C       2.056544        -1.649563       -0.779220
C       0.937411        0.535211        -0.305920
H       2.019185        -2.706178       -0.511911
H       1.925210        -1.558567       -1.859147
C       3.359939        -1.039685       -0.376988
O       0.532528        1.083670        -1.315987
O       1.531195        1.168511        0.696813
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N       3.901468        0.024925        -1.069898
C       4.124868        -1.314255       0.727345
C       4.968768        0.384610        -0.384126
N       5.144470        -0.395450       0.705183
H       4.029527        -2.054028       1.504452
H       5.645834        1.184515        -0.636923
H       5.899604        -0.319928       1.370789
C       1.786749        2.579464        0.501756
H       2.434542        2.713021        -0.362620
H       0.847268        3.109152        0.360964
H       2.283047        2.906440        1.409463
###
43
TyrHisOMe6 m052x E=-1141.19900456 au
N       -2.891064       -3.773067       -0.084885
H       -2.172856       -4.407453       -0.418272
H       -2.949208       -3.899491       0.921198
C       -2.491503       -2.397145       -0.355076
H       -2.369156       -2.273549       -1.432226
C       -3.579078       -1.431329       0.140586
C       -1.186108       -2.026726       0.338231
H       -4.487673       -1.653743       -0.424042
H       -3.774032       -1.656087       1.193515
C       -3.183814       0.017603        -0.007746
O       -1.026529       -2.237521       1.551730
C       -2.755665       0.772119        1.089941
C       -3.164094       0.641394        -1.262378
H       -2.755134       0.315645        2.075834
C       -2.333485       2.092269        0.953102
C       -2.738637       1.956144        -1.417615
H       -3.489396       0.083524        -2.136560
H       -2.010092       2.651810        1.825348
C       -2.303493       2.736445        -0.311520
H       -2.734532       2.414714        -2.401349
O       -1.899755       3.979318        -0.453376
N       -0.242201       -1.472999       -0.440893
H       -0.472974       -1.278576       -1.406787
C       1.005290        -0.929378       0.064446
H       1.118902        -1.248954       1.097221
C       2.174702        -1.410172       -0.800858
C       0.938398        0.591644        0.011446
H       2.218572        -2.498954       -0.722649
H       1.963980        -1.159568       -1.842769
C       3.479470        -0.785687       -0.411625
O       0.814786        1.210691        -1.031156
O       1.039338        1.164736        1.203312
N       4.442454        -0.485036       -1.354497
C       3.930659        -0.442116       0.838497
C       5.452299        0.025633        -0.676821
N       5.189370        0.072526        0.646402
H       3.485676        -0.518697       1.816367
H       6.381890        0.376042        -1.094697
H       5.807216        0.431583        1.359310
C       1.089595        2.613391        1.206862
H       2.007911        2.935152        0.718240
H       0.220652        3.018225        0.694191
H       1.090402        2.896082        2.254332
###
27
ValGly1 m052x E=-610.832848800 au
N       -2.736197       -1.302900       -0.856575
H       -2.848610       -1.769842       0.047521
H       -2.444044       -2.012440       -1.532702
H       -3.638658       -0.924782       -1.153687
C       -1.721253       -0.213623       -0.756983
H       -1.490829       0.099782        -1.773965
C       -2.296658       0.977936        0.034722
C       -0.497965       -0.841387       -0.103205
H       -3.269882       1.181925        -0.423277
C       -2.496883       0.671953        1.519033
C       -1.424120       2.220063        -0.148534
O       -0.619353       -1.822905       0.644625
H       -1.536013       0.513681        2.015602
H       -2.983595       1.524569        1.995597
H       -3.124760       -0.205347       1.690553
H       -1.219726       2.412709        -1.204080
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H       -1.943580       3.086190        0.264156
H       -0.473793       2.120233        0.380314
N       0.674502        -0.274064       -0.377027
H       0.729497        0.534855        -0.983571
C       1.885629        -0.734081       0.262129
C       3.013341        0.210280        -0.063260
H       1.765308        -0.765393       1.347980
H       2.156768        -1.737458       -0.075196
O       2.871503        1.238018        -0.694048
O       4.219348        -0.137790       0.388839
H       4.209247        -0.985370       0.861219
###
26
ValGly2 m052x E=-610.385623671 au
N       -2.721749       -1.257249       -0.847500
H       -2.841482       -1.715440       0.060064
H       -2.458305       -1.980349       -1.520950
H       -3.612158       -0.849491       -1.140670
C       -1.667250       -0.205071       -0.757654
H       -1.425168       0.090570        -1.777114
C       -2.202913       1.011864        0.021918
C       -0.466899       -0.868898       -0.094440
H       -3.166988       1.246807        -0.440497
C       -2.418387       0.725169        1.507987
C       -1.286237       2.221102        -0.166807
O       -0.633087       -1.843051       0.661296
H       -1.465183       0.534585        2.007911
H       -2.873620       1.599173        1.977011
H       -3.079504       -0.126447       1.685250
H       -1.074574       2.400593        -1.223308
H       -1.774096       3.107860        0.240772
H       -0.340044       2.089143        0.362731
N       0.718981        -0.341797       -0.365370
H       0.801794        0.472839        -0.961849
C       1.934447        -0.787253       0.288290
C       3.091566        0.161607        -0.022209
H       1.791712        -0.814904       1.370206
H       2.204847        -1.791844       -0.040669
O       2.849973        1.193223        -0.704062
O       4.211387        -0.177783       0.446352
###
25
ValGly3 m052x E=-609.923207635 au
N       -2.569366       -1.322431       -1.137729
H       -2.804780       -1.802708       -0.275379
H       -3.431168       -0.919210       -1.490985
C       -1.647509       -0.231869       -0.824073
H       -1.272265       0.180978        -1.762591
C       -2.291078       0.938494        -0.039353
C       -0.469815       -0.823490       -0.070056
H       -3.147935       1.236597        -0.654273
C       -2.809836       0.535806        1.340456
C       -1.346848       2.135882        0.073219
O       -0.629223       -1.722218       0.780831
H       -1.983322       0.298143        2.014947
H       -3.371177       1.364545        1.777888
H       -3.475081       -0.329437       1.293631
H       -0.924690       2.405057        -0.898770
H       -1.885607       3.002571        0.462041
H       -0.521525       1.922188        0.757503
N       0.733776        -0.329862       -0.360406
H       0.827721        0.429537        -1.022056
C       1.927732        -0.714147       0.363883
C       3.112755        0.169269        -0.021060
H       1.767482        -0.623043       1.440080
H       2.191796        -1.752938       0.154815
O       2.939563        1.062200        -0.893634
O       4.193069        -0.078219       0.581802
###
28
AlaGlyGly1 m052x E=-740.229452294 au
N       5.019785        0.526018        -0.624372
H       5.155318        1.179525        0.151697
H       4.838361        1.075742        -1.467136
H       5.881338        -0.006586       -0.761953
C       3.889412        -0.395940       -0.322015
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H       3.721319        -1.002545       -1.209359
C       4.249962        -1.258225       0.880400
C       2.675478        0.472987        -0.028238
H       4.407794        -0.633050       1.761123
H       3.440388        -1.958976       1.080757
H       5.157292        -1.825129       0.669086
O       2.814741        1.647730        0.344631
N       1.494878        -0.122310       -0.167338
H       1.438727        -1.098824       -0.432051
C       0.267193        0.546786        0.203101
C       -0.895082       -0.393151       -0.039694
H       0.278209        0.818751        1.261493
H       0.134651        1.459278        -0.379555
O       -0.720942       -1.594318       -0.294386
N       -2.106559       0.156298        0.061234
H       -2.206279       1.143694        0.259856
C       -3.298481       -0.647136       -0.084869
C       -4.514242       0.228592        0.004556
H       -3.315366       -1.156699       -1.050353
H       -3.364557       -1.409243       0.694660
O       -4.489513       1.437267        0.132518
O       -5.637750       -0.483749       -0.073321
H       -6.401661       0.115106        -0.019907
###
27
AlaGlyGly2 m052x E=-739.779032174 au
N       5.009488        0.439733        -0.450358
H       5.068245        1.186177        0.247399
H       4.922465        0.880480        -1.368681
H       5.876993        -0.100881       -0.429938
C       3.843955        -0.440768       -0.158042
H       3.762325        -1.151450       -0.977970
C       4.067148        -1.152258       1.169970
C       2.617728        0.458903        -0.100365
H       4.141906        -0.427490       1.982562
H       3.232628        -1.824350       1.365778
H       4.983995        -1.740941       1.123794
O       2.738745        1.675418        0.113964
N       1.445663        -0.147816       -0.252505
H       1.393904        -1.143489       -0.432482
C       0.202021        0.579442        -0.121397
C       -0.955559       -0.393406       -0.241570
H       0.156675        1.087391        0.843304
H       0.114613        1.334976        -0.904989
O       -0.767830       -1.596146       -0.497798
N       -2.162756       0.133268        -0.065626
H       -2.271806       1.114036        0.160597
C       -3.375639       -0.654904       -0.156744
C       -4.603190       0.200767        0.150306
H       -3.489402       -1.072874       -1.158804
H       -3.346671       -1.485817       0.550276
O       -4.431178       1.417839        0.427163
O       -5.711164       -0.399452       0.097374
###
26
AlaGlyGly3 m052x E=-739.318520710 au
N       4.949942        -0.164303       -0.892893
H       5.200183        0.814476        -0.788573
H       4.587008        -0.270808       -1.834519
C       3.900526        -0.476486       0.072539
H       3.615585        -1.521500       -0.052799
C       4.417690        -0.256644       1.491281
C       2.665534        0.394326        -0.120200
H       4.747747        0.778023        1.611579
H       3.639311        -0.462374       2.227960
H       5.262922        -0.919405       1.679467
O       2.763751        1.629081        -0.257097
N       1.482007        -0.223624       -0.104906
H       1.428914        -1.232112       -0.048544
C       0.242725        0.509219        -0.237762
C       -0.923107       -0.458100       -0.183981
H       0.146312        1.252832        0.554670
H       0.208692        1.035558        -1.195063
O       -0.754399       -1.686543       -0.287680
N       -2.122163       0.099809        -0.044602
H       -2.218772       1.102089        0.058812
```

```
C       -3.344959       -0.676969       -0.039614
C       -4.563510       0.230374        0.124486
H       -3.449962       -1.235466       -0.971497
H       -3.339786       -1.396892       0.781090
O       -4.372815       1.469020        0.256209
O       -5.682294       -0.351798       0.117783
###
46
AlaLysAla1 m052x E=-992.596905138 au
N       4.013040        -2.914266       -0.820594
H       4.045992        -2.457067       -1.735944
H       3.380357        -3.713910       -0.895377
C       3.552850        -1.948742       0.216574
H       3.452612        -2.500150       1.149096
C       4.569634        -0.821795       0.344942
C       2.201314        -1.417301       -0.241400
H       4.639797        -0.263195       -0.590044
H       4.265887        -0.146961       1.143872
H       5.547180        -1.236303       0.594206
O       1.880710        -1.461804       -1.437088
N       1.446507        -0.875735       0.715515
H       1.745511        -0.929163       1.681579
C       0.155780        -0.267759       0.421490
H       0.223589        0.179492        -0.568378
C       -0.968836       -1.314328       0.437631
C       -0.072931       0.778149        1.506151
H       -0.663683       -2.117938       -0.237231
H       -1.039423       -1.730309       1.446262
C       -2.317771       -0.753654       -0.007274
O       0.073112        0.455306        2.691845
H       -2.630068       0.059614        0.656257
C       -3.393944       -1.837833       -0.008772
H       -3.084662       -2.664874       -0.655005
H       -3.523036       -2.233262       1.003029
C       -4.712691       -1.277728       -0.506074
H       -5.074441       -0.470297       0.126854
H       -4.637962       -0.924882       -1.532355
N       -5.764442       -2.342433       -0.490369
H       -5.907377       -2.693040       0.458444
H       -6.655953       -1.983912       -0.836379
H       -5.488724       -3.131208       -1.078239
N       -0.411804       2.034511        1.159556
H       -0.578810       2.661152        1.939698
C       -0.675875       2.553939        -0.175214
H       -1.256375       1.840238        -0.758180
C       -1.466449       3.858318        -0.054746
C       0.592480        2.829516        -0.975751
H       -0.904578       4.591317        0.526908
H       -1.660284       4.261446        -1.047031
H       -2.416354       3.656738        0.439653
O       1.754377        2.887619        -0.323068
O       0.554102        3.021847        -2.174940
H       1.631742        2.716428        0.625855
H       4.948092        -3.257720       -0.591541
H       -2.221899       -0.335198       -1.014102
###
45
AlaLysAla2 m052x E=-992.148322456 au
N       3.455902        -3.583183       -0.824709
H       3.701526        -3.042535       -1.658994
H       2.712548        -4.236643       -1.081932
C       3.019839        -2.660137       0.261234
H       2.669842        -3.273495       1.088894
C       4.193683        -1.782551       0.672519
C       1.894259        -1.810682       -0.313626
H       4.537913        -1.188905       -0.176152
H       3.884442        -1.113171       1.474215
H       5.011620        -2.405652       1.035462
O       1.897666        -1.516585       -1.517108
N       0.979617        -1.401619       0.566575
H       1.032586        -1.735792       1.521264
C       -0.133350       -0.525667       0.214094
H       0.052387        -0.156851       -0.790318
C       -1.462628       -1.279439       0.246362
C       -0.129411       0.608599        1.238115
H       -1.388348       -2.107090       -0.463555
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H       -1.606716       -1.701643       1.244182
C       -2.644312       -0.384403       -0.121223
O       -0.465821       0.355761        2.412318
H       -2.693238       0.471117        0.560857
C       -3.961565       -1.154643       -0.053482
H       -3.935943       -1.996148       -0.752495
H       -4.100220       -1.560034       0.953473
C       -5.131702       -0.251585       -0.393509
H       -5.216814       0.577162        0.305890
H       -5.064412       0.136054        -1.407643
N       -6.412592       -1.022233       -0.309189
H       -6.531742       -1.419868       0.624128
H       -7.218045       -0.426878       -0.507601
H       -6.414268       -1.792254       -0.980445
N       0.261809        1.825210        0.863634
H       0.308751        2.528900        1.593216
C       0.785464        2.252040        -0.431030
H       1.403876        1.460617        -0.854865
C       -0.332435       2.629619        -1.405579
C       1.704513        3.467716        -0.219027
H       -0.907554       3.469511        -1.010117
H       0.092967        2.912791        -2.368255
H       -1.006571       1.784747        -1.553514
O       1.684189        4.047905        0.899432
O       2.396318        3.805905        -1.217219
H       4.273002        -4.120790       -0.527490
H       -2.503683       0.012539        -1.130874
###
44
AlaLysAla3 m052x E=-991.688537135 au
N       3.129177        -4.093819       -0.403147
H       3.240381        -3.942377       -1.401193
H       2.260027        -4.603461       -0.282738
C       3.025828        -2.794133       0.250266
H       2.877883        -2.955117       1.318822
C       4.308015        -1.995756       0.028232
C       1.862119        -1.966748       -0.286123
H       4.479526        -1.856304       -1.041853
H       4.245640        -1.014596       0.501558
H       5.154204        -2.537576       0.451712
O       1.638950        -1.890473       -1.507344
N       1.134406        -1.305060       0.624594
H       1.306934        -1.474911       1.606627
C       0.002911        -0.457920       0.264990
H       0.177334        -0.093660       -0.744008
C       -1.315398       -1.233371       0.308999
C       -0.010214       0.684539        1.276370
H       -1.213188       -2.090815       -0.361413
H       -1.463621       -1.614733       1.322517
C       -2.510282       -0.382667       -0.115843
O       -0.312337       0.431491        2.460405
H       -2.563189       0.525291        0.495073
C       -3.819117       -1.157905       0.022873
H       -3.760069       -2.088080       -0.550763
H       -3.982515       -1.421441       1.072166
C       -4.988483       -0.332523       -0.479406
H       -5.105590       0.589055        0.086702
H       -4.889398       -0.096817       -1.536611
N       -6.265026       -1.099036       -0.323748
H       -6.431580       -1.321248       0.659621
H       -7.063118       -0.564842       -0.669685
H       -6.223019       -1.979711       -0.840582
N       0.330962        1.911753        0.886837
H       0.359610        2.623654        1.609370
C       0.798975        2.353472        -0.424490
H       1.462408        1.600598        -0.849383
C       -0.357253       2.645298        -1.384181
C       1.625927        3.638781        -0.247927
H       -0.990033       3.437402        -0.978101
H       0.034773        2.964221        -2.350082
H       -0.966137       1.753013        -1.531021
O       1.530590        4.266311        0.840842
O       2.316502        3.983359        -1.244634
H       -2.381704       -0.066315       -1.155203
###
43
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AlaLysAla4 m052x E=-991.220812629 au
N 3.148973 -4.044211 -0.401526
H 3.258030 -3.891180 -1.399566
H 2.285930 -4.564187 -0.280990
C 3.028870 -2.745721 0.251987
H 2.883621 -2.908703 1.320591
C 4.300200 -1.930451 0.029676
C 1.853457 -1.935373 -0.284494
H 4.469627 -1.788387 -1.040375
H 4.225026 -0.950362 0.503429
H 5.153496 -2.461300 0.452853
O 1.637946 -1.851997 -1.506848
N 1.106480 -1.297565 0.627282
H 1.275973 -1.473974 1.608633
C -0.039422 -0.469009 0.268828
H 0.129147 -0.102470 -0.740245
C -1.346307 -1.263291 0.312429
C -0.068196 0.673739 1.279318
H -1.227283 -2.123303 -0.352299
H -1.491668 -1.642533 1.327418
C -2.553814 -0.435145 -0.122264
O -0.369088 0.418952 2.463367
H -2.616275 0.480186 0.478263
C -3.860144 -1.215250 0.015140
H -3.783153 -2.161074 -0.533450
H -4.029754 -1.465016 1.068568
C -5.058785 -0.432766 -0.511486
H -5.131532 0.519495 0.018884
H -4.900999 -0.197292 -1.566351
N -6.346364 -1.125738 -0.384706
H -6.495278 -1.351147 0.593741
H -6.281028 -2.016915 -0.866389
N 0.261543 1.904207 0.889640
H 0.280117 2.617535 1.610948
C 0.725374 2.348982 -0.422052
H 1.396063 1.601939 -0.845928
C -0.433752 2.628590 -1.382093
C 1.539321 3.642704 -0.247320
H -1.073949 3.415150 -0.976853
H -0.045156 2.949755 -2.348668
H -1.034596 1.730457 -1.527156
O 1.431906 4.274730 0.837760
O 2.231874 3.989416 -1.242019
H -2.422704 -0.124396 -1.163983
###
29
CysGlyGly1 m052x E=-1138.39122171 au
N 4.617674 -1.231140 0.462261
H 4.496498 -1.960696 1.169561
H 5.505387 -0.755873 0.641105
H 4.662785 -1.683542 -0.456558
C 3.485478 -0.262306 0.490009
H 3.372885 0.093726 1.511775
C 3.823106 0.881662 -0.469667
C 2.253286 -1.011800 0.002624
H 4.757171 1.342552 -0.147703
H 3.955246 0.493047 -1.479493
S 2.589746 2.219695 -0.466656
O 2.361294 -1.836618 -0.915604
H 1.605560 1.539891 -1.082364
N 1.102886 -0.682724 0.582360
H 1.085725 0.053250 1.278816
C -0.166722 -1.087297 0.016996
C -1.223813 -0.071652 0.405355
H -0.089110 -1.119980 -1.071244
H -0.461452 -2.078511 0.366004
O -0.939529 0.963402 1.025746
N -2.467960 -0.370736 0.029132
H -2.658805 -1.226754 -0.476058
C -3.561077 0.532501 0.304983
C -4.846797 -0.064529 -0.188892
H -3.658255 0.719449 1.376206
H -3.416787 1.495346 -0.190358
O -4.940276 -1.134330 -0.758650
O -5.886603 0.726597 0.073768
H -6.700848 0.313288 -0.259988

```
###
28
CysGlyGly2 m052x E=-1137.94148125 au
N       4.240238        -1.596276       0.778490
H       3.840079        -2.241259       1.464255
H       5.169202        -1.317100       1.104433
H       4.339074        -2.097303       -0.110395
C       3.365840        -0.401339       0.587902
H       3.165566        0.023646        1.568926
C       4.112598        0.589910        -0.306020
C       2.096616        -0.907112       -0.088029
H       5.049143        0.861785        0.181786
H       4.339213        0.131690        -1.268665
S       3.207011        2.148753        -0.552809
O       2.186484        -1.729868       -1.012803
H       2.287430        1.664422        -1.404930
N       0.950283        -0.409308       0.354306
H       0.933821        0.282885        1.094523
C       -0.309546       -0.742395       -0.273845
C       -1.412149       0.056346        0.396199
H       -0.281779       -0.493078       -1.337003
H       -0.516862       -1.809636       -0.180654
O       -1.155334       0.908072        1.265668
N       -2.645616       -0.216180       -0.014792
H       -2.810614       -0.913447       -0.730367
C       -3.806187       0.483664        0.497774
C       -5.081483       0.002011        -0.190979
H       -3.911251       0.319685        1.571600
H       -3.708768       1.558118        0.331790
O       -4.982694       -0.875282       -1.090348
O       -6.150320       0.536501        0.211934
###
27
CysGlyGly3 m052x E=-1137.47673242 au
N       -4.543367       -1.431613       0.047342
H       -4.365421       -2.300053       -0.462052
H       -5.474170       -1.082673       -0.186536
H       -4.523791       -1.651426       1.046522
C       -3.511680       -0.399196       -0.285741
H       -3.661671       -0.138869       -1.333942
C       -3.724468       0.831248        0.594865
C       -2.159273       -1.092522       -0.142315
H       -4.798329       1.027001        0.613604
H       -3.415745       0.588632        1.615055
S       -2.842955       2.313109        -0.031518
O       -2.103625       -2.334847       -0.067983
N       -1.086238       -0.312249       -0.129290
H       -1.217295       0.707440        -0.152792
C       0.234016        -0.893913       -0.023443
C       1.288783        0.191957        -0.099468
H       0.346371        -1.434116       0.919331
H       0.399569        -1.606396       -0.834134
O       0.992100        1.389585        -0.251890
N       2.544681        -0.235036       0.007218
H       2.749572        -1.219300       0.124707
C       3.680321        0.661976        -0.057817
C       4.990968        -0.111638       0.080655
H       3.694231        1.197295        -1.009064
H       3.631997        1.404284        0.741056
O       4.935575        -1.362000       0.227184
O       6.041503        0.585168        0.035843
###
26
CysGlyGly4 m052x E=-1137.00839267 au
C       3.654575        0.670544        -0.844766
S       3.546841        2.149986        0.236909
C       3.518845        -0.644264       -0.083026
C       2.220614        -0.707267       0.718120
N       1.079721        -0.588586       0.031849
C       -0.212308       -0.629799       0.674482
C       -1.286602       -0.322632       -0.351607
N       -2.516197       -0.172207       0.132016
C       -3.655859       0.103368        -0.719265
C       -4.926114       0.284748        0.110287
O       -5.970479       0.547945        -0.546495
N       3.666029        -1.778182       -1.004551
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O       2.221166        -0.923028       1.947504
O       -1.021191       -0.232599       -1.564192
O       -4.848200       0.158876        1.361541
H       3.519164        -2.650137       -0.506477
H       2.952218        -1.724592       -1.724718
H       4.312529        -0.701421       0.661546
H       4.619312        0.640650        -1.355020
H       2.885341        0.709983        -1.623660
H       1.095182        -0.389787       -0.959804
H       -0.405938       -1.617623       1.099857
H       -0.265309       0.099716        1.485467
H       -2.691002       -0.225959       1.127415
H       -3.488750       1.011288        -1.301229
H       -3.818339       -0.716799       -1.421340
###
31
GlyAlaAla1 m052x E=-779.538748335 au
N       3.184211        -2.471237       0.199038
H       3.474519        -2.256887       1.156323
C       3.102972        -1.229415       -0.604704
H       3.855273        -3.122087       -0.212327
H       2.273317        -2.933406       0.250274
C       2.251234        -0.228034       0.147570
H       4.109461        -0.833643       -0.728603
H       2.680262        -1.466793       -1.577824
O       1.995683        -0.387885       1.346660
N       1.824561        0.823162        -0.560657
H       2.060174        0.890506        -1.542675
C       1.070822        1.896570        0.065082
H       1.577395        2.196051        0.983213
C       0.973920        3.082058        -0.891474
C       -0.332843       1.473414        0.487467
H       0.471915        2.788454        -1.815345
H       0.409104        3.885271        -0.420465
H       1.974123        3.446258        -1.126868
O       -0.937150       2.147820        1.336673
N       -0.872851       0.412847        -0.118353
H       -0.329032       -0.124472       -0.780519
C       -2.210305       -0.045400       0.199920
H       -2.369833       0.057189        1.275362
C       -3.287574       0.743375        -0.557400
C       -2.294033       -1.516523       -0.152338
H       -3.186737       0.586489        -1.631929
H       -4.285163       0.437137        -0.240937
H       -3.162275       1.802756        -0.335930
O       -1.457275       -2.098802       -0.814208
O       -3.375392       -2.176868       0.270207
H       -3.956031       -1.636630       0.828672
###
30
GlyAlaAla2 m052x E=-779.090870959 au
N       3.128485        -2.416408       0.228856
H       3.405858        -2.195481       1.188610
C       3.061650        -1.179639       -0.584166
H       3.802909        -3.072131       -0.168840
H       2.215222        -2.875221       0.270208
C       2.210258        -0.168371       0.156008
H       4.071455        -0.790114       -0.700831
H       2.646626        -1.421344       -1.559461
O       1.983624        -0.298018       1.365112
N       1.754020        0.855067        -0.572953
H       1.959148        0.889508        -1.563453
C       0.975596        1.925151        0.029340
H       1.478409        2.254673        0.939187
C       0.855046        3.087146        -0.952668
C       -0.418578       1.477970        0.464820
H       0.360317        2.762700        -1.870237
H       0.271636        3.887912        -0.500441
H       1.846709        3.469103        -1.196184
O       -1.032675       2.167712        1.300878
N       -0.929581       0.391547        -0.106420
H       -0.361913       -0.177252       -0.720991
C       -2.225544       -0.162988       0.252889
H       -2.340145       -0.100639       1.336739
C       -3.374596       0.586727        -0.425065
C       -2.260009       -1.647345       -0.140006
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H       -3.324453       0.458735        -1.508346
H       -4.330580       0.203788        -0.068575
H       -3.314339       1.650339        -0.192267
O       -1.297902       -2.111054       -0.812866
O       -3.278078       -2.292130       0.229574
###
29
GlyAlaAla3 m052x E=-778.631301575 au
N       3.488261        -2.422714       0.176830
H       4.113587        -2.040320       0.877455
C       2.957305        -1.338691       -0.626650
H       2.727184        -2.856066       0.687805
C       2.213581        -0.269087       0.158150
H       3.764142        -0.856106       -1.179816
H       2.259873        -1.738148       -1.365834
O       2.000367        -0.363009       1.376042
N       1.780032        0.782919        -0.559463
H       1.981865        0.815767        -1.549928
C       1.025156        1.867821        0.038641
H       1.527012        2.188773        0.952362
C       0.936640        3.033933        -0.943067
C       -0.383813       1.459975        0.463431
H       0.439695        2.720590        -1.863571
H       0.370566        3.850099        -0.496219
H       1.938684        3.390867        -1.182576
O       -0.996982       2.177720        1.277723
N       -0.910741       0.374283        -0.095249
H       -0.342603       -0.218717       -0.686084
C       -2.226670       -0.139558       0.249726
H       -2.360320       -0.053319       1.329694
C       -3.342711       0.627070        -0.464334
C       -2.295805       -1.629714       -0.113999
H       -3.275597       0.478299        -1.544012
H       -4.315250       0.275791        -0.120000
H       -3.258818       1.692857        -0.249500
O       -1.342013       -2.132290       -0.769940
O       -3.333246       -2.240205       0.261676
###
40
GlyGlyAspAla1 m052x E=-1175.67678423 au
N       -7.775565       -0.501851       -0.455233
H       -7.968329       -0.361620       0.538882
C       -6.499660       0.143810        -0.841231
H       -7.738604       -1.509656       -0.622705
H       -8.548762       -0.110285       -0.995948
C       -5.385007       -0.457644       -0.008385
H       -6.330318       -0.034441       -1.900939
H       -6.586057       1.212838        -0.659938
O       -5.624375       -1.344739       0.824174
N       -4.169090       0.029070        -0.236723
H       -4.019385       0.754070        -0.928293
C       -3.018725       -0.472450       0.481084
C       -1.774147       0.228561        -0.024437
H       -3.121832       -0.288006       1.552459
H       -2.913155       -1.548439       0.332015
O       -1.830920       1.126758        -0.877269
N       -0.629578       -0.196594       0.516369
H       -0.631242       -0.936918       1.207379
C       0.654096        0.353091        0.130196
H       0.657100        0.515491        -0.947537
C       0.918757        1.685706        0.846785
C       1.715899        -0.683763       0.495709
H       -0.001083       2.276978        0.849718
H       1.206915        1.528438        1.888307
C       1.957940        2.530987        0.169725
O       1.488653        -1.532863       1.376085
O       2.261164        3.620071        0.884006
O       2.465008        2.297436        -0.913208
N       2.866077        -0.591169       -0.161987
H       3.009227        0.166788        -0.820160
C       4.005793        -1.453596       0.115386
H       4.102342        -1.564291       1.196906
C       3.830614        -2.831838       -0.526406
C       5.286774        -0.784948       -0.404429
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H       2.898874        -3.284936       -0.186403
O       5.176793        0.275033        -1.077858
O       6.365797        -1.375414       -0.125456
H       2.909868        4.153109        0.393758
###
39
GlyGlyAspAla2 m052x E=-1175.22238680 au
N       -7.739806       -0.537182       -0.591002
H       -7.925305       -0.760005       0.390216
C       -6.514512       0.288430        -0.704200
H       -7.636269       -1.421243       -1.093983
H       -8.543567       -0.038758       -0.976656
C       -5.399021       -0.399063       0.056446
H       -6.272432       0.416020        -1.755818
H       -6.717403       1.258533        -0.253595
O       -5.654178       -1.276223       0.895586
N       -4.169747       0.020810        -0.222171
H       -4.011225       0.739994        -0.917990
C       -3.020182       -0.492973       0.488920
C       -1.775123       0.207959        -0.018746
H       -3.120082       -0.312606       1.561243
H       -2.920647       -1.568662       0.334146
O       -1.842010       1.123491        -0.854675
N       -0.627274       -0.231691       0.496716
H       -0.622591       -0.993881       1.163280
C       0.654273        0.334264        0.115711
H       0.646451        0.524888        -0.956727
C       0.932291        1.649828        0.857975
C       1.722136        -0.708929       0.433378
H       0.007977        2.233798        0.872820
H       1.207044        1.454379        1.896700
C       1.993052        2.546228        0.218987
O       1.481975        -1.648165       1.215879
O       2.379685        3.530339        0.910140
O       2.390978        2.279780        -0.950670
N       2.899536        -0.522938       -0.154421
H       3.042622        0.315941        -0.710580
C       4.047549        -1.381526       0.093967
H       4.115735        -1.573597       1.166665
C       3.924144        -2.710058       -0.656388
C       5.331126        -0.656849       -0.333655
H       3.929692        -2.534229       -1.734275
H       4.756948        -3.364449       -0.400329
H       2.992076        -3.206407       -0.384992
O       5.226893        0.454508        -0.919004
O       6.411359        -1.255802       -0.074549
###
43
GlyGlyGluAla1 m052x E=-1214.98572362 au
N       7.813669        -0.671569       0.339964
H       7.963286        -0.571520       -0.666563
C       6.552040        -0.010567       0.746753
H       7.787456        -1.671571       0.550523
H       8.606908        -0.257799       0.833148
C       5.420289        -0.582422       -0.083250
H       6.396675        -0.181564       1.809060
H       6.651074        1.056633        0.558023
O       5.657581        -1.289271       -1.074097
N       4.194040        -0.254622       0.311474
H       4.044660        0.299662        1.145817
C       3.030494        -0.707630       -0.417233
C       1.784062        -0.159854       0.249550
H       3.068262        -0.364744       -1.452537
H       2.981899        -1.798636       -0.423528
O       1.838742        0.466203        1.317629
N       0.642786        -0.420332       -0.396481
H       0.679546        -0.853225       -1.311281
C       -0.632651       0.132130        0.030948
H       -0.685239       0.085649        1.118557
C       -0.771020       1.588767        -0.434970
C       -1.723142       -0.730196       -0.588621
H       0.057151        2.148951        0.003897
H       -0.674409       1.625973        -1.521882
C       -2.113529       2.202079        -0.005186
O       -1.653087       -1.043646       -1.791324
H       -2.938400       1.781541        -0.577458
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H       -2.283349       2.023045        1.060171
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O       -2.648739       4.227023        -1.198091
O       -1.401597       4.442698        0.606324
N       -2.720572       -1.089757       0.213052
H       -2.754664       -0.745678       1.164953
C       -3.892488       -1.812141       -0.260206
H       -4.169122       -1.415744       -1.238600
C       -3.616768       -3.313435       -0.374780
C       -5.065481       -1.563391       0.698675
H       -3.394776       -3.732516       0.608729
H       -4.487410       -3.821554       -0.788650
H       -2.764584       -3.486573       -1.032619
O       -4.832895       -0.973412       1.788890
O       -6.185806       -1.997647       0.317183
H       -1.022843       3.915414        1.326522
###
42
GlyGlyGluAla2 m052x E=-1214.53173593 au
N       7.797959        -0.646047       0.354164
H       7.946299        -0.543543       -0.652320
C       6.535468        0.012014        0.763001
H       7.773727        -1.646470       0.562871
H       8.590816        -0.231767       0.847480
C       5.404438        -0.557534       -0.069660
H       6.380061        -0.162247       1.824746
H       6.633327        1.079895        0.577403
O       5.642993        -1.248896       -1.071231
N       4.177874        -0.242797       0.334109
H       4.029295        0.289999        1.182450
C       3.013055        -0.693406       -0.394717
C       1.767983        -0.150275       0.279098
H       3.051728        -0.349402       -1.429167
H       2.962101        -1.784644       -0.401866
O       1.818462        0.398850        1.389685
N       0.635275        -0.334354       -0.405265
H       0.686683        -0.687136       -1.352778
C       -0.638117       0.220741        0.035047
H       -0.697178       0.121894        1.118658
C       -0.756776       1.696953        -0.367075
C       -1.732017       -0.602233       -0.628009
H       0.070278        2.228163        0.106095
H       -0.627700       1.772196        -1.449665
C       -2.085887       2.309043        0.054680
O       -1.705344       -0.786798       -1.859760
H       -2.917073       1.863085        -0.497491
H       -2.276381       2.113521        1.115586
C       -2.181675       3.821482        -0.140696
O       -3.325433       4.339367        0.036619
O       -1.143332       4.472924        -0.446305
N       -2.686184       -1.077019       0.166766
H       -2.686770       -0.849579       1.153255
C       -3.851233       -1.790151       -0.335394
H       -4.211238       -1.279340       -1.230022
C       -3.519028       -3.246558       -0.673283
C       -4.963434       -1.748825       0.721001
H       -3.226678       -3.786070       0.229979
H       -4.389680       -3.734753       -1.110831
H       -2.697609       -3.286241       -1.388974
O       -4.668386       -1.359085       1.883667
O       -6.097102       -2.148055       0.340103
###
25
GlyGlyGly1 m052x E=-700.915686095 au
N       5.441157        0.050488        0.081991
H       5.494697        0.940744        -0.418977
C       4.193094        -0.664729       -0.272440
H       5.474803        0.258975        1.082210
C       3.021355        0.268765        -0.048338
H       4.244510        -0.937645       -1.324915
H       4.116611        -1.562902       0.334625
O       3.198589        1.491080        0.061935
N       1.825465        -0.310530       -0.014806
H       1.734218        -1.317673       -0.071285
C       0.616590        0.473291        0.114889
C       -0.579569       -0.454647       0.077059
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H       0.608339        1.015444        1.063062
H       0.542957        1.204047        -0.692005
O       -0.451825       -1.687912       0.098662
N       -1.770000       0.146655        0.034250
H       -1.835946       1.156519        0.019249
C       -2.987690       -0.629690       0.049947
C       -4.174826       0.284429        -0.041510
H       -3.024439       -1.323453       -0.792394
H       -3.075322       -1.214980       0.968016
O       -4.113078       1.496316        -0.115026
O       -5.319007       -0.399080       -0.033618
H       6.257421        -0.514233       -0.158568
H       -6.065366       0.221130        -0.092335
###
24
GlyGlyGly2 m052x E=-700.465446048 au
N       -5.374250       0.083736        -0.086873
H       -5.412716       0.981716        0.401543
C       -4.136393       -0.644982       0.276362
H       -5.406151       0.279072        -1.089784
C       -2.952366       0.271524        0.045733
H       -4.193378       -0.906542       1.331421
H       -4.070908       -1.550083       -0.321570
O       -3.115199       1.495270        -0.075106
N       -1.763982       -0.322168       0.019241
H       -1.685089       -1.330232       0.078306
C       -0.544589       0.444050        -0.119966
C       0.643216        -0.497141       -0.070546
H       -0.530314       0.972205        -1.076023
H       -0.464647       1.185773        0.675932
O       0.496200        -1.731531       -0.115095
N       1.832174        0.092335        0.001705
H       1.908790        1.101268        0.037786
C       3.072688        -0.655926       -0.021024
C       4.274918        0.285378        0.038553
H       3.127100        -1.337793       0.829543
H       3.144031        -1.252310       -0.932543
O       4.060913        1.525166        0.108897
O       5.405508        -0.273004       0.014994
H       -6.198536       -0.465008       0.162686
###
23
GlyGlyGly3 m052x E=-700.005533226 au
N       -5.503839       0.013765        -0.173835
H       -5.626998       0.678407        0.581737
C       -4.223852       -0.651063       -0.015238
H       -5.491582       0.559757        -1.028474
C       -3.022251       0.280301        0.038168
H       -4.225725       -1.225157       0.913366
H       -4.073924       -1.362487       -0.827816
O       -3.142356       1.511765        0.164188
N       -1.825226       -0.310599       -0.038855
H       -1.754363       -1.317753       -0.105686
C       -0.599556       0.444348        0.089668
C       0.586145        -0.498839       0.040197
H       -0.512372       1.183817        -0.708073
H       -0.574992       0.978719        1.042682
O       0.441407        -1.733870       0.082358
N       1.776778        0.089812        -0.029671
H       1.853251        1.098840        -0.058209
C       3.017344        -0.657607       0.001195
C       4.219678        0.284719        -0.037301
H       3.079231        -1.260434       0.909271
H       3.082585        -1.333764       -0.853161
O       4.006178        1.525233        -0.095474
O       5.350501        -0.273372       -0.009727
###
45
GlyGlyHisAla1 m052x E=-1212.59790312 au
N       -8.184021       0.178061        -0.282857
H       -8.336748       -0.820124       -0.118907
C       -6.852970       0.401700        -0.893807
H       -8.922016       0.531437        -0.894033
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H -3.419782 -1.656155 0.152692
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O 1.201992 -1.620191 1.513639
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44
GlyGlyHisAla2 m052x E=-1212.14176659 au
N -8.151073 0.140885 -0.281167
H -8.312459 -0.843934 -0.056786
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H       4.340925        -3.782674       -0.004064
H       2.576286        -3.682981       0.130015
O       4.557489        -0.296170       -1.606102
O       5.905370        -1.540118       -0.310400
H       4.359801        3.340449        -1.063135
###
48
GlyGlyLysAla1 m052x E=-1160.39540755 au
N       8.176696        0.324076        0.324413
H       8.414701        -0.635483       0.098813
C       6.830328        0.358451        0.864008
H       8.193283        0.831082        -0.553817
C       5.764176        -0.229867       -0.048650
H       6.797980        -0.203374       1.799490
H       6.552698        1.385978        1.101253
O       6.048192        -0.871242       -1.075443
N       4.499345        -0.026909       0.334025
H       4.298643        0.485867        1.182689
C       3.383603        -0.575901       -0.401562
C       2.087827        -0.149891       0.260717
H       3.394136        -0.226496       -1.435360
H       3.424584        -1.667932       -0.416662
O       2.075453        0.433328        1.355803
N       0.979899        -0.473873       -0.411653
H       1.060022        -0.878935       -1.335891
C       -0.348057       -0.090388       0.040115
H       -0.377659       -0.162878       1.127174
C       -0.687626       1.341784        -0.402645
C       -1.339537       -1.062559       -0.577708
H       0.064358        2.003321        0.035359
H       -0.588483       1.395945        -1.490644
C       -2.084682       1.790202        0.019417
O       -1.235127       -1.380418       -1.777449
H       -2.842332       1.182543        -0.484843
H       -2.212133       1.640787        1.096852
C       -2.316893       3.260173        -0.327189
H       -1.584081       3.884283        0.192568
H       -2.181527       3.408862        -1.402863
C       -3.718030       3.685683        0.067859
H       -4.476012       3.107470        -0.455995
H       -3.878355       3.601827        1.140487
N       -3.944690       5.120974        -0.292736
H       -3.818321       5.265012        -1.296487
H       -4.889731       5.418860        -0.046455
H       -3.281693       5.726056        0.195337
N       -2.312369       -1.497115       0.218679
H       -2.391445       -1.130909       1.159538
C       -3.453499       -2.254203       -0.275140
H       -3.724219       -1.864153       -1.258014
C       -3.136893       -3.747304       -0.388847
C       -4.650740       -2.037812       0.661425
H       -2.922085       -4.164727       0.596947
H       -3.986034       -4.276340       -0.820968
H       -2.268092       -3.894655       -1.031151
O       -4.454173       -1.446301       1.758031
O       -5.753123       -2.496902       0.256901
###
47
GlyGlyLysAla2 m052x E=-1159.92731242 au
N       8.178388        0.325474        0.310825
H       8.417586        -0.633504       0.084101
C       6.834105        0.356450        0.856158
H       8.190118        0.832705        -0.567346
C       5.766587        -0.238476       -0.050432
H       6.807698        -0.204459       1.792412
H       6.554103        1.383309        1.093389
O       6.049946        -0.900826       -1.064147
N       4.501956        -0.020664       0.324094
H       4.299756        0.521387        1.154049
C       3.385251        -0.571786       -0.408045
C       2.089586        -0.140869       0.252303
H       3.392842        -0.223759       -1.442765
```

```
H       3.428072        -1.663397       -0.422358
O       2.079709        0.511076        1.308011
N       0.980415        -0.532647       -0.380482
H       1.056499        -1.000273       -1.275172
C       -0.349376       -0.135570       0.051508
H       -0.379327       -0.147931       1.141234
C       -0.702714       1.270902        -0.463790
C       -1.332373       -1.151188       -0.505609
H       0.065275        1.950433        -0.084476
H       -0.631787       1.265427        -1.555645
C       -2.083031       1.757653        -0.025296
O       -1.166440       -1.629025       -1.643496
H       -2.863444       1.149626        -0.494617
H       -2.188617       1.630302        1.058538
C       -2.307328       3.224518        -0.389416
H       -1.542374       3.844268        0.091729
H       -2.197217       3.355698        -1.471949
C       -3.687450       3.715879        0.034959
H       -4.453688       3.099528        -0.440576
H       -3.801465       3.586018        1.113619
N       -3.965279       5.120229        -0.288412
H       -3.859343       5.248485        -1.289612
H       -3.250197       5.698454        0.141244
N       -2.369280       -1.448334       0.274162
H       -2.501234       -0.933979       1.136780
C       -3.520762       -2.197652       -0.205485
H       -3.667410       -1.959105       -1.260716
C       -3.314975       -3.705549       -0.051111
C       -4.777715       -1.737589       0.548487
H       -3.226199       -3.970732       1.004331
H       -4.156940       -4.246021       -0.482694
H       -2.402964       -4.007833       -0.567435
O       -4.642627       -0.918207       1.497941
O       -5.867083       -2.233442       0.151348
###
47
GlyGlyTyrAla1 m052x E=-1292.92268125 au
N       8.603502        -0.714438       -0.234515
H       8.912217        0.250801        -0.201892
C       7.269035        -0.759281       -0.805548
H       8.559430        -1.026828       0.729398
C       6.245005        0.100404        -0.081227
H       7.303430        -0.404804       -1.837878
H       6.911918        -1.788754       -0.832480
O       6.579808        1.051239        0.647664
N       4.963432        -0.210267       -0.297243
H       4.717354        -0.980645       -0.905074
C       3.886504        0.571332        0.265372
C       2.560480        -0.030841       -0.153636
H       3.950881        0.593131        1.354536
H       3.926381        1.603270        -0.092419
O       2.492937        -0.927804       -1.007973
N       1.487894        0.496582        0.443196
H       1.607125        1.190436        1.170587
C       0.136681        0.066137        0.136268
H       0.080766        -0.184072       -0.923041
C       -0.269651       -1.165698       0.980508
C       -0.807338       1.211523        0.459914
H       0.437591        -1.963560       0.746653
H       -0.161973       -0.904588       2.035483
C       -1.684221       -1.601193       0.692178
O       -0.636967       1.890069        1.489372
C       -2.742173       -1.176111       1.500131
C       -1.979187       -2.373630       -0.435726
H       -2.534881       -0.568634       2.375175
C       -4.061431       -1.506078       1.196713
C       -3.290767       -2.714081       -0.753536
H       -1.171528       -2.712341       -1.076125
H       -4.877386       -1.168088       1.826043
C       -4.329176       -2.272741       0.064523
H       -3.517678       -3.312003       -1.627671
O       -5.612772       -2.622015       -0.290383
H       -6.240716       -2.236144       0.334721
N       -1.823723       1.385471        -0.382290
H       -1.958657       0.712570        -1.128119
C       -2.991885       2.182850        -0.037574
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H       -3.152441       2.107469        1.039520
C       -2.816788       3.652205        -0.426054
C       -4.224572       1.594236        -0.738996
H       -2.715318       3.748989        -1.508864
H       -3.681219       4.229366        -0.097596
H       -1.923090       4.056965        0.050313
O       -4.043796       0.751703        -1.659064
O       -5.340839       2.029537        -0.344013
###
46
GlyGlyTyrAla2 m052x E=-1292.44583065 au
N       8.603077        -0.478210       -0.517984
H       8.720827        0.455451        -0.895767
C       7.217493        -0.879635       -0.673992
H       8.814276        -0.408113       0.471219
C       6.209788        0.041847        -0.002522
H       6.969081        -0.951698       -1.733310
H       7.076313        -1.874267       -0.246613
O       6.553233        0.920846        0.807319
N       4.929060        -0.170160       -0.321418
H       4.680224        -0.883683       -0.994331
C       3.854577        0.580982        0.285288
C       2.527610        -0.011198       -0.147198
H       3.931172        0.551202        1.373447
H       3.884318        1.628897        -0.023480
O       2.462549        -0.894247       -1.016866
N       1.453266        0.506904        0.453708
H       1.570834        1.186612        1.194534
C       0.103991        0.065013        0.147973
H       0.051063        -0.183502       -0.911709
C       -0.295062       -1.171879       0.988566
C       -0.849513       1.200882        0.471470
H       0.427874        -1.957805       0.758461
H       -0.189167       -0.908185       2.043911
C       -1.703134       -1.626840       0.700159
O       -0.692359       1.874445        1.507029
C       -2.777776       -1.216567       1.498608
C       -1.998806       -2.401578       -0.427970
H       -2.580643       -0.605072       2.375477
C       -4.090572       -1.561092       1.191607
C       -3.305368       -2.756271       -0.748185
H       -1.186312       -2.733042       -1.069248
H       -4.904144       -1.226750       1.827547
C       -4.407461       -2.343847       0.048824
H       -3.505223       -3.360659       -1.627146
O       -5.644874       -2.666154       -0.252855
N       -1.858642       1.376799        -0.379377
H       -1.988339       0.701392        -1.123817
C       -3.034390       2.164892        -0.040005
H       -3.211541       2.073646        1.033362
C       -2.859086       3.640372        -0.404379
C       -4.253919       1.582740        -0.769611
H       -2.738298       3.752930        -1.483712
H       -3.731840       4.209227        -0.083532
H       -1.976027       4.042391        0.093709
O       -4.055087       0.752130        -1.696803
O       -5.377462       2.012577        -0.389738
###
35
GlyHisGly2 m052x E=-965.271461569 au
N       -5.826568       -0.211707       -0.635352
H       -5.793297       0.784102        -0.866982
C       -4.752512       -0.553417       0.325564
H       -6.742111       -0.428254       -0.237798
H       -5.719181       -0.733683       -1.507908
C       -3.431432       -0.064229       -0.230718
H       -4.962943       -0.047016       1.266046
H       -4.752226       -1.628767       0.483425
O       -3.402531       0.735087        -1.174808
N       -2.344776       -0.540893       0.381110
H       -2.440431       -1.171071       1.168586
C       -1.013638       -0.085146       0.035904
H       -0.967540       0.092098        -1.037903
C       -0.673583       1.225441        0.789388
C       -0.018071       -1.158496       0.441165
H       -1.396286       1.982585        0.487059
```

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H       -0.775785       1.052319        1.862320
C       0.702036        1.716354        0.489827
O       -0.178270       -1.800166       1.493381
N       1.817666        1.304103        1.197547
C       1.166685        2.550451        -0.481954
H       1.815996        0.650935        1.973672
C       2.912707        1.849598        0.681483
N       2.534288        2.617863        -0.332130
H       0.644307        3.094363        -1.249494
H       3.921349        1.703104        1.028916
N       1.037539        -1.294947       -0.357548
H       1.147243        -0.663124       -1.143323
C       2.243550        -1.984216       0.062543
C       3.463050        -1.437155       -0.681655
H       2.394630        -1.844275       1.134116
H       2.174337        -3.056563       -0.129268
O       3.276703        -0.573876       -1.579940
O       4.574313        -1.913526       -0.324794
H       3.170417        3.157037        -0.906857
###
34
GlyHisGly3 m052x E=-964.815779015 au
N       -5.803207       -0.251613       -0.626658
H       -5.775894       0.743866        -0.860204
C       -4.721900       -0.585669       0.329074
H       -6.715409       -0.472483       -0.224053
H       -5.697173       -0.774262       -1.498883
C       -3.405861       -0.090762       -0.236052
H       -4.930429       -0.078245       1.269361
H       -4.715596       -1.660689       0.489136
O       -3.389604       0.698893        -1.190314
N       -2.314877       -0.550760       0.376562
H       -2.405819       -1.168196       1.174510
C       -0.986051       -0.068354       0.044460
H       -0.932387       0.095324        -1.031399
C       -0.677180       1.256095        0.781963
C       0.017719        -1.127035       0.464792
H       -1.423999       1.984032        0.461317
H       -0.794395       1.089182        1.854265
C       0.704385        1.754433        0.503477
O       -0.156295       -1.782248       1.508263
N       1.759630        1.493991        1.355448
C       1.153902        2.439389        -0.596932
C       2.821640        2.013116        0.769659
N       2.503186        2.600883        -0.404365
H       0.644120        2.816792        -1.467644
H       3.828603        1.998967        1.154472
N       1.081390        -1.264038       -0.323081
H       1.213579        -0.606425       -1.083106
C       2.272470        -1.972636       0.105042
C       3.506321        -1.465437       -0.642132
H       2.428816        -1.826852       1.174784
H       2.179772        -3.045351       -0.075077
O       3.351156        -0.586758       -1.531505
O       4.601181        -1.988863       -0.297950
H       3.149190        3.058049        -1.030872
###
50
GlyHisLys3 m052x E=-1178.33361389 au
N       -5.935161       -3.304719       -0.483253
H       -6.582380       -2.514026       -0.449815
C       -4.729473       -3.035711       0.332623
H       -6.417572       -4.135990       -0.136571
H       -5.686083       -3.455473       -1.463230
C       -4.035759       -1.805838       -0.218315
H       -5.037984       -2.873129       1.363002
H       -4.075760       -3.903433       0.280527
O       -4.507553       -1.189696       -1.181911
N       -2.904456       -1.467831       0.404105
H       -2.594763       -1.987182       1.216897
C       -2.141774       -0.296431       0.026991
H       -2.163540       -0.190051       -1.057226
C       -2.740777       0.974283        0.682654
C       -0.715366       -0.484975       0.519602
H       -3.776304       1.059135        0.355109
H       -2.727102       0.850667        1.766946
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C       -2.009940       2.217689        0.305831
O       -0.496797       -1.067877       1.595408
N       -0.921135       2.696804        1.013401
C       -2.174651       3.071037        -0.743442
C       -0.433405       3.780803        0.421577
N       -1.188571       4.027901        -0.640992
H       -2.901583       3.075644        -1.536945
H       0.414090        4.357870        0.750720
H       -1.045116       4.804758        -1.274361
N       0.228268        0.071692        -0.236194
H       -0.041910       0.566632        -1.078187
C       1.597025        0.281624        0.222110
H       1.597104        0.260796        1.311363
C       2.529631        -0.811391       -0.317570
C       2.048380        1.673309        -0.249765
H       2.154449        -1.771114       0.049927
H       2.460170        -0.823639       -1.409345
C       3.984008        -0.626968       0.108832
O       1.653515        2.045188        -1.389484
O       2.793765        2.329603        0.525204
H       4.396827        0.271860        -0.357765
H       4.035504        -0.481036       1.192516
C       4.836965        -1.833362       -0.281759
H       4.482394        -2.724328       0.245072
H       4.747689        -2.021075       -1.356161
C       6.291577        -1.584104       0.066221
H       6.701177        -0.749634       -0.498480
H       6.423796        -1.398381       1.130029
N       7.122232        -2.783316       -0.268440
H       7.057064        -3.002148       -1.264433
H       8.105236        -2.626189       -0.041189
H       6.800926        -3.600015       0.254349
H       -0.516638       2.268226        1.839581
###
49
GlyHisLys4 m052x E=-1177.87822496 au
N       5.887380        -3.335235       0.507637
H       6.467120        -2.524953       0.738610
C       4.784453        -2.941705       -0.400115
H       6.473204        -4.048180       0.069749
H       5.522055        -3.713307       1.384712
C       4.057344        -1.758989       0.210554
H       5.216120        -2.652553       -1.356520
H       4.124162        -3.793871       -0.539101
O       4.548771        -1.143842       1.166818
N       2.896274        -1.447504       -0.364820
H       2.580506        -1.965565       -1.176057
C       2.152367        -0.253721       -0.006742
H       2.192020        -0.122092       1.074343
C       2.748529        0.993844        -0.703780
C       0.716918        -0.442599       -0.466028
H       3.782075        1.086507        -0.367456
H       2.749658        0.815647        -1.780821
C       1.981349        2.241332        -0.405808
O       0.472177        -1.044557       -1.527453
N       0.999346        2.714312        -1.254046
C       2.055362        3.037354        0.708981
C       0.493491        3.773447        -0.651982
N       1.104063        4.010691        0.529836
H       2.685351        2.997869        1.581952
H       -0.294679       4.402821        -1.032445
H       0.892550        4.767825        1.163294
N       -0.213929       0.117245        0.303048
H       0.078649        0.653511        1.110957
C       -1.584395       0.331411        -0.146821
H       -1.584828       0.380972        -1.235487
C       -2.502113       -0.808180       0.319073
C       -2.066021       1.679027        0.410942
H       -2.108712       -1.738560       -0.100785
H       -2.439798       -0.883534       1.408842
C       -3.955530       -0.620797       -0.108988
O       -1.688600       1.982986        1.577035
O       -2.827412       2.365704        -0.321162
H       -4.380858       0.251305        0.395588
H       -3.999653       -0.424118       -1.185110
C       -4.803597       -1.849387       0.217110
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H       -4.427749       -2.718672       -0.330787
H       -4.740251       -2.072730       1.286577
C       -6.250828       -1.598669       -0.159943
H       -6.674697       -0.773840       0.408390
H       -6.359362       -1.396190       -1.223335
N       -7.086824       -2.803918       0.137273
H       -7.040653       -3.039010       1.130607
H       -8.065290       -2.643312       -0.106351
H       -6.754558       -3.611639       -0.392496
###
48
GlyHisLys5 m052x E=-1177.41910438 au
N       5.946917        -3.498425       0.367539
H       6.608045        -2.729460       0.365061
C       4.738526        -3.086212       -0.320345
H       5.728169        -3.676913       1.341488
C       4.058536        -1.854525       0.262229
H       4.966730        -2.866978       -1.365020
H       4.015695        -3.903202       -0.319371
O       4.547179        -1.208900       1.203617
N       2.893753        -1.522189       -0.313929
H       2.580298        -2.037321       -1.126725
C       2.176791        -0.306814       0.016116
H       2.214147        -0.153453       1.094702
C       2.799027        0.918091        -0.699238
C       0.738182        -0.464917       -0.443499
H       3.833952        0.993868        -0.363207
H       2.797367        0.722961        -1.773466
C       2.056614        2.185074        -0.420885
O       0.478267        -1.064601       -1.503144
N       1.090595        2.669447        -1.281236
C       2.134494        2.988101        0.688810
C       0.597504        3.741295        -0.691071
N       1.201621        3.976541        0.494404
H       2.755107        2.943329        1.568220
H       -0.175997       4.381690        -1.083193
H       0.996999        4.741290        1.120925
N       -0.182743       0.118460        0.321429
H       0.118505        0.651943        1.127702
C       -1.548692       0.352769        -0.130909
H       -1.546269       0.404245        -1.219545
C       -2.482125       -0.776000       0.330126
C       -2.014124       1.705802        0.427014
H       -2.094579       -1.710955       -0.084979
H       -2.428710       -0.850254       1.420461
C       -3.930376       -0.576022       -0.109511
O       -1.635503       2.004855        1.594009
O       -2.765602       2.402415        -0.306216
H       -4.352903       0.299200        0.392078
H       -3.964243       -0.378702       -1.185901
C       -4.789566       -1.798778       0.209167
H       -4.414623       -2.670113       -0.336101
H       -4.735769       -2.023143       1.278968
C       -6.232561       -1.540054       -0.178653
H       -6.656256       -0.713163       0.386799
H       -6.332555       -1.337133       -1.242790
N       -7.076668       -2.741236       0.112806
H       -7.036467       -2.977611       1.106098
H       -8.053067       -2.575194       -0.135362
H       -6.746002       -3.550130       -0.416187
###
47
GlyHisLys6 m052x E=-1176.95090992 au
N       6.018619        -3.319958       0.158621
H       6.518939        -2.569491       -0.305445
C       4.601194        -3.190517       -0.129037
H       6.164829        -3.181646       1.152370
C       3.984544        -1.874442       0.320755
H       4.425973        -3.320310       -1.196884
H       4.053642        -3.983723       0.384626
O       4.491462        -1.189939       1.225840
N       2.841416        -1.530547       -0.288074
H       2.514813        -2.069838       -1.079314
C       2.128041        -0.308149       0.023922
H       2.166746        -0.139398       1.100282
C       2.753766        0.905151        -0.707520
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C       0.688591        -0.468489       -0.432983
H       3.790546        0.978955        -0.377148
H       2.745732        0.699763        -1.779791
C       2.017089        2.176730        -0.434776
O       0.427400        -1.080740       -1.485357
N       1.048999        2.659560        -1.293492
C       2.099157        2.982728        0.672525
C       0.558317        3.733228        -0.704533
N       1.166188        3.971129        0.478507
H       2.721912        2.939339        1.550495
H       -0.216418       4.372723        -1.095695
H       0.964038        4.737681        1.103634
N       -0.230249       0.125429        0.325490
H       0.071688        0.665910        1.126738
C       -1.599688       0.347786        -0.123925
H       -1.600981       0.387995        -1.213112
C       -2.524476       -0.782046       0.351965
C       -2.069571       1.703584        0.422189
H       -2.118343       -1.719889       -0.038771
H       -2.478398       -0.833049       1.444295
C       -3.972610       -0.620841       -0.104994
O       -1.688792       2.015219        1.585443
O       -2.825794       2.391092        -0.314945
H       -4.415304       0.261847        0.366772
H       -3.996080       -0.449480       -1.187039
C       -4.818660       -1.847899       0.232056
H       -4.394478       -2.733204       -0.255275
H       -4.792306       -2.030269       1.312687
C       -6.269484       -1.684376       -0.209801
H       -6.701662       -0.810457       0.282647
H       -6.300067       -1.490389       -1.284402
N       -7.129602       -2.840397       0.070766
H       -7.093636       -3.034042       1.066559
H       -6.730245       -3.655273       -0.383861
###
29
GlySerGly1 m052x E=-815.436975178 au
N       4.987689        -1.239874       -0.177164
H       5.137153        -1.028821       0.812039
C       4.015125        -0.296240       -0.774063
H       5.883940        -1.180609       -0.664129
H       4.648187        -2.202274       -0.236549
C       2.717390        -0.383202       0.004797
H       4.427252        0.708691        -0.709833
H       3.867036        -0.563254       -1.817725
O       2.634318        -1.087472       1.017937
N       1.711030        0.343411        -0.488911
H       1.864942        0.942617        -1.290993
C       0.436405        0.447199        0.198327
H       0.203884        -0.518054       0.643752
C       0.529770        1.512984        1.292739
C       -0.600629       0.868556        -0.834188
H       1.332561        1.232749        1.977427
H       0.761195        2.477346        0.834127
O       -0.724068       1.557199        1.965304
O       -0.291912       1.723571        -1.680996
H       -0.680642       2.239760        2.645851
N       -1.818645       0.323189        -0.792342
H       -2.475047       0.667213        -1.481939
C       -2.273225       -0.691666       0.144159
C       -3.743012       -0.986295       0.016402
H       -1.754598       -1.639787       -0.007584
H       -2.115762       -0.373758       1.175217
O       -4.388497       -0.233550       -0.871395
O       -4.282764       -1.846248       0.685305
H       -5.328175       -0.484920       -0.889023
###
28
GlySerGly2 m052x E=-814.990119818 au
N       4.889274        -1.354401       -0.093466
H       5.022009        -1.152899       0.900115
C       3.968778        -0.369542       -0.706417
H       5.798351        -1.327667       -0.558989
H       4.513673        -2.302113       -0.167495
C       2.668872        -0.371618       0.073028
H       4.432112        0.613418        -0.647356
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H       3.813366        -0.638052       -1.748221
O       2.584795        -0.961433       1.157533
N       1.668481        0.305925        -0.493719
H       1.821010        0.801732        -1.363839
C       0.393000        0.500713        0.173141
H       0.157397        -0.395061       0.743413
C       0.487992        1.707877        1.108605
C       -0.646298       0.781572        -0.903382
H       1.260911        1.508520        1.853778
H       0.764867        2.588746        0.524231
O       -0.783757       1.885633        1.722929
O       -0.340351       1.541889        -1.843516
H       -0.755058       2.688244        2.256969
N       -1.847439       0.224831        -0.794400
H       -2.536220       0.467881        -1.498602
C       -2.314149       -0.688963       0.237335
C       -3.796546       -1.009760       0.033749
H       -1.762188       -1.629649       0.206454
H       -2.201744       -0.252553       1.229142
O       -4.399175       -0.479411       -0.936383
O       -4.295334       -1.800016       0.880079
###
27
GlySerGly3 m052x E=-814.530682784 au
N       5.001015        -1.403625       -0.191117
H       4.603103        -2.335080       -0.240158
C       4.025136        -0.445085       -0.673568
H       5.180938        -1.224690       0.790578
C       2.714509        -0.425497       0.100137
H       4.441161        0.562627        -0.609537
H       3.808974        -0.633523       -1.725414
O       2.591222        -0.976147       1.205157
N       1.711812        0.244807        -0.490168
H       1.882060        0.724933        -1.364586
C       0.441849        0.488950        0.167458
H       0.184440        -0.383860       0.763158
C       0.556833        1.718354        1.070387
C       -0.594556       0.761583        -0.913295
H       1.326824        1.526594        1.820504
H       0.846713        2.579754        0.463681
O       -0.711735       1.933803        1.682561
O       -0.285319       1.505115        -1.866246
H       -0.668479       2.749828        2.194767
N       -1.800975       0.215872        -0.797432
H       -2.486339       0.451881        -1.507128
C       -2.276085       -0.676814       0.248587
C       -3.760813       -0.989566       0.049552
H       -1.731740       -1.622299       0.235256
H       -2.161104       -0.224637       1.233139
O       -4.359330       -0.470547       -0.929329
O       -4.266182       -1.762532       0.908008
###
58
PheAlaArg1 m052x E=-1333.18358341 au
N       6.367198        -1.007016       -0.021533
H       6.518239        -0.778033       0.965824
H       6.816212        -0.282299       -0.586814
H       6.818175        -1.901825       -0.224970
C       4.905620        -1.080423       -0.298775
H       4.774713        -1.198298       -1.372428
C       4.314622        -2.275296       0.465926
C       4.290644        0.216033        0.203713
H       4.812518        -3.177565       0.104705
H       4.538988        -2.152358       1.528185
C       2.823723        -2.370314       0.252241
O       4.715800        0.733633        1.247573
C       1.937282        -1.851158       1.200153
C       2.314860        -2.924339       -0.925316
H       2.329207        -1.413143       2.112312
C       0.561563        -1.888029       0.976137
C       0.939627        -2.964698       -1.150362
H       2.998797        -3.327607       -1.664656
H       -0.116625       -1.480632       1.716845
C       0.060437        -2.447154       -0.199446
H       0.555865        -3.400994       -2.064572
H       -1.008625       -2.477259       -0.374570
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N       3.272416        0.690951        -0.508747
H       2.930830        0.164314        -1.304948
C       2.422358        1.751065        0.006042
H       2.374331        1.652621        1.091956
C       2.951758        3.141041        -0.359496
C       1.028272        1.543291        -0.571318
H       2.944450        3.278530        -1.441810
H       2.337453        3.912889        0.105022
H       3.973818        3.240542        0.006580
O       0.843225        0.869824        -1.594954
N       0.047453        2.177324        0.081779
H       0.262950        2.649358        0.950290
C       -1.337826       2.102452        -0.356318
H       -1.357255       2.070520        -1.444147
C       -2.035062       0.854875        0.213174
C       -2.089435       3.345463        0.061316
H       -1.464958       -0.004210       -0.146077
H       -1.960973       0.877021        1.303489
C       -3.493847       0.725194        -0.217342
O       -1.755266       3.772352        1.280870
O       -2.948127       3.871029        -0.619419
H       -4.101669       1.505177        0.248419
H       -3.576065       0.837363        -1.302061
C       -4.026148       -0.638452       0.196382
H       -3.471515       -1.424044       -0.322824
H       -3.899073       -0.776232       1.273242
N       -5.445666       -0.739035       -0.141494
H       -5.897478       0.054627        -0.574591
C       -6.184388       -1.818087       0.093767
N       -5.646396       -2.895455       0.662310
N       -7.473519       -1.834238       -0.254313
H       -4.672839       -2.925329       0.918284
H       -6.215331       -3.711036       0.830096
H       -7.909243       -1.000412       -0.616826
H       -8.053464       -2.620453       -0.006613
H       -2.281236       4.557557        1.511215
###
57
PheAlaArg2 m052x E=-1332.73562766 au
N       6.328549        -1.063053       -0.084272
H       6.504482        -0.744071       0.873866
H       6.779656        -0.405828       -0.724865
H       6.755985        -1.983296       -0.210067
C       4.859577        -1.124312       -0.321693
H       4.698947        -1.285396       -1.385723
C       4.267561        -2.275086       0.507646
C       4.280770        0.204412        0.139436
H       4.745421        -3.199864       0.177337
H       4.514811        -2.109163       1.558967
C       2.771650        -2.359002       0.326057
O       4.752043        0.764080        1.141716
C       1.908637        -1.797385       1.271229
C       2.235106        -2.947958       -0.822036
H       2.322057        -1.331264       2.159614
C       0.528608        -1.827293       1.073935
C       0.855623        -2.980897       -1.020467
H       2.901202        -3.383125       -1.559610
H       -0.131368       -1.386971       1.812133
C       -0.000254       -2.421714       -0.071775
H       0.450406        -3.443773       -1.912104
H       -1.072625       -2.446100       -0.226074
N       3.244840        0.659802        -0.558028
H       2.869567        0.104118        -1.318594
C       2.431573        1.764428        -0.077363
H       2.426318        1.734433        1.013107
C       2.971445        3.115830        -0.553657
C       1.013028        1.548306        -0.591535
H       2.921432        3.180996        -1.641784
H       2.391072        3.929429        -0.117698
H       4.009738        3.217773        -0.236774
O       0.795691        0.855794        -1.601808
N       0.061175        2.185257        0.086595
H       0.303846        2.722859        0.909417
C       -1.342183       2.180976        -0.305922
H       -1.401601       2.237604        -1.392566
C       -2.029004       0.897081        0.184652
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C       -2.022856       3.416540        0.298391
H       -1.472410       0.053449        -0.230121
H       -1.941007       0.849676        1.274187
C       -3.495373       0.788691        -0.224859
O       -1.613286       3.801931        1.428365
O       -2.963338       3.931630        -0.363230
H       -4.090775       1.552542        0.280385
H       -3.595694       0.943582        -1.303029
C       -4.027188       -0.588186       0.143115
H       -3.476763       -1.357456       -0.404437
H       -3.895641       -0.762364       1.214265
N       -5.449304       -0.678039       -0.190083
H       -5.899725       0.124588        -0.607756
C       -6.189037       -1.760446       0.023320
N       -5.651771       -2.850157       0.568892
N       -7.478557       -1.769810       -0.326114
H       -4.678391       -2.884831       0.824735
H       -6.221594       -3.668041       0.721367
H       -7.915729       -0.924795       -0.659935
H       -8.061118       -2.554120       -0.078359
###
56
PheAlaArg3 m052x E=-1332.27752411 au
N       6.294878        -1.293193       -0.502834
H       6.667662        -0.565449       -1.103704
H       6.616677        -1.081920       0.437240
C       4.839731        -1.226744       -0.513249
H       4.484990        -1.376260       -1.534302
C       4.269102        -2.342358       0.382852
C       4.305239        0.101152        0.008706
H       4.643166        -3.291503       -0.004677
H       4.663941        -2.203628       1.393107
C       2.760673        -2.346702       0.410338
O       4.789309        0.628110        1.027010
C       2.057476        -1.708300       1.437107
C       2.040901        -2.940023       -0.631440
H       2.607182        -1.239057       2.246615
C       0.663312        -1.664469       1.424173
C       0.647216        -2.904935       -0.644445
H       2.578089        -3.435245       -1.433681
H       0.132114        -1.163558       2.225226
C       -0.045440       -2.268685       0.385697
H       0.103555        -3.376097       -1.454642
H       -1.128832       -2.242592       0.378759
N       3.274267        0.630415        -0.658849
H       2.854443        0.097884        -1.411081
C       2.483626        1.716359        -0.106362
H       2.496209        1.630849        0.981787
C       3.026750        3.088905        -0.515839
C       1.051178        1.542245        -0.599695
H       2.942894        3.224098        -1.595573
H       2.476685        3.883953        -0.011305
H       4.076901        3.155306        -0.229931
O       0.796801        0.862723        -1.610635
N       0.122964        2.197772        0.095172
H       0.386587        2.719249        0.921629
C       -1.285686       2.219733        -0.277117
H       -1.361384       2.332148        -1.358717
C       -1.970738       0.914134        0.155072
C       -1.954443       3.425646        0.394808
H       -1.409302       0.093988        -0.296680
H       -1.883680       0.816291        1.241507
C       -3.435219       0.812842        -0.262469
O       -1.510562       3.779329        1.522333
O       -2.923332       3.951720        -0.215657
H       -4.039284       1.547340        0.274558
H       -3.534681       1.014821        -1.333022
C       -3.952240       -0.585454       0.041365
H       -3.390783       -1.324179       -0.536107
H       -3.824023       -0.804152       1.104738
N       -5.372128       -0.678620       -0.301032
H       -5.823883       0.124608        -0.716029
C       -6.103627       -1.771739       -0.115389
N       -5.561426       -2.867125       0.413568
N       -7.390630       -1.785591       -0.474766
H       -4.586554       -2.902468       0.663456
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H       -6.124970       -3.693002       0.544803
H       -7.835225       -0.934337       -0.781852
H       -7.968546       -2.577389       -0.240002
###
55
PheAlaArg4 m052x E=-1331.79791680 au
N       6.258330        -1.282641       -0.538997
H       6.620312        -0.565744       -1.159191
H       6.591261        -1.050995       0.392353
C       4.802885        -1.222657       -0.531893
H       4.435523        -1.395346       -1.544811
C       4.248570        -2.321133       0.395489
C       4.268474        0.113796        -0.032329
H       4.618233        -3.277410       0.021488
H       4.658695        -2.161498       1.396508
C       2.740830        -2.326330       0.446740
O       4.764342        0.666903        0.966300
C       2.053483        -1.673340       1.474981
C       2.005340        -2.933236       -0.576080
H       2.615411        -1.193968       2.270034
C       0.659314        -1.627542       1.481625
C       0.611716        -2.895708       -0.569678
H       2.530335        -3.440233       -1.379045
H       0.140337        -1.115510       2.283633
C       -0.065115       -2.243637       0.461176
H       0.055651        -3.376687       -1.365545
H       -1.148348       -2.215756       0.469041
N       3.223773        0.621259        -0.695508
H       2.798150        0.071229        -1.431631
C       2.434645        1.714065        -0.154121
H       2.459749        1.648521        0.935180
C       2.965367        3.082003        -0.594578
C       0.997707        1.528023        -0.629372
H       2.863498        3.199311        -1.674879
H       2.418258        3.882010        -0.094707
H       4.019472        3.158807        -0.326478
O       0.737503        0.852804        -1.641881
N       0.074029        2.171449        0.081942
H       0.346111        2.683538        0.911491
C       -1.340730       2.192856        -0.268983
H       -1.433324       2.313447        -1.348354
C       -2.019138       0.884379        0.164723
C       -1.997529       3.395551        0.420619
H       -1.499010       0.070259        -0.344640
H       -1.864830       0.752708        1.240167
C       -3.509733       0.815127        -0.156555
O       -1.549713       3.727983        1.553476
O       -2.960042       3.942301        -0.181355
H       -4.065370       1.524137        0.461740
H       -3.681672       1.084573        -1.203747
C       -4.030762       -0.593532       0.093770
H       -3.525008       -1.295249       -0.577651
H       -3.795737       -0.881175       1.121417
N       -5.480931       -0.631725       -0.110057
H       -5.822343       0.046653        -0.777341
C       -6.162726       -1.819975       -0.212084
N       -5.576133       -2.895186       0.416239
N       -7.270540       -1.871355       -0.882543
H       -4.978148       -2.699238       1.205353
H       -6.186437       -3.686992       0.554335
H       -7.682788       -2.794171       -0.785261
###
## AMINO ACIDS optimized with m062x
## opt(tight) freq m062x/6-31+G(d,p) scf=(xqc,tight) integral=ultrafine scrf(smd,solvent=water)
###
14
Ala1 m062x E=-324.103609736 au
N       -1.448773       -1.008321       -0.138890
H       -1.439118       -1.250966       0.859329
H       -1.114629       -1.826488       -0.659737
H       -2.418994       -0.820757       -0.413329
C       -0.602983       0.189586        -0.401538
H       -0.641285       0.382247        -1.476447
C       -1.125144       1.383197        0.385793
C       0.820115        -0.174703       -0.032823
H       -1.060649       1.194236        1.460722
```

```
H       -0.533893       2.265910        0.140023
H       -2.165743       1.572074        0.113197
O       1.142585        -1.255079       0.416023
O       1.657549        0.828857        -0.259281
H       2.562730        0.563286        -0.014051
###
12
Ala3 m062x E=-323.190103346 au
N       -1.444328       -1.057396       -0.359491
H       -1.016185       -1.781082       -0.933734
H       -1.405555       -1.416200       0.593872
C       -0.612997       0.142865        -0.419008
H       -0.626069       0.517519        -1.447115
C       -1.192345       1.212621        0.504977
C       0.864859        -0.068912       -0.039684
H       -1.197302       0.851267        1.540094
H       -0.600653       2.130591        0.463698
H       -2.221032       1.447562        0.218575
O       1.167880        -1.061444       0.679066
O       1.684619        0.803027        -0.453649
###
13
AlaZW m062x E=-323.656704712 au
N       -1.335603       -1.065904       -0.164473
H       -0.939803       -1.850378       -0.690522
H       -1.295352       -1.319890       0.828437
C       -0.556702       0.186745        -0.407760
H       -0.623868       0.391852        -1.478193
C       -1.162440       1.322656        0.400856
C       0.916359        -0.063610       -0.043389
H       -1.095397       1.111117        1.472590
H       -0.617122       2.243603        0.189965
H       -2.211606       1.471285        0.132324
O       1.209575        -1.181259       0.453156
O       1.698691        0.891973        -0.274289
H       -2.317059       -0.946720       -0.432469
###
28
Arg1 m062x E=-607.291468007 au
N       3.508827        -1.515050       -0.287628
H       3.617345        -1.678424       0.720940
H       4.426215        -1.249293       -0.663201
H       3.225063        -2.395780       -0.731042
C       2.486605        -0.461926       -0.540750
H       2.462843        -0.273138       -1.615448
C       1.128093        -0.958137       -0.036627
C       2.945871        0.785113        0.191059
H       0.927209        -1.907596       -0.545924
H       1.203944        -1.162403       1.038020
C       -0.007711       0.022086        -0.315251
O       3.666168        0.751201        1.167062
H       0.128971        0.941120        0.263692
H       -0.014295       0.292281        -1.377549
C       -1.343021       -0.605846       0.056840
H       -1.507094       -1.513492       -0.534592
H       -1.349144       -0.877780       1.118565
N       -2.417553       0.348165        -0.207649
H       -2.172359       1.279419        -0.525934
C       -3.701344       0.105584        0.042655
N       -4.087689       -1.085000       0.497978
N       -4.612521       1.057897        -0.171067
H       -3.429350       -1.842647       0.613039
H       -5.068984       -1.266973       0.662376
H       -4.322979       1.990687        -0.433090
H       -5.584137       0.893354        0.055007
O       2.451546        1.891479        -0.346180
H       2.726625        2.665891        0.179092
###
27
Arg2 m062x E=-606.846415198 au
N       3.567341        -1.429011       -0.289182
H       3.721907        -1.488506       0.724478
H       4.459363        -1.170224       -0.721888
H       3.291070        -2.349729       -0.644871
C       2.519152        -0.399496       -0.560813
H       2.502294        -0.228219       -1.637979
```

```
C       1.175861        -0.937935       -0.069299
C       2.921224        0.890110        0.178761
H       0.976536        -1.881671       -0.591400
H       1.254038        -1.160739       1.002314
C       0.028591        0.035863        -0.320462
O       3.560066        0.738894        1.252941
H       0.166758        0.945299        0.273583
H       0.013529        0.328143        -1.377186
C       -1.303129       -0.601940       0.046313
H       -1.466614       -1.502422       -0.556356
H       -1.306329       -0.888367       1.104270
N       -2.382478       0.351367        -0.203435
H       -2.140015       1.286678        -0.511739
C       -3.665291       0.101719        0.042212
N       -4.047915       -1.095074       0.484782
N       -4.580209       1.052553        -0.164556
H       -3.386053       -1.850508       0.593904
H       -5.028668       -1.283196       0.645084
H       -5.550323       0.884280        0.064978
O       2.543574        1.971155        -0.334115
H       -4.292232       1.990012        -0.411337
###
26
Arg3 m062x E=-606.381786546 au
N       3.700002        -1.410172       -0.303168
H       3.764611        -1.545181       0.704807
H       3.433652        -2.312298       -0.693790
C       2.613597        -0.458444       -0.553448
H       2.586380        -0.236976       -1.624315
C       1.239486        -0.990519       -0.120423
C       2.902827        0.849297        0.193375
H       1.048118        -1.918337       -0.674824
H       1.290378        -1.252497       0.944908
C       0.097363        -0.006128       -0.359110
O       3.251622        0.751941        1.404057
H       0.245277        0.898098        0.244035
H       0.083890        0.301430        -1.412308
C       -1.244038       -0.624707       0.003320
H       -1.423440       -1.517024       -0.607112
H       -1.247199       -0.922361       1.058181
N       -2.313853       0.344951        -0.229881
H       -2.062088       1.276252        -0.543100
C       -3.595078       0.115048        0.039189
N       -3.987335       -1.074385       0.493339
N       -4.501772       1.076118        -0.161885
H       -3.333470       -1.837350       0.597924
H       -4.967207       -1.246817       0.674882
H       -4.201882       2.012761        -0.397383
H       -5.464447       0.929715        0.109999
O       2.733777        1.936523        -0.427576
###
25
Arg4 m062x E=-605.904048612 au
N       -3.614557       1.489636        0.047836
H       -3.635689       1.431439        1.065282
H       -3.344970       2.446212        -0.175584
C       -2.558708       0.588550        -0.425666
H       -2.565155       0.594882        -1.519452
C       -1.160148       0.987479        0.065864
C       -2.871346       -0.839921       0.035866
H       -0.944271       1.993371        -0.317981
H       -1.186433       1.057201        1.161719
C       -0.055166       0.024404        -0.363366
O       -3.157235       -0.999336       1.256625
H       -0.208578       -0.953712       0.112217
H       -0.095287       -0.134006       -1.448533
C       1.318966        0.552795        0.019434
H       1.503868        1.483847        -0.525152
H       1.340906        0.786005        1.093504
N       2.350885        -0.428665       -0.323188
H       2.068781        -1.384860       -0.132199
C       3.668468        -0.230259       0.035744
N       4.066082        1.087099        0.110672
N       4.422779        -1.251358       0.289965
H       3.564046        1.752234        -0.464316
H       5.068300        1.228731        0.110842
```

```
H       5.380477        -0.940505       0.447191
O       -2.789605       -1.767677       -0.818098
###
18
Asn1 m062x E=-492.767386121 au
N       -1.822826       -1.567096       -0.009444
H       -2.670918       -1.345127       0.524970
H       -1.536805       -2.525759       0.218998
H       -2.068192       -1.532116       -1.006635
C       -0.731810       -0.610231       0.309497
H       -0.513437       -0.702701       1.376694
C       0.513776        -0.925692       -0.514413
C       -1.263317       0.785260        0.041470
H       0.713553        -2.001653       -0.452936
H       0.358910        -0.666228       -1.565371
C       1.737539        -0.233171       0.059698
O       -2.400013       1.011893        -0.313027
O       1.924939        -0.179831       1.282142
N       2.600075        0.263834        -0.832181
H       3.458640        0.690950        -0.506849
H       2.415246        0.220124        -1.824920
O       -0.330025       1.704974        0.241442
H       -0.694085       2.592066        0.065444
###
16
Asn3 m062x E=-491.858475554 au
N       1.963188        -1.526330       0.031214
H       2.759492        -1.295569       -0.560045
H       2.239268        -1.257473       0.975090
C       0.836452        -0.686264       -0.361751
H       0.599546        -0.887182       -1.409654
C       -0.379305       -1.066005       0.500396
C       1.075966        0.829367        -0.213377
H       -0.584714       -2.131077       0.361491
H       -0.141945       -0.889862       1.554991
C       -1.617290       -0.303896       0.087692
O       1.805368        1.219915        0.739464
O       -2.173417       -0.524606       -1.001347
N       -2.077949       0.613219        0.949794
H       -2.879256       1.178196        0.697717
H       -1.591118       0.807883        1.813649
O       0.481439        1.583146        -1.035374
###
17
AsnZW m062x E=-492.322640644 au
N       1.826001        1.519534        -0.096076
H       2.706241        1.204468        0.326095
H       1.613833        2.471291        0.217967
H       1.970362        1.539563        -1.111828
C       0.738001        0.567981        0.271420
H       0.558396        0.700257        1.341525
C       -0.524605       0.893051        -0.512564
C       1.240541        -0.871922       0.043566
H       -0.724955       1.970025        -0.456580
H       -0.404088       0.623532        -1.565830
C       -1.733561       0.209973        0.093014
O       2.482232        -1.026911       -0.077314
O       -1.910580       0.184103        1.319902
N       -2.618932       -0.298562       -0.772640
H       -3.461337       -0.736687       -0.421854
H       -2.440124       -0.298353       -1.767030
O       0.354590        -1.759119       0.025653
###
17
Asp1 m062x E=-512.625252348 au
N       -1.830886       -1.551024       0.058280
H       -2.660491       -1.303239       0.610266
H       -1.556474       -2.510319       0.299311
H       -2.101039       -1.530916       -0.933100
C       -0.716640       -0.607838       0.331753
H       -0.478947       -0.680844       1.395990
C       0.494939        -0.968454       -0.528544
C       -1.225407       0.792873        0.040450
H       0.725796        -2.030918       -0.384870
H       0.287013        -0.795251       -1.586471
C       1.743475        -0.207569       -0.156658
```

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O       -2.365273       1.037154        -0.288120
O       1.937491        -0.135436       1.161440
O       2.520909        0.249255        -0.969791
O       -0.261352       1.689988        0.188344
H       -0.599182       2.583770        -0.005364
H       2.767119        0.343118        1.339290
###
16
Asp2 m062x E=-512.181975902 au
N       1.849703        1.494759        -0.022534
H       2.705441        1.152275        0.428160
H       1.652541        2.448729        0.295012
H       2.031896        1.520572        -1.032357
C       0.725150        0.569614        0.294417
H       0.527848        0.678125        1.363733
C       -0.501647       0.952388        -0.523480
C       1.180211        -0.879883       0.032020
H       -0.733376       2.013766        -0.369904
H       -0.328165       0.782461        -1.588409
C       -1.731215       0.183848        -0.121036
O       2.416447        -1.079001       -0.062709
O       -1.905549       0.132601        1.204492
O       -2.531969       -0.285555       -0.906792
O       0.257388        -1.726524       -0.038822
H       -2.729635       -0.347205       1.400632
###
15
Asp3 m062x E=-511.726209107 au
N       1.720361        1.566084        -0.027364
H       2.606437        1.270105        0.395513
H       1.465054        2.495584        0.318129
H       1.876662        1.630534        -1.039111
C       0.660179        0.559754        0.283838
H       0.452096        0.650727        1.352911
C       -0.594308       0.857265        -0.521514
C       1.234846        -0.846384       0.024356
H       -0.816705       1.930012        -0.457940
H       -0.439822       0.607023        -1.574550
C       -1.833616       0.128654        0.011265
O       2.484960        -0.938527       -0.094593
O       -1.973736       0.046625        1.262709
O       -2.659526       -0.295028       -0.843957
O       0.399696        -1.780858       -0.023043
###
14
Asp4 m062x E=-511.259172596 au
N       -1.875674       1.571966        -0.063110
H       -2.669657       1.321918        -0.649825
H       -2.167476       1.362510        0.891047
C       -0.758068       0.687146        -0.389424
H       -0.496501       0.832555        -1.440945
C       0.450689        1.069549        0.478619
C       -1.050494       -0.810901       -0.183015
H       0.700834        2.114574        0.272889
H       0.171729        0.972300        1.533073
C       1.665193        0.192886        0.178180
O       -1.780055       -1.139531       0.794348
O       2.278375        0.404693        -0.908498
O       1.975096        -0.700410       1.017691
O       -0.505058       -1.619714       -0.987369
###
15
Cys1 m062x E=-722.251652919 au
N       -1.471727       1.641550        -0.249638
H       -2.311778       1.466345        -0.813869
H       -1.109255       2.569587        -0.498941
H       -1.749774       1.658751        0.740414
C       -0.433713       0.595964        -0.482956
H       -0.261748       0.531473        -1.557918
C       0.834527        1.009204        0.266918
C       -0.992386       -0.714166       0.051323
H       1.168539        1.977731        -0.110993
H       0.613260        1.108744        1.333737
S       2.179498        -0.206903       0.142688
O       -1.589841       -0.778552       1.105084
H       2.334614        -0.119997       -1.190226
```

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O       -0.739614       -1.740801       -0.744086
H       -1.068665       -2.564230       -0.337429
###
14
Cys2 m062x E=-721.805398624 au
N       -1.546025       1.535211        -0.247116
H       -1.879386       1.441407        0.720170
H       -2.346331       1.360160        -0.863426
H       -1.220444       2.494708        -0.403420
C       -0.464599       0.534753        -0.489049
H       -0.258240       0.525733        -1.559793
C       0.759924        0.980620        0.306565
C       -0.980178       -0.843598       -0.024031
H       1.064232        1.972462        -0.034895
H       0.508664        1.026811        1.369893
S       2.152826        -0.178590       0.043704
O       -1.827052       -0.832932       0.906161
H       3.083716        0.654895        0.535889
O       -0.481215       -1.841551       -0.593010
###
13
Cys3 m062x E=-721.337292178 au
N       -1.428057       1.597628        -0.232220
H       -1.698506       1.555842        0.757588
H       -2.271467       1.453673        -0.796277
H       -1.058140       2.531589        -0.434302
C       -0.392367       0.537427        -0.495317
H       -0.233944       0.503290        -1.573438
C       0.882103        0.935182        0.245503
C       -0.992551       -0.787911       0.010486
H       1.174931        1.924851        -0.125441
H       0.624696        1.049530        1.306074
S       2.253839        -0.254585       0.038168
O       -1.487352       -0.748727       1.170972
O       -0.960861       -1.780898       -0.756395
###
12
Cys4 m062x E=-720.868958369 au
N       -1.443070       1.679028        -0.249779
H       -1.616361       1.742554        0.752946
H       -1.037272       2.573749        -0.519544
C       -0.429527       0.630033        -0.463972
H       -0.248502       0.549388        -1.539574
C       0.895485        0.920979        0.245181
C       -1.038387       -0.693086       0.013730
H       1.246179        1.896457        -0.115872
H       0.679240        1.037959        1.315288
S       2.194801        -0.351838       -0.010903
O       -1.337319       -0.773960       1.241683
O       -1.238184       -1.609971       -0.834181
###
21
Gln1 m062x E=-532.064600613 au
N       2.127236        -1.668775       -0.467813
H       2.263715        -1.899932       0.524156
H       3.053290        -1.526320       -0.886308
H       1.687252        -2.472340       -0.930091
C       1.270816        -0.457636       -0.609484
H       1.226036        -0.203955       -1.670318
C       -0.123115       -0.772010       -0.056674
C       1.956142        0.658383        0.155594
H       -0.486217       -1.656337       -0.590903
H       -0.036188       -1.031605       1.003193
C       -1.108772       0.376234        -0.246483
O       2.762442        0.458549        1.040181
H       -0.843417       1.230594        0.385967
H       -1.107564       0.727726        -1.282626
C       -2.508561       -0.035401       0.155729
O       -2.712829       -0.906151       1.015369
N       -3.509994       0.617786        -0.450519
H       -4.466431       0.429000        -0.178689
H       -3.327516       1.323276        -1.150704
O       1.554144        1.856914        -0.242902
H       1.967237        2.544907        0.311372
###
19
```

Gln3 m062x E=-531.153640092 au
N -2.314757 1.590995 -0.545241
H -2.406097 1.833212 0.440565
H -1.892491 2.399636 -0.998252
C -1.380352 0.465318 -0.639786
H -1.326187 0.147363 -1.684981
C 0.032090 0.820521 -0.154516
C -1.925131 -0.710057 0.182188
H 0.403866 1.645759 -0.773717
H -0.034120 1.189275 0.875756
C 1.001076 -0.355200 -0.227892
O -2.304276 -0.455153 1.360227
H 0.710179 -1.138665 0.484496
H 0.983927 -0.814348 -1.222325
C 2.422148 0.031253 0.117205
O 2.689145 1.013890 0.827669
N 3.384485 -0.767833 -0.370773
H 4.350699 -0.593918 -0.125825
H 3.158886 -1.565784 -0.948096
O -1.926836 -1.855697 -0.350237
###
20
GlnZW m062x E=-531.618862853 au
N 2.197537 -1.575495 -0.491628
H 2.408083 -1.709118 0.505075
H 3.088642 -1.433388 -0.977141
H 1.757354 -2.422763 -0.864538
C 1.307207 -0.383926 -0.638620
H 1.275517 -0.127820 -1.698538
C -0.081800 -0.760999 -0.122781
C 1.928425 0.772017 0.168195
H -0.439116 -1.619735 -0.702459
H -0.000526 -1.075922 0.923259
C -1.078561 0.386568 -0.248695
O 2.630155 0.446846 1.161337
H -0.800286 1.215123 0.412893
H -1.092953 0.782038 -1.268998
C -2.471469 -0.041426 0.157152
O -2.664641 -0.908819 1.023833
N -3.484563 0.591109 -0.452790
H -4.437817 0.387054 -0.180827
H -3.314278 1.292635 -1.159870
O 1.652205 1.933122 -0.218850
###
20
Glu1 m062x E=-551.920643966 au
N -2.013959 1.798005 -0.017107
H -2.951135 1.805359 -0.435489
H -1.538470 2.668832 -0.278559
H -2.126936 1.781740 1.004102
C -1.225056 0.623261 -0.478696
H -1.211370 0.639001 -1.569983
C 0.193247 0.728048 0.089173
C -1.946522 -0.618375 0.010685
H 0.594075 1.696722 -0.227395
H 0.142512 0.719579 1.183946
C 1.104344 -0.397653 -0.421485
O -2.693863 -0.615853 0.966124
H 0.810313 -1.360503 0.006888
H 1.060502 -0.462453 -1.510177
C 2.534130 -0.110369 -0.037803
O 2.866423 -0.262964 1.254373
O 3.385112 0.271763 -0.816697
O -1.643241 -1.686642 -0.712399
H -2.086161 -2.473405 -0.343334
H 2.128066 -0.600796 1.787291
###
19
Glu2 m062x E=-551.475655415 au
N -2.075823 1.722605 0.003758
H -2.250428 1.593573 1.007670
H -2.987928 1.756954 -0.462341
H -1.599993 2.617506 -0.147114
C -1.260947 0.576538 -0.499040
H -1.247450 0.636636 -1.588181
C 0.150962 0.712328 0.071674

```
C       -1.938022       -0.730316       -0.044727
H       0.546908        1.688848        -0.229102
H       0.098463        0.691542        1.167008
C       1.082557        -0.395737       -0.440328
O       -2.628024       -0.667167       1.005270
H       0.789808        -1.365120       -0.026138
H       1.050914        -0.450433       -1.530108
C       2.504282        -0.100247       -0.039240
O       2.821824        -0.252248       1.257821
O       3.365080        0.289178        -0.804805
O       -1.706476       -1.745655       -0.744234
H       2.078247        -0.596004       1.779551
###
18
Glu3 m062x E=-551.021876516 au
N       -2.148910       1.613731        -0.338420
H       -2.332534       1.671460        0.670891
H       -3.052016       1.515700        -0.812485
H       -1.710596       2.484763        -0.654205
C       -1.266269       0.433813        -0.598052
H       -1.265617       0.257472        -1.674555
C       0.137128        0.765026        -0.089639
C       -1.870877       -0.774651       0.139362
H       0.485872        1.660240        -0.616199
H       0.075362        1.013193        0.976635
C       1.125306        -0.372642       -0.307784
O       -2.461086       -0.526789       1.223848
H       0.842665        -1.254280       0.278666
H       1.124536        -0.689062       -1.357209
C       2.567065        -0.030637       0.074554
O       2.808784        1.081944        0.619350
O       3.438283        -0.915340       -0.174155
O       -1.695907       -1.899947       -0.388199
###
17
Glu4 m062x E=-550.554292950 au
N       -2.160776       1.727599        -0.323841
H       -2.260580       1.821065        0.685973
H       -1.678456       2.567139        -0.640036
C       -1.293176       0.572886        -0.577361
H       -1.249878       0.402490        -1.657045
C       0.135297        0.769971        -0.048251
C       -1.905679       -0.673919       0.070858
H       0.544996        1.670525        -0.524274
H       0.083491        0.966054        1.029784
C       1.061504        -0.418764       -0.321023
O       -2.337705       -0.555494       1.252713
H       0.726769        -1.289787       0.255743
H       1.030823        -0.685664       -1.381642
C       2.501401        -0.115393       0.086779
O       2.710174        0.195042        1.296526
O       3.403072        -0.186472       -0.798493
O       -1.909019       -1.747289       -0.596700
###
11
Gly1 m062x E=-284.804637056 au
N       1.831381        0.081288        0.000002
H       1.852151        0.686986        -0.827866
C       0.626474        -0.776821       0.000000
H       2.679800        -0.494345       -0.000037
H       1.852189        0.686930        0.827909
C       -0.599252       0.097723        0.000000
H       0.637954        -1.407626       -0.889549
H       0.637954        -1.407629       0.889547
O       -0.557760       1.309854        -0.000009
O       -1.711786       -0.625395       0.000007
H       -2.486678       -0.034416       0.000004
###
Gly3 m062x E=-283.892699957 au
###
10
GlyZW m062x E=-284.357902554 au
N       -1.768616       0.079466        0.015585
C       -0.563146       -0.788900       -0.022096
C       0.709756        0.058817        -0.001223
O       1.787356        -0.587762       0.016662
```

O 0.570252 1.307705 -0.010606
H -1.796933 0.618081 0.886533
H -0.601893 -1.383773 -0.934879
H -0.591697 -1.453778 0.840918
H -1.741452 0.756323 -0.753094
H -2.628236 -0.472161 -0.057099
###
22
His1 m062x E=-549.520426314 au
N 2.555173 -1.475363 0.025908
H 3.332616 -1.241454 -0.602479
H 2.323489 -2.467713 -0.094747
H 2.884696 -1.336914 0.989566
C 1.366078 -0.630052 -0.260952
H 1.034647 -0.866857 -1.275597
C 0.254562 -0.947995 0.754661
C 1.824848 0.815889 -0.229988
H 0.223977 -2.033705 0.881033
H 0.498360 -0.503801 1.724591
C -1.098325 -0.499937 0.311431
O 2.981006 1.143748 -0.072319
N -1.713157 0.645759 0.776017
C -1.981552 -1.074783 -0.553564
H -1.299646 1.316209 1.418776
C -2.913196 0.776780 0.222699
N -3.091181 -0.260694 -0.588881
H -1.914105 -1.983089 -1.130722
H -3.613772 1.577514 0.401473
O 0.813091 1.653936 -0.397146
H 1.137390 2.573373 -0.375905
H -3.930762 -0.422358 -1.137292
###
21
His2 m062x E=-549.081050286 au
N -2.409754 1.556669 -0.267718
H -3.230119 1.179838 -0.756007
H -2.127426 2.444062 -0.694517
H -2.694282 1.737989 0.701882
C -1.306387 0.553974 -0.317768
H -0.948171 0.542318 -1.351245
C -0.187687 0.993797 0.636210
C -1.913222 -0.835166 -0.012171
H -0.118069 2.085231 0.626349
H -0.437414 0.687653 1.657884
C 1.161007 0.477470 0.258510
O -3.156457 -0.939732 -0.114328
N 1.428302 -0.861684 0.059567
C 2.340262 1.133804 0.065096
H 0.675774 -1.565003 0.112661
C 2.708519 -1.027185 -0.247899
N 3.280425 0.173954 -0.243510
H 2.585680 2.182032 0.122332
H 3.198888 -1.963118 -0.466501
O -1.102720 -1.752344 0.284830
H 4.260794 0.342870 -0.447099
###
20
His3 m062x E=-548.623872177 au
N -2.727954 -1.168260 -0.000429
H -3.044476 -0.711161 -0.865297
H -3.437997 -0.995194 0.717992
H -2.662554 -2.179355 -0.155316
C -1.409427 -0.582854 0.388826
H -1.210638 -0.871256 1.421469
C -0.341895 -1.152934 -0.556804
C -1.518997 0.948474 0.268776
H -0.331540 -2.240926 -0.431906
H -0.634714 -0.934326 -1.589400
C 1.020311 -0.590531 -0.301042
O -2.290765 1.380878 -0.627573
N 1.576722 0.384495 -1.104321
C 1.878611 -0.897065 0.724493
C 2.749948 0.656425 -0.564510
N 2.973744 -0.090654 0.540372
H 1.807291 -1.596744 1.543349
H 3.469184 1.372034 -0.934817

```
O       -0.808108       1.626082        1.049060
H       3.807536        -0.066908       1.114233
###
19
His4 m062x E=-548.158557776 au
N       2.715654        -1.195615       -0.557190
H       2.582037        -2.059356       -1.080310
H       2.898992        -1.476785       0.405706
C       1.451680        -0.445429       -0.567814
H       1.254073        -0.131548       -1.596656
C       0.273447        -1.272020       -0.045704
C       1.672141        0.816153        0.283725
H       0.202560        -2.184580       -0.652345
H       0.499002        -1.590720       0.979183
C       -1.037947       -0.548965       -0.060116
O       1.857364        0.635977        1.520960
N       -2.136435       -1.034072       0.625422
C       -1.375349       0.614462        -0.706452
C       -3.109577       -0.174078       0.392809
N       -2.699385       0.835998        -0.405723
H       -0.813068       1.287501        -1.335231
H       -4.117381       -0.235620       0.776727
O       1.686647        1.937695        -0.295585
H       -3.263512       1.616817        -0.716320
###
23
Ile1 m062x E=-441.989194334 au
N       1.372109        -1.697965       -0.590574
H       1.584421        -1.937687       0.385166
H       2.267629        -1.622962       -1.086495
H       0.837598        -2.467975       -1.006607
C       0.596805        -0.426309       -0.681565
H       0.482419        -0.199829       -1.744055
C       -0.788725       -0.586931       -0.016968
C       1.446594        0.645481        -0.028345
H       -1.152187       -1.570338       -0.345740
C       -0.699303       -0.574786       1.510592
C       -1.772623       0.461242        -0.553896
O       2.402060        0.397606        0.678802
H       -0.456914       0.429922        1.877783
H       -1.656411       -0.869138       1.946149
H       0.054623        -1.270114       1.893978
H       -1.737914       0.442055        -1.649411
H       -1.452831       1.460782        -0.240111
C       -3.205107       0.212995        -0.086846
H       -3.311633       0.359968        0.991531
H       -3.892734       0.903454        -0.582885
H       -3.523700       -0.808158       -0.323424
O       1.013366        1.867595        -0.304025
H       1.563614        2.524006        0.162094
###
22
Ile2 m062x E=-441.542376985 au
N       1.448643        -1.533334       -0.740289
H       1.851629        -1.675647       0.193717
H       2.233265        -1.448432       -1.393302
H       0.893591        -2.352394       -1.006696
C       0.626792        -0.281220       -0.735858
H       0.518304        0.029992        -1.776149
C       -0.758392       -0.573238       -0.129448
C       1.412016        0.788192        0.047612
H       -1.138506       -1.455402       -0.665399
C       -0.674472       -0.904057       1.362037
C       -1.730586       0.579819        -0.409284
O       2.286697        0.372348        0.852973
H       -0.395408       -0.015784       1.940687
H       -1.641021       -1.256799       1.729772
H       0.056839        -1.691265       1.572966
H       -1.662391       0.849098        -1.470250
H       -1.422289       1.461751        0.163004
C       -3.177923       0.228309        -0.071153
H       -3.316195       0.060678        1.000809
H       -3.849225       1.039925        -0.365817
H       -3.494369       -0.678611       -0.598205
O       1.093387        1.982577        -0.168793
###
```

```
21
Ile3 m062x E=-441.075390326 au
N       1.493904        -1.522699       -0.920144
H       1.816302        -1.800047       0.004719
H       0.901983        -2.277886       -1.261476
C       0.680181        -0.312837       -0.776683
H       0.540409        0.125799        -1.770081
C       -0.732795       -0.574881       -0.193049
C       1.435521        0.720040        0.071200
H       -1.143351       -1.391126       -0.808080
C       -0.689174       -1.051399       1.259517
C       -1.661843       0.632707        -0.363564
O       2.197029        0.293364        0.984652
H       -0.422825       -0.226978       1.932283
H       -1.662133       -1.439153       1.574013
H       0.042700        -1.853616       1.400682
H       -1.600215       0.980989        -1.402654
H       -1.305141       1.457952        0.264669
C       -3.119034       0.327759        -0.020011
H       -3.247015       0.116351        1.045905
H       -3.764521       1.176315        -0.266174
H       -3.479806       -0.542134       -0.580746
O       1.226615        1.942148        -0.179216
###
23
Leu1 m062x E=-441.989906932 au
N       -1.714708       -1.669320       0.473995
H       -1.979422       -1.869624       -0.498508
H       -2.573867       -1.484164       1.003720
H       -1.268654       -2.505521       0.867428
C       -0.775550       -0.512577       0.526546
H       -0.610855       -0.271942       1.577699
C       0.525561        -0.907783       -0.184005
C       -1.463573       0.643371        -0.171747
H       0.922363        -1.784582       0.343978
H       0.271466        -1.218988       -1.205186
C       1.606653        0.177986        -0.227040
O       -2.301306       0.487857        -1.036845
H       1.219176        1.037498        -0.788322
C       2.006976        0.642364        1.173099
C       2.820819        -0.370841       -0.976549
H       2.343024        -0.210707       1.775043
H       2.831529        1.359609        1.114838
H       1.182734        1.129614        1.702620
H       2.551437        -0.701654       -1.984715
H       3.598560        0.393734        -1.064508
H       3.247171        -1.226384       -0.439568
O       -1.025570       1.820886        0.250000
H       -1.441998       2.533283        -0.269550
###
21
Leu3 m062x E=-441.077484630 au
N       1.756422        -1.650945       -0.686951
H       2.648587        -1.345026       -1.071028
H       1.956979        -1.961305       0.263098
C       0.855791        -0.495952       -0.599474
H       0.705488        -0.112126       -1.612155
C       -0.481541       -0.953387       -0.012434
C       1.426533        0.648641        0.257713
H       -0.906792       -1.713514       -0.681925
H       -0.273757       -1.449041       0.946541
C       -1.519306       0.151972        0.209449
O       1.841733        0.351461        1.415110
H       -1.089574       0.900708        0.891030
C       -1.896967       0.849117        -1.098197
C       -2.763604       -0.433177       0.877327
H       -2.281875       0.117857        -1.820339
H       -2.679885       1.595652        -0.927772
H       -1.043899       1.359405        -1.555163
H       -2.513872       -0.921333       1.825262
H       -3.505548       0.345778        1.081109
H       -3.231182       -1.181168       0.225247
O       1.432633        1.813219        -0.235303
###
22
LeuZW m062x E=-441.543315594 au
```

```
N       -1.781374       -1.563612       0.524008
H       -2.108257       -1.679668       -0.443058
H       -2.600987       -1.366255       1.106129
H       -1.355394       -2.437663       0.847965
C       -0.803282       -0.432535       0.561996
H       -0.642838       -0.180928       1.610653
C       0.485827        -0.901416       -0.117417
C       -1.436614       0.754007        -0.187065
H       0.875759        -1.758144       0.449387
H       0.227854        -1.261713       -1.122119
C       1.583212        0.162494        -0.225885
O       -2.193128       0.459848        -1.150400
H       1.194478        1.003137        -0.815306
C       2.009577        0.683099        1.146736
C       2.781142        -0.428814       -0.968777
H       2.346950        -0.146598       1.780270
H       2.839236        1.390359        1.048016
H       1.194855        1.197637        1.664849
H       2.493025        -0.801157       -1.957284
H       3.566085        0.322021        -1.102835
H       3.207882        -1.265131       -0.402145
O       -1.117897       1.903700        0.201637
###
26
Lys1 m062x E=-497.790111172 au
N       2.726193        -1.589083       -0.108258
H       2.841381        -1.610753       0.912705
H       3.644421        -1.398615       -0.524683
H       2.421703        -2.518673       -0.418707
C       1.723616        -0.556548       -0.496510
H       1.717091        -0.488790       -1.585129
C       0.350704        -0.963656       0.046164
C       2.188346        0.756213        0.103856
H       0.111034        -1.940818       -0.388531
H       0.428184        -1.088215       1.133390
C       -0.750740       0.037499        -0.293757
O       2.808367        0.821162        1.145398
H       -0.561863       0.991742        0.211323
H       -0.750327       0.235126        -1.372601
C       -2.117485       -0.493842       0.132743
H       -2.333864       -1.431754       -0.392872
H       -2.110756       -0.709746       1.208199
C       -3.206796       0.518328        -0.170120
H       -3.051283       1.453413        0.369399
H       -3.279067       0.728769        -1.237960
N       -4.539229       -0.009857       0.257220
H       -4.544767       -0.217255       1.261157
H       -5.285136       0.666314        0.068748
H       -4.764184       -0.876185       -0.242271
O       1.816422        1.801787        -0.621011
H       2.084505        2.626456        -0.174261
###
25
Lys2 m062x E=-497.344864335 au
N       2.768635        -1.518263       -0.091791
H       2.949692        -1.401459       0.913023
H       3.657120        -1.384555       -0.584360
H       2.441614        -2.473665       -0.266743
C       1.754610        -0.503725       -0.514027
H       1.755275        -0.472642       -1.604187
C       0.391086        -0.934815       0.025675
C       2.184482        0.858803        0.059375
H       0.152116        -1.915265       -0.404366
H       0.467296        -1.059841       1.113659
C       -0.723965       0.054013        -0.305077
O       2.765631        0.833662        1.176316
H       -0.539112       1.008515        0.200760
H       -0.730384       0.256741        -1.383336
C       -2.085672       -0.488244       0.123881
H       -2.298804       -1.424903       -0.405658
H       -2.073218       -0.710542       1.198154
C       -3.183834       0.517309        -0.167674
H       -3.034363       1.449150        0.379122
H       -3.260969       0.736057        -1.233522
N       -4.511507       -0.024131       0.259246
H       -4.511874       -0.239630       1.261435
```

```
H       -5.262810       0.648207        0.078986
H       -4.731831       -0.888001       -0.246370
O       1.884385        1.872407        -0.616528
###
23
Lys3 m062x E=-496.413646951 au
N       2.758632        -1.605601       -0.100190
H       3.684871        -1.311596       -0.404413
H       2.798930        -1.634607       0.917923
C       1.782146        -0.581423       -0.481831
H       1.779744        -0.502054       -1.573114
C       0.392087        -1.011800       -0.009484
C       2.101386        0.814977        0.080563
H       0.154310        -1.969265       -0.488738
H       0.437334        -1.195943       1.073466
C       -0.713544       -0.001673       -0.309306
O       2.381104        0.899060        1.311222
H       -0.514131       0.937830        0.223610
H       -0.708548       0.238546        -1.381628
C       -2.093057       -0.519895       0.090387
H       -2.303604       -1.458655       -0.437981
H       -2.096098       -0.752062       1.164897
C       -3.203307       0.477496        -0.202910
H       -2.957809       1.435762        0.278185
H       -3.249008       0.665030        -1.280772
N       -4.506586       -0.047525       0.224736
H       -4.496982       -0.151110       1.237776
H       -5.227399       0.640855        0.022327
O       2.036371        1.796322        -0.714704
###
24
LysZW m062x E=-496.879653909 au
N       -2.895697       1.517355        -0.115688
H       -2.952478       1.533093        0.901857
H       -2.607161       2.453351        -0.395655
C       -1.833053       0.575489        -0.484433
H       -1.799900       0.504174        -1.575340
C       -0.447849       0.992185        0.028376
C       -2.181808       -0.813139       0.064349
H       -0.207898       1.971232        -0.407001
H       -0.507651       1.127276        1.117059
C       0.659067        -0.004793       -0.309080
O       -2.494035       -0.884922       1.287284
H       0.459863        -0.962957       0.188420
H       0.659680        -0.202533       -1.389215
C       2.036361        0.499603        0.116028
H       2.268771        1.435640        -0.406796
H       2.036161        0.713530        1.192228
C       3.109332        -0.528672       -0.190213
H       2.940831        -1.461435       0.349589
H       3.174488        -0.740867       -1.258241
N       4.453291        -0.023498       0.231749
H       4.464504        0.186866        1.234924
H       5.186915        -0.712947       0.043839
H       4.691552        0.837391        -0.270768
O       -2.101356       -1.797935       -0.723221
###
21
Met1 m062x E=-800.845425551 au
N       2.437957        -1.585283       -0.238740
H       2.579597        -1.687770       0.773769
H       3.348905        -1.378050       -0.663588
H       2.107937        -2.482636       -0.612361
C       1.444918        -0.513896       -0.528096
H       1.374572        -0.408391       -1.612086
C       0.094253        -0.916348       0.076534
C       1.979995        0.765918        0.082947
H       -0.163298       -1.893227       -0.348335
H       0.213357        -1.037142       1.159357
C       -1.010737       0.088039        -0.232286
O       2.752340        0.779411        1.018777
H       -0.845113       1.032033        0.293474
H       -1.056612       0.288906        -1.307480
S       -2.607701       -0.599502       0.310902
C       -3.665031       0.804749        -0.130749
H       -3.624498       0.994524        -1.205642
```

```
H       -4.688896       0.545637        0.145058
H       -3.365098       1.701143        0.416527
O       1.485971        1.845247        -0.506147
H       1.809798        2.645944        -0.053082
###
19
Met3 m062x E=-799.935113354 au
N       2.608059        -1.510264       -0.272417
H       2.747132        -1.543087       0.736427
H       2.273627        -2.432445       -0.546184
C       1.553489        -0.530786       -0.541325
H       1.459151        -0.407551       -1.623979
C       0.187465        -0.952792       0.027471
C       1.949061        0.825404        0.054977
H       -0.074028       -1.918721       -0.422625
H       0.292647        -1.110525       1.108597
C       -0.916495       0.062041        -0.248818
O       2.450898        0.821422        1.214438
H       -0.736021       0.994111        0.296225
H       -0.965558       0.293909        -1.318520
S       -2.530192       -0.600474       0.277747
C       -3.559471       0.841492        -0.108491
H       -3.512882       1.073805        -1.174999
H       -4.590075       0.595853        0.154813
H       -3.241498       1.710293        0.472392
O       1.710334        1.860031        -0.629697
###
20
MetZW m062x E=-800.399932128 au
N       2.517317        -1.487251       -0.176122
H       2.719947        -1.401954       0.827806
H       3.393376        -1.327037       -0.683274
H       2.198033        -2.440412       -0.376914
C       1.486722        -0.469868       -0.544071
H       1.453275        -0.412685       -1.632483
C       0.141581        -0.924944       0.024806
C       1.923709        0.882122        0.050338
H       -0.105928       -1.891953       -0.429132
H       0.246167        -1.076973       1.105921
C       -0.968300       0.081686        -0.255274
O       2.544686        0.832891        1.144037
H       -0.808528       1.004438        0.309829
H       -1.005557       0.328861        -1.321263
S       -2.570191       -0.626979       0.245095
C       -3.609944       0.828559        -0.046353
H       -3.556007       1.138272        -1.092426
H       -4.639715       0.553085        0.188762
H       -3.307604       1.655127        0.600532
O       1.589285        1.908148        -0.589375
###
24
Phe1 m062x E=-555.070575159 au
N       -3.027720       -1.080989       -0.124286
H       -3.319231       -0.582489       -0.974923
H       -3.719977       -0.887861       0.608695
H       -3.039090       -2.088502       -0.320429
C       -1.663900       -0.646357       0.287332
H       -1.450211       -1.081503       1.264331
C       -0.649961       -1.116979       -0.768964
C       -1.687653       0.868402        0.378582
H       -0.682930       -2.210985       -0.782814
H       -0.976304       -0.747419       -1.747091
C       0.744884        -0.627867       -0.465463
O       -2.370791       1.558193        -0.350034
C       1.253517        0.499315        -1.117239
C       1.524363        -1.264636       0.505728
H       0.649144        0.997501        -1.872036
C       2.522852        0.985643        -0.803070
C       2.793019        -0.780353       0.821235
H       1.133758        -2.142874       1.014361
H       2.907727        1.861116        -1.317030
C       3.294112        0.347303        0.168029
H       3.391285        -1.282995       1.575037
H       4.282258        0.724251        0.413067
O       -0.867046       1.331236        1.309645
H       -0.867090       2.306428        1.294931
```

```
###
22
Phe3 m062x E=-554.160731778 au
N       -3.068697       -1.126627       -0.217651
H       -3.751784       -0.902751       0.503294
H       -3.329837       -0.564760       -1.027467
C       -1.749732       -0.678592       0.229297
H       -1.501427       -1.201489       1.157401
C       -0.712826       -1.048159       -0.845082
C       -1.668958       0.833911        0.504688
H       -0.729410       -2.136414       -0.965024
H       -1.033459       -0.600852       -1.793924
C       0.679478        -0.579026       -0.505059
O       -2.169797       1.606697        -0.361054
C       1.191679        0.601517        -1.054131
C       1.465894        -1.289470       0.410190
H       0.589120        1.162737        -1.764821
C       2.459920        1.063481        -0.699036
C       2.733236        -0.831733       0.768317
H       1.078870        -2.208933       0.843915
H       2.842124        1.980677        -1.137218
C       3.234078        0.348223        0.214424
H       3.331525        -1.395783       1.477762
H       4.221394        0.705366        0.490906
O       -1.084311       1.209262        1.560688
###
23
PheZW m062x E=-554.624760814 au
N       -3.012734       -1.082385       -0.158812
H       -3.323277       -0.479873       -0.931164
H       -3.699850       -0.994962       0.596334
H       -3.001376       -2.058140       -0.472584
C       -1.658929       -0.632742       0.284601
H       -1.434588       -1.135626       1.225947
C       -0.649700       -1.022518       -0.805292
C       -1.707394       0.893955        0.486595
H       -0.673185       -2.112417       -0.913586
H       -0.975838       -0.579760       -1.753279
C       0.748005        -0.561124       -0.476367
O       -2.470226       1.530288        -0.287152
C       1.264751        0.602514        -1.053639
C       1.531982        -1.269492       0.440690
H       0.658698        1.159395        -1.764687
C       2.542703        1.052827        -0.721054
C       2.808817        -0.821392       0.776410
H       1.137737        -2.176734       0.892732
H       2.931916        1.957314        -1.178584
C       3.317158        0.342149        0.195851
H       3.408272        -1.380802       1.488263
H       4.312139        0.690894        0.454770
O       -0.959258       1.367505        1.374747
###
18
Pro1 m062x E=-401.489760856 au
N       0.759320        -1.035487       0.560790
H       0.208181        -1.853451       0.270851
H       1.155090        -1.224181       1.486311
C       1.871821        -0.736234       -0.411411
C       -0.114293       0.186670        0.630676
H       1.489046        -0.958864       -1.408904
H       2.722462        -1.374378       -0.179614
C       2.086905        0.752762        -0.207990
C       0.655429        1.290471        -0.130433
H       -0.268357       0.439824        1.680777
C       -1.449204       -0.135500       0.000861
H       2.653507        1.193958        -1.028651
H       2.622765        0.929579        0.729521
H       0.243487        1.405143        -1.136910
H       0.574306        2.243049        0.391888
O       -1.726439       -1.210629       -0.490208
O       -2.262505       0.911520        0.037017
H       -3.108122       0.691575        -0.395489
###
16
Pro3 m062x E=-400.571896356 au
N       0.747302        -0.951926       0.828577
```

H 1.282784 -0.785901 1.679011
C 1.703276 -0.843008 -0.287422
C -0.150897 0.208423 0.675327
H 1.224102 -1.216657 -1.199355
H 2.588819 -1.451832 -0.093777
C 1.993406 0.652537 -0.417474
C 0.611429 1.277413 -0.176331
H -0.396191 0.601620 1.664453
C -1.479779 -0.110554 -0.017657
H 2.418319 0.929702 -1.386006
H 2.696609 0.954178 0.366781
H 0.097176 1.440835 -1.129238
H 0.664307 2.239145 0.338228
O -1.617227 -1.186439 -0.660230
O -2.366729 0.791880 0.072881
###
17
ProZW m062x E=-401.043637343 au
N 0.664029 -1.031419 0.538061
H 0.072776 -1.772334 0.135179
H 0.946856 -1.306340 1.481642
C 1.875220 -0.761356 -0.315606
C -0.167061 0.228692 0.588084
H 1.609186 -1.029452 -1.339469
H 2.699808 -1.382118 0.030677
C 2.072437 0.738019 -0.164373
C 0.636974 1.264900 -0.217588
H -0.264194 0.520255 1.634429
C -1.554647 -0.040430 -0.008163
H 2.703520 1.141541 -0.957723
H 2.533215 0.962340 0.802875
H 0.284118 1.283503 -1.254007
H 0.522501 2.262441 0.206891
O -1.747273 -1.167117 -0.536894
O -2.369418 0.912260 0.061763
###
15
Ser1 m062x E=-399.297937081 au
N -0.326741 1.911474 -0.260883
H -0.578587 2.063163 0.724479
H -1.161022 2.100759 -0.828172
H 0.397362 2.591401 -0.521161
C 0.162149 0.524120 -0.470712
H 0.349435 0.381326 -1.535801
C 1.451436 0.340735 0.335012
C -0.924467 -0.420081 0.009843
H 2.174744 1.089338 -0.007675
H 1.239743 0.504252 1.399260
O 1.911581 -0.973439 0.094576
O -1.732630 -0.109413 0.859979
H 2.731702 -1.103237 0.590168
O -0.861982 -1.601937 -0.583541
H -1.536651 -2.197647 -0.207890
###
13
Ser3 m062x E=-398.390421934 au
N -0.248745 1.944744 -0.323187
H -0.464910 2.085022 0.662737
H 0.547392 2.543970 -0.533945
C 0.149039 0.547690 -0.501499
H 0.318010 0.357198 -1.564571
C 1.426973 0.220481 0.266281
C -0.976526 -0.375561 -0.016732
H 2.238420 0.859656 -0.104089
H 1.269819 0.434051 1.332200
O 1.745446 -1.155205 0.073825
O -1.480710 -0.113174 1.111536
H 2.569086 -1.347905 0.540893
O -1.306425 -1.344229 -0.755263
###
14
SerZW m062x E=-398.852402449 au
N -0.596814 1.795697 -0.267828
H -0.979181 1.819026 0.685703
H -1.383739 1.910014 -0.914274
H 0.044243 2.584989 -0.400296

```
C       0.078879        0.486046        -0.486753
H       0.302837        0.394142        -1.549894
C       1.367387        0.485678        0.332807
C       -0.877349       -0.631944       -0.026216
H       1.986197        1.336863        0.023911
H       1.122538        0.593691        1.397691
O       2.028462        -0.741168       0.082368
O       -1.667476       -0.329890       0.905950
H       2.859594        -0.744071       0.575644
O       -0.759524       -1.741844       -0.596158
###
18
Thr1 m062x E=-438.603863250 au
N       0.231972        1.715611        -0.015435
H       -0.585081       2.321807        -0.151482
H       1.042396        2.161393        -0.458852
H       0.409380        1.650488        0.995657
C       -0.008983       0.363289        -0.586244
H       0.010872        0.441151        -1.675626
C       1.060434        -0.616656       -0.102868
C       -1.392564       -0.073433       -0.140832
H       0.834045        -1.581071       -0.570307
C       2.468656        -0.183420       -0.470396
O       0.872315        -0.691952       1.306273
O       -2.122541       0.615258        0.539576
H       2.741946        0.754192        0.023434
H       3.175683        -0.952698       -0.149501
H       2.559313        -0.060027       -1.553051
H       1.554257        -1.264554       1.685893
O       -1.693153       -1.283718       -0.589562
H       -2.584839       -1.535337       -0.286367
###
16
Thr3 m062x E=-437.692216848 au
N       0.104217        1.798715        -0.112670
H       1.057033        2.106901        -0.289534
H       -0.036633       1.819083        0.894982
C       -0.059368       0.426249        -0.578454
H       -0.016922       0.418928        -1.672276
C       1.012872        -0.566763       -0.097984
C       -1.432344       -0.136190       -0.173455
H       0.792338        -1.534996       -0.566136
C       2.427748        -0.148455       -0.461001
O       0.865076        -0.687663       1.321534
O       -2.065766       0.431394        0.756106
H       2.707525        0.783479        0.040449
H       3.136760        -0.923327       -0.153010
H       2.520634        -0.010201       -1.542639
H       1.554023        -1.281002       1.650895
O       -1.816526       -1.171097       -0.791224
###
17
ThrZW m062x E=-438.158350315 au
N       0.093813        1.680991        0.027178
H       -0.802995       2.177388        -0.012299
H       0.815233        2.229316        -0.449575
H       0.349843        1.596256        1.018574
C       -0.068960       0.324668        -0.574583
H       -0.037122       0.438895        -1.660329
C       1.066193        -0.580773       -0.113886
C       -1.452130       -0.231315       -0.172887
H       0.887984        -1.560108       -0.570681
C       2.443440        -0.070447       -0.506108
O       0.924783        -0.669223       1.303913
O       -2.212962       0.540684        0.463930
H       2.663466        0.892256        -0.033421
H       3.204474        -0.786024       -0.182502
H       2.513699        0.040822        -1.591686
H       1.671791        -1.169191       1.661484
O       -1.693611       -1.406379       -0.538472
###
28
Trp1 m062x E=-686.609966419 au
N       3.345716        1.423555        -0.508450
H       3.952506        0.709109        -0.929882
H       3.851110        1.843361        0.280087
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H 3.175726 2.156269 -1.206898
C 2.056744 0.817874 -0.070629
H 1.485092 1.584860 0.453373
C 1.300292 0.300993 -1.307986
C 2.390692 -0.322570 0.870812
H 1.120138 1.166449 -1.956347
H 1.953597 -0.396895 -1.843470
C 0.018578 -0.375455 -0.942094
O 3.394816 -0.995787 0.757582
C -0.227006 -1.724348 -0.969797
C -1.168918 0.245421 -0.415981
H 0.415034 -2.533330 -1.291679
N -1.493497 -1.980974 -0.502183
C -2.094896 -0.794927 -0.153291
C -1.536252 1.576449 -0.144209
H -1.915663 -2.897016 -0.432574
C -3.370877 -0.545423 0.367770
C -2.797972 1.828185 0.373019
H -0.842864 2.390840 -0.337839
H -4.065936 -1.356772 0.560583
C -3.705436 0.775123 0.627362
H -3.097612 2.849068 0.588597
H -4.685573 1.005234 1.033548
O 1.457284 -0.507383 1.793108
H 1.682421 -1.281832 2.341556
###
26
Trp3 m062x E=-685.698996943 au
N -3.338917 -1.545023 -0.556553
H -3.858504 -1.906704 0.240938
H -3.937135 -0.833248 -0.975001
C -2.126868 -0.882336 -0.071584
H -1.510517 -1.623886 0.444842
C -1.346409 -0.327979 -1.275165
C -2.398956 0.270442 0.910009
H -1.120766 -1.167899 -1.942786
H -2.006042 0.358025 -1.821110
C -0.087790 0.384565 -0.887389
O -3.284817 1.111693 0.582888
C 0.120073 1.739297 -0.842434
C 1.127237 -0.222826 -0.407278
H -0.548276 2.546556 -1.111143
N 1.387357 2.011836 -0.373313
C 2.028601 0.828106 -0.100587
C 1.537605 -1.555050 -0.214585
H 1.785693 2.934329 -0.265223
C 3.319791 0.586537 0.386541
C 2.814451 -1.799535 0.268700
H 0.863117 -2.377033 -0.440918
H 3.995471 1.405398 0.614099
C 3.696824 -0.736313 0.565784
H 3.146225 -2.821756 0.422656
H 4.690150 -0.959841 0.942882
O -1.708414 0.321921 1.968081
###
27
TrpZW m062x E=-686.163547975 au
N 3.341169 1.424333 -0.498361
H 3.983787 0.672256 -0.777869
H 3.793096 1.957301 0.251250
H 3.187022 2.051855 -1.294020
C 2.063234 0.806883 -0.029357
H 1.490750 1.580033 0.484068
C 1.307846 0.278003 -1.258739
C 2.415592 -0.337468 0.937811
H 1.118392 1.127151 -1.927312
H 1.959993 -0.426591 -1.788059
C 0.025801 -0.398066 -0.891002
O 3.473066 -0.972337 0.681247
C -0.217187 -1.747266 -0.890436
C -1.171321 0.229963 -0.395332
H 0.431693 -2.562300 -1.182015
N -1.490438 -1.998033 -0.433427
C -2.099111 -0.806263 -0.120751
C -1.546369 1.565854 -0.160909
H -1.910264 -2.913440 -0.346337

```
C       -3.382994       -0.547413       0.375971
C       -2.816183       1.827218        0.331569
H       -0.851775       2.377128        -0.363361
H       -4.078830       -1.355717       0.578812
C       -3.724865       0.778230        0.598125
H       -3.121280       2.852264        0.517963
H       -4.711374       1.015405        0.984457
O       1.605311        -0.559849       1.869159
###
25
Tyr1 m062x E=-630.280285160 au
N       3.479144        -0.940225       0.029676
H       4.138083        -0.680848       -0.713400
H       3.553172        -1.951785       0.186827
H       3.766154        -0.456454       0.890134
C       2.080542        -0.572818       -0.328852
H       1.861757        -0.993025       -1.311355
C       1.128126        -1.131720       0.742842
C       2.014014        0.941981        -0.377181
H       1.235609        -2.221020       0.729435
H       1.460136        -0.765134       1.720297
C       -0.304626       -0.732524       0.494861
O       2.693304        1.651783        0.335981
C       -0.877665       0.333371        1.192213
C       -1.070889       -1.387946       -0.475219
H       -0.294717       0.855457        1.947479
C       -2.184869       0.742387        0.933792
C       -2.376446       -0.991883       -0.746108
H       -0.640239       -2.220240       -1.026681
H       -2.627451       1.571027        1.479865
C       -2.929854       0.077082        -0.038958
H       -2.973350       -1.500625       -1.496520
O       -4.220581       0.434506        -0.338597
H       -4.489743       1.184283        0.212012
O       1.118437        1.381109        -1.248856
H       1.057295        2.353173        -1.198375
###
23
Tyr3 m062x E=-629.370051406 au
N       -3.537467       -0.959293       -0.085146
H       -4.170294       -0.661637       0.654987
H       -3.793228       -0.407291       -0.903391
C       -2.171040       -0.593409       0.288880
H       -1.922116       -1.096107       1.227999
C       -1.207071       -1.079006       -0.807041
C       -1.969296       0.918088        0.498133
H       -1.303612       -2.167471       -0.879090
H       -1.534714       -0.650666       -1.762286
C       0.227252        -0.696335       -0.541320
O       -2.450514       1.692933        -0.377252
C       0.809201        0.408779        -1.168073
C       0.994401        -1.403864       0.392762
H       0.232934        0.975806        -1.895484
C       2.116378        0.802111        -0.879829
C       2.299419        -1.025932       0.694331
H       0.562093        -2.266423       0.894935
H       2.561224        1.661126        -1.375241
C       2.857377        0.081888        0.054789
H       2.891153        -1.578265       1.417909
O       4.150080        0.421435        0.380904
H       4.417378        1.205382        -0.120561
O       -1.314351       1.288966        1.513905
###
22
Tyr4 m062x E=-628.892619136 au
N       -3.489018       -0.999539       -0.094537
H       -4.132848       -0.700779       0.635603
H       -3.745111       -0.461599       -0.922003
C       -2.130125       -0.608418       0.286258
H       -1.880620       -1.101125       1.230703
C       -1.147117       -1.080621       -0.798037
C       -1.961585       0.906708        0.489741
H       -1.236557       -2.170677       -0.870537
H       -1.477915       -0.659978       -1.756695
C       0.283568        -0.682436       -0.531439
O       -2.441765       1.667817        -0.399187
```

```
C       0.866736        0.427615        -1.154417
C       1.067161        -1.374633       0.402276
H       0.284565        0.990553        -1.883301
C       2.170172        0.830444        -0.870305
C       2.369433        -0.985477       0.699451
H       0.644462        -2.242149       0.908413
H       2.595649        1.693617        -1.377855
C       2.977899        0.137909        0.072262
H       2.954136        -1.546837       1.425242
O       4.208831        0.504140        0.344716
O       -1.337001       1.299194        1.516653
###
24
TyrZW m062x E=-629.834327038 au
N       -3.459160       0.972429        0.025736
H       -3.773860       0.400389        0.819051
H       -4.105884       0.806031        -0.751940
H       -3.507368       1.963857        0.281459
C       -2.067815       0.566141        -0.336530
H       -1.824644       1.033846        -1.291333
C       -1.123472       1.050831        0.772736
C       -2.044887       -0.968244       -0.464658
H       -1.215859       2.140418        0.841746
H       -1.459424       0.621530        1.723743
C       0.309919        0.664922        0.507956
O       -2.799865       -1.600048       0.320943
C       0.863191        -0.479761       1.087315
C       1.104962        1.423236        -0.358345
H       0.260180        -1.085117       1.760235
C       2.175010        -0.864382       0.815058
C       2.416299        1.053777        -0.642081
H       0.692738        2.318358        -0.817980
H       2.600147        -1.754398       1.271144
C       2.948031        -0.093785       -0.052500
H       3.033860        1.645300        -1.310756
O       4.247116        -0.420541       -0.357797
H       4.498402        -1.232422       0.106169
O       -1.256201       -1.452063       -1.311320
###
20
Val1 m062x E=-402.694789049 au
N       -0.704718       1.782172        -0.624204
H       -0.856423       2.066428        0.350574
H       -1.609189       1.844758        -1.104792
H       -0.060187       2.450135        -1.060864
C       -0.146525       0.401148        -0.705386
H       -0.119387       0.128642        -1.762526
C       1.278543        0.359046        -0.111504
C       -1.119867       -0.503320       0.023704
H       1.797190        1.212946        -0.564991
C       1.290021        0.518693        1.409606
C       2.010978        -0.913998       -0.533731
O       -1.969470       -0.088275       0.785419
H       0.804849        -0.335303       1.896794
H       2.324819        0.556548        1.760110
H       0.795166        1.434998        1.748025
H       1.958058        -1.067350       -1.615701
H       3.063640        -0.832198       -0.250150
H       1.596728        -1.795426       -0.036919
O       -0.918735       -1.783566       -0.254091
H       -1.535498       -2.334066       0.263115
###
18
Val3 m062x E=-401.781047957 au
N       -0.650362       1.713486        -0.915570
H       -0.884009       2.059107        0.012970
H       0.120316        2.286430        -1.254601
C       -0.186073       0.330797        -0.779493
H       -0.175141       -0.129395       -1.772933
C       1.250105        0.212875        -0.208289
C       -1.180852       -0.464824       0.077328
H       1.857714        0.873522        -0.843617
C       1.360663        0.707337        1.234061
C       1.815034        -1.201499       -0.334207
O       -1.785985       0.147799        1.001859
H       0.833240        0.033405        1.918997
```

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H       2.410142        0.741204        1.543429
H       0.942853        1.711959        1.358467
H       1.707886        -1.586366       -1.354094
H       2.879596        -1.208627       -0.078623
H       1.304065        -1.892853       0.344091
O       -1.313689       -1.696662       -0.177045
###
19
ValZW m062x E=-402.248025079 au
N       0.817724        -1.662995       -0.689523
H       1.690056        -1.673487       -1.227034
H       1.064399        -1.901109       0.277669
C       0.185218        -0.307005       -0.729500
H       0.137978        -0.013138       -1.779496
C       -1.236063       -0.387082       -0.142663
C       1.099737        0.660883        0.042866
H       -1.717473       -1.237930       -0.642712
C       -1.234951       -0.638871       1.366142
C       -2.042016       0.866038        -0.480753
O       1.908393        0.145284        0.858703
H       -0.796151       0.211622        1.900243
H       -2.262951       -0.761061       1.718993
H       -0.681699       -1.540902       1.648189
H       -2.014368       1.081438        -1.553435
H       -3.085698       0.718466        -0.188642
H       -1.660043       1.738817        0.056267
O       0.938863        1.883980        -0.189930
H       0.192282        -2.379637       -1.070124
###
# PEPTIDES optimized with m062x
# opt(tight) freq m062x/6-31+G(d,p) scf=(xqc,tight) integral=ultrafine scrf(smd,solvent=water)
###
24
AlaAla1 m062x E=-571.354247040 au
N       3.502976        -0.481482       0.112938
H       3.561710        -0.688988       -0.890897
H       3.448061        -1.378243       0.607940
H       4.361626        -0.000981       0.400257
C       2.315898        0.373216        0.397683
H       2.272708        0.510339        1.480058
C       2.467411        1.707342        -0.320495
C       1.091370        -0.401825       -0.078609
H       2.480291        1.559168        -1.404139
H       1.635310        2.364475        -0.061455
H       3.396479        2.191475        -0.010179
O       1.218149        -1.417342       -0.771838
N       -0.089075       0.108919        0.284572
H       -0.130900       0.961834        0.835415
C       -1.338943       -0.491311       -0.144066
H       -1.238657       -0.799175       -1.190685
C       -1.720910       -1.704290       0.713342
C       -2.414494       0.577092        -0.067877
H       -1.893247       -1.399679       1.748743
H       -2.622069       -2.186287       0.326757
H       -0.903417       -2.427497       0.685035
O       -2.258015       1.644602        0.488363
O       -3.593814       0.286826        -0.620871
H       -3.597756       -0.572530       -1.074511
###
23
AlaAla2 m062x E=-570.905954968 au
N       3.412823        0.487308        -0.383205
H       3.493186        0.935334        0.537692
H       3.308818        1.230817        -1.081685
H       4.278274        -0.025067       -0.580341
C       2.243055        -0.436660       -0.391905
H       2.100502        -0.768035       -1.421443
C       2.520324        -1.610215       0.537272
C       1.042259        0.369782        0.093562
H       2.654092        -1.259092       1.564669
H       1.681330        -2.307543       0.506817
H       3.421348        -2.137613       0.214468
O       1.218053        1.372759        0.802698
N       -0.150209       -0.105639       -0.254456
H       -0.224452       -0.965073       -0.792682
C       -1.400624       0.463088        0.229406
```

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H       -1.295683       0.667571        1.300109
C       -1.749263       1.757464        -0.507210
C       -2.526952       -0.571033       0.054212
H       -1.928090       1.553599        -1.567526
H       -2.649042       2.202874        -0.077417
H       -0.929767       2.475011        -0.420641
O       -2.271032       -1.622185       -0.591849
O       -3.637221       -0.264201       0.562849
###
22
AlaAla3 m062x E=-570.446188044 au
N       -3.297060       0.400185        0.942533
H       -2.874182       0.938165        1.696695
H       -3.583507       1.075672        0.235038
C       -2.291204       -0.481003       0.353513
H       -1.951305       -1.175602       1.126971
C       -2.901732       -1.267567       -0.801245
C       -1.084083       0.290529        -0.175022
H       -3.283981       -0.580394       -1.563493
H       -2.159600       -1.923147       -1.265719
H       -3.730530       -1.879381       -0.436729
O       -1.236870       1.275253        -0.922757
N       0.119484        -0.162704       0.187669
H       0.198980        -0.989100       0.771216
C       1.371036        0.415822        -0.275278
H       1.302811        0.577760        -1.356170
C       1.671081        1.745497        0.421180
C       2.518197        -0.575228       -0.013938
H       1.816992        1.585361        1.494160
H       2.577466        2.192030        0.006078
H       0.842302        2.443090        0.279367
O       2.279902        -1.582186       0.705903
O       3.630445        -0.279958       -0.527407
###
21
AlaGly1 m062x E=-532.059248852 au
N       -3.299802       -0.409347       -0.593788
H       -3.456988       -1.041586       0.200248
H       -3.145835       -0.987717       -1.426606
H       -4.144350       0.153486        -0.739710
C       -2.130373       0.473519        -0.319967
H       -1.939210       1.045808        -1.229186
C       -2.447912       1.390668        0.853220
C       -0.955533       -0.445191       -0.007837
H       -2.633970       0.804650        1.757832
H       -1.604739       2.060987        1.030249
H       -3.329365       1.994676        0.624853
O       -1.147331       -1.601309       0.387735
N       0.256888        0.089932        -0.161504
H       0.360997        1.048666        -0.481102
C       1.445492        -0.662815       0.169938
C       2.665257        0.183146        -0.071745
H       1.440871        -0.970135       1.221149
H       1.521472        -1.569415       -0.439039
O       2.639434        1.332762        -0.462079
O       3.784920        -0.485056       0.198641
H       4.553753        0.089347        0.032317
###
20
AlaGly2 m062x E=-531.608653932 au
N       -3.308824       -0.401733       -0.345773
H       -3.427707       -0.852387       0.568571
H       -3.258023       -1.145448       -1.049740
H       -4.133294       0.176438        -0.537359
C       -2.075987       0.437144        -0.355255
H       -1.972871       0.834345        -1.367123
C       -2.216650       1.561015        0.661965
C       -0.908120       -0.495713       -0.044404
H       -2.303153       1.154204        1.673672
H       -1.343294       2.214178        0.616450
H       -3.102822       2.159100        0.435707
O       -1.116687       -1.667489       0.305568
N       0.306004        0.033526        -0.164242
H       0.432548        1.005367        -0.433288
C       1.508458        -0.718842       0.135142
C       2.755609        0.151530        -0.039332
```

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H       1.482236        -1.086384       1.166063
H       1.590890        -1.588875       -0.523412
O       2.596208        1.358103        -0.361158
O       3.854900        -0.428601       0.164574
###
19
AlaGly3 m062x E=-531.148970082 au
N       -3.232055       -0.184378       -0.936276
H       -2.907581       -0.603048       -1.805911
H       -3.521595       -0.960474       -0.342248
C       -2.118280       0.497017        -0.285216
H       -1.765254       1.290659        -0.950062
C       -2.582437       1.110885        1.033598
C       -0.948334       -0.440256       0.007594
H       -2.951687       0.327080        1.703782
H       -1.765577       1.638447        1.533293
H       -3.393321       1.819161        0.846779
O       -1.139706       -1.604171       0.407357
N       0.277719        0.063237        -0.159598
H       0.403909        1.020692        -0.471458
C       1.479858        -0.677785       0.161168
C       2.732034        0.175662        -0.053549
H       1.462817        -1.004442       1.206547
H       1.557279        -1.576346       -0.459066
O       2.582722        1.373229        -0.412618
O       3.830024        -0.406168       0.158748
###
32
AlaHis1 m062x E=-796.774348384 au
N       -4.392202       -1.463987       -0.456615
H       -4.321043       -1.950378       0.445506
H       -3.983037       -2.073831       -1.172261
H       -5.383818       -1.324823       -0.677467
C       -3.688505       -0.152097       -0.384050
H       -3.695962       0.275692        -1.387639
C       -4.404103       0.752040        0.610092
C       -2.262172       -0.441446       0.067425
H       -4.384760       0.310904        1.610794
H       -3.909035       1.724229        0.640195
H       -5.441148       0.898688        0.299122
O       -2.000185       -1.458716       0.716069
N       -1.359597       0.495684        -0.248017
H       -1.629123       1.297760        -0.811115
C       0.018485        0.396370        0.182881
H       0.046026        -0.002657       1.201558
C       0.818422        -0.541232       -0.757022
C       0.612595        1.796606        0.159619
H       0.304814        -1.505703       -0.758912
H       0.792606        -0.137049       -1.772707
C       2.235238        -0.730534       -0.329753
O       0.209143        2.661538        -0.588365
O       1.644981        2.039915        0.966729
N       3.306432        -0.236783       -1.050471
C       2.771865        -1.332288       0.770980
H       3.241156        0.269009        -1.930542
C       4.446560        -0.522269       -0.429819
N       4.137915        -1.185110       0.679047
H       2.302655        -1.847475       1.593921
H       5.439057        -0.266213       -0.766781
H       1.831640        1.305453        1.575978
H       4.820322        -1.535021       1.345168
###
31
AlaHis2 m062x E=-796.329701439 au
N       4.349711        -1.376545       0.631858
H       4.237775        -2.023068       -0.158809
H       3.946992        -1.826321       1.461393
H       5.350582        -1.227816       0.797594
C       3.669908        -0.084209       0.327573
H       3.697306        0.517940        1.236583
C       4.388832        0.609937        -0.820737
C       2.234026        -0.421366       -0.058544
H       4.353089        -0.008011       -1.722724
H       3.906416        1.567333        -1.026020
H       5.431385        0.796034        -0.551660
O       1.974138        -1.505386       -0.599669
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N       1.336042        0.532586        0.182751
H       1.613472        1.401745        0.631509
C       -0.054121       0.429907        -0.221028
H       -0.105364       0.017748        -1.233051
C       -0.816252       -0.510937       0.742888
C       -0.686964       1.834348        -0.214389
H       -0.300625       -1.474245       0.755917
H       -0.783382       -0.092918       1.753903
C       -2.233710       -0.727562       0.338257
O       -0.123003       2.716158        0.486123
O       -1.741585       1.971349        -0.884541
N       -3.287884       -0.026395       0.890910
C       -2.783273       -1.537521       -0.611116
H       -3.204240       0.687328        1.609898
C       -4.428349       -0.372033       0.303085
N       -4.139936       -1.292448       -0.610151
H       -2.328407       -2.251562       -1.278711
H       -5.408605       0.016830        0.530946
H       -4.828896       -1.741741       -1.205572
###
30
AlaHis3 m062x E=-795.873985470 au
N       -4.370404       -1.407068       -0.475963
H       -4.308479       -1.902600       0.421659
H       -3.969854       -2.018289       -1.194990
H       -5.358151       -1.246360       -0.698201
C       -3.638027       -0.111028       -0.386841
H       -3.625903       0.322759        -1.387804
C       -4.348702       0.800926        0.603326
C       -2.221537       -0.437199       0.078193
H       -4.348189       0.355059        1.602248
H       -3.836491       1.763719        0.644432
H       -5.379933       0.968419        0.283029
O       -2.000984       -1.479902       0.712008
N       -1.300449       0.482629        -0.201603
H       -1.545526       1.300355        -0.753053
C       0.088377        0.369440        0.220113
H       0.115284        -0.050596       1.228569
C       0.865106        -0.557413       -0.742627
C       0.711754        1.775234        0.237887
H       0.371099        -1.533835       -0.728361
H       0.780534        -0.152255       -1.756035
C       2.308812        -0.702292       -0.382882
O       0.326827        2.575528        -0.658056
O       1.575121        2.007769        1.122813
N       3.297678        0.048357        -0.989110
C       2.862032        -1.507651       0.580707
C       4.422068        -0.302219       -0.393733
N       4.208396        -1.237131       0.560240
H       2.427149        -2.226329       1.258610
H       5.406810        0.081246        -0.617251
H       4.918100        -1.662758       1.143228
###
29
AlaHis4 m062x E=-795.414494643 au
N       -4.316147       -1.258723       -0.970902
H       -3.745993       -1.565692       -1.756600
H       -4.311479       -2.024287       -0.298163
C       -3.694063       -0.096468       -0.343225
H       -3.658698       0.713292        -1.077785
C       -4.521432       0.345344        0.859418
C       -2.271662       -0.386199       0.132246
H       -4.588854       -0.470258       1.587284
H       -4.071846       1.212698        1.350880
H       -5.531786       0.609044        0.537304
O       -2.014527       -1.411776       0.789320
N       -1.344256       0.532052        -0.165028
H       -1.588298       1.327722        -0.745420
C       0.049358        0.416134        0.234071
H       0.091799        0.019865        1.251632
C       0.803975        -0.541937       -0.715857
C       0.692862        1.811382        0.207411
H       0.292662        -1.508830       -0.680335
H       0.720193        -0.154105       -1.736270
C       2.246955        -0.708876       -0.362834
O       0.333162        2.584340        -0.722758
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O       1.548746        2.066828        1.094573
N       3.245842        0.024949        -0.973638
C       2.792048        -1.527517       0.594240
C       4.367779        -0.349732       -0.388384
N       4.143454        -1.283513       0.564177
H       2.348629        -2.240936       1.272169
H       5.358036        0.015317        -0.618298
H       4.849412        -1.725107       1.139744
###
34
AlaLys3 m062x E=-744.135383967 au
N       3.929215        -2.171143       0.731282
H       3.854557        -2.701010       -0.136255
H       3.201122        -2.529369       1.346403
C       3.663127        -0.766867       0.430687
H       3.694161        -0.202744       1.367493
C       4.729849        -0.229708       -0.518324
C       2.294970        -0.561704       -0.217766
H       4.727235        -0.804333       -1.450710
H       4.551379        0.822222        -0.757640
H       5.715856        -0.321644       -0.056233
O       1.919898        -1.288284       -1.157175
N       1.556368        0.448477        0.254177
H       1.889644        0.994211        1.041769
C       0.251407        0.807645        -0.281716
H       0.280238        0.695251        -1.369060
C       -0.840145       -0.106398       0.300728
C       -0.036948       2.278622        0.060073
H       -0.544696       -1.142335       0.095929
H       -0.852215       0.020454        1.390877
C       -2.231952       0.147945        -0.271007
O       0.416418        2.711279        1.155219
O       -0.733247       2.932225        -0.761204
H       -2.565982       1.159131        -0.012111
H       -2.193675       0.094297        -1.366970
C       -3.248126       -0.863813       0.255475
H       -2.927348       -1.882779       0.006224
H       -3.307058       -0.793625       1.348949
C       -4.620738       -0.611312       -0.338813
H       -4.983158       0.392402        -0.112848
H       -4.627550       -0.759332       -1.419412
N       -5.617986       -1.568194       0.234551
H       -5.712364       -1.430914       1.245693
H       -6.541396       -1.444276       -0.189576
H       -5.325134       -2.537802       0.076670
###
33
AlaLys4 m062x E=-743.668870515 au
N       -3.865785       -2.153900       -0.753943
H       -3.780396       -2.702461       0.100902
H       -3.136339       -2.489227       -1.380425
C       -3.614213       -0.753682       -0.422525
H       -3.654485       -0.169562       -1.346613
C       -4.682719       -0.249512       0.541982
C       -2.245310       -0.550175       0.224666
H       -4.671411       -0.845331       1.460923
H       -4.512375       0.798141        0.805172
H       -5.669593       -0.339643       0.081393
O       -1.866191       -1.285562       1.155800
N       -1.510433       0.466040        -0.239523
H       -1.845031       1.014394        -1.024679
C       -0.195652       0.811129        0.283201
H       -0.212161       0.688896        1.369710
C       0.882066        -0.105308       -0.321225
C       0.098254        2.282877        -0.048412
H       0.581616        -1.140427       -0.118034
H       0.875455        0.026808        -1.410953
C       2.286867        0.131413        0.226759
O       -0.359637       2.726590        -1.137528
O       0.802452        2.927402        0.773516
H       2.631346        1.136058        -0.047491
H       2.260101        0.095338        1.324422
C       3.284414        -0.900894       -0.294819
H       2.947624        -1.908980       -0.015069
H       3.313065        -0.867263       -1.391731
C       4.687808        -0.679711       0.247177
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H       5.049634        0.304533        -0.068187
H       4.647708        -0.668313       1.346450
N       5.616103        -1.693428       -0.269439
H       6.542646        -1.523727       0.114012
H       5.331316        -2.604485       0.085395
###
25
AsnGly1 m062x E=-700.721606936 au
N       -2.716161       -1.915875       -0.333491
H       -2.406127       -2.711723       -0.901415
H       -3.652150       -1.637453       -0.648184
H       -2.778124       -2.241297       0.638397
C       -1.763227       -0.779127       -0.449536
H       -1.713114       -0.503384       -1.504448
C       -2.278490       0.393363        0.384048
C       -0.406881       -1.303247       0.023546
H       -3.348113       0.530621        0.181819
H       -2.166744       0.188657        1.453741
C       -1.595270       1.697850        0.016468
O       -0.326081       -2.390058       0.607468
O       -0.956479       1.823461        -1.039776
N       -1.751029       2.695567        0.889815
H       -1.354828       3.604066        0.683342
H       -2.269265       2.566492        1.748628
N       0.643123        -0.518539       -0.223414
H       0.518997        0.366098        -0.713261
C       1.964772        -0.899887       0.215380
C       2.929396        0.226251        -0.057843
H       1.974844        -1.113605       1.290161
H       2.315562        -1.798626       -0.304867
O       2.600591        1.293775        -0.530976
O       4.206408        -0.001365       0.256241
H       4.350209        -0.895648       0.609687
###
24
AsnGly2 m062x E=-700.273531629 au
N       -2.812635       -1.716827       -0.439234
H       -2.562602       -2.515085       -1.033037
H       -3.720000       -1.353375       -0.750358
H       -2.902583       -2.067420       0.522054
C       -1.769719       -0.657799       -0.505963
H       -1.639934       -0.390793       -1.555460
C       -2.234982       0.552986        0.300999
C       -0.488875       -1.262898       0.067711
H       -3.242506       0.835301        -0.028157
H       -2.283728       0.310230        1.366841
C       -1.344707       1.757253        0.056319
O       -0.552767       -2.242779       0.824997
O       -0.765781       1.920179        -1.028138
N       -1.255134       2.629134        1.064083
H       -0.732696       3.486762        0.934489
H       -1.738801       2.472958        1.938093
N       0.640104        -0.654450       -0.278883
H       0.616561        0.180209        -0.861991
C       1.923924        -1.012902       0.291262
C       2.986656        0.025380        -0.081688
H       1.851484        -1.067623       1.381815
H       2.247981        -1.994162       -0.069461
O       2.634640        1.000773        -0.795760
O       4.142245        -0.192438       0.369097
###
23
AsnGly3 m062x E=-699.816855917 au
N       -2.591234       -1.957835       -0.770567
H       -2.085369       -2.712622       -1.230159
H       -2.809906       -2.293103       0.166914
C       -1.710773       -0.803610       -0.649830
H       -1.395513       -0.497162       -1.650801
C       -2.481950       0.353169        0.000832
C       -0.472977       -1.093672       0.202249
H       -3.355245       0.575889        -0.618965
H       -2.826119       0.051599        0.995095
C       -1.638690       1.606843        0.070182
O       -0.569959       -1.731068       1.267182
O       -1.164473       2.114800        -0.959131
N       -1.421092       2.121474        1.287044
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H       -0.869544       2.965372        1.381556
H       -1.819907       1.698762        2.113984
N       0.687181        -0.602779       -0.238266
H       0.722118        -0.049685       -1.089609
C       1.919623        -0.709424       0.514958
C       3.047432        0.073117        -0.162218
H       1.782318        -0.314689       1.527436
H       2.226024        -1.756197       0.608417
O       2.782392        0.702027        -1.220346
O       4.168434        0.020150        0.411247
###
24
AspGly1 m062x E=-720.582817577 au
N       -2.661351       -1.953452       -0.391847
H       -2.330356       -2.731495       -0.972925
H       -3.596842       -1.683020       -0.715169
H       -2.732245       -2.302162       0.571550
C       -1.723534       -0.801014       -0.467221
H       -1.662800       -0.499908       -1.515075
C       -2.275843       0.337803        0.390445
C       -0.367716       -1.317951       0.020308
H       -3.355005       0.436553        0.222087
H       -2.130384       0.139856        1.457766
C       -1.667756       1.672099        0.050330
O       -0.295007       -2.389029       0.633174
O       -2.126578       2.637495        0.844626
O       -0.865326       1.869365        -0.843061
N       0.683743        -0.543945       -0.245962
H       0.557244        0.334495        -0.744545
C       2.002663        -0.892133       0.232088
C       2.947214        0.244693        -0.048162
H       1.992443        -1.081186       1.310517
H       2.384154        -1.793329       -0.259348
O       2.624295        1.288991        -0.577671
O       4.185497        -0.033032       0.354554
H       -1.723369       3.486834        0.589833
H       4.767201        0.723826        0.160270
###
23
AspGly2 m062x E=-720.132281881 au
N       -2.590181       -1.964460       -0.439084
H       -2.245116       -2.729750       -1.028638
H       -3.522360       -1.694096       -0.771121
H       -2.670526       -2.331269       0.516685
C       -1.656875       -0.806152       -0.478436
H       -1.572037       -0.494243       -1.521211
C       -2.235155       0.322029        0.375252
C       -0.310180       -1.318226       0.040882
H       -3.311652       0.416056        0.186843
H       -2.108911       0.119895        1.444093
C       -1.629769       1.661967        0.052032
O       -0.258024       -2.389186       0.663982
O       -2.092187       2.617324        0.857919
O       -0.829204       1.873075        -0.839244
N       0.742179        -0.548467       -0.207713
H       0.633762        0.332073        -0.706555
C       2.068633        -0.866414       0.284095
C       3.046510        0.268481        -0.033214
H       2.047118        -1.019026       1.367887
H       2.438625        -1.789742       -0.171966
O       2.590038        1.304314        -0.584225
O       4.244489        0.061937        0.296166
H       -1.692775       3.470764        0.611111
###
22
AspGly3 m062x E=-719.680420555 au
N       -2.707660       -1.831377       -0.364204
H       -2.415746       -2.618717       -0.952402
H       -3.631955       -1.514937       -0.674978
H       -2.785784       -2.184094       0.596228
C       -1.721931       -0.714552       -0.435938
H       -1.666872       -0.404445       -1.480793
C       -2.203268       0.441814        0.437698
C       -0.378968       -1.293318       0.011574
H       -3.285260       0.560113        0.310962
H       -2.025152       0.223436        1.496058
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C       -1.574971       1.800617        0.097325
O       -0.327610       -2.425325       0.521413
O       -1.916852       2.761334        0.835410
O       -0.787103       1.872636        -0.886150
N       0.679212        -0.513298       -0.173735
H       0.550091        0.421517        -0.563629
C       2.010352        -0.909100       0.237736
C       3.018728        0.213946        -0.018180
H       2.025375        -1.152968       1.305130
H       2.332647        -1.801804       -0.307681
O       2.590680        1.301823        -0.484183
O       4.216154        -0.054445       0.270434
###
21
AspGly4 m062x E=-719.216911479 au
N       -2.769705       -1.865936       -0.265308
H       -2.441299       -2.704437       -0.738464
H       -3.612257       -1.564825       -0.749145
C       -1.768442       -0.808767       -0.411026
H       -1.657561       -0.476141       -1.451737
C       -2.198350       0.394883        0.435234
C       -0.405685       -1.352573       0.017342
H       -3.283048       0.512177        0.324085
H       -2.019440       0.194555        1.497757
C       -1.592510       1.758655        0.090048
O       -0.267086       -2.506042       0.464556
O       -1.929476       2.718098        0.839269
O       -0.824215       1.862101        -0.909014
N       0.629890        -0.521577       -0.131213
H       0.470045        0.415916        -0.499702
C       1.978266        -0.896048       0.234815
C       2.963492        0.246149        -0.021550
H       2.032287        -1.165173       1.295308
H       2.306801        -1.770679       -0.336891
O       2.516291        1.331476        -0.476028
O       4.169805        -0.003457       0.251874
###
35
AspHis0 m062x E=-985.301142735 au
N       -3.204902       -2.669851       -0.507083
H       -2.637124       -3.188035       -1.187278
H       -4.193461       -2.794349       -0.752120
H       -3.037467       -3.086044       0.417185
C       -2.844456       -1.225615       -0.503127
H       -2.964187       -0.856961       -1.523109
C       -3.777076       -0.487138       0.455416
C       -1.384365       -1.140000       -0.056458
H       -4.812037       -0.807240       0.286565
H       -3.533803       -0.709500       1.499522
C       -3.752344       1.003329        0.244674
O       -0.890843       -2.042631       0.625837
O       -4.458498       1.644466        1.174993
O       -3.184461       1.570767        -0.669300
N       -0.728435       -0.038169       -0.430929
H       -1.217444       0.690739        -0.946673
C       0.623279        0.219196        0.017034
H       0.717998        -0.070867       1.069389
C       1.647823        -0.585239       -0.820952
C       0.868657        1.711823        -0.088124
H       1.288007        -1.616190       -0.856932
H       1.668802        -0.198363       -1.843721
C       3.022448        -0.570911       -0.242978
O       0.094309        2.490659        -0.605270
O       2.038055        2.063740        0.435558
N       4.078735        0.104124        -0.822207
C       3.517646        -1.131756       0.896881
H       4.030968        0.640271        -1.684810
C       5.171110        -0.027304       -0.076422
N       4.845685        -0.774483       0.972614
H       3.042114        -1.741712       1.648277
H       6.143121        0.391133        -0.287110
H       5.493034        -1.042997       1.707863
H       -4.440086       2.601645        0.994150
H       2.169171        3.022810        0.321829
###
34
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AspHis2 m062x E=-984.846937799 au
N 2.804376 -2.735939 -0.740356
H 2.011953 -3.364620 -0.556945
H 3.670617 -3.165779 -0.399429
H 2.878276 -2.618765 -1.758161
C 2.563541 -1.429276 -0.068266
H 2.669339 -1.613905 1.005258
C 3.604760 -0.412967 -0.550443
C 1.092325 -1.082885 -0.325907
H 4.562706 -0.928467 -0.663394
H 3.313174 0.017247 -1.510444
C 3.804734 0.701396 0.448576
O 0.300250 -2.002918 -0.572239
O 4.550416 0.325748 1.486969
O 3.331218 1.815641 0.334693
N 0.726944 0.192320 -0.212463
H 1.399082 0.952273 -0.116208
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H 4.628763 1.062538 2.120295
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33
AspHis3 m062x E=-984.402277184 au
N -3.303396 2.634341 0.291793
H -2.731188 3.249202 0.880147
H -4.284798 2.733102 0.570781
H -3.202595 2.958594 -0.676805
C -2.871359 1.212725 0.414337
H -2.983004 0.931933 1.462883
C -3.760559 0.341987 -0.470517
C -1.397981 1.170055 0.008953
H -4.800635 0.669869 -0.359918
H -3.493617 0.468152 -1.525061
C -3.739892 -1.152907 -0.124006
O -0.870127 2.159662 -0.521500
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O -3.103130 -1.526517 0.900044
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C 0.604993 -0.203713 -0.163239
H 0.754414 0.215245 -1.162906
C 1.573564 0.496503 0.819641
C 0.888464 -1.716114 -0.206619
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H 3.195406 2.036881 -1.265284
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H 5.608260 1.212008 -1.325271
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32
AspHis4 m062x E=-983.945702048 au
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H       -4.291147       2.688104        0.602498
H       -3.283555       2.907847        -0.706916
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H       -2.908836       0.936495        1.461759
C       -3.764108       0.284843        -0.416706
C       -1.397161       1.179315        -0.066676
H       -4.804410       0.596905        -0.268860
H       -3.546990       0.384133        -1.485269
C       -3.700558       -1.198831       -0.028274
O       -0.914535       2.176989        -0.626507
O       -4.370647       -1.982170       -0.750733
O       -3.016292       -1.530563       0.979275
N       -0.736600       0.046157        0.152513
H       -1.218411       -0.725767       0.616266
C       0.650301        -0.143790       -0.241229
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O       0.305405        -2.386002       0.507766
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C       3.657267        1.129439        -0.668063
C       5.092066        -0.130526       0.421649
N       4.966809        0.717026        -0.624214
H       3.294934        1.818887        -1.415405
H       6.032039        -0.594930       0.681204
H       5.710294        1.003764        -1.248640
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31
AspHis5 m062x E=-983.483212099 au
N       -4.898882       0.645491        0.797440
C       -3.605935       1.110162        0.805171
C       -3.012745       0.572995        -0.309978
N       -3.925725       -0.205819       -0.994455
C       -5.043886       -0.136016       -0.296448
C       -1.592676       0.714494        -0.756841
C       -0.591122       -0.085029       0.108751
C       -0.902841       -1.588589       0.038329
O       -1.708216       -2.046847       0.891757
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O       1.062032        2.096921        0.752899
C       2.941664        1.212019        -0.483242
C       3.795990        0.303048        0.414242
C       3.571371        -1.203389       0.243359
O       3.117818        -1.621418       -0.860365
N       3.400052        2.598321        -0.529980
O       3.898491        -1.942418       1.214245
O       -0.353020       -2.244602       -0.888067
H       4.393326        2.595743        -0.751031
H       3.312838        2.996759        0.403540
H       2.962165        0.806540        -1.497616
H       4.849925        0.481988        0.164716
H       3.666934        0.574708        1.467484
H       1.210306        -0.596501       -0.899828
H       -0.671631       0.247626        1.147344
H       -1.282887       1.764022        -0.724625
H       -1.504710       0.372168        -1.792937
H       -3.230748       1.759675        1.581426
H       -5.977477       -0.620702       -0.541839
H       -5.618858       0.854253        1.477861
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34
AspHis m062x E=-984.851638501 au
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H       -2.828389       3.288560        0.650812
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H       -3.386860       2.855602        -0.842317
C       -2.913206       1.217150        0.363170
H       -2.959501       1.021572        1.436342
C       -3.813462       0.242748        -0.394951
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H       -4.856294       0.549616        -0.257278
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H 0.767213 0.377708 -1.214726
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29
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H -3.344801 -2.186133 1.025679
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O -1.206235 -1.249752 1.440187
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H 1.181529 -0.941515 0.986204
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28
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27
CysAsn3 m062x E=-1137.26106635 au
N       3.170567        -2.245029       -0.200518
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C       2.578838        -0.954577       0.277292
H       2.653721        -0.969917       1.368371
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H       4.438976        -0.047203       -0.210167
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S       3.074872        1.791082        0.603054
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H       0.921076        1.001276        0.203781
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N       -4.239818       -0.470133       1.131239
H       -5.190102       -0.709727       0.878516
H       -4.074614       0.069511        1.969097
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26
CysAsn4 m062x E=-1136.79559491 au
N       3.269783        -2.290501       -0.166822
H       2.648317        -3.072892       0.029818
H       3.353536        -2.267811       -1.183238
C       2.608391        -1.057114       0.261109
H       2.633816        -1.021884       1.357618
C       3.381891        0.155696        -0.275013
C       1.120473        -1.056463       -0.123961
H       4.441641        -0.110625       -0.222606
H       3.138453        0.275663        -1.339354
S       3.115916        1.734137        0.627818
O       0.554658        -2.113346       -0.467394
N       0.453097        0.102042        -0.039215
H       0.973691        0.954770        0.200901
C       -0.964139       0.175385        -0.342932
H       -1.156034       -0.387675       -1.262852
C       -1.807903       -0.443953       0.785381
C       -1.412632       1.626665        -0.584900
H       -1.341554       -1.388367       1.086543
H       -1.824810       0.220233        1.654417
C       -3.207773       -0.790694       0.334270
O       -0.564368       2.548409        -0.475428
O       -2.634299       1.772661        -0.863968
O       -3.408704       -1.436310       -0.708031
N       -4.209969       -0.419307       1.143152
H       -5.163254       -0.653314       0.896691
H       -4.036992       0.131631        1.972005
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42
DLeuTyr3 m062x E=-994.505962714 au
C       -2.776714       -0.839637       -1.417469
C       -3.384278       -1.759196       -0.340503
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C       -1.370042       -0.454753       -0.970946
H       -4.428753       -1.955009       -0.620940
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C       -3.332303       -1.271356       1.114633
O       -0.480539       -1.325811       -0.880672
H       -2.280848       -1.079070       1.375502
C       -4.129238       0.011871        1.357816
C       -3.844472       -2.385555       2.029407
H       -5.169210       -0.114592       1.030547
H       -4.140795       0.254205        2.425856
H       -3.709275       0.867074        0.822035
H       -3.265487       -3.305981       1.901669
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H       -4.893884       -2.612506       1.804190
N       -1.165774       0.823998        -0.660904
H       -1.965420       1.450427        -0.689544
C       0.064926        1.305188        -0.062196
H       0.290324        0.678952        0.812179
C       1.270594        1.239308        -1.040052
C       -0.163451       2.731413        0.479435
H       0.920471        0.830362        -1.991419
H       1.620099        2.258407        -1.237021
C       2.427393        0.401629        -0.545063
O       -1.315216       3.231776        0.374403
O       0.836454        3.287347        1.005442
C       2.881974        -0.699571       -1.275037
C       3.077820        0.705642        0.658415
H       2.389108        -0.962912       -2.207837
C       3.953821        -1.475292       -0.830968
C       4.146275        -0.058293       1.118584
H       2.741617        1.555745        1.246662
H       4.299425        -2.330266       -1.406153
C       4.583619        -1.150458       0.368508
H       4.646771        0.183722        2.051269
O       5.643277        -1.877421       0.860876
H       5.860230        -2.595858       0.249173
N       -3.604670       0.336166        -1.699545
H       -3.579517       0.542733        -2.693896
H       -4.572607       0.136890        -1.463181
H       -2.635380       -1.451022       -2.317257
###
41
DLeuTyr4 m062x E=-994.028480847 au
C       -2.728067       -0.853201       -1.404016
C       -3.386395       -1.734398       -0.325271
C       -1.327203       -0.480126       -0.928254
H       -4.422447       -1.925220       -0.638518
H       -2.870059       -2.700318       -0.337955
C       -3.380302       -1.208894       1.117356
O       -0.455096       -1.363798       -0.797951
H       -2.337202       -1.013943       1.407463
C       -4.180083       0.082626        1.300117
C       -3.925855       -2.296865       2.044397
H       -5.211250       -0.052968       0.949396
H       -4.219297       0.358422        2.359294
H       -3.744922       0.919643        0.748131
H       -3.345567       -3.221543       1.960966
H       -3.898785       -1.970790       3.089021
H       -4.968116       -2.527962       1.791772
N       -1.110027       0.801866        -0.643475
H       -1.898428       1.439329        -0.710124
C       0.122783        1.290126        -0.052650
H       0.344197        0.685415        0.837253
C       1.334107        1.195943        -1.025397
C       -0.103271       2.730897        0.448127
H       0.975295        0.778350        -1.970707
H       1.684474        2.211775        -1.240449
C       2.486314        0.352106        -0.527876
O       -1.240987       3.249409        0.286472
O       0.884874        3.285727        0.998216
C       2.886508        -0.805738       -1.205105
C       3.206215        0.692985        0.626646
H       2.348530        -1.104494       -2.103999
C       3.951675        -1.588420       -0.763290
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H       2.926827        1.586853        1.181604
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N       -3.525850       0.328529        -1.742797
H       -3.450927       0.517950        -2.738165
H       -4.506280       0.144050        -1.549638
H       -2.570140       -1.490980       -2.282668
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41
GluHisOMe2 m062x E=-1063.87631983 au
N       -3.176569       -3.139458       -0.051446
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H       -2.648389       -3.959704       -0.368916
H       -4.138454       -3.222296       -0.399193
C       -2.555624       -1.871602       -0.531965
H       -2.427899       -1.957148       -1.612623
C       -3.482201       -0.708265       -0.171383
C       -1.213353       -1.737585       0.178196
H       -4.417713       -0.840092       -0.722659
H       -3.708646       -0.754847       0.899386
C       -2.858441       0.638812        -0.508769
O       -1.120017       -1.992473       1.380437
H       -1.968432       0.834495        0.102112
H       -2.540162       0.687431        -1.558066
C       -3.810463       1.779938        -0.267126
O       -4.965508       1.657723        0.087344
O       -3.318906       3.013547        -0.467062
N       -0.191777       -1.299010       -0.574584
H       -0.374832       -1.016440       -1.533658
C       1.072350        -0.907812       0.027102
H       1.358799        -1.662659       0.763212
C       2.127346        -0.790617       -1.072797
C       0.894628        0.407984        0.787103
H       2.234321        -1.768584       -1.552526
H       1.788266        -0.078584       -1.832471
C       3.446985        -0.342352       -0.538024
O       1.057330        0.528601        1.984284
N       4.391853        0.266503        -1.341640
C       4.007971        -0.424240       0.702352
C       5.483173        0.544897        -0.635061
N       5.265629        0.132549        0.607552
H       3.630052        -0.827161       1.628741
H       6.376626        1.024939        -1.002927
H       5.934198        0.221569        1.367219
O       0.522480        1.396203        -0.018646
C       0.256657        2.665339        0.608196
H       -0.563581       2.560128        1.321314
H       1.154131        3.022106        1.115873
H       -0.017998       3.338174        -0.201679
H       4.275246        0.481201        -2.328596
H       -2.386073       2.990641        -0.737790
###
40
GluHisOMe3 m062x E=-1063.42294497 au
N       -3.260625       -3.082599       -0.069146
H       -3.277350       -3.114847       0.958043
H       -2.761561       -3.912988       -0.406139
H       -4.227119       -3.127038       -0.410437
C       -2.605728       -1.823606       -0.528235
H       -2.477383       -1.897674       -1.609682
C       -3.499089       -0.636420       -0.158561
C       -1.260126       -1.737471       0.179203
H       -4.417901       -0.719463       -0.746429
H       -3.769632       -0.717439       0.900555
C       -2.817975       0.700455        -0.421937
O       -1.158132       -2.052294       1.366659
H       -1.988333       0.856770        0.277864
H       -2.383861       0.726598        -1.429685
C       -3.734269       1.919702        -0.285639
O       -4.956049       1.742464        -0.029626
O       -3.180640       3.046415        -0.443782
N       -0.241541       -1.275331       -0.566021
H       -0.443911       -0.931639       -1.501236
C       1.028483        -0.898600       0.031732
H       1.299789        -1.649617       0.776999
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C       2.086548        -0.813156       -1.067826
C       0.868231        0.428752        0.775116
H       2.183235        -1.800354       -1.530289
H       1.758282        -0.110037       -1.840418
C       3.408762        -0.370958       -0.534986
O       0.984618        0.550723        1.978171
N       4.359309        0.227307        -1.339590
C       3.965774        -0.448570       0.707463
C       5.450420        0.503442        -0.631765
N       5.227239        0.099736        0.612677
H       3.582844        -0.843529       1.635267
H       6.347682        0.975865        -1.000129
H       5.894478        0.189013        1.373443
O       0.560394        1.422641        -0.049374
C       0.298976        2.700724        0.561317
H       -0.536544       2.612348        1.258575
H       1.192126        3.048211        1.083220
H       0.047062        3.369145        -0.258766
H       4.245853        0.437531        -2.327866
###
39
GluHisOMe4 m062x E=-1062.97060551 au
N       -3.201230       -3.094448       -0.056806
H       -3.204816       -3.116318       0.970805
H       -2.698834       -3.923596       -0.391774
H       -4.171313       -3.150804       -0.385738
C       -2.562029       -1.833881       -0.535574
H       -2.444720       -1.917118       -1.617662
C       -3.460011       -0.651576       -0.162059
C       -1.211648       -1.728854       0.161525
H       -4.402863       -0.766490       -0.705916
H       -3.682623       -0.706440       0.909487
C       -2.812613       0.686450        -0.494861
O       -1.109113       -2.012482       1.358141
H       -1.925861       0.850076        0.129379
H       -2.466988       0.708493        -1.535213
C       -3.713163       1.903309        -0.271303
O       -4.844162       1.738123        0.262005
O       -3.237488       3.018910        -0.632463
N       -0.194532       -1.285725       -0.593347
H       -0.392437       -0.975585       -1.540842
C       1.079305        -0.896529       -0.005465
H       1.360255        -1.645556       0.738392
C       2.135877        -0.788929       -1.103389
C       0.898671        0.424096        0.743217
H       2.227843        -1.772555       -1.576932
H       1.788610        -0.087262       -1.869373
C       3.460983        -0.328759       -0.579743
O       1.000462        0.547447        1.948102
N       4.390945        0.261270        -1.411292
C       3.965241        -0.419689       0.694128
C       5.435283        0.516835        -0.646598
N       5.224911        0.124644        0.629570
H       3.559105        -0.813400       1.613640
H       6.355283        0.984953        -0.964355
H       5.875804        0.222753        1.398927
O       0.577077        1.417553        -0.079341
C       0.279431        2.685918        0.533202
H       -0.563969       2.577053        1.218303
H       1.156589        3.052115        1.069260
H       0.024103        3.352745        -0.287308
###
21
GlyAla1 m062x E=-532.057702087 au
N       -3.778958       -0.186292       0.007906
H       -3.848073       0.179847        -0.947704
C       -2.484777       -0.878628       0.206886
H       -3.872217       0.610042        0.647408
H       -4.561107       -0.827219       0.173409
C       -1.363789       0.082783        -0.144015
H       -2.420349       -1.208219       1.243645
H       -2.455315       -1.747383       -0.452706
O       -1.606306       1.155047        -0.708690
N       -0.136482       -0.332284       0.180987
H       -0.008654       -1.230518       0.637427
C       1.043837        0.452093        -0.133630
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H       0.941080        0.848365        -1.149524
C       1.258741        1.608956        0.847246
C       2.234792        -0.481817       -0.127904
H       1.438299        1.226104        1.855336
H       2.111371        2.215519        0.536359
H       0.366392        2.237992        0.859026
O       2.192053        -1.649183       0.206548
O       3.350267        0.133838        -0.514886
H       4.095719        -0.492429       -0.480201
###
20
GlyAla2 m062x E=-531.606966343 au
N       -3.697418       -0.328702       -0.232432
H       -3.826424       0.684222        -0.129359
C       -2.440287       -0.752692       0.428651
H       -4.503576       -0.810358       0.176714
H       -3.673329       -0.535266       -1.236559
C       -1.316251       0.149408        -0.051199
H       -2.567453       -0.632453       1.505886
H       -2.257998       -1.801586       0.197326
O       -1.579932       1.246129        -0.567071
N       -0.085141       -0.311074       0.152279
H       0.063725        -1.244088       0.526550
C       1.110675        0.456646        -0.167515
H       0.989083        0.886140        -1.166752
C       1.347934        1.577052        0.847509
C       2.323160        -0.489342       -0.199367
H       1.524571        1.155221        1.841769
H       2.218039        2.169096        0.555445
H       0.477904        2.236654        0.894854
O       2.178334        -1.651794       0.264979
O       3.386846        -0.003783       -0.667068
###
19
GlyAla3 m062x E=-531.147850033 au
N       -3.838810       -0.334261       0.049701
H       -3.928606       0.451709        0.689884
C       -2.496798       -0.876784       0.159413
H       -3.956112       0.057433        -0.882013
C       -1.376864       0.111378        -0.151186
H       -2.340266       -1.272568       1.166366
H       -2.387153       -1.719629       -0.530144
O       -1.608152       1.225827        -0.651221
N       -0.139051       -0.313143       0.129819
H       0.004587        -1.245871       0.503848
C       1.057702        0.462170        -0.153915
H       0.957041        0.906110        -1.149454
C       1.268764        1.572452        0.879152
C       2.282509        -0.467314       -0.169968
H       1.428080        1.138668        1.871505
H       2.139595        2.176538        0.613734
H       0.391489        2.223056        0.918233
O       2.154547        -1.626560       0.308199
O       3.344167        0.026354        -0.636926
###
24
GlyAsp1 m062x E=-720.583429560 au
N       4.314923        -0.631869       -0.292172
H       4.051842        -1.623987       -0.290462
C       3.318648        0.165670        0.460664
H       4.365623        -0.329747       -1.270914
C       1.937598        -0.173289       -0.066963
H       3.383788        -0.110551       1.514483
H       3.554562        1.223300        0.346392
O       1.746197        -1.206608       -0.715014
N       0.971753        0.698292        0.245362
H       1.191373        1.558338        0.739307
C       -0.402663       0.464668        -0.142897
H       -0.427068       0.148730        -1.192811
C       -1.038101       -0.635966       0.731197
C       -1.144517       1.794872        -0.045378
H       -0.290662       -1.407411       0.928677
H       -1.357606       -0.235010       1.700635
C       -2.226935       -1.294770       0.092648
O       -0.620540       2.808122        0.373301
O       -2.407463       1.794129        -0.443166
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O -2.911766 -0.787544 -0.787024
O -2.482489 -2.496832 0.586704
H 5.245625 -0.536486 0.124611
H -3.285040 -2.859698 0.168798
H -2.694876 0.890309 -0.735089
###
23
GlyAsp2 m062x E=-720.134916699 au
N 4.375614 -0.578151 -0.163132
H 4.125186 -1.574019 -0.161019
C 3.334784 0.204003 0.545578
H 4.455364 -0.283785 -1.142137
C 1.977324 -0.219592 0.013641
H 3.396197 -0.033460 1.609046
H 3.527174 1.266099 0.396785
O 1.843268 -1.320968 -0.536786
N 0.981039 0.641879 0.215950
H 1.167453 1.572156 0.579883
C -0.377838 0.367796 -0.208764
H -0.352822 -0.034211 -1.228084
C -1.059676 -0.654221 0.711814
C -1.194930 1.674763 -0.236542
H -0.396250 -1.515413 0.848129
H -1.271106 -0.215683 1.689030
C -2.320660 -1.183809 0.088260
O -0.596601 2.754572 -0.000435
O -2.419233 1.531655 -0.489617
O -2.391758 -1.623602 -1.045713
O -3.367362 -1.182698 0.922625
H 5.289044 -0.462882 0.284923
H -4.137356 -1.570205 0.469215
###
22
GlyAsp3 m062x E=-719.676713166 au
N 4.327570 -0.531763 -0.175839
H 4.080997 -1.528607 -0.185131
C 3.278493 0.236466 0.536539
H 5.238743 -0.416163 0.276472
H 4.408816 -0.227204 -1.151521
C 1.925949 -0.198719 -0.000255
H 3.341676 -0.007263 1.598455
H 3.461366 1.300936 0.394076
O 1.808710 -1.303352 -0.552196
N 0.922718 0.652523 0.193385
H 1.088782 1.569756 0.597633
C -0.442046 0.354115 -0.210513
H -0.421479 -0.086682 -1.211697
C -1.107921 -0.634261 0.758801
C -1.253270 1.659641 -0.267283
H -0.401972 -1.450667 0.951112
H -1.321545 -0.136978 1.709142
C -2.380192 -1.268355 0.192653
O -0.726107 2.705540 0.197383
O -2.409924 1.562875 -0.754206
O -2.307295 -1.778985 -0.961340
O -3.409568 -1.280549 0.925230
###
21
GlyAsp4 m062x E=-719.216966131 au
N 4.469367 -0.592961 0.038336
H 4.308220 -1.487089 0.496496
C 3.367585 0.299016 0.350740
H 4.458979 -0.791348 -0.959821
C 1.990511 -0.204803 -0.069717
H 3.342620 0.483950 1.428593
H 3.532436 1.267922 -0.129610
O 1.830669 -1.319977 -0.594367
N 0.974344 0.636770 0.160308
H 1.153585 1.560795 0.540254
C -0.397045 0.349327 -0.219711
H -0.402782 -0.078820 -1.227121
C -1.053692 -0.649951 0.746697
C -1.208899 1.655666 -0.244299
H -0.349884 -1.474332 0.909049
H -1.241832 -0.167536 1.710188
C -2.343205 -1.264015 0.199590

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O       -0.679348       2.695018        0.233557
O       -2.371717       1.570289        -0.721228
O       -2.298617       -1.767569       -0.959519
O       -3.360843       -1.269216       0.949266
###
18
GlyGly1 m062x E=-492.760127487 au
N       3.627956        0.189833        -0.189714
H       3.657629        -0.047548       -1.186997
C       2.338526        0.825596        0.169718
H       3.751694        -0.682995       0.336387
C       1.244849        -0.222083       0.073886
H       2.410511        1.185633        1.197404
H       2.161363        1.667176        -0.498774
O       1.525018        -1.425919       0.047786
N       -0.002851       0.249038        0.046658
H       -0.178256       1.249383        0.054143
C       -1.138162       -0.644462       0.021931
C       -2.406717       0.162578        -0.026528
H       -1.108852       -1.297403       -0.856656
H       -1.162780       -1.283383       0.910738
O       -2.447662       1.376146        -0.050351
H       4.412207        0.815863        0.016929
O       -3.485191       -0.617999       -0.039462
H       -4.287548       -0.066416       -0.069607
###
17
GlyGly2 m062x E=-492.309600536 au
N       -3.561146       0.215633        0.196438
H       -3.592500       -0.010655       1.196095
C       -2.263185       0.830092        -0.171400
H       -3.692986       -0.661800       -0.319647
C       -1.183885       -0.234490       -0.076905
H       -2.336289       1.186282        -1.200295
H       -2.072041       1.672308        0.492163
O       -1.492551       -1.435911       -0.066881
N       0.066018        0.214399        -0.035105
H       0.265366        1.210899        -0.033721
C       1.211064        -0.673852       -0.011565
C       2.515951        0.125882        0.029021
H       1.172693        -1.324104       0.867932
H       1.218894        -1.314984       -0.898590
O       2.440057        1.382356        0.031090
O       3.572648        -0.559212       0.056869
H       -4.338134       0.848162        -0.016800
###
16
GlyGly3 m062x E=-491.850587401 au
N       -3.660606       -0.367846       -0.234238
H       -3.607948       -0.118185       -1.219748
C       -2.346651       -0.799902       0.211647
H       -3.902974       0.490540        0.255720
C       -1.253693       0.252445        0.085003
H       -2.396469       -1.070367       1.271778
H       -2.047694       -1.700007       -0.330427
O       -1.519250       1.467823        0.069603
N       0.000764        -0.205221       0.026449
H       0.187956        -1.202551       0.032802
C       1.153560        0.670035        -0.003044
C       2.456393        -0.132232       -0.031306
H       1.126804        1.314310        -0.888015
H       1.166337        1.322711        0.876129
O       2.382445        -1.389152       -0.028408
O       3.516208        0.550447        -0.055885
###
27
GlyHis2 m062x E=-756.575010495 au
N       -4.871964       -0.943951       0.058807
H       -4.529046       -1.908734       -0.011053
C       -3.884155       -0.007574       -0.527144
H       -5.022623       -0.744661       1.053200
C       -2.517107       -0.323901       0.055329
H       -3.864668       -0.166081       -1.606714
H       -4.196865       1.014139        -0.314812
O       -2.319478       -1.407188       0.624252
N       -1.590634       0.617341        -0.115585
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H       -1.819268       1.480308        -0.600900
C       -0.200176       0.433867        0.274492
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C       0.540126        -0.415733       -0.783369
C       0.460887        1.814459        0.414892
H       -0.006108       -1.358767       -0.886120
H       0.490286        0.108118        -1.743505
C       1.971289        -0.678402       -0.440348
O       0.052026        2.721531        -0.360439
O       1.379224        1.923121        1.267988
N       3.009155        0.006583        -1.041359
C       2.470661        -1.552468       0.492492
C       4.109622        -0.452427       -0.475530
N       3.834388        -1.392248       0.456775
H       1.989402        -2.252314       1.158642
H       5.119266        -0.145847       -0.706359
H       4.515546        -1.892953       1.013972
H       -5.772223       -0.874346       -0.424662
###
28
GlyHis3 m062x E=-757.030639754 au
N       4.768392        -1.193794       0.191691
H       4.592363        -1.749683       -0.652623
C       3.962163        0.048569        0.163130
H       4.521314        -1.776205       0.998438
H       5.767759        -0.974613       0.244274
C       2.519546        -0.314840       -0.140650
H       4.062528        0.556499        1.121628
H       4.353276        0.688689        -0.629556
O       2.238077        -1.431544       -0.595989
N       1.629737        0.651019        0.087818
H       1.927377        1.554772        0.446090
C       0.226475        0.523184        -0.259293
H       0.142737        0.025733        -1.229950
C       -0.510626       -0.325519       0.804020
C       -0.403706       1.924909        -0.353004
H       0.057103        -1.247305       0.952709
H       -0.524133       0.219363        1.753494
C       -1.901562       -0.688204       0.409107
O       0.208195        2.874287        0.203809
O       -1.507238       1.994560        -0.951087
N       -3.019695       0.004105        0.833586
C       -2.366078       -1.680190       -0.403491
H       -3.006084       0.828876        1.427513
C       -4.117401       -0.524104       0.302485
N       -3.737166       -1.549778       -0.451590
H       -1.842867       -2.455489       -0.939836
H       -5.129915       -0.185201       0.457266
H       -4.375474       -2.147551       -0.967671
###
26
GlyHis4 m062x E=-756.116123418 au
N       -5.017609       -0.917075       -0.026180
H       -4.764954       -1.890821       -0.178986
C       -3.941882       -0.073382       -0.514616
H       -5.090624       -0.805367       0.982611
C       -2.568756       -0.376383       0.073738
H       -3.851894       -0.191789       -1.599481
H       -4.183053       0.976686        -0.331280
O       -2.328203       -1.448796       0.653482
N       -1.644693       0.579409        -0.095758
H       -1.885941       1.430589        -0.593228
C       -0.250191       0.418100        0.281086
H       -0.202474       -0.091584       1.246557
C       0.497463        -0.425022       -0.777736
C       0.399285        1.804501        0.410753
H       -0.039184       -1.373950       -0.876778
H       0.438057        0.096245        -1.738882
C       1.932775        -0.671535       -0.439984
O       -0.010474       2.702009        -0.375987
O       1.313741        1.932339        1.266995
N       2.961803        0.022149        -1.046660
C       2.444677        -1.536338       0.494835
C       4.069020        -0.422653       -0.482374
N       3.806642        -1.361802       0.454283
H       1.972860        -2.238446       1.165356
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H       5.074538        -0.105703       -0.717217
H       4.494802        -1.852769       1.011407
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33
GlyLys1 m062x E=-705.742754798 au
N       -4.592775       -1.946190       -0.009789
C       -3.918962       -0.746241       -0.557990
H       -5.501697       -2.082964       -0.462201
H       -4.742134       -1.851678       1.000385
C       -2.590634       -0.566326       0.152053
H       -3.776007       -0.887547       -1.629769
H       -4.561879       0.118420        -0.388121
O       -2.269308       -1.302864       1.090096
N       -1.838766       0.441434        -0.303448
H       -2.140955       0.975077        -1.113489
C       -0.536216       0.739811        0.266986
H       -0.587603       0.573986        1.346845
C       0.560508        -0.152097       -0.345842
C       -0.242616       2.204420        -0.015730
H       0.253894        -1.188191       -0.164745
H       0.567041        0.009311        -1.430282
C       1.951550        0.085325        0.235875
O       -0.603657       2.754813        -1.036033
O       0.472900        2.880070        0.883889
H       2.295082        1.099098        -0.003539
H       1.909881        0.009396        1.330493
C       2.962005        -0.920900       -0.310720
H       2.639779        -1.941815       -0.072792
H       3.014623        -0.834821       -1.403118
C       4.337467        -0.676234       0.280754
H       4.700161        0.329141        0.062810
H       4.348027        -0.834724       1.359816
N       5.330303        -1.628717       -0.305978
H       5.420853        -1.482135       -1.316247
H       6.255665        -1.509183       0.115349
H       5.037740        -2.599665       -0.155685
H       0.662995        2.357218        1.680993
H       -4.024897       -2.787312       -0.158139
###
32
GlyLys2 m062x E=-705.295573050 au
N       4.699888        -1.745323       -0.088813
C       3.819815        -0.837341       0.685266
H       5.490174        -2.061483       0.480751
H       5.070769        -1.278589       -0.923180
C       2.539844        -0.619343       -0.103931
H       3.581165        -1.322670       1.633371
H       4.353919        0.092632        0.876447
O       2.216672        -1.418015       -0.995856
N       1.825391        0.444807        0.252833
H       2.154934        1.058024        0.992759
C       0.523422        0.760393        -0.322091
H       0.565758        0.576032        -1.398927
C       -0.570361       -0.115484       0.311533
C       0.235328        2.252490        -0.082552
H       -0.280199       -1.163004       0.166076
H       -0.582011       0.073528        1.392446
C       -1.961494       0.113296        -0.272546
O       0.703145        2.762359        0.972232
O       -0.471701       2.841098        -0.941296
H       -2.291818       1.137363        -0.065670
H       -1.924984       0.002819        -1.364168
C       -2.980525       -0.866360       0.306569
H       -2.673459       -1.897636       0.093376
H       -3.025109       -0.752279       1.396974
C       -4.357295       -0.620930       -0.281035
H       -4.712197       0.389868        -0.075708
H       -4.374504       -0.794279       -1.357802
N       -5.354817       -1.558399       0.323090
H       -5.437778       -1.398680       1.331982
H       -6.281742       -1.436622       -0.093930
H       -5.070467       -2.533224       0.183053
H       4.166985        -2.563271       -0.405547
###
31
GlyLys3 m062x E=-704.834152913 au
```

```
N       -4.868740       -1.603899       0.164268
C       -3.824957       -1.024913       -0.673067
H       -5.634393       -1.898091       -0.435330
H       -5.244821       -0.883282       0.776234
C       -2.553333       -0.762653       0.116749
H       -3.555601       -1.750561       -1.447639
H       -4.125075       -0.102391       -1.184718
O       -2.168500       -1.518251       1.025273
N       -1.863209       0.322785        -0.257207
H       -2.215215       0.916067        -1.000635
C       -0.573231       0.686835        0.309761
H       -0.602056       0.501259        1.386856
C       0.553390        -0.146867       -0.323620
C       -0.334826       2.187043        0.072423
H       0.300072        -1.204275       -0.180544
H       0.560784        0.044167        -1.404371
C       1.934424        0.130631        0.263759
O       -0.795654       2.679125        -0.994362
O       0.331075        2.806040        0.944185
H       2.229724        1.165861        0.057679
H       1.898451        0.019450        1.355419
C       2.988048        -0.813906       -0.310999
H       2.710233        -1.854780       -0.104099
H       3.037502        -0.694693       -1.400634
C       4.352791        -0.531937       0.287974
H       4.684958        0.486431        0.081933
H       4.364230        -0.700794       1.365552
N       5.378005        -1.448015       -0.303207
H       5.462012        -1.294806       -1.313005
H       6.298976        -1.297699       0.117479
H       5.118639        -2.428678       -0.155797
###
30
GlyLys4 m062x E=-704.367556288 au
N       -4.829004       -1.582823       0.176247
C       -3.789443       -0.999332       -0.663449
H       -5.601503       -1.865678       -0.420026
H       -5.195984       -0.867157       0.799467
C       -2.509032       -0.753940       0.117726
H       -3.531694       -1.716345       -1.449881
H       -4.089044       -0.068811       -1.160641
O       -2.122540       -1.521109       1.015943
N       -1.814142       0.329945        -0.251412
H       -2.167225       0.931915        -0.987286
C       -0.514220       0.676752        0.304752
H       -0.531840       0.474359        1.379033
C       0.600561        -0.153758       -0.353642
C       -0.270506       2.178926        0.088738
H       0.343316        -1.211541       -0.218045
H       0.591560        0.047649        -1.432644
C       1.992583        0.109138        0.215089
O       -0.735315       2.688846        -0.968246
O       0.402092        2.783047        0.965884
H       2.296074        1.140742        -0.002256
H       1.962741        0.013140        1.309058
C       3.036072        -0.850458       -0.352774
H       2.747899        -1.884862       -0.118673
H       3.061796        -0.766300       -1.447065
C       4.427857        -0.586410       0.200159
H       4.746315        0.422439        -0.082244
H       4.385440        -0.611455       1.299171
N       5.401089        -1.541087       -0.345141
H       6.319366        -1.338142       0.041635
H       5.160044        -2.473985       -0.015705
###
31
GlyPhe1 m062x E=-763.026355178 au
N       5.084645        -1.065005       -0.035970
H       4.715616        -2.017855       0.060619
C       4.134590        -0.085067       0.539316
H       5.992127        -1.011279       0.436508
H       5.231066        -0.891823       -1.036032
C       2.754696        -0.364788       -0.026357
H       4.115567        -0.222579       1.621888
H       4.479704        0.921484        0.305687
O       2.498523        -1.454136       -0.549257
```

```
N       1.870519        0.629964        0.106234
H       2.142109        1.490008        0.574285
C       0.474837        0.455109        -0.250609
H       0.411990        -0.114896       -1.180706
C       -0.294109       -0.282788       0.873913
C       -0.125789       1.827902        -0.464394
H       0.233224        -1.227525       1.038806
H       -0.216463       0.316773        1.786519
C       -1.740186       -0.540781       0.535751
O       0.245124        2.820680        0.130939
C       -2.751676       0.258984        1.076275
C       -2.087293       -1.564904       -0.352627
H       -2.487932       1.059209        1.764157
C       -4.087810       0.038911        0.739497
C       -3.421017       -1.786459       -0.692429
H       -1.305958       -2.192750       -0.775393
H       -4.863398       0.665495        1.169533
C       -4.425138       -0.984183       -0.146642
H       -3.677633       -2.587124       -1.379491
H       -5.464307       -1.158676       -0.408028
O       -1.125122       1.818437        -1.340566
H       -1.526700       2.705364        -1.389301
###
30
GlyPhe2 m062x E=-762.578325539 au
N       1.190731        3.631386        -0.396283
C       0.307148        2.806493        0.460531
H       1.983155        3.073155        -0.732558
H       1.548171        4.437478        0.124894
C       -0.069175       1.545522        -0.298466
H       0.862157        2.535311        1.361107
H       -0.566777       3.396775        0.735099
O       0.585270        1.202810        -1.292511
N       -1.108759       0.880289        0.206171
H       -1.623170       1.276353        0.987437
C       -1.558509       -0.419188       -0.263364
H       -1.328253       -0.500006       -1.328888
C       -0.866610       -1.572288       0.502355
C       -3.080624       -0.548384       -0.067162
H       -1.159760       -1.508783       1.556577
H       -1.250624       -2.512850       0.096984
C       0.632718        -1.515434       0.372797
O       -3.642368       0.265888        0.712261
C       1.409540        -0.850436       1.327191
C       1.265939        -2.056947       -0.752109
H       0.931205        -0.437971       2.212471
C       2.786873        -0.706946       1.150869
C       2.641264        -1.919257       -0.930435
H       0.670816        -2.578257       -1.498635
H       3.375007        -0.183520       1.899048
C       3.405634        -1.235950       0.018195
H       3.117569        -2.342556       -1.809811
H       4.476475        -1.124003       -0.121879
O       -3.635547       -1.500194       -0.676468
H       0.686199        3.975997        -1.219725
###
29
GlyPhe3 m062x E=-762.116116066 au
C       3.575933        -0.858796       -0.019079
C       2.922798        -0.383838       1.118154
C       1.569821        -0.664284       1.316956
C       0.850918        -1.415581       0.381657
C       1.519610        -1.898884       -0.749447
C       2.871098        -1.624668       -0.950509
C       -0.631719       -1.631484       0.534980
C       -1.451439       -0.568035       -0.234341
C       -2.947569       -0.882229       -0.056709
O       -3.382159       -1.880286       -0.691843
N       -1.164574       0.776727        0.226843
C       -0.234588       1.581803        -0.312352
O       0.433990        1.271681        -1.310328
C       -0.042229       2.901573        0.416476
N       0.526873        3.923829        -0.451750
O       -3.612841       -0.158382       0.731145
H       -0.163488       4.186820        -1.151661
H       0.698762        4.755389        0.106730
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H       0.660342        2.699637        1.233008
H       -0.994125       3.188992        0.880099
H       -1.734256       1.118646        0.993065
H       -1.204426       -0.627094       -1.297688
H       -0.916317       -1.588029       1.592547
H       -0.914361       -2.613800       0.144848
H       1.066449        -0.295113       2.207247
H       0.969486        -2.485275       -1.482226
H       3.465547        0.204372        1.852342
H       3.374628        -2.005042       -1.834361
H       4.627948        -0.640950       -0.176106
###
32
GlyTyr1 m062x E=-838.237441307 au
N       5.584295        -0.302930       -0.515192
H       5.492571        -0.842158       -1.382910
C       4.516000        -0.654609       0.448851
H       6.507100        -0.490748       -0.112141
H       5.532098        0.690680        -0.765664
C       3.177964        -0.267840       -0.146732
H       4.568239        -1.723687       0.654393
H       4.689821        -0.099322       1.371997
O       3.107938        0.423886        -1.167640
N       2.098501        -0.704403       0.512346
H       2.206894        -1.258388       1.355957
C       0.764431        -0.381291       0.042364
H       0.585745        -0.850200       -0.930420
C       -0.271946       -0.886042       1.064361
C       0.591137        1.114304        -0.170515
H       -0.102882       -1.960661       1.186511
H       -0.079540       -0.398878       2.026074
C       -1.688629       -0.627964       0.617828
O       1.141220        1.852898        0.793985
O       -0.045382       1.584084        -1.092252
C       -2.383299       0.504826        1.049430
C       -2.323908       -1.499239       -0.274315
H       -1.905893       1.195524        1.741048
C       -3.679520       0.767687        0.608579
C       -3.617180       -1.252889       -0.723930
H       -1.799190       -2.387121       -0.619038
H       -4.215229       1.649545        0.949532
C       -4.293030       -0.115230       -0.279738
H       -4.111134       -1.932392       -1.411395
O       -5.568628       0.084361        -0.748428
H       -5.940802       0.893101        -0.367334
H       0.959325        2.793940        0.620889
###
31
GlyTyr2 m062x E=-837.781530513 au
N       3.472996        -3.089784       -0.520106
H       2.631306        -3.570279       -0.182243
C       3.563603        -1.741343       0.088269
H       4.295379        -3.653358       -0.285854
H       3.402774        -3.028041       -1.541069
C       2.223496        -1.047014       -0.084116
H       3.777465        -1.862191       1.151641
H       4.375801        -1.192359       -0.386505
O       1.199708        -1.712236       -0.300974
N       2.242957        0.275957        0.044743
H       3.121928        0.776586        0.144833
C       1.046542        1.095495        -0.075968
H       0.562313        0.857072        -1.031032
C       0.034522        0.848232        1.076999
C       1.472654        2.576084        -0.157919
H       0.477897        0.138584        1.781203
H       -0.113537       1.788023        1.618920
C       -1.307360       0.321657        0.622948
O       2.701296        2.843143        -0.084724
O       0.539327        3.408366        -0.295709
C       -1.777909       -0.921359       1.053006
C       -2.118264       1.068571        -0.241707
H       -1.164235       -1.524342       1.717898
C       -3.018193       -1.411716       0.643114
C       -3.356842       0.594459        -0.663980
H       -1.774484       2.039254        -0.591271
H       -3.373863       -2.380549       0.984052
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C       -3.805043       -0.649153       -0.217060
H       -3.981766       1.178226        -1.332937
O       -5.035479       -1.079782       -0.656593
H       -5.230689       -1.949244       -0.277613
###
30
GlyTyr3 m062x E=-837.322554095 au
N       3.601413        -3.203808       -0.481878
H       2.844954        -3.738298       -0.060198
C       3.564680        -1.852672       0.050172
H       3.394040        -3.170277       -1.477843
C       2.234560        -1.130028       -0.125862
H       3.769734        -1.882256       1.125276
H       4.357132        -1.253030       -0.404978
O       1.180417        -1.746222       -0.359835
N       2.272203        0.199198        0.019779
H       3.159405        0.677646        0.139372
C       1.094695        1.043892        -0.083300
H       0.596694        0.830948        -1.037630
C       0.082046        0.802006        1.071856
C       1.540723        2.518908        -0.144167
H       0.514423        0.071506        1.761396
H       -0.043385       1.735668        1.630360
C       -1.274263       0.310937        0.620730
O       2.771677        2.772907        -0.058929
O       0.619239        3.367080        -0.276063
C       -1.775083       -0.920177       1.051205
C       -2.069236       1.078217        -0.240854
H       -1.174602       -1.539237       1.713330
C       -3.028287       -1.379194       0.644521
C       -3.320660       0.635533        -0.659992
H       -1.702208       2.040130        -0.590826
H       -3.406349       -2.339599       0.985120
C       -3.798144       -0.597167       -0.213497
H       -3.932402       1.235177        -1.327117
O       -5.039753       -0.997690       -0.651104
H       -5.251569       -1.866234       -0.278981
###
29
GlyTyr4 m062x E=-836.849690166 au
N       -5.490404       -1.234981       0.029468
H       -5.161584       -2.187967       -0.109797
C       -4.494709       -0.318063       -0.499341
H       -5.550627       -1.107535       1.037370
C       -3.084349       -0.525718       0.037509
H       -4.433464       -0.437948       -1.586314
H       -4.804807       0.712239        -0.310778
O       -2.716245       -1.623478       0.491004
N       -2.272527       0.537063        -0.035494
H       -2.614572       1.402726        -0.440085
C       -0.854416       0.483130        0.290223
H       -0.726075       -0.107346       1.201009
C       -0.058538       -0.170509       -0.863885
C       -0.348946       1.912711        0.536367
H       -0.528480       -1.139354       -1.067785
H       -0.189506       0.454677        -1.755066
C       1.407133        -0.351684       -0.566225
O       -0.828698       2.817534        -0.202417
O       0.528117        2.074098        1.425268
C       2.364144        0.571872        -1.004611
C       1.864661        -1.436047       0.194415
H       2.039664        1.429656        -1.593175
C       3.716698        0.422364        -0.709812
C       3.212427        -1.600044       0.499893
H       1.144823        -2.172138       0.551606
H       4.437241        1.152760        -1.071603
C       4.198930        -0.676360       0.053764
H       3.538527        -2.457308       1.085008
O       5.473222        -0.834022       0.322647
###
27
GlyVal1 m062x E=-610.648221903 au
N       -4.165833       0.006019        -0.089665
H       -4.121962       1.017238        -0.259549
C       -2.937306       -0.456465       0.597140
H       -4.995223       -0.200933       0.474998
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H       -4.272654       -0.451427       -1.000955
C       -1.733426       0.054983        -0.173174
H       -2.934295       -0.043741       1.607296
H       -2.953194       -1.544788       0.649940
O       -1.867883       0.920508        -1.044163
N       -0.561275       -0.491713       0.170589
H       -0.529892       -1.159284       0.934513
C       0.685477        -0.015860       -0.408444
H       0.492554        0.247116        -1.451604
C       1.222569        1.240488        0.328207
C       1.727474        -1.113682       -0.420363
H       0.350999        1.902970        0.396335
C       1.707151        0.911599        1.739080
C       2.304501        1.949983        -0.481785
O       2.693786        -1.100610       -1.156481
H       2.617399        0.300391        1.709123
H       1.947406        1.833967        2.275370
H       0.950745        0.372533        2.318652
H       1.968646        2.152394        -1.503687
H       2.552711        2.903870        -0.007244
H       3.220602        1.353292        -0.532227
O       1.512271        -2.068113       0.486805
H       2.231889        -2.724289       0.449319
###
26
GlyVal2 m062x E=-610.198501381 au
N       -4.131501       -0.010430       -0.122570
H       -4.068306       0.995193        -0.320497
C       -2.909079       -0.464029       0.583306
H       -4.967717       -0.191043       0.440431
H       -4.236877       -0.491936       -1.021524
C       -1.698508       0.085437        -0.152628
H       -2.932941       -0.060664       1.596958
H       -2.909303       -1.552601       0.624549
O       -1.828144       1.049980        -0.921966
N       -0.544991       -0.520318       0.112949
H       -0.517153       -1.325205       0.732491
C       0.729494        -0.072394       -0.433269
H       0.579658        0.179874        -1.487565
C       1.238018        1.185945        0.314321
C       1.736839        -1.233571       -0.348841
H       0.361128        1.840147        0.400809
C       1.731271        0.849862        1.721037
C       2.305095        1.936398        -0.479358
O       2.764223        -1.139442       -1.070266
H       2.646710        0.247251        1.679565
H       1.962361        1.767392        2.270684
H       0.982626        0.292965        2.294262
H       1.970541        2.139117        -1.502137
H       2.523982        2.894118        0.003160
H       3.236986        1.365689        -0.531293
O       1.477041        -2.174406       0.449736
###
25
GlyVal3 m062x E=-609.739439862 au
N       -4.256316       -0.069571       -0.023268
H       -4.300928       0.945294        -0.081199
C       -2.979084       -0.445038       0.557149
H       -4.291632       -0.402233       -0.984464
C       -1.758193       0.094577        -0.179265
H       -2.924634       -0.066729       1.583205
H       -2.905166       -1.533789       0.618469
O       -1.846613       1.050326        -0.970294
N       -0.598337       -0.512967       0.097897
H       -0.579240       -1.298793       0.739684
C       0.682491        -0.073023       -0.433642
H       0.546534        0.182065        -1.489216
C       1.192696        1.183645        0.317270
C       1.689869        -1.232747       -0.344413
H       0.316157        1.838681        0.400868
C       1.678107        0.844852        1.726151
C       2.265150        1.934639        -0.468625
O       2.716844        -1.144684       -1.069420
H       2.594818        0.243722        1.688803
H       1.904111        1.760675        2.280921
H       0.926746        0.284418        2.292446
```

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H       1.934871        2.143545        -1.491646
H       2.486581        2.889494        0.018705
H       3.195420        1.361034        -0.520711
O       1.436358        -2.169524       0.461463
###
29
HisGly1 m062x E=-757.477734223 au
N       -3.497464       -1.054778       -0.372412
H       -3.572838       -1.889339       -0.965609
H       -4.262379       -0.416405       -0.619758
H       -3.619171       -1.349986       0.605417
C       -2.176303       -0.393910       -0.541546
H       -2.020187       -0.219645       -1.607093
C       -2.188002       0.937348        0.231968
C       -1.122282       -1.328925       0.039560
H       -2.935122       1.592929        -0.221772
H       -2.478296       0.747086        1.271059
C       -0.859921       1.615310        0.197826
O       -1.370742       -1.983717       1.055887
N       0.127159        1.381170        1.139640
C       -0.330460       2.506649        -0.685867
H       0.050707        0.746498        1.931766
C       1.211673        2.091396        0.847224
N       0.945784        2.788812        -0.250833
H       -0.754521       2.964165        -1.565441
H       2.134141        2.106307        1.406960
H       1.601487        3.423654        -0.696761
N       0.056952        -1.321194       -0.589686
H       0.188150        -0.693318       -1.378897
C       1.241397        -1.899662       0.001108
C       2.435523        -1.024631       -0.301964
H       1.119268        -1.968706       1.086821
H       1.440411        -2.908169       -0.378160
O       2.369466        0.007327        -0.935203
O       3.610726        -1.451192       0.163358
H       3.535984        -2.293946       0.642313
###
28
HisGly2 m062x E=-757.031416395 au
N       -3.551144       -0.770088       -0.418291
H       -3.695364       -1.588335       -1.020823
H       -4.251496       -0.061384       -0.664758
H       -3.704068       -1.064422       0.555509
C       -2.172577       -0.232781       -0.566345
H       -1.983052       -0.077886       -1.629488
C       -2.078305       1.099706        0.204026
C       -1.216067       -1.253071       0.039700
H       -2.746291       1.822338        -0.270686
H       -2.412978       0.942867        1.235320
C       -0.689229       1.644107        0.204798
O       -1.562529       -1.900454       1.037275
N       0.244171        1.312662        1.171808
C       -0.039981       2.453538        -0.678747
H       0.079465        0.701701        1.969270
C       1.412461        1.880407        0.890430
N       1.252208        2.589018        -0.221227
H       -0.387800       2.939388        -1.576545
H       2.320754        1.790391        1.466649
H       1.990220        3.123992        -0.669783
N       -0.010114       -1.313164       -0.520614
H       0.219451        -0.673451       -1.279138
C       1.132888        -1.891849       0.162396
C       2.428892        -1.215195       -0.300342
H       1.025161        -1.751849       1.242592
H       1.210410        -2.966744       -0.027124
O       2.347942        -0.343370       -1.204712
O       3.479743        -1.603024       0.273910
###
27
HisGly3 m062x E=-756.579234144 au
N       -3.462619       -1.009453       -0.428984
H       -3.526371       -1.856987       -1.003845
H       -4.213513       -0.370593       -0.711876
H       -3.611784       -1.281714       0.551181
C       -2.130073       -0.357659       -0.565158
H       -1.933522       -0.219445       -1.629593
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C       -2.161331       0.997256        0.164582
C       -1.106829       -1.288598       0.072666
H       -2.867056       1.645471        -0.362776
H       -2.535249       0.837101        1.181881
C       -0.807938       1.630298        0.223580
O       -1.419190       -1.956824       1.069624
N       0.068386        1.368602        1.257641
C       -0.213303       2.455125        -0.697130
C       1.170416        2.028358        0.958040
N       1.043864        2.705727        -0.206535
H       -0.568325       2.878945        -1.624209
H       2.075090        2.056714        1.548260
N       0.101995        -1.285857       -0.484142
H       0.304017        -0.609941       -1.218314
C       1.266496        -1.813329       0.201036
C       2.540625        -1.114882       -0.285466
H       1.166412        -1.657074       1.279319
H       1.373199        -2.889290       0.031046
O       2.434089        -0.260446       -1.204285
O       3.606524        -1.468609       0.284531
H       1.755954        3.281291        -0.638803
###
26
HisGly4 m062x E=-756.120989261 au
N       -3.535203       -0.967421       -0.534444
H       -3.535105       -1.859637       -1.024901
H       -3.765413       -1.179350       0.435758
C       -2.193151       -0.402905       -0.570993
H       -1.905716       -0.248082       -1.615499
C       -2.194253       0.963811        0.143097
C       -1.147532       -1.293819       0.094391
H       -2.889213       1.612461        -0.397558
H       -2.588036       0.821796        1.156649
C       -0.842632       1.601291        0.216549
O       -1.407543       -1.923061       1.135254
N       0.024981        1.366409        1.266168
C       -0.237526       2.411345        -0.711596
C       1.129135        2.023827        0.966321
N       1.014247        2.677863        -0.211972
H       -0.581789       2.814582        -1.651965
H       2.026656        2.067509        1.566609
N       0.057458        -1.325990       -0.489327
H       0.242125        -0.667288       -1.241617
C       1.236625        -1.812507       0.198305
C       2.497021        -1.093025       -0.291608
H       1.135561        -1.646486       1.275098
H       1.373307        -2.888226       0.044942
O       2.383416        -0.262917       -1.231818
O       3.566692        -1.403465       0.299263
H       1.730609        3.244131        -0.648871
###
44
HisLys0 m062x E=-970.462312715 au
N       2.670499        3.431402        -0.300594
H       2.027841        3.956496        -0.904813
H       2.460277        3.677027        0.676033
C       2.509742        1.966733        -0.497736
H       2.576163        1.759808        -1.567016
C       3.627373        1.236327        0.271182
C       1.151019        1.575626        0.071469
H       4.587530        1.499372        -0.178776
H       3.626059        1.572758        1.313354
C       3.450053        -0.244192       0.225810
O       0.731240        2.121461        1.096298
N       2.737093        -0.936866       1.188192
C       3.830341        -1.171662       -0.697793
C       2.675047        -2.226359       0.869826
N       3.342717        -2.385718       -0.267335
H       4.401196        -1.068828       -1.606847
H       2.190304        -3.003439       1.441144
H       3.462918        -3.277558       -0.739116
N       0.536616        0.573801        -0.563630
H       0.968293        0.165588        -1.389353
C       -0.592267       -0.130523       0.021745
H       -0.521984       -0.045536       1.112147
C       -1.932672       0.455523        -0.457339
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C       -0.449493       -1.592497       -0.378516
H       -1.924308       1.511235        -0.164124
H       -1.958333       0.414281        -1.552179
C       -3.161742       -0.237831       0.125856
O       0.078801        -1.934842       -1.416769
O       -0.948193       -2.512323       0.446431
H       -3.247125       -1.255425       -0.274723
H       -3.055605       -0.326583       1.215162
C       -4.436823       0.537621        -0.197714
H       -4.386170       1.535215        0.255006
H       -4.527067       0.670296        -1.282911
C       -5.661248       -0.192594       0.321261
H       -5.791882       -1.161032       -0.163403
H       -5.620402       -0.336473       1.401902
N       -6.896460       0.601601        0.038029
H       -7.000538       0.768868        -0.967901
H       -7.734455       0.113799        0.367356
H       -6.857863       1.514078        0.503568
H       3.629118        3.728566        -0.515580
H       2.299982        -0.524415       2.010337
H       -1.287969       -2.129035       1.272108
###
43
HisLys1 m062x E=-970.017628869 au
N       2.793688        3.383965        -0.276517
H       2.162051        3.949777        -0.855012
H       2.622215        3.630063        0.707319
C       2.545065        1.932694        -0.480744
H       2.589760        1.731487        -1.552157
C       3.630616        1.137612        0.269393
C       1.169712        1.618933        0.099510
H       4.602322        1.382069        -0.166783
H       3.635024        1.441068        1.321802
C       3.412478        -0.335160       0.170440
O       0.775744        2.230490        1.102080
N       2.641136        -1.044212       1.075288
C       3.821446        -1.241480       -0.761555
C       2.573014        -2.321161       0.713493
N       3.293407        -2.459385       -0.393388
H       4.438472        -1.121622       -1.637755
H       2.043009        -3.105096       1.232998
H       3.417389        -3.338075       -0.887975
N       0.516757        0.622679        -0.495143
H       0.948012        0.144213        -1.283647
C       -0.617577       -0.058809       0.118252
H       -0.572830       0.113804        1.197318
C       -1.944378       0.481026        -0.434160
C       -0.465684       -1.568462       -0.150976
H       -1.969479       1.557909        -0.227168
H       -1.947674       0.356050        -1.524136
C       -3.174108       -0.191522       0.169971
O       0.070931        -1.900476       -1.242913
O       -0.906718       -2.351862       0.729096
H       -3.207321       -1.245247       -0.130640
H       -3.104227       -0.173883       1.265359
C       -4.464938       0.497742        -0.267889
H       -4.461082       1.542413        0.066620
H       -4.533074       0.500538        -1.362964
C       -5.676483       -0.210419       0.309189
H       -5.748189       -1.241203       -0.040079
H       -5.669252       -0.201869       1.400008
N       -6.933978       0.478886        -0.118116
H       -7.018708       0.483768        -1.139530
H       -7.762006       0.015437        0.267035
H       -6.940318       1.452972        0.201119
H       3.760597        3.630589        -0.515828
H       2.163609        -0.649866       1.883569
###
42
HisLys2 m062x E=-969.565988704 au
N       -2.749330       3.377435        0.301851
H       -2.114656       3.916149        0.901466
H       -2.551895       3.630319        -0.674822
C       -2.551866       1.912432        0.484862
H       -2.614639       1.699347        1.553153
C       -3.648223       1.157825        -0.287961
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C       -1.177000       1.569470        -0.073498
H       -4.610497       1.404509        0.169924
H       -3.656140       1.517246        -1.322790
C       -3.423312       -0.320826       -0.273040
O       -0.753214       2.170997        -1.071958
N       -2.658242       -0.947652       -1.236648
C       -3.838649       -1.234188       0.662604
C       -2.615974       -2.216725       -0.879639
N       -3.321016       -2.437771       0.253885
H       -4.443433       -1.135348       1.551159
H       -2.107875       -3.010002       -1.408796
H       -3.433870       -3.330503       0.718194
N       -0.539825       0.578573        0.546068
H       -1.011739       0.089121        1.302881
C       0.585210        -0.125934       -0.056534
H       0.518518        -0.009634       -1.142306
C       1.919831        0.452981        0.437447
C       0.454465        -1.621349       0.288020
H       1.910919        1.526757        0.213125
H       1.967212        0.347639        1.528610
C       3.145789        -0.194423       -0.200037
O       -0.089769       -1.909608       1.389074
O       0.926871        -2.440393       -0.542526
H       3.203598        -1.249812       0.089517
H       3.050628        -0.168137       -1.293354
C       4.435086        0.510478        0.216925
H       4.412591        1.556875        -0.111252
H       4.522469        0.507774        1.310730
C       5.645072        -0.180485       -0.383090
H       5.726374        -1.215728       -0.049348
H       5.627215        -0.156435       -1.473524
N       6.902531        0.509933        0.042778
H       6.996457        0.499143        1.063340
H       7.729590        0.057329        -0.357237
H       6.900300        1.488941        -0.261042
H       -3.713641       3.647322        0.523756
###
41
HisLys3 m062x E=-969.108227560 au
N       -2.846096       3.415576        0.403522
H       -2.131287       3.923164        0.921328
H       -2.744137       3.701059        -0.569672
C       -2.570526       1.988152        0.489470
H       -2.607791       1.686525        1.540628
C       -3.654645       1.207238        -0.281076
C       -1.209372       1.601403        -0.083763
H       -4.617052       1.440624        0.182822
H       -3.679590       1.580022        -1.312115
C       -3.429284       -0.272083       -0.289958
O       -0.772240       2.142891        -1.114886
N       -2.674313       -0.895030       -1.265685
C       -3.832010       -1.194747       0.642989
C       -2.624529       -2.166741       -0.916926
N       -3.316605       -2.396755       0.222213
H       -4.426558       -1.103425       1.539351
H       -2.121872       -2.955953       -1.457377
H       -3.422478       -3.292255       0.682274
N       -0.556090       0.627833        0.563532
H       -1.032082       0.155582        1.327132
C       0.554162        -0.103127       -0.032005
H       0.482769        -0.008701       -1.119665
C       1.900751        0.470036        0.437320
C       0.416818        -1.591204       0.336324
H       1.897417        1.540275        0.195965
H       1.958576        0.383569        1.529849
C       3.117470        -0.194956       -0.199606
O       -0.120167       -1.863706       1.445405
O       0.878389        -2.427735       -0.484661
H       3.168403        -1.247511       0.101496
H       3.016549        -0.180141       -1.292701
C       4.414823        0.503745        0.202720
H       4.397125        1.548127        -0.132214
H       4.509931        0.507876        1.295898
C       5.616404        -0.198622       -0.400811
H       5.692822        -1.232825       -0.062676
H       5.592626        -0.179444       -1.491218
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N       6.880681        0.485435        0.015115
H       6.979984        0.478127        1.035213
H       7.702829        0.026473        -0.387663
H       6.882543        1.463270        -0.292463
###
40
HisLys4 m062x E=-968.641617725 au
N       -2.813220       3.410489        0.399216
H       -2.100431       3.920458        0.917497
H       -2.710538       3.695675        -0.574006
C       -2.532932       1.983969        0.486153
H       -2.569698       1.682958        1.537504
C       -3.614054       1.199057        -0.284372
C       -1.169984       1.601902        -0.086183
H       -4.577608       1.430197        0.178295
H       -3.639173       1.570355        -1.315939
C       -3.384353       -0.279586       -0.291137
O       -0.734796       2.145168        -1.117427
N       -2.629261       -0.902037       -1.267067
C       -3.782979       -1.201788       0.644020
C       -2.575565       -2.173070       -0.916400
N       -3.265015       -2.403069       0.224318
H       -4.376137       -1.110576       1.541318
H       -2.071478       -2.961782       -1.456228
H       -3.367593       -3.298070       0.686097
N       -0.513463       0.631353        0.561697
H       -0.987571       0.158559        1.326071
C       0.604040        -0.092801       -0.029383
H       0.541458        0.010793        -1.116675
C       1.945943        0.477449        0.456969
C       0.464685        -1.583752       0.325413
H       1.943446        1.549595        0.222802
H       1.990319        0.385156        1.549915
C       3.171690        -0.180996       -0.169997
O       -0.067341       -1.864941       1.435017
O       0.918921        -2.414713       -0.505425
H       3.218241        -1.236204       0.125785
H       3.075495        -0.164949       -1.264240
C       4.470621        0.509552        0.240227
H       4.449848        1.558133        -0.088097
H       4.553571        0.519142        1.334832
C       5.696534        -0.171897       -0.347884
H       5.745561        -1.204383       0.013270
H       5.585251        -0.220289       -1.441187
N       6.928948        0.514504        0.060915
H       7.726532        0.048348        -0.364724
H       6.918430        1.455845        -0.327724
###
44
LeuTyr1 m062x E=-995.424544612 au
N       -4.186337       -2.363613       -0.046017
H       -4.084494       -2.508378       0.966220
H       -3.787979       -3.180502       -0.522287
H       -5.185301       -2.313994       -0.272971
C       -3.495993       -1.102863       -0.448132
H       -3.519833       -1.058460       -1.538056
C       -4.230498       0.077000        0.194367
C       -2.067867       -1.220812       0.068493
H       -5.278791       0.028871        -0.128808
H       -4.210114       -0.066260       1.282304
C       -3.662352       1.456346        -0.158445
O       -1.840977       -1.764741       1.155705
H       -2.607332       1.489226        0.142503
C       -3.758487       1.747765        -1.656380
C       -4.414916       2.520840        0.639594
H       -4.801611       1.685273        -1.989311
H       -3.394926       2.757204        -1.871843
H       -3.170843       1.049718        -2.261521
H       -4.340074       2.338240        1.716330
H       -4.011377       3.516730        0.433152
H       -5.477291       2.523208        0.368219
N       -1.103617       -0.693052       -0.692222
H       -1.346442       -0.210853       -1.552230
C       0.276455        -0.689340       -0.243988
H       0.651244        -1.715891       -0.184128
C       1.127345        0.122561        -1.238455
```

```
C       0.418452        -0.108091       1.154794
H       1.005558        -0.348282       -2.219237
H       0.721231        1.138324        -1.295276
C       2.582793        0.159314        -0.846663
O       -0.344287       0.963820        1.363739
O       1.202387        -0.542513       1.974786
C       3.115415        1.258438        -0.168641
C       3.420411        -0.930663       -1.110301
H       2.480048        2.114330        0.047324
C       4.448730        1.278744        0.238594
C       4.753038        -0.927568       -0.711150
H       3.023952        -1.795173       -1.637508
H       4.857031        2.138470        0.762925
C       5.263449        0.180847        -0.033299
H       5.403138        -1.771620       -0.919131
O       6.584152        0.142075        0.341293
H       6.814764        0.954944        0.814457
H       -0.176932       1.307283        2.260029
###
43
LeuTyr2 m062x E=-994.968297456 au
N       -2.510711       -2.275241       -1.936007
H       -1.855566       -2.939998       -1.505481
H       -2.127309       -1.993801       -2.844782
H       -3.403094       -2.754281       -2.096631
C       -2.698429       -1.100577       -1.031554
H       -3.276523       -0.358865       -1.584346
C       -3.420872       -1.575187       0.230342
C       -1.300868       -0.590557       -0.695582
H       -4.394076       -1.982866       -0.072819
H       -2.835777       -2.396113       0.664183
C       -3.638353       -0.487681       1.288651
O       -0.417743       -1.403918       -0.380952
H       -2.658422       -0.088349       1.585607
C       -4.502358       0.660536        0.764948
C       -4.283879       -1.120134       2.521618
H       -5.464446       0.276840        0.404229
H       -4.704355       1.380247        1.564274
H       -4.028556       1.207420        -0.056518
H       -3.670300       -1.935090       2.918562
H       -4.419340       -0.377362       3.313593
H       -5.269650       -1.528348       2.268488
N       -1.121284       0.725171        -0.739740
H       -1.895554       1.348570        -0.954802
C       0.109741        1.361853        -0.297798
H       0.339421        0.995811        0.711299
C       1.309135        1.049342        -1.233869
C       -0.143002       2.877858        -0.165198
H       0.945837        0.453280        -2.075869
H       1.682702        1.992686        -1.645744
C       2.445687        0.314867        -0.560457
O       -1.295767       3.309440        -0.432923
O       0.839052        3.566424        0.213316
C       2.890275        -0.920643       -1.037168
C       3.086493        0.856299        0.561696
H       2.406358        -1.364810       -1.903595
C       3.940024        -1.603738       -0.421537
C       4.131585        0.187556        1.191817
H       2.760917        1.818003        0.951301
H       4.276139        -2.565340       -0.800756
C       4.555811        -1.046295       0.697059
H       4.623642        0.610235        2.062443
O       5.590210        -1.672718       1.353124
H       5.779959        -2.522187       0.929258
###
42
LeuTyr3 m062x E=-994.509286287 au
N       -2.620317       -1.957449       -2.253661
H       -2.058474       -2.742626       -1.926469
H       -2.106239       -1.542801       -3.028782
C       -2.726207       -0.985330       -1.165227
H       -3.292168       -0.125878       -1.535632
C       -3.460619       -1.623623       0.015222
C       -1.350951       -0.507209       -0.704605
H       -4.451535       -1.936068       -0.339103
H       -2.915134       -2.535240       0.295963
```

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C       -3.625780       -0.731829       1.250778
O       -0.477133       -1.324657       -0.356979
H       -2.627802       -0.423733       1.596207
C       -4.442689       0.524977        0.945121
C       -4.285867       -1.530689       2.374710
H       -5.429057       0.249060        0.551776
H       -4.595294       1.116023        1.853894
H       -3.956152       1.172569        0.208632
H       -3.700684       -2.420694       2.628342
H       -4.390700       -0.923400       3.279392
H       -5.287361       -1.860216       2.072094
N       -1.136259       0.811564        -0.704451
H       -1.891944       1.453939        -0.923013
C       0.094485        1.410086        -0.217881
H       0.313668        0.991427        0.772820
C       1.301010        1.133312        -1.157769
C       -0.128647       2.921252        -0.012377
H       0.933670        0.600790        -2.039702
H       1.701287        2.091600        -1.505817
C       2.417048        0.331170        -0.529054
O       -1.246772       3.406806        -0.330036
O       0.845166        3.557911        0.469240
C       2.841714        -0.873193       -1.095139
C       3.063762        0.775967        0.631432
H       2.350633        -1.244195       -1.991501
C       3.881154        -1.615574       -0.533856
C       4.100206        0.047026        1.207902
H       2.752063        1.709855        1.093497
H       4.202812        -2.550397       -0.985261
C       4.508723        -1.150683       0.619826
H       4.598996        0.396851        2.106613
O       5.539871        -1.835800       1.220938
H       5.732328        -2.643714       0.723049
###
41
LeuTyr4 m062x E=-994.031969913 au
N       -2.696004       -1.927885       -2.227570
H       -2.166547       -2.731613       -1.891745
H       -2.165319       -1.541873       -3.006133
C       -2.764759       -0.940587       -1.149603
H       -3.292444       -0.062358       -1.532504
C       -3.530889       -1.534302       0.033962
C       -1.371388       -0.518418       -0.687724
H       -4.534545       -1.803487       -0.319958
H       -3.028513       -2.467474       0.324163
C       -3.656846       -0.624955       1.261362
O       -0.539900       -1.370789       -0.320431
H       -2.646120       -0.364301       1.608617
C       -4.409623       0.667997        0.941755
C       -4.359199       -1.380759       2.389271
H       -5.407338       0.437513        0.547721
H       -4.535735       1.274004        1.844749
H       -3.889521       1.284049        0.201178
H       -3.819601       -2.296629       2.651879
H       -4.436304       -0.761900       3.288951
H       -5.375089       -1.662334       2.086251
N       -1.094350       0.788210        -0.709178
H       -1.820115       1.459459        -0.941334
C       0.162059        1.338701        -0.228731
H       0.372844        0.908788        0.758405
C       1.356653        1.019366        -1.177582
C       -0.005514       2.856854        -0.027539
H       0.965090        0.443873        -2.022332
H       1.737156        1.962649        -1.585435
C       2.488115        0.244642        -0.540690
O       -1.092548       3.389501        -0.379045
O       0.979621        3.456674        0.478156
C       2.748453        -1.084852       -0.893981
C       3.323072        0.819135        0.428883
H       2.119904        -1.563613       -1.643782
C       3.785673        -1.813210       -0.315577
C       4.362159        0.105142        1.018828
H       3.156446        1.852500        0.728373
H       3.960582        -2.843944       -0.616790
C       4.638860        -1.246303       0.669342
H       4.993435        0.581408        1.766193
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O       5.620734        -1.922597       1.218683
###
36
LysAla1 m062x E=-745.042030542 au
N       -0.389939       3.651342        -0.218827
H       -0.491615       3.776351        0.796340
H       -1.261252       3.960083        -0.663855
H       0.369751        4.255911        -0.549386
C       -0.097574       2.221106        -0.523800
H       -0.161113       2.096049        -1.606207
C       1.301704        1.873666        -0.009368
C       -1.155329       1.392055        0.194120
H       2.016590        2.510891        -0.542075
H       1.356499        2.125346        1.057013
C       1.659829        0.403461        -0.221386
O       -1.561937       1.741439        1.307950
H       1.019331        -0.233616       0.401098
H       1.473404        0.124264        -1.266770
C       3.121181        0.134555        0.130078
H       3.776467        0.746520        -0.501399
H       3.307066        0.415678        1.173800
C       3.456220        -1.331950       -0.067184
H       2.844557        -1.976509       0.565697
H       3.337934        -1.636802       -1.107803
N       4.881991        -1.594589       0.301987
H       5.048978        -1.374218       1.288998
H       5.128676        -2.576965       0.151461
H       5.518702        -1.019323       -0.259036
N       -1.547086       0.281484        -0.438914
H       -1.116090       0.041950        -1.327582
C       -2.328994       -0.743573       0.225452
H       -2.206205       -0.617255       1.306063
C       -3.816005       -0.664141       -0.135777
C       -1.752494       -2.096812       -0.157802
H       -3.955718       -0.805107       -1.210558
H       -4.386186       -1.426159       0.401622
H       -4.193826       0.320058        0.149068
O       -0.981785       -2.262787       -1.080331
O       -2.160277       -3.143718       0.563436
H       -2.739944       -2.884476       1.299343
###
35
LysAla2 m062x E=-744.594852555 au
N       0.198295        3.534691        0.439987
H       0.283478        3.753664        -0.560757
H       1.066200        3.823878        0.903827
H       -0.573646       4.084909        0.831358
C       -0.054184       2.073952        0.611544
H       0.028465        1.849050        1.676376
C       -1.452893       1.745022        0.088542
C       1.015175        1.345865        -0.196088
H       -2.172265       2.325035        0.677955
H       -1.528314       2.076130        -0.954561
C       -1.777819       0.256744        0.194380
O       1.338563        1.784563        -1.310969
H       -1.136159       -0.316684       -0.485417
H       -1.566217       -0.094682       1.212735
C       -3.239547       -0.018016       -0.150810
H       -3.895198       0.554362        0.516560
H       -3.443973       0.307093        -1.178186
C       -3.552866       -1.496079       -0.014558
H       -2.937868       -2.105786       -0.677871
H       -3.423077       -1.841964       1.011725
N       -4.978196       -1.761256       -0.384117
H       -5.153402       -1.506397       -1.361363
H       -5.213905       -2.751088       -0.268439
H       -5.616695       -1.213713       0.201901
N       1.510197        0.239228        0.351133
H       1.130450        -0.106324       1.229100
C       2.357914        -0.686210       -0.388300
H       1.975496        -0.755717       -1.412588
C       3.813213        -0.217469       -0.417773
C       2.253925        -2.083625       0.248259
H       4.229057        -0.209992       0.594520
H       4.410280        -0.887724       -1.039638
H       3.876610        0.792102        -0.831387
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O       1.615693        -2.196187       1.329211
O       2.842133        -3.011613       -0.366498
###
34
LysAla3 m062x E=-744.136907105 au
N       0.030301        3.450373        0.621658
H       0.995953        3.661113        0.867670
H       -0.091254       3.759034        -0.342169
C       -0.175466       2.003247        0.666012
H       -0.009862       1.665660        1.693875
C       -1.610807       1.672764        0.257500
C       0.793898        1.264761        -0.255031
H       -2.281715       2.170884        0.966345
H       -1.800729       2.108267        -0.732736
C       -1.909076       0.175399        0.226625
O       0.873404        1.563315        -1.462418
H       -1.310070       -0.309847       -0.555483
H       -1.616234       -0.280348       1.181769
C       -3.387845       -0.098925       -0.036904
H       -3.994561       0.337102        0.766321
H       -3.690958       0.379296        -0.976683
C       -3.660913       -1.588800       -0.121757
H       -3.115732       -2.054206       -0.943794
H       -3.411180       -2.100891       0.808544
N       -5.115775       -1.834965       -0.374388
H       -5.411801       -1.393183       -1.250666
H       -5.321177       -2.836293       -0.437125
H       -5.686422       -1.441462       0.380647
N       1.534475        0.301824        0.302549
H       1.373244        0.038943        1.269794
C       2.448837        -0.541619       -0.451391
H       1.968285        -0.813772       -1.397739
C       3.766015        0.178935        -0.745776
C       2.711117        -1.842408       0.328394
H       4.295801        0.400020        0.186072
H       4.404748        -0.444405       -1.375252
H       3.572390        1.118753        -1.269103
O       2.240585        -1.942873       1.493079
O       3.402724        -2.711118       -0.267543
###
33
LysAla4 m062x E=-743.671107619 au
N       -0.083467       3.439904        0.628455
H       0.874725        3.672101        0.884051
H       -0.202471       3.747011        -0.336169
C       -0.257773       1.988369        0.667850
H       -0.091403       1.651541        1.695897
C       -1.683131       1.626895        0.249130
C       0.733243        1.274337        -0.248902
H       -2.367813       2.112559        0.953945
H       -1.874830       2.061666        -0.741440
C       -1.956252       0.124650        0.213712
O       0.821930        1.586676        -1.452234
H       -1.338611       -0.347937       -0.562811
H       -1.656834       -0.325353       1.170629
C       -3.424930       -0.191908       -0.059804
H       -4.049608       0.242628        0.732814
H       -3.733406       0.279544        -1.003295
C       -3.696900       -1.690447       -0.141772
H       -3.081009       -2.128384       -0.934674
H       -3.387527       -2.167742       0.794419
N       -5.095116       -2.052564       -0.398775
H       -5.389382       -1.605944       -1.265627
H       -5.674382       -1.639538       0.330042
N       1.482082        0.316252        0.306593
H       1.311949        0.039339        1.268391
C       2.409424        -0.512496       -0.447843
H       1.936552        -0.784350       -1.398245
C       3.720688        0.222905        -0.731453
C       2.681596        -1.815192       0.325571
H       4.244380        0.442949        0.204081
H       4.368042        -0.390401       -1.361966
H       3.520540        1.164083        -1.249760
O       2.200442        -1.930482       1.484493
O       3.391480        -2.670143       -0.268900
###
```

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34
LysDAla3 m062x E=-744.137164341 au
N       -0.004289       3.465548       -0.242336
H       -0.976863       3.705205       -0.425096
H       0.156139        3.657045       0.745970
C       0.191546        2.034029       -0.470110
H       -0.036273       1.819478       -1.518879
C       1.645233        1.660267       -0.182633
C       -0.723428       1.192767       0.416501
H       2.281512        2.252960       -0.849206
H       1.881934        1.960472       0.847074
C       1.943710        0.173837       -0.365324
O       -0.687781       1.317325       1.656124
H       1.323122        -0.421929      0.318160
H       1.678274        -0.132886      -1.385622
C       3.413809        -0.143863      -0.100448
H       4.050926        0.435193       -0.780268
H       3.672509        0.148792       0.924801
C       3.694496        -1.622733      -0.287406
H       3.082999        -2.239274      0.373033
H       3.536470        -1.938733      -1.319348
N       5.122451        -1.925422      0.043844
H       5.322712        -1.704545      1.024388
H       5.337652        -2.914968      -0.107349
H       5.758642        -1.371060      -0.538257
N       -1.546831       0.340056       -0.199906
H       -1.569854       0.293820       -1.213331
C       -2.441232       -0.560012      0.510836
C       -3.520900       -1.080624      -0.452589
O       -3.365914       -0.873297      -1.686126
O       -4.475321       -1.709533      0.078372
C       -1.678913       -1.737698      1.125226
H       -1.217656       -2.344689      0.339843
H       -0.894787       -1.373023      1.793653
H       -2.940441       0.002727       1.305989
H       -2.360129       -2.367646      1.701946
###
33
LysDAla4 m062x E=-743.671594537 au
N       0.139065        3.515107       -0.338405
H       -0.818585       3.795728       -0.540752
H       0.296184        3.731542       0.645230
C       0.265901        2.069269       -0.514062
H       0.045387        1.830528       -1.559216
C       1.695276        1.628844       -0.190967
C       -0.699007       1.295839       0.381220
H       2.369369        2.155390       -0.876087
H       1.938654        1.964236       0.826581
C       1.917755        0.121737       -0.303360
O       -0.734601       1.512345       1.608127
H       1.295617        -0.403396      0.435097
H       1.587807        -0.223561      -1.293330
C       3.377511        -0.271464      -0.088425
H       4.010057        0.228407       -0.834944
H       3.711652        0.077727       0.898570
C       3.595087        -1.778324      -0.181767
H       2.966870        -2.282252      0.560818
H       3.263977        -2.132870      -1.164008
N       4.979707        -2.219512      0.018173
H       5.294193        -1.894060      0.930694
H       5.571230        -1.743281      -0.660493
N       -1.477807       0.387781       -0.214710
H       -1.418147       0.247727       -1.218111
C       -2.366134       -0.505755      0.511573
C       -3.362229       -1.151891      -0.465004
O       -3.143603       -1.036292      -1.700857
O       -4.317530       -1.783755      0.061483
C       -1.580620       -1.599577      1.241475
H       -1.057463       -2.233168      0.517736
H       -0.844621       -1.153237      1.914961
H       -2.936169       0.082573       1.237251
H       -2.258144       -2.222112      1.830492
###
42
LysGlu1 m062x E=-972.863450006 au
N       -2.362516       -3.446334      -0.801217
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H       -2.477615       -3.682249       0.192704
H       -1.668148       -4.087101       -1.200885
H       -3.256769       -3.603126       -1.278107
C       -1.938032       -2.022174       -0.938591
H       -1.703590       -1.850809       -1.990760
C       -3.075160       -1.116646       -0.468248
C       -0.704403       -1.854249       -0.061077
H       -3.941938       -1.310185       -1.110330
H       -3.346282       -1.395734       0.557348
C       -2.699678       0.361630        -0.527202
O       -0.671006       -2.354123       1.068619
H       -1.894490       0.569401        0.187340
H       -2.317633       0.605847        -1.526778
C       -3.899030       1.250485        -0.206878
H       -4.689402       1.091157        -0.950291
H       -4.308088       0.984387        0.775482
C       -3.492555       2.712142        -0.203423
H       -2.759856       2.926564        0.575645
H       -3.089128       3.021683        -1.168350
N       -4.678335       3.582712        0.069589
H       -5.096427       3.355643        0.977508
H       -4.417252       4.573052        0.080548
H       -5.399556       3.453846        -0.647327
N       0.303036        -1.132849       -0.565307
H       0.206889        -0.699453       -1.478430
C       1.473976        -0.851035       0.240731
H       1.980267        -1.792115       0.484474
C       2.420363        0.060358        -0.546011
C       1.045895        -0.162887       1.540425
H       2.666375        -0.455898       -1.479604
H       1.896193        0.989412        -0.795684
C       3.703822        0.372602        0.235078
O       0.181653        0.685946        1.583129
O       1.709420        -0.491450       2.651095
H       3.492760        0.965244        1.127505
H       4.197246        -0.558830       0.534400
C       4.645221        1.178645        -0.622561
O       4.822086        2.375243        -0.501727
O       5.300929        0.525389        -1.595405
H       5.106382        -0.426137       -1.591268
H       2.357604        -1.200560       2.504264
###
41
LysGlu2 m062x E=-972.414877282 au
N       -1.198353       3.540481        0.567257
H       -1.052906       3.773703        -0.423142
H       -0.367802       3.841047        1.088563
H       -2.005519       4.068984        0.914785
C       -1.428904       2.072908        0.704809
H       -1.409964       1.836013        1.770368
C       -2.783137       1.721950        0.088456
C       -0.283104       1.387254        -0.032304
H       -3.550379       2.276886        0.640723
H       -2.800616       2.069195        -0.951957
C       -3.079501       0.225357        0.148282
O       0.122446        1.858894        -1.105576
H       -2.388534       -0.317184       -0.507843
H       -2.914579       -0.143947       1.168629
C       -4.513916       -0.076279       -0.279538
H       -5.218123       0.424212        0.395872
H       -4.689479       0.310926        -1.290688
C       -4.769615       -1.571869       -0.260987
H       -4.121586       -2.100506       -0.961195
H       -4.636686       -1.992502       0.736572
N       -6.177979       -1.864984       -0.670651
H       -6.362706       -1.505810       -1.612675
H       -6.363681       -2.872339       -0.673224
H       -6.844431       -1.422239       -0.030280
N       0.192085        0.282310        0.535609
H       -0.211331       -0.057684       1.404567
C       1.197358        -0.565255       -0.088733
H       1.020533        -0.582179       -1.168148
C       2.601259        -0.003570       0.191219
C       1.051813        -1.995137       0.465427
H       2.626759        1.024014        -0.187967
H       2.759806        0.033059        1.274671
```

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C       3.712230        -0.833071       -0.469856
O       0.578764        -2.112155       1.627861
O       1.442733        -2.930139       -0.278991
H       3.785119        -1.821801       -0.016190
H       3.507663        -0.946418       -1.540432
C       5.040114        -0.148853       -0.290280
O       5.878382        -0.475781       0.528587
O       5.289683        0.914817        -1.073867
H       4.564533        1.074226        -1.699604
###
40
LysGlu3 m062x E=-971.959330419 au
N       -1.121707       3.490757        0.546449
H       -0.969741       3.722276        -0.443418
H       -0.286018       3.773934        1.069338
H       -1.918482       4.034996        0.893419
C       -1.381972       2.027163        0.680654
H       -1.372587       1.788798        1.746015
C       -2.740433       1.708874        0.057309
C       -0.244418       1.323509        -0.053365
H       -3.494747       2.294734        0.595300
H       -2.738579       2.043005        -0.987503
C       -3.088466       0.224514        0.135522
O       0.156467        1.782516        -1.134658
H       -2.406993       -0.354274       -0.498716
H       -2.955703       -0.131565       1.165138
C       -4.525791       -0.029040       -0.313456
H       -5.217903       0.541947        0.317401
H       -4.658394       0.312941        -1.347212
C       -4.865361       -1.504717       -0.222541
H       -4.232265       -2.109052       -0.873627
H       -4.783901       -1.874868       0.800196
N       -6.277829       -1.737853       -0.656559
H       -6.413530       -1.433616       -1.626021
H       -6.527255       -2.729508       -0.597944
H       -6.932542       -1.211276       -0.069385
N       0.232305        0.225404        0.524357
H       -0.161589       -0.101600       1.402315
C       1.258154        -0.611170       -0.085645
H       1.077409        -0.650630       -1.163804
C       2.651698        -0.016170       0.180761
C       1.143402        -2.031858       0.494172
H       2.630414        1.025779        -0.160442
H       2.828085        -0.006291       1.262304
C       3.781225        -0.762710       -0.533754
O       0.679050        -2.137865       1.662180
O       1.546586        -2.975826       -0.233321
H       3.898986        -1.762602       -0.104291
H       3.546287        -0.869644       -1.596683
C       5.100123        -0.009627       -0.372094
O       5.581220        0.070985        0.796340
O       5.628014        0.502157        -1.401476
###
39
LysGlu4 m062x E=-971.500995253 au
N       -1.216492       3.498636        0.671564
H       -0.303076       3.711262        1.067766
H       -1.173441       3.768472        -0.310506
C       -1.452988       2.057846        0.742837
H       -1.438367       1.758318        1.795598
C       -2.822823       1.730978        0.147044
C       -0.380412       1.268452        -0.004052
H       -3.577250       2.262115        0.738235
H       -2.863247       2.135394        -0.873217
C       -3.137408       0.237036        0.118991
O       -0.144516       1.499711        -1.205435
H       -2.429152       -0.280516       -0.541449
H       -3.006935       -0.187629       1.123058
C       -4.557861       -0.038292       -0.369233
H       -5.282796       0.423899        0.311850
H       -4.703006       0.408626        -1.360687
C       -4.820428       -1.530023       -0.450361
H       -4.151063       -2.018858       -1.159465
H       -4.725474       -2.014250       0.522366
N       -6.215364       -1.786472       -0.926896
H       -6.364366       -1.369783       -1.851026
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H       -6.408164       -2.789924       -0.996857
H       -6.901016       -1.376587       -0.284971
N       0.262070        0.325922        0.692543
H       0.033515        0.178250        1.669866
C       1.259682        -0.562226       0.113540
H       0.959199        -0.795898       -0.911641
C       2.642865        0.110055        0.102371
C       1.294948        -1.864404       0.930635
H       2.542824        1.056834        -0.441766
H       2.922888        0.351777        1.133429
C       3.727085        -0.748040       -0.549894
O       1.076463        -1.768751       2.169654
O       1.568943        -2.923896       0.307463
H       3.923486        -1.633177       0.067026
H       3.398890        -1.095379       -1.533899
C       5.046215        0.009752        -0.694128
O       5.514110        0.569649        0.339870
O       5.602723        0.024992        -1.830388
###
38
LysGlu5 m062x E=-971.034331861 au
N       -1.232712       3.428611        0.814840
H       -0.310242       3.612408        1.204918
H       -1.202159       3.749916        -0.152176
C       -1.476155       1.986825        0.808273
H       -1.443700       1.629000        1.842177
C       -2.857919       1.696300        0.221896
C       -0.417884       1.241237        -0.001300
H       -3.596170       2.210837        0.847699
H       -2.911965       2.144563        -0.779603
C       -3.190486       0.207984        0.139949
O       -0.182116       1.561666        -1.182021
H       -2.497003       -0.289326       -0.552430
H       -3.037517       -0.255247       1.124734
C       -4.622156       -0.049435       -0.325014
H       -5.328173       0.419597        0.374008
H       -4.781698       0.421321        -1.305087
C       -4.939837       -1.537489       -0.431801
H       -4.235325       -2.008502       -1.125795
H       -4.785194       -2.013520       0.542520
N       -6.300203       -1.852941       -0.881211
H       -6.454634       -1.402741       -1.781473
H       -6.962343       -1.417784       -0.241282
N       0.217494        0.241365        0.618593
H       -0.007457       0.022220        1.583431
C       1.227966        -0.588027       -0.020864
H       0.955119        -0.718117       -1.071550
C       2.607742        0.086340        0.070444
C       1.246772        -1.965648       0.662295
H       2.514574        1.085459        -0.370806
H       2.863608        0.213970        1.129537
C       3.719531        -0.688911       -0.644090
O       0.991156        -1.997294       1.897650
O       1.548272        -2.955570       -0.055354
H       3.854649        -1.668538       -0.178797
H       3.450200        -0.831242       -1.695809
C       5.025768        0.096352        -0.552746
O       5.807089        -0.171218       0.406330
O       5.233515        0.995330        -1.419358
###
48
PheArg1 m062x E=-1085.51791848 au
N       3.189176        3.602548        -0.165614
H       2.556822        4.148659        -0.761478
H       2.973097        3.824803        0.814930
C       3.022373        2.141135        -0.395694
H       3.099502        1.959486        -1.469415
C       4.116201        1.381932        0.376908
C       1.654601        1.748638        0.144145
H       5.083824        1.671193        -0.044513
H       4.081641        1.701974        1.424037
C       3.917765        -0.112376       0.283451
O       1.224357        2.269055        1.178781
C       3.248569        -0.800906       1.301470
C       4.336575        -0.815111       -0.850551
H       2.912975        -0.257087       2.182197
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C       3.007204        -2.170690       1.191554
C       4.096508        -2.184931       -0.962573
H       4.853917        -0.285460       -1.647094
H       2.487803        -2.693036       1.989404
C       3.432034        -2.865629       0.058502
H       4.428468        -2.719937       -1.847186
H       3.243492        -3.931227       -0.030154
N       1.031356        0.780070        -0.534049
H       1.501803        0.366610        -1.335228
C       -0.061223       0.020817        0.051772
H       0.010899        0.084843        1.141672
C       -1.427377       0.553158        -0.412996
C       0.132975        -1.424551       -0.366704
H       -1.461124       1.608981        -0.122219
H       -1.464068       0.507889        -1.507456
C       -2.617464       -0.192246       0.184054
O       0.650751        -1.752612       -1.416319
O       -0.352460       -2.287042       0.520897
H       -2.635169       -1.229423       -0.167898
H       -2.538810       -0.213193       1.277515
C       -3.915505       0.488192        -0.222682
H       -3.939116       1.514483        0.161201
H       -3.988154       0.526648        -1.315800
N       -5.055658       -0.257120       0.308319
H       -4.877188       -1.081853       0.870643
C       -6.321836       0.058348        0.051964
N       -6.612333       1.138588        -0.670555
N       -7.311488       -0.721778       0.498206
H       -5.886522       1.749050        -1.018239
H       -7.576475       1.368049        -0.871593
H       -7.101831       -1.499736       1.109442
H       -8.269906       -0.406582       0.429068
H       4.152606        3.894635        -0.362789
H       -0.245441       -3.195819       0.184213
###
47
PheArg2 m062x E=-1085.06842372 au
N       3.093774        3.601846        -0.202964
H       2.447866        4.115399        -0.812506
H       2.863697        3.835620        0.771668
C       2.970891        2.130705        -0.402188
H       3.051954        1.929213        -1.471936
C       4.091915        1.422651        0.378395
C       1.612095        1.714034        0.147113
H       5.048482        1.747622        -0.042634
H       4.043136        1.747842        1.423469
C       3.951849        -0.077983       0.292388
O       1.169420        2.264113        1.166605
C       3.294316        -0.784866       1.305031
C       4.408795        -0.770007       -0.833343
H       2.928537        -0.248958       2.178630
C       3.096572        -2.161195       1.195470
C       4.212683        -2.146785       -0.945003
H       4.918521        -0.225956       -1.625131
H       2.580685        -2.697108       1.986530
C       3.554487        -2.844782       0.068364
H       4.571649        -2.673422       -1.824071
H       3.396373        -3.915175       -0.021246
N       1.017946        0.712321        -0.496316
H       1.499011        0.271581        -1.276937
C       -0.078515       -0.055325       0.081471
H       -0.006820       0.009360        1.171650
C       -1.431497       0.506745        -0.381105
C       0.092313        -1.528145       -0.338778
H       -1.461360       1.564529        -0.093225
H       -1.470895       0.463860        -1.476454
C       -2.633963       -0.223434       0.209175
O       0.641754        -1.744836       -1.452493
O       -0.357903       -2.399042       0.450188
H       -2.649721       -1.263710       -0.132604
H       -2.565717       -0.236594       1.303808
C       -3.927281       0.456374        -0.212675
H       -3.954639       1.485343        0.163931
H       -3.991370       0.487471        -1.306636
N       -5.072814       -0.284579       0.314086
H       -4.897802       -1.110975       0.875074
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C       -6.336951       0.030064        0.049189
N       -6.623407       1.109126        -0.677063
N       -7.329843       -0.748892       0.491511
H       -5.894851       1.713262        -1.029997
H       -7.586064       1.335453        -0.888239
H       -7.123663       -1.521884       1.110245
H       -8.287314       -0.431840       0.418309
H       4.048285        3.920131        -0.401895
###
46
PheArg3 m062x E=-1084.61126975 au
N       3.201027        3.638990        -0.292081
H       2.471243        4.118634        -0.815621
H       3.068422        3.902196        0.683696
C       3.003454        2.200741        -0.406833
H       3.076499        1.918462        -1.461966
C       4.108596        1.465651        0.380173
C       1.655734        1.729749        0.135394
H       5.068517        1.756852        -0.056531
H       4.081909        1.824452        1.416089
C       3.943208        -0.033855       0.346985
O       1.192498        2.197088        1.190932
C       3.278261        -0.702692       1.381374
C       4.374779        -0.770519       -0.761656
H       2.934161        -0.138565       2.245890
C       3.040797        -2.075595       1.306714
C       4.143201        -2.144160       -0.838401
H       4.891591        -0.260649       -1.571696
H       2.516331        -2.577872       2.114322
C       3.471311        -2.799991       0.194345
H       4.482825        -2.701319       -1.706513
H       3.282855        -3.867487       0.131858
N       1.051256        0.757873        -0.559293
H       1.541500        0.351405        -1.350801
C       -0.028112       -0.050175       -0.008092
H       0.060201        -0.045523       1.083282
C       -1.395596       0.524072        -0.410826
C       0.137427        -1.499023       -0.504058
H       -1.416324       1.571498        -0.086432
H       -1.468286       0.520270        -1.505495
C       -2.583013       -0.223071       0.188620
O       0.678807        -1.664478       -1.631247
O       -0.308674       -2.409446       0.243025
H       -2.603708       -1.255779       -0.174830
H       -2.491388       -0.258584       1.281103
C       -3.885423       0.463777        -0.191777
H       -3.902287       1.487105        0.200759
H       -3.975136       0.512338        -1.283368
N       -5.021785       -0.282367       0.348422
H       -4.837977       -1.109266       0.905820
C       -6.289558       0.035258        0.105960
N       -6.585498       1.118687        -0.610028
N       -7.276759       -0.745036       0.558274
H       -5.861537       1.729793        -0.960368
H       -7.550986       1.350572        -0.801199
H       -7.062695       -1.525121       1.165168
H       -8.234856       -0.426766       0.500561
###
45
PheArg4 m062x E=-1084.13530867 au
N       3.045515        3.678946        -0.281843
H       2.335992        4.124642        -0.860144
H       2.837150        3.947068        0.679372
C       2.909615        2.233252        -0.391682
H       3.047131        1.945736        -1.438867
C       3.998943        1.547220        0.460100
C       1.554648        1.714348        0.083636
H       4.969721        1.854408        0.059982
H       3.915991        1.928299        1.485015
C       3.871172        0.043687        0.455208
O       1.019662        2.170658        1.109730
C       3.183841        -0.616942       1.480095
C       4.351494        -0.705857       -0.624301
H       2.801753        -0.042279       2.321331
C       2.969284        -1.994394       1.422907
C       4.143390        -2.084124       -0.683087
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H       4.885203        -0.202257       -1.427303
H       2.425754        -2.490258       2.221864
C       3.446542        -2.731747       0.338381
H       4.519498        -2.651475       -1.529285
H       3.274938        -3.802754       0.288743
N       1.025830        0.713735        -0.631122
H       1.570308        0.321348        -1.393641
C       -0.052934       -0.126516       -0.128308
H       -0.001623       -0.134147       0.965773
C       -1.418866       0.422508        -0.569027
C       0.163045        -1.564405       -0.635308
H       -1.467368       1.467639        -0.239636
H       -1.456803       0.425198        -1.665650
C       -2.611068       -0.346235       -0.007149
O       0.735363        -1.702860       -1.751083
O       -0.275633       -2.495570       0.090434
H       -2.627850       -1.366242       -0.405705
H       -2.521589       -0.423822       1.084527
C       -3.916931       0.353145        -0.354861
H       -3.908893       1.374888        0.051043
H       -4.012415       0.433339        -1.444153
N       -5.050619       -0.396023       0.171752
H       -4.843125       -0.992892       0.964984
C       -6.311680       0.146071        0.144229
N       -6.681607       1.164534        -0.563334
N       -7.250638       -0.550982       0.884787
H       -5.893511       1.533326        -1.090774
H       -6.898922       -1.025803       1.707783
H       -8.088824       -0.013324       1.065421
###
22
SerGly1 m062x E=-607.253874083 au
N       -3.232933       -0.835607       0.069270
H       -3.148697       -1.776597       -0.332612
H       -4.110728       -0.411190       -0.248725
H       -3.277556       -0.945066       1.089870
C       -2.072413       -0.002108       -0.335871
H       -2.170625       0.186187        -1.409395
C       -2.116424       1.326684        0.415019
C       -0.814248       -0.840396       -0.108974
H       -3.130018       1.736752        0.341826
H       -1.867582       1.172731        1.471124
O       -1.179181       2.184742        -0.215529
O       -0.901834       -2.065117       0.041883
H       -1.053544       2.966893        0.339225
N       0.339819        -0.174360       -0.122372
H       0.334940        0.839491        -0.223315
C       1.600156        -0.862214       0.031875
C       2.720834        0.147938        0.014886
H       1.641069        -1.412406       0.978783
H       1.760511        -1.582303       -0.778204
O       2.546762        1.344858        -0.078726
O       3.958537        -0.341129       0.110695
H       3.972317        -1.310970       0.174946
###
21
SerGly2 m062x E=-606.805699352 au
N       -3.193095       -0.803464       0.058807
H       -3.099650       -1.754727       -0.316647
H       -4.060939       -0.384121       -0.290924
H       -3.263256       -0.887830       1.080202
C       -2.016600       0.013222        -0.337471
H       -2.105484       0.202804        -1.411504
C       -2.049915       1.341668        0.413535
C       -0.772503       -0.845877       -0.103023
H       -3.060340       1.760365        0.340778
H       -1.803410       1.184533        1.469831
O       -1.105942       2.193961        -0.214303
O       -0.890963       -2.074838       0.026792
H       -0.977182       2.974848        0.341347
N       0.389323        -0.204481       -0.088908
H       0.414654        0.809222        -0.182519
C       1.652924        -0.898859       0.059533
C       2.823579        0.087242        0.019946
H       1.685171        -1.442312       1.009188
H       1.782956        -1.630730       -0.743718
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O       2.563633        1.312960        -0.104181
O       3.969393        -0.427184       0.116637
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20
SerGly3 m062x E=-606.348147408 au
N       -3.310334       -0.744581       0.050064
H       -3.304771       -1.648621       -0.416230
H       -3.266975       -0.956353       1.046800
C       -2.098291       -0.029416       -0.325214
H       -2.139063       0.175117        -1.402553
C       -2.079453       1.316167        0.395068
C       -0.827432       -0.865164       -0.100967
H       -3.076025       1.759989        0.310158
H       -1.847402       1.174188        1.458241
O       -1.111576       2.165651        -0.218575
O       -0.894532       -2.102270       0.022568
H       -1.017165       2.963343        0.318881
N       0.337991        -0.213761       -0.088834
H       0.350394        0.799672        -0.172718
C       1.607542        -0.894504       0.054502
C       2.774132        0.095737        0.022164
H       1.648959        -1.446224       0.999743
H       1.748086        -1.622061       -0.751626
O       2.514116        1.322452        -0.095888
O       3.923414        -0.414281       0.117819
###
34
SerLeu1 m062x E=-764.438295278 au
N       3.627855        -1.762699       -0.396962
H       3.103885        -2.645948       -0.398022
H       4.535597        -1.909066       0.056322
H       3.791848        -1.507225       -1.378528
C       2.850597        -0.711114       0.307493
H       2.813045        -0.990182       1.364787
C       3.569166        0.627715        0.160083
C       1.427441        -0.760464       -0.250450
H       4.631121        0.483573        0.389886
H       3.472411        0.992901        -0.868734
O       2.969726        1.523439        1.081949
O       1.049178        -1.753070       -0.884572
H       3.249721        2.423605        0.865553
N       0.657254        0.294948        0.020202
H       1.043137        1.069408        0.557516
C       -0.747811       0.318741        -0.350914
H       -0.852196       -0.158355       -1.328806
C       -1.596266       -0.417573       0.707785
C       -1.167343       1.775454        -0.441237
H       -1.140052       -1.408020       0.832345
H       -1.479887       0.119930        1.656737
C       -3.083075       -0.594414       0.384452
O       -0.666743       2.641958        0.246980
O       -2.152637       2.090966        -1.283353
H       -3.539423       0.395969        0.250407
C       -3.296299       -1.415037       -0.888911
C       -3.769268       -1.272669       1.570403
H       -2.802189       -2.390111       -0.796184
H       -4.363233       -1.592445       -1.056675
H       -2.900540       -0.923512       -1.783939
H       -3.646027       -0.690362       2.489071
H       -4.840830       -1.392964       1.383491
H       -3.342029       -2.268456       1.739561
H       -2.449164       1.335337        -1.817720
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33
SerLeu2 m062x E=-763.989309002 au
N       3.620513        -1.760109       -0.374192
H       3.093237        -2.641643       -0.371383
H       4.526077        -1.903378       0.083848
H       3.788782        -1.512019       -1.356853
C       2.836576        -0.704105       0.317851
H       2.818439        -0.961846       1.380987
C       3.537090        0.639245        0.131932
C       1.405545        -0.787240       -0.220966
H       4.604729        0.511775        0.345786
H       3.419459        0.982311        -0.902396
O       2.945877        1.549493        1.044817
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O       1.034481        -1.818734       -0.803849
H       3.212870        2.446843        0.802301
N       0.634397        0.270868        0.003576
H       1.018823        1.080455        0.486487
C       -0.772016       0.315870        -0.377854
H       -0.877815       -0.173264       -1.348680
C       -1.625557       -0.404626       0.682080
C       -1.198480       1.786355        -0.508268
H       -1.211523       -1.414998       0.804687
H       -1.488086       0.119941        1.636470
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O       -0.608139       2.624050        0.227779
O       -2.130439       2.037912        -1.316465
H       -3.543372       0.488280        0.291630
C       -3.372179       -1.261631       -0.942509
C       -3.818732       -1.241046       1.527241
H       -2.878140       -2.241473       -0.926916
H       -4.443810       -1.428265       -1.093664
H       -2.997433       -0.707152       -1.807982
H       -3.648863       -0.726291       2.478772
H       -4.898981       -1.296585       1.358850
H       -3.439492       -2.265664       1.625143
###
32
SerLeu3 m062x E=-763.531612357 au
N       3.762180        -1.785388       -0.291358
H       3.315400        -2.691874       -0.176554
H       3.799361        -1.630738       -1.298477
C       2.901338        -0.770262       0.298704
H       2.834447        -0.959461       1.377412
C       3.556763        0.596441        0.112117
C       1.460204        -0.835212       -0.236252
H       4.622002        0.494922        0.341944
H       3.451612        0.927047        -0.928925
O       2.950556        1.536611        0.997368
O       1.051422        -1.847402       -0.834402
H       3.235347        2.425152        0.745263
N       0.681259        0.224351        0.002938
H       1.072970        1.025169        0.492050
C       -0.723341       0.285221        -0.377213
H       -0.835298       -0.185380       -1.356550
C       -1.589468       -0.445627       0.665639
C       -1.145712       1.758625        -0.482179
H       -1.212032       -1.474453       0.744278
H       -1.420362       0.036811        1.637111
C       -3.093129       -0.490043       0.375682
O       -0.598176       2.572896        0.311688
O       -2.034969       2.040185        -1.329226
H       -3.471983       0.540152        0.343052
C       -3.399958       -1.163056       -0.962883
C       -3.806046       -1.223126       1.512781
H       -2.974365       -2.174432       -0.986561
H       -4.481373       -1.251028       -1.111004
H       -2.993198       -0.604491       -1.810890
H       -3.604992       -0.751002       2.480210
H       -4.889603       -1.230555       1.356345
H       -3.466583       -2.264662       1.568426
###
49
TyrArg1 m062x E=-1160.72837946 au
N       2.814354        3.955786        -0.137196
H       2.169381        4.456804        -0.758242
H       2.541669        4.155159        0.833905
C       2.769862        2.487090        -0.380550
H       2.912397        2.322324        -1.450122
C       3.882886        1.803429        0.438609
C       1.410435        1.984910        0.083834
H       4.844230        2.130306        0.030849
H       3.808249        2.152098        1.474652
C       3.749308        0.301116        0.390807
O       0.883552        2.461798        1.094655
C       3.058084        -0.375854       1.401965
C       4.209281        -0.430047       -0.707737
H       2.690161        0.178930        2.262391
C       2.816017        -1.744066       1.318712
C       3.978585        -1.801069       -0.805127
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H 4.747220 0.077952 -1.504551
H 2.272237 -2.266312 2.099926
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H 4.332289 -2.366359 -1.663421
O 2.984039 -3.792217 0.148313
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H 1.450198 0.595688 -1.396815
C -0.151162 0.127046 -0.087852
H -0.096060 0.152528 1.005352
C -1.543286 0.596451 -0.544628
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O 0.699161 -1.550719 -1.596941
O -0.337797 -2.209066 0.282454
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H 3.358979 -4.175502 -0.658325
H 3.760503 4.320774 -0.292245
H -0.165652 -3.097876 -0.080272
###
48
TyrArg2 m062x E=-1160.27850960 au
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H 2.089333 4.433485 -0.828314
H 2.379891 4.162492 0.784661
C 2.709183 2.484456 -0.383846
H 2.864073 2.302876 -1.448830
C 3.834319 1.845717 0.453109
C 1.356500 1.961484 0.082492
H 4.789119 2.207304 0.059072
H 3.733047 2.192300 1.487697
C 3.758738 0.339850 0.401710
O 0.815969 2.464496 1.078991
C 3.084153 -0.368197 1.402677
C 4.259256 -0.367593 -0.694245
H 2.681577 0.168651 2.259032
C 2.901330 -1.744775 1.313213
C 4.087709 -1.746753 -0.797971
H 4.783719 0.164927 -1.484058
H 2.369378 -2.291644 2.085590
C 3.398784 -2.430469 0.204607
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O 3.180511 -3.784332 0.148293
N 0.876908 0.921654 -0.596888
H 1.435908 0.520945 -1.346392
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H -0.119506 0.093031 1.029175
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C 0.092794 -1.381402 -0.530768
H -1.640750 1.607435 -0.236114
H -1.608473 0.499194 -1.613254
C -2.712655 -0.233900 0.096717
O 0.685213 -1.527880 -1.634143
O -0.331876 -2.303545 0.212412
H -2.689948 -1.274137 -0.244020
H -2.615640 -0.242224 1.189474
C -4.047332 0.386653 -0.286477
H -4.100356 1.423230 0.066317
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H       -7.770457       1.156316        -0.724892
H       -7.089055       -1.647899       1.284990
H       -8.331691       -0.681862       0.552727
H       3.562440        -4.149377       -0.663538
H       3.656252        4.345673        -0.275869
###
47
TyrArg3 m062x E=-1159.82122259 au
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H       2.112826        4.431907        -0.777367
H       2.674315        4.226913        0.737806
C       2.751396        2.543259        -0.379371
H       2.878332        2.283163        -1.435088
C       3.872398        1.864336        0.436919
C       1.418159        1.978464        0.104790
H       4.828091        2.196806        0.020665
H       3.806054        2.229506        1.468986
C       3.768889        0.359449        0.414799
O       0.887871        2.397530        1.148845
C       3.109755        -0.327824       1.440682
C       4.220708        -0.373630       -0.686729
H       2.745341        0.223930        2.304597
C       2.890290        -1.701275       1.368796
C       4.013549        -1.749256       -0.774225
H       4.733937        0.138788        -1.497258
H       2.368148        -2.228574       2.161469
C       3.337635        -2.408284       0.253034
H       4.362182        -2.312114       -1.636384
O       3.085504        -3.758612       0.212373
N       0.901339        0.979795        -0.623366
H       1.445981        0.613179        -1.398598
C       -0.137721       0.097080        -0.109623
H       -0.062385       0.077628        0.982884
C       -1.532322       0.603063        -0.511207
C       0.111806        -1.327351       -0.639894
H       -1.607541       1.645565        -0.179420
H       -1.606296       0.601952        -1.605833
C       -2.675415       -0.207768       0.090737
O       0.669152        -1.434195       -1.766477
O       -0.290454       -2.280151       0.078657
H       -2.647503       -1.238250       -0.278269
H       -2.570494       -0.244607       1.182270
C       -4.017196       0.411968        -0.267049
H       -4.070209       1.443531        0.100330
H       -4.142939       0.427001        -1.355812
N       -5.098066       -0.371098       0.331108
H       -4.853693       -1.143466       0.941393
C       -6.387188       -0.087929       0.177366
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H       -6.085515       1.532685        -1.034059
H       -7.745435       1.163520        -0.677066
H       -7.037802       -1.653355       1.304251
H       -8.289371       -0.689682       0.585653
H       3.436398        -4.133644       -0.608624
###
46
TyrArg4 m062x E=-1159.34436788 au
N       2.878087        3.951621        -0.241281
H       2.136504        4.389013        -0.784703
H       2.695552        4.192931        0.732132
C       2.784423        2.503658        -0.376373
H       2.921548        2.239384        -1.429893
C       3.898372        1.828730        0.453228
C       1.448374        1.937956        0.096420
H       4.856136        2.170877        0.047180
H       3.819313        2.202101        1.482438
C       3.803446        0.323375        0.438482
O       0.907519        2.358932        1.135067
C       3.134988        -0.372876       1.453748
C       4.248152        -0.421037       -0.662080
H       2.768988        0.177782        2.320180
C       2.904363        -1.743908       1.375037
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C       3.331646        -2.511353       0.255915
H       4.383506        -2.342613       -1.624431
O       3.098195        -3.797702       0.159334
N       0.934049        0.940874        -0.635981
H       1.490189        0.565685        -1.398815
C       -0.114323       0.065143        -0.128779
H       -0.032971       0.027168        0.963025
C       -1.504808       0.596054        -0.513195
C       0.108763        -1.354315       -0.683121
H       -1.561917       1.636773        -0.172488
H       -1.589309       0.604804        -1.607054
C       -2.653145       -0.204088       0.092931
O       0.655209        -1.451542       -1.815866
O       -0.303377       -2.312046       0.023225
H       -2.635811       -1.234236       -0.277331
H       -2.543487       -0.243316       1.183952
C       -3.992002       0.426011        -0.257469
H       -4.037274       1.456996        0.112560
H       -4.122689       0.443956        -1.345585
N       -5.074493       -0.352657       0.343788
H       -4.830993       -1.125828       0.953430
C       -6.363064       -0.066335       0.192389
N       -6.741012       0.942523        -0.591690
N       -7.289420       -0.784251       0.838418
H       -6.059273       1.552742        -1.020372
H       -7.719724       1.187836        -0.660810
H       -7.015496       -1.630690       1.319541
H       -8.265869       -0.663775       0.603589
###
45
TyrArg5 m062x E=-1158.86583284 au
N       -2.737946       3.970578        0.341348
H       -1.992412       4.374799        0.904513
H       -2.537045       4.230843        -0.623503
C       -2.684807       2.517691        0.441988
H       -2.831739       2.232690        1.488633
C       -3.815933       1.894753        -0.405016
C       -1.364303       1.926214        -0.043499
H       -4.764684       2.249588        0.011234
H       -3.727479       2.294809        -1.423371
C       -3.757601       0.387802        -0.433313
O       -0.816775       2.351285        -1.077189
C       -3.103450       -0.293467       -1.467799
C       -4.219089       -0.377729       0.645643
H       -2.725210       0.273787        -2.318083
C       -2.901824       -1.670681       -1.428015
C       -4.029570       -1.755350       0.700136
H       -4.729051       0.121190        1.469288
H       -2.381009       -2.169128       -2.243075
C       -3.345295       -2.459847       -0.330594
H       -4.395591       -2.322655       1.553257
O       -3.138183       -3.752974       -0.270662
N       -0.872843       0.904295        0.669520
H       -1.432581       0.532540        1.431254
C       0.154172        0.012244        0.145811
H       0.062789        -0.013602       -0.945619
C       1.557612        0.514070        0.520450
C       -0.094465       -1.408051       0.686232
H       1.636775        1.545857        0.156587
H       1.640609        0.547425        1.613832
C       2.693780        -0.320094       -0.065047
O       -0.637225       -1.507627       1.820853
O       0.293560        -2.366174       -0.033016
H       2.718464        -1.310883       0.403377
H       2.531006        -0.471933       -1.139328
C       4.034407        0.367075        0.148888
H       4.025302        1.333523        -0.365971
H       4.179857        0.560219        1.222190
N       5.113726        -0.456459       -0.390581
H       4.955882        -1.455682       -0.321764
C       6.440103        -0.135448       -0.220439
N       6.707817        1.202386        -0.020260
N       7.341672        -1.058308       -0.350632
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H       5.994236        1.767384        0.422146
H       7.643379        1.398497        0.311819
H       8.268076        -0.647890       -0.245622
###
32
TyrGly1 m062x E=-838.237920689 au
N       3.993827        -0.432394       -0.373126
H       4.416503        0.272190        -0.987367
H       4.400548        -1.345325       -0.603723
H       4.241887        -0.197332       0.596673
C       2.511935        -0.461701       -0.518621
H       2.281496        -0.556858       -1.581336
C       1.951649        -1.655001       0.277533
C       1.973886        0.840839        0.055151
H       2.345481        -2.569960       -0.175556
H       2.326265        -1.587820       1.305214
C       0.442992        -1.657757       0.273469
O       2.503807        1.348788        1.049088
C       -0.271557       -1.071648       1.322453
C       -0.269216       -2.166101       -0.817608
H       0.266366        -0.663313       2.175497
C       -1.662251       -0.990310       1.290569
C       -1.658712       -2.095596       -0.864452
H       0.269992        -2.623188       -1.643803
H       -2.213019       -0.530971       2.107270
C       -2.352079       -1.501756       0.190757
H       -2.212090       -2.490539       -1.710685
O       -3.719633       -1.441383       0.094627
H       -4.087176       -0.998692       0.873562
N       0.884702        1.329125        -0.546286
H       0.448666        0.782510        -1.285144
C       0.051293        2.311417        0.109781
C       -1.360874       2.191670        -0.410209
H       0.041359        2.142381        1.193096
H       0.404184        3.333598        -0.066634
O       -1.699251       1.398962        -1.263334
O       -2.255427       3.027323        0.120490
H       -1.858529       3.622346        0.778911
###
31
TyrGly2 m062x E=-837.789918490 au
N       3.969196        -0.522522       -0.373504
H       4.416849        0.157775        -0.997089
H       4.342003        -1.453056       -0.590109
H       4.223673        -0.281717       0.593247
C       2.486640        -0.496321       -0.518121
H       2.251282        -0.586420       -1.580092
C       1.882869        -1.665834       0.282786
C       1.996887        0.825378        0.056817
H       2.240561        -2.597193       -0.166946
H       2.262117        -1.609212       1.309456
C       0.374771        -1.613576       0.282710
O       2.547276        1.299388        1.061581
C       -0.312905       -0.960759       1.310467
C       -0.361484       -2.137463       -0.784621
H       0.243836        -0.540608       2.145711
C       -1.698729       -0.821992       1.276969
C       -1.747443       -2.013269       -0.831153
H       0.156061        -2.647587       -1.593468
H       -2.227515       -0.305611       2.073924
C       -2.411893       -1.345899       0.198145
H       -2.319130       -2.418054       -1.660412
O       -3.775568       -1.226089       0.098720
H       -4.118261       -0.717248       0.848183
N       0.931241        1.354194        -0.540851
H       0.480860        0.832998        -1.290429
C       0.073569        2.317976        0.125049
C       -1.366205       2.192663        -0.387596
H       0.087210        2.141626        1.204667
H       0.413450        3.343870        -0.051584
O       -1.571360       1.475707        -1.401182
O       -2.231913       2.847658        0.251719
###
30
TyrGly3 m062x E=-837.331994732 au
N       4.018929        -0.567264       -0.467201
```

```
H       4.428771        0.213040        -0.976598
H       4.302966        -0.451625       0.504899
C       2.567081        -0.471221       -0.530605
H       2.255458        -0.513925       -1.578957
C       1.940783        -1.665061       0.222473
C       2.016181        0.806158        0.096434
H       2.285012        -2.578249       -0.272066
H       2.338723        -1.662738       1.244689
C       0.432801        -1.613470       0.253548
O       2.478441        1.244180        1.164330
C       -0.243300       -0.989321       1.307063
C       -0.323755       -2.103432       -0.817053
H       0.323681        -0.597585       2.149230
C       -1.629335       -0.839733       1.293333
C       -1.709870       -1.971068       -0.844699
H       0.180213        -2.593112       -1.647135
H       -2.145354       -0.342214       2.110632
C       -2.358567       -1.327417       0.209159
H       -2.293144       -2.349226       -1.678680
O       -3.724282       -1.193912       0.128522
H       -4.051831       -0.701016       0.894988
N       0.980219        1.378023        -0.532775
H       0.567175        0.880853        -1.317618
C       0.072821        2.282785        0.148279
C       -1.351013       2.143210        -0.401726
H       0.061990        2.060213        1.219568
H       0.381424        3.327471        0.031410
O       -1.519113       1.466112        -1.449414
O       -2.249056       2.749146        0.243843
###
29
TyrGly4 m062x E=-836.854551993 au
N       3.991224        -0.527968       -0.490490
H       4.386039        0.269718        -0.984596
H       4.279115        -0.428561       0.482291
C       2.536572        -0.454475       -0.542403
H       2.219294        -0.486008       -1.589537
C       1.930198        -1.667435       0.195943
C       1.974073        0.808184        0.101859
H       2.295228        -2.566281       -0.311902
H       2.338189        -1.672255       1.215218
C       0.422232        -1.648483       0.239507
O       2.448262        1.251949        1.163051
C       -0.268238       -1.061350       1.308097
C       -0.344209       -2.117102       -0.835565
H       0.298357        -0.678108       2.157015
C       -1.654828       -0.938542       1.308340
C       -1.732095       -2.007919       -0.849887
H       0.160815        -2.577003       -1.684509
H       -2.160741       -0.471503       2.150950
C       -2.446848       -1.401276       0.220723
H       -2.299151       -2.382867       -1.699250
O       -3.752256       -1.275603       0.206147
N       0.921657        1.369886        -0.508423
H       0.489219        0.859949        -1.274468
C       0.033972        2.286059        0.181858
C       -1.387594       2.205923        -0.384818
H       -0.000563       2.040054        1.248189
H       0.378545        3.322131        0.095067
O       -1.583776       1.494551        -1.404404
O       -2.256471       2.886080        0.225957
###
46
TyrHisOMe3 m062x E=-1142.23908011 au
N       -3.332159       -3.485003       -0.210492
H       -3.154611       -3.787036       0.755829
H       -2.884011       -4.159477       -0.840452
H       -4.343778       -3.509617       -0.380375
C       -2.799994       -2.109738       -0.417885
H       -2.906367       -1.866964       -1.477010
C       -3.596620       -1.125394       0.457563
C       -1.342337       -2.111788       0.018063
H       -4.636873       -1.149814       0.118243
H       -3.562499       -1.485223       1.491935
C       -3.040490       0.275725        0.377299
O       -0.987352       -2.778102       0.994133
```

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C       -2.135417       0.742010        1.336096
C       -3.373521       1.117046        -0.689281
H       -1.854260       0.097766        2.166704
C       -1.586049       2.020501        1.248250
C       -2.833622       2.395974        -0.792746
H       -4.071059       0.769908        -1.447703
H       -0.887909       2.379821        2.000508
C       -1.943132       2.847299        0.182312
H       -3.098310       3.050859        -1.616954
O       -1.444751       4.117737        0.043515
H       -0.848698       4.323407        0.779223
N       -0.532375       -1.301655       -0.678511
H       -0.932314       -0.734018       -1.422184
C       0.741065        -0.869090       -0.141559
H       0.746825        -1.028942       0.939705
C       1.919174        -1.647782       -0.778797
C       0.888654        0.615452        -0.426380
H       1.791137        -2.702158       -0.524556
H       1.869750        -1.544046       -1.866841
C       3.239553        -1.167070       -0.282354
O       0.410788        1.163400        -1.400623
O       1.656747        1.214182        0.472129
N       3.962555        -0.181424       -0.928885
C       3.928588        -1.447166       0.859523
H       3.699528        0.267295        -1.803478
C       5.036506        0.141475        -0.215620
N       5.033521        -0.623798       0.870660
H       3.723064        -2.146339       1.654059
H       5.781469        0.876109        -0.478853
H       5.751901        -0.601218       1.588523
C       1.992674        2.589920        0.207704
H       2.562155        2.655541        -0.721907
H       1.082207        3.187581        0.136433
H       2.598210        2.907740        1.053384
###
45
TyrHisOMe4 m062x E=-1141.78719080 au
N       -3.378499       -3.432177       -0.199382
H       -3.242306       -3.715715       0.779225
H       -2.927436       -4.132382       -0.798332
H       -4.383922       -3.433253       -0.403945
C       -2.801085       -2.076412       -0.417280
H       -2.855177       -1.859740       -1.485901
C       -3.610540       -1.050239       0.395548
C       -1.363895       -2.106488       0.081601
H       -4.635025       -1.058400       0.010123
H       -3.632541       -1.383270       1.439218
C       -3.018010       0.335460        0.305520
O       -1.074508       -2.749722       1.096114
C       -2.147808       0.806482        1.293517
C       -3.285436       1.158096        -0.793819
H       -1.916300       0.176077        2.149564
C       -1.572557       2.073295        1.204072
C       -2.718204       2.424807        -0.899695
H       -3.953877       0.806302        -1.575966
H       -0.903407       2.436490        1.980202
C       -1.866999       2.883230        0.106732
H       -2.933478       3.066104        -1.748649
O       -1.344842       4.144283        -0.033505
H       -0.784903       4.360049        0.727342
N       -0.502773       -1.352031       -0.610030
H       -0.851993       -0.813224       -1.398629
C       0.785721        -0.960689       -0.069031
H       0.780738        -1.132221       1.009802
C       1.947989        -1.754706       -0.713856
C       0.963766        0.524934        -0.330333
H       1.854675        -2.791606       -0.379917
H       1.822061        -1.727932       -1.800558
C       3.277976        -1.184369       -0.344793
O       0.558320        1.081773        -1.333796
O       1.642739        1.124757        0.637032
N       3.833235        -0.147838       -1.069229
C       4.048214        -1.449289       0.758359
C       4.914792        0.206028        -0.403232
N       5.087595        -0.553236       0.703442
H       3.945855        -2.168325       1.556832
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H 5.607770 0.986521 -0.682158
H 5.853670 -0.478741 1.361119
C 2.002358 2.498311 0.405676
H 2.652330 2.565680 -0.469125
H 1.104357 3.099403 0.253384
H 2.530638 2.815732 1.302072
###
44
TyrHisOMe5 m062x E=-1141.33092820 au
N -3.423115 -3.489719 -0.256415
H -2.869050 -4.189898 -0.745322
H -3.397493 -3.743729 0.730427
C -2.796706 -2.184557 -0.412703
H -2.779869 -1.928100 -1.476729
C -3.623796 -1.125367 0.341849
C -1.375373 -2.129676 0.138470
H -4.630730 -1.136487 -0.086146
H -3.700227 -1.442734 1.388845
C -3.038642 0.264163 0.266459
O -1.094488 -2.638330 1.233002
C -2.213173 0.759657 1.281286
C -3.274777 1.078282 -0.847619
H -2.006091 0.142101 2.152827
C -1.654756 2.035881 1.203978
C -2.726111 2.354273 -0.942296
H -3.908382 0.711191 -1.651787
H -1.020989 2.415247 2.002015
C -1.922118 2.834240 0.092199
H -2.920603 2.986182 -1.803420
O -1.416437 4.105493 -0.035886
H -0.892942 4.333963 0.746631
N -0.476537 -1.462313 -0.609501
H -0.802968 -1.004878 -1.455586
C 0.796677 -1.017088 -0.080070
H 0.809929 -1.203868 0.995459
C 1.986973 -1.749619 -0.746289
C 0.923403 0.477838 -0.320272
H 1.935287 -2.797151 -0.437839
H 1.856942 -1.701960 -1.832101
C 3.295995 -1.138442 -0.366808
O 0.516060 1.036169 -1.322374
O 1.572889 1.089197 0.662793
N 3.817219 -0.072600 -1.073821
C 4.069091 -1.389366 0.737892
C 4.880676 0.312379 -0.395807
N 5.073835 -0.453749 0.702605
H 3.988296 -2.121733 1.526664
H 5.546077 1.121678 -0.659595
H 5.833306 -0.360648 1.365504
C 1.907398 2.471039 0.446453
H 2.565645 2.558136 -0.420438
H 1.000950 3.057810 0.289125
H 2.420357 2.791486 1.350772
###
43
TyrHisOMe6 m062x E=-1140.85336418 au
N -3.133258 -3.643905 -0.070649
H -2.456508 -4.335642 -0.386346
H -3.205549 -3.750379 0.940380
C -2.631463 -2.305440 -0.357506
H -2.493326 -2.210172 -1.439059
C -3.653895 -1.254545 0.109721
C -1.305090 -2.012360 0.339046
H -4.567977 -1.412856 -0.472394
H -3.889519 -1.462585 1.161031
C -3.153408 0.161792 -0.031512
O -1.161010 -2.223886 1.551504
C -2.655906 0.870497 1.069074
C -3.092586 0.793905 -1.281749
H -2.685019 0.405448 2.053810
C -2.128829 2.153269 0.939328
C -2.561991 2.071230 -1.430295
H -3.469436 0.269997 -2.159708
H -1.756087 2.678778 1.816391
C -2.051743 2.805603 -0.322027
H -2.526798 2.535981 -2.413367

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O       -1.541744       4.004963       -0.456537
N       -0.325946       -1.512739       -0.440509
H       -0.545571       -1.299521       -1.408747
C       0.931730        -1.005272       0.074356
H       1.036849        -1.345098       1.105545
C       2.093881        -1.499776       -0.795719
C       0.911266        0.519974        0.047066
H       2.126802        -2.591722       -0.718373
H       1.875713        -1.250747       -1.839825
C       3.409077        -0.887122       -0.422116
O       0.796386        1.161197        -0.981109
O       1.068419        1.065670        1.247156
N       4.372842        -0.618788       -1.374121
C       3.865745        -0.517023       0.819105
C       5.389133        -0.101124       -0.711079
N       5.129661        -0.019511       0.612762
H       3.422163        -0.564870       1.802069
H       6.323171        0.231229        -1.139520
H       5.753910        0.351371        1.318293
C       1.235711        2.496778        1.273698
H       2.195962        2.748549        0.816711
H       0.421271        2.989004        0.739975
H       1.230659        2.771966        2.326300
###
27
ValGly1 m062x E=-610.648339876 au
N       -2.756294       -1.288899       -0.841996
H       -2.844618       -1.769406       0.061938
H       -2.491836       -1.995040       -1.537749
H       -3.668515       -0.901243       -1.105474
C       -1.727686       -0.210501       -0.758824
H       -1.502825       0.094639        -1.782849
C       -2.279967       0.992639        0.033046
C       -0.505265       -0.848434       -0.107626
H       -3.251333       1.215594        -0.427211
C       -2.490439       0.684601        1.515357
C       -1.384250       2.217946        -0.149218
O       -0.634759       -1.816691       0.652054
H       -1.533029       0.503809        2.016538
H       -2.963776       1.543575        1.998773
H       -3.136237       -0.183716       1.682375
H       -1.176975       2.410544        -1.206543
H       -1.884235       3.096648        0.266598
H       -0.431447       2.099398        0.377141
N       0.674427        -0.295149       -0.395118
H       0.734737        0.511634        -1.009730
C       1.884110        -0.750693       0.249414
C       3.009833        0.204224        -0.061218
H       1.754387        -0.791475       1.336933
H       2.164427        -1.754197       -0.089894
O       2.862185        1.235480        -0.683018
O       4.216705        -0.136548       0.392634
H       4.213277        -0.989048       0.860008
###
26
ValGly2 m062x E=-610.200329357 au
N       -2.736502       -1.245531       -0.838679
H       -2.833087       -1.720502       0.067318
H       -2.496901       -1.961882       -1.532794
H       -3.636728       -0.829860       -1.099437
C       -1.672226       -0.201501       -0.759990
H       -1.434127       0.088513        -1.785299
C       -2.189619       1.023402        0.020783
C       -0.472873       -0.873981       -0.097955
H       -3.151849       1.274332        -0.444195
C       -2.415410       0.732232        1.504300
C       -1.255570       2.219366        -0.164567
O       -0.646381       -1.838127       0.665066
H       -1.466380       0.519542        2.008911
H       -2.858166       1.610715        1.981745
H       -3.092785       -0.111198       1.674967
H       -1.039379       2.399926        -1.222306
H       -1.729049       3.115640        0.244914
H       -0.308251       2.073602        0.364983
N       0.718713        -0.355939       -0.376186
H       0.805288        0.459354        -0.977097
```

```
C       1.933046        -0.797858       0.281410
C       3.091271        0.157408        -0.020912
H       1.783168        -0.831405       1.365364
H       2.207644        -1.804900       -0.046952
O       2.844780        1.188928        -0.699390
O       4.209528        -0.179050       0.450014
###
25
ValGly3 m062x E=-609.739637951 au
N       -2.600461       -1.312274       -1.116989
H       -2.829715       -1.787002       -0.245619
H       -3.466859       -0.898139       -1.455653
C       -1.658998       -0.233263       -0.821717
H       -1.289076       0.167284        -1.771359
C       -2.269985       0.955024        -0.035327
C       -0.479643       -0.836813       -0.075354
H       -3.131563       1.267283        -0.641772
C       -2.779905       0.565333        1.351407
C       -1.303722       2.136284        0.057602
O       -0.643106       -1.728527       0.778465
H       -1.949393       0.311621        2.019556
H       -3.322263       1.404474        1.798204
H       -3.462839       -0.289705       1.315288
H       -0.886591       2.392821        -0.922553
H       -1.820723       3.018654        0.446745
H       -0.470755       1.914538        0.734336
N       0.729167        -0.353004       -0.375743
H       0.824800        0.409155        -1.039211
C       1.924511        -0.735793       0.346264
C       3.105506        0.166397        -0.019887
H       1.756046        -0.666597       1.425929
H       2.199085        -1.772635       0.124533
O       2.924464        1.064739        -0.883915
O       4.183933        -0.075940       0.585796
###
28
AlaGlyGly1 m062x E=-740.013845537 au
N       5.027123        0.525595        -0.618322
H       5.146174        1.199081        0.147815
H       4.854889        1.059828        -1.476702
H       5.898915        -0.001747       -0.732816
C       3.897542        -0.398090       -0.314008
H       3.733345        -1.009418       -1.202772
C       4.255614        -1.256335       0.891663
C       2.679836        0.473446        -0.029217
H       4.410275        -0.628195       1.773875
H       3.445313        -1.959221       1.093628
H       5.165897        -1.825073       0.687079
O       2.817923        1.649551        0.331662
N       1.497304        -0.125999       -0.164413
H       1.441075        -1.107147       -0.424211
C       0.267117        0.546543        0.189620
C       -0.896842       -0.394904       -0.049518
H       0.271713        0.835694        1.246671
H       0.138737        1.455850        -0.404908
O       -0.722876       -1.592279       -0.310229
N       -2.111341       0.154581        0.060360
H       -2.212117       1.143919        0.265253
C       -3.304205       -0.646753       -0.085347
C       -4.521906       0.229714        0.010461
H       -3.322604       -1.156905       -1.053967
H       -3.367892       -1.415578       0.692199
O       -4.493480       1.436546        0.144381
O       -5.644914       -0.482271       -0.068981
H       -6.411478       0.115581        -0.011101
###
27
AlaGlyGly2 m062x E=-739.562645303 au
N       5.014029        0.449375        -0.451420
H       5.068113        1.198807        0.248447
H       4.927280        0.893302        -1.371732
H       5.888380        -0.085944       -0.430470
C       3.851241        -0.437421       -0.162496
H       3.770812        -1.142547       -0.991510
C       4.079010        -1.161590       1.157715
C       2.621334        0.461077        -0.097688
```

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H       4.154645        -0.444233       1.980038
H       3.244916        -1.838581       1.350927
H       4.998221        -1.750135       1.106005
O       2.741352        1.674934        0.118143
N       1.446958        -0.149127       -0.247072
H       1.395311        -1.147839       -0.428309
C       0.202285        0.574896        -0.111650
C       -0.957246       -0.397460       -0.237379
H       0.156923        1.080753        0.857784
H       0.115109        1.339640        -0.890738
O       -0.768803       -1.598192       -0.490835
N       -2.167709       0.131858        -0.067324
H       -2.277773       1.115885        0.158696
C       -3.381523       -0.654018       -0.159135
C       -4.612299       0.202686        0.147731
H       -3.493655       -1.075806       -1.163237
H       -3.351917       -1.489358       0.547558
O       -4.436195       1.418361        0.423929
O       -5.719620       -0.396066       0.094347
###
26
AlaGlyGly3 m062x E=-739.103674583 au
N       4.949604        -0.128462       -0.925858
H       5.191363        0.853313        -0.796833
H       4.576201        -0.208200       -1.869672
C       3.909428        -0.474449       0.039088
H       3.620414        -1.515924       -0.127904
C       4.445314        -0.320588       1.459575
C       2.670062        0.404775        -0.105837
H       4.785778        0.707354        1.623132
H       3.674576        -0.552929       2.199601
H       5.290112        -0.996637       1.611503
O       2.765573        1.640106        -0.211600
N       1.483601        -0.215189       -0.085490
H       1.429622        -1.228005       -0.056060
C       0.242267        0.518179        -0.186226
C       -0.923894       -0.452745       -0.165272
H       0.146408        1.235973        0.634076
H       0.205763        1.083665        -1.124489
O       -0.750370       -1.676588       -0.285625
N       -2.129127       0.101490        -0.033591
H       -2.230939       1.104969        0.083956
C       -3.350507       -0.676341       -0.058619
C       -4.576704       0.224637        0.111768
H       -3.442657       -1.218412       -1.005318
H       -3.350676       -1.418682       0.746080
O       -4.387936       1.460511        0.261885
O       -5.692306       -0.360551       0.089045
###
46
AlaLysAla1 m062x E=-992.290968482 au
N       4.041264        -2.882685       -0.819206
H       4.063595        -2.427405       -1.739575
H       3.414013        -3.691098       -0.889581
C       3.578385        -1.918200       0.219004
H       3.483773        -2.472864       1.153966
C       4.588369        -0.785367       0.346378
C       2.218928        -1.397939       -0.236660
H       4.651679        -0.220991       -0.588506
H       4.284201        -0.112365       1.149738
H       5.572712        -1.192344       0.590690
O       1.893679        -1.453031       -1.428205
N       1.462891        -0.852315       0.721458
H       1.764838        -0.895762       1.690597
C       0.166875        -0.256953       0.426229
H       0.235140        0.196078        -0.565498
C       -0.948324       -1.314002       0.429025
C       -0.079987       0.785343        1.513987
H       -0.631197       -2.115478       -0.247483
H       -1.019172       -1.738119       1.437584
C       -2.301727       -0.767345       -0.017988
O       0.071992        0.465960        2.697156
H       -2.617614       0.054129        0.639252
C       -3.373897       -1.854765       -0.008918
H       -3.062790       -2.687435       -0.651767
H       -3.495303       -2.248244       1.007602
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C       -4.700462       -1.309245       -0.501698
H       -5.067065       -0.498763       0.129699
H       -4.634359       -0.957059       -1.531951
N       -5.744520       -2.380803       -0.477313
H       -5.884345       -2.729794       0.476070
H       -6.642839       -2.030664       -0.823499
H       -5.465897       -3.174222       -1.063216
N       -0.442151       2.038039        1.163820
H       -0.625832       2.664273        1.944715
C       -0.713708       2.548379        -0.173121
H       -1.298201       1.825609        -0.748381
C       -1.505321       3.852064        -0.062610
C       0.554128        2.811016        -0.985313
H       -0.941368       4.594716        0.509276
H       -1.705656       4.246916        -1.059476
H       -2.455302       3.657417        0.439341
O       1.719778        2.876001        -0.340156
O       0.511605        2.984597        -2.186026
H       1.605124        2.724779        0.614839
H       4.983743        -3.219680       -0.597454
H       -2.210254       -0.353417       -1.030334
###
45
AlaLysAla2 m062x E=-991.841553389 au
N       3.485921        -3.564553       -0.799261
H       3.713019        -3.024220       -1.642850
H       2.773219        -4.256409       -1.055529
C       3.000530        -2.649356       0.272581
H       2.684577        -3.271546       1.111690
C       4.123165        -1.702273       0.674463
C       1.822980        -1.874175       -0.308147
H       4.426773        -1.087550       -0.177953
H       3.779240        -1.049439       1.478832
H       4.982654        -2.273863       1.033041
O       1.746006        -1.682573       -1.527083
N       0.952931        -1.403944       0.591567
H       1.082567        -1.638529       1.571904
C       -0.160242       -0.529613       0.235186
H       0.028338        -0.168906       -0.776175
C       -1.498448       -1.265909       0.267553
C       -0.141346       0.618038        1.248523
H       -1.430849       -2.108932       -0.429130
H       -1.657455       -1.673339       1.272417
C       -2.661370       -0.356700       -0.123251
O       -0.512491       0.395742        2.415537
H       -2.693849       0.515881        0.543254
C       -3.998423       -1.090127       -0.052344
H       -3.993550       -1.942655       -0.742729
H       -4.150595       -1.484724       0.959935
C       -5.146974       -0.163666       -0.403900
H       -5.215459       0.676000        0.289041
H       -5.067069       0.217620        -1.422753
N       -6.447056       -0.900313       -0.318543
H       -6.581810       -1.289080       0.619969
H       -7.240200       -0.285865       -0.524692
H       -6.468419       -1.678501       -0.984973
N       0.309806        1.813821        0.864008
H       0.374563        2.528887        1.585474
C       0.856989        2.200244        -0.433234
H       1.461802        1.380673        -0.832882
C       -0.243891       2.576870        -1.426848
C       1.805480        3.400930        -0.239675
H       -0.799524       3.445989        -1.060531
H       0.192520        2.819727        -2.398188
H       -0.945213       1.747205        -1.554757
O       1.798519        3.992709        0.871745
O       2.500408        3.711710        -1.242918
H       4.327104        -4.062423       -0.489893
H       -2.503844       0.022644        -1.140610
###
44
AlaLysAla3 m062x E=-991.383391621 au
N       3.175307        -4.064359       -0.412478
H       3.276524        -3.907502       -1.414438
H       2.309434        -4.586161       -0.291417
C       3.054386        -2.767372       0.244775
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H       2.906002        -2.937555       1.315185
C       4.328296        -1.953172       0.033730
C       1.877555        -1.951496       -0.287436
H       4.505646        -1.803374       -1.036493
H       4.254008        -0.973110       0.512795
H       5.182231        -2.486515       0.458058
O       1.653591        -1.868303       -1.505349
N       1.137726        -1.306227       0.630806
H       1.313369        -1.479229       1.615110
C       -0.001567       -0.467841       0.277062
H       0.170705        -0.100779       -0.735446
C       -1.316957       -1.248085       0.316255
C       -0.022581       0.678001        1.288950
H       -1.210260       -2.111429       -0.350216
H       -1.469741       -1.628630       1.332766
C       -2.510744       -0.401109       -0.117468
O       -0.337041       0.430137        2.467999
H       -2.560333       0.517127        0.484373
C       -3.824556       -1.166181       0.023115
H       -3.768504       -2.105343       -0.541483
H       -3.993339       -1.422422       1.076239
C       -4.991339       -0.343266       -0.489608
H       -5.109104       0.586658        0.068453
H       -4.887840       -0.113287       -1.550748
N       -6.270959       -1.103794       -0.334197
H       -6.444685       -1.321073       0.652412
H       -7.069066       -0.568468       -0.687459
H       -6.231823       -1.990909       -0.846682
N       0.330157        1.904313        0.896248
H       0.354891        2.623212        1.616512
C       0.794148        2.339921        -0.418446
H       1.467407        1.586088        -0.835849
C       -0.365079       2.604419        -1.381934
C       1.609900        3.638424        -0.254321
H       -1.012435       3.392825        -0.984954
H       0.021152        2.919897        -2.353977
H       -0.965298       1.701765        -1.522511
O       1.507211        4.270360        0.830079
O       2.294294        3.982412        -1.253896
H       -2.377779       -0.091623       -1.161600
###
43
AlaLysAla4 m062x E=-990.917912046 au
N       3.203439        -4.003084       -0.414398
H       3.306543        -3.841705       -1.415458
H       2.344333        -4.537161       -0.298332
C       3.060668        -2.709593       0.246234
H       2.912922        -2.885228       1.315794
C       4.321947        -1.874998       0.040581
C       1.871343        -1.913089       -0.286959
H       4.499703        -1.719199       -1.028680
H       4.231296        -0.897687       0.522556
H       5.182889        -2.396428       0.465635
O       1.663102        -1.812225       -1.506594
N       1.100954        -1.307808       0.632939
H       1.272504        -1.490620       1.616142
C       -0.051468       -0.486386       0.281001
H       0.115913        -0.116962       -0.731323
C       -1.357109       -1.282429       0.318663
C       -0.085934       0.659624        1.292241
H       -1.235603       -2.147808       -0.343020
H       -1.508635       -1.661675       1.336122
C       -2.560645       -0.453742       -0.124661
O       -0.402663       0.411150        2.470611
H       -2.617020       0.471079        0.468108
C       -3.875184       -1.218707       0.011383
H       -3.805108       -2.171222       -0.532079
H       -4.050372       -1.465084       1.067532
C       -5.067551       -0.430781       -0.521645
H       -5.133990       0.527632        0.004693
H       -4.903259       -0.197277       -1.579084
N       -6.363081       -1.107937       -0.400161
H       -6.518126       -1.333905       0.580840
H       -6.304725       -2.004155       -0.880755
N       0.261564        1.887857        0.900173
H       0.278543        2.607933        1.619346
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C       0.724994        2.324491        -0.414282
H       1.403078        1.573735        -0.829672
C       -0.434691       2.580967        -1.379585
C       1.533074        3.627787        -0.251094
H       -1.086212       3.367190        -0.985105
H       -0.049417       2.895662        -2.352279
H       -1.030843       1.675163        -1.517828
O       1.422990        4.262544        0.830966
O       2.219243        3.972793        -1.249222
H       -2.422596       -0.148444       -1.170359
###
29
CysGlyGly1 m062x E=-1138.16482417 au
N       4.637599        -1.210843       0.442777
H       4.534531        -1.941353       1.156405
H       5.527014        -0.726640       0.606476
H       4.674734        -1.669617       -0.477007
C       3.494893        -0.254515       0.483603
H       3.390613        0.098311        1.510666
C       3.806815        0.898796        -0.475535
C       2.263590        -1.018603       0.010171
H       4.738145        1.374787        -0.158372
H       3.943396        0.513060        -1.489174
S       2.555935        2.219056        -0.468049
O       2.371214        -1.853196       -0.895963
H       1.579919        1.527744        -1.085655
N       1.110462        -0.684261       0.589618
H       1.091558        0.064146        1.277757
C       -0.159322       -1.090725       0.026329
C       -1.218486       -0.073547       0.411541
H       -0.081323       -1.130622       -1.064926
H       -0.454413       -2.084381       0.377760
O       -0.935841       0.956508        1.036219
N       -2.464258       -0.370337       0.026898
H       -2.655066       -1.226172       -0.485123
C       -3.559257       0.529996        0.302775
C       -4.846268       -0.068499       -0.193109
H       -3.655969       0.717781        1.377039
H       -3.415165       1.497816        -0.189810
O       -4.934396       -1.135411       -0.766761
O       -5.886979       0.718944        0.074377
H       -6.703333       0.306153        -0.259929
###
28
CysGlyGly2 m062x E=-1137.71404389 au
N       4.278813        -1.571722       0.758210
H       3.903863        -2.222998       1.456863
H       5.213498        -1.277732       1.064300
H       4.367254        -2.078588       -0.132318
C       3.378685        -0.393778       0.581899
H       3.183332        0.024470        1.570355
C       4.092460        0.618571        -0.318233
C       2.107992        -0.923557       -0.078281
H       5.032396        0.908537        0.158937
H       4.321276        0.164444        -1.285916
S       3.158489        2.160779        -0.555557
O       2.197598        -1.762184       -0.985465
H       2.224972        1.655487        -1.381020
N       0.959187        -0.417657       0.358365
H       0.941943        0.285977        1.092211
C       -0.302177       -0.758052       -0.262201
C       -1.405063       0.051631        0.398383
H       -0.275324       -0.526550       -1.332669
H       -0.510333       -1.827060       -0.154763
O       -1.146187       0.909402        1.257880
N       -2.641951       -0.222776       -0.011265
H       -2.809139       -0.928501       -0.722555
C       -3.802068       0.481433        0.495200
C       -5.081668       -0.001627       -0.191268
H       -3.906120       0.326715        1.573720
H       -3.700616       1.558052        0.324873
O       -4.980910       -0.883313       -1.084793
O       -6.148517       0.536425        0.208220
###
27
CysGlyGly3 m062x E=-1137.25098271 au
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N       -4.547448       -1.434613       0.048324
H       -4.347367       -2.315778       -0.437313
H       -5.481360       -1.104731       -0.212463
H       -4.546991       -1.633648       1.055442
C       -3.517975       -0.399975       -0.287623
H       -3.667547       -0.148444       -1.341519
C       -3.733213       0.838155        0.582974
C       -2.163132       -1.094221       -0.141135
H       -4.809923       1.036916        0.590984
H       -3.441378       0.592928        1.611293
S       -2.838472       2.314589        -0.030710
O       -2.108096       -2.334242       -0.067061
N       -1.087603       -0.311890       -0.126395
H       -1.215540       0.711323        -0.148869
C       0.232526        -0.892195       -0.018741
C       1.288889        0.194254        -0.096124
H       0.344979        -1.434132       0.926817
H       0.398439        -1.611116       -0.827894
O       0.990938        1.389776        -0.244126
N       2.548100        -0.234009       0.006031
H       2.754436        -1.221769       0.119233
C       3.684815        0.660892        -0.058951
C       4.998576        -0.113770       0.078730
H       3.696940        1.200618        -1.011408
H       3.635300        1.407058        0.740556
O       4.938700        -1.362959       0.225211
O       6.048621        0.581438        0.032976
###
26
CysGlyGly4 m062x E=-1136.78620180 au
N       -4.671140       -1.406823       0.006137
H       -4.479175       -2.283460       -0.474727
H       -4.637379       -1.634832       0.999851
C       -3.588194       -0.467393       -0.284169
H       -3.668223       -0.174573       -1.338362
C       -3.756507       0.794473        0.575116
C       -2.209895       -1.128828       -0.130327
H       -4.830166       1.000252        0.604169
H       -3.453486       0.555297        1.603271
S       -2.878044       2.293689        -0.022981
O       -2.098123       -2.366753       -0.032761
N       -1.135447       -0.330794       -0.141322
H       -1.276293       0.689380        -0.167751
C       0.190582        -0.893166       -0.029684
C       1.243730        0.195919        -0.103180
H       0.309426        -1.435444       0.915524
H       0.370312        -1.612663       -0.836129
O       0.948633        1.392295        -0.252522
N       2.504697        -0.229646       0.003843
H       2.712566        -1.216979       0.116339
C       3.639084        0.668130        -0.056036
C       4.955299        -0.102338       0.080622
H       3.651355        1.211905        -1.006261
H       3.586881        1.411391        0.746116
O       4.900395        -1.352476       0.221055
O       6.003035        0.597029        0.040602
###
31
GlyAlaAla1 m062x E=-779.308811756 au
N       3.153030        -2.488180       0.209143
H       3.429031        -2.271512       1.173700
C       3.082048        -1.247775       -0.598238
H       3.831469        -3.143178       -0.190692
H       2.239178        -2.952784       0.249679
C       2.234583        -0.237115       0.149874
H       4.093972        -0.858987       -0.723913
H       2.659743        -1.485911       -1.574453
O       1.958412        -0.401650       1.341431
N       1.833774        0.828046        -0.558911
H       2.086265        0.900242        -1.539678
C       1.081665        1.905607        0.062390
H       1.589014        2.204016        0.984876
C       0.990755        3.092354        -0.892073
C       -0.324977       1.483282        0.486330
H       0.486767        2.803316        -1.819191
H       0.427947        3.900036        -0.420968
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H       1.993380        3.455594        -1.128896
O       -0.930145       2.154339        1.333878
N       -0.864656       0.419387        -0.121965
H       -0.319275       -0.120438       -0.785774
C       -2.199574       -0.043751       0.200398
H       -2.350369       0.049532        1.281641
C       -3.283998       0.753502        -0.536732
C       -2.282631       -1.515366       -0.160770
H       -3.197646       0.607320        -1.616479
H       -4.281267       0.446270        -0.212440
H       -3.156850       1.813638        -0.308117
O       -1.442428       -2.091978       -0.821350
O       -3.363958       -2.180794       0.252410
H       -3.948665       -1.645696       0.814812
###
30
GlyAlaAla2 m062x E=-778.864611370 au
N       -0.209945       3.230541        0.081302
H       -0.251383       3.306748        1.102438
C       -1.415894       2.537339        -0.430164
H       -0.135282       4.170631        -0.315175
H       0.633403        2.668445        -0.173505
C       -1.497524       1.191829        0.264310
H       -2.298151       3.132599        -0.187708
H       -1.328580       2.434791        -1.511440
O       -1.066568       1.053986        1.413506
N       -2.045530       0.186173        -0.435780
H       -2.268901       0.331221        -1.415543
C       -2.010376       -1.174217       0.086515
H       -2.558314       -1.207908       1.032100
C       -2.634685       -2.138655       -0.914202
C       -0.574862       -1.589686       0.435412
H       -2.108757       -2.097483       -1.872497
H       -2.576457       -3.157195       -0.524797
H       -3.685421       -1.886422       -1.074687
O       -0.369677       -2.362843       1.381477
N       0.396431        -1.092087       -0.344033
H       0.127596        -0.378231       -1.014422
C       1.778210        -0.973562       0.099706
H       1.800815        -1.167099       1.176687
C       2.710982        -1.953900       -0.609217
C       2.243784        0.481461        -0.114264
H       2.724757        -1.762195       -1.686607
H       3.727387        -1.855801       -0.221415
H       2.369197        -2.978209       -0.439478
O       1.485614        1.252820        -0.777902
O       3.356079        0.792295        0.371299
###
29
GlyAlaAla3 m062x E=-778.402290878 au
N       3.459454        -2.439134       0.179817
H       4.083599        -2.060947       0.888794
C       2.939778        -1.347639       -0.621241
H       2.689785        -2.867310       0.689293
C       2.195033        -0.274840       0.160891
H       3.754407        -0.868166       -1.171094
H       2.244263        -1.741189       -1.369583
O       1.955952        -0.378638       1.370816
N       1.787013        0.792602        -0.555677
H       2.011100        0.835472        -1.544234
C       1.031414        1.879566        0.038690
H       1.532097        2.198491        0.958319
C       0.949787        3.048499        -0.939191
C       -0.381417       1.471365        0.461458
H       0.452108        2.740796        -1.864108
H       0.384950        3.868332        -0.491874
H       1.954367        3.405210        -1.178520
O       -0.999673       2.188048        1.268935
N       -0.903467       0.379364        -0.097416
H       -0.327402       -0.219123       -0.680369
C       -2.216385       -0.142022       0.247550
H       -2.345038       -0.061448       1.332613
C       -3.338124       0.628139        -0.452105
C       -2.278747       -1.635711       -0.120076
H       -3.279218       0.489077        -1.536077
H       -4.310636       0.271721        -0.105620
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H       -3.258290       1.695375        -0.230381
O       -1.300282       -2.139406       -0.735660
O       -3.330386       -2.242537       0.215897
###
40
GlyGlyAspAla1 m062x E=-1175.33985273 au
N       -7.788116       -0.494608       -0.458771
H       -7.983531       -0.357199       0.538564
C       -6.510562       0.150806        -0.841106
H       -7.752146       -1.505536       -0.627638
H       -8.564355       -0.102017       -1.000018
C       -5.396456       -0.456025       -0.008000
H       -6.340545       -0.022848       -1.904331
H       -6.596512       1.222324        -0.657504
O       -5.637952       -1.345502       0.817703
N       -4.177188       0.032840        -0.232989
H       -4.026193       0.765123        -0.921291
C       -3.027024       -0.470760       0.483054
C       -1.779484       0.230554        -0.019230
H       -3.131049       -0.291112       1.558421
H       -2.923191       -1.549987       0.333295
O       -1.835599       1.135496        -0.861649
N       -0.632003       -0.204659       0.515158
H       -0.632533       -0.955226       1.199771
C       0.652172        0.343891        0.129099
H       0.652616        0.509298        -0.952119
C       0.919261        1.677182        0.844145
C       1.716166        -0.696498       0.487796
H       -0.000997       2.272628        0.847953
H       1.203582        1.518960        1.889596
C       1.965142        2.521258        0.169812
O       1.484371        -1.559185       1.350481
O       2.258451        3.615060        0.879467
O       2.482444        2.278542        -0.905204
N       2.875165        -0.587839       -0.158077
H       3.023508        0.183099        -0.805118
C       4.016871        -1.448880       0.114777
H       4.112494        -1.563688       1.199789
C       3.843756        -2.826156       -0.528487
C       5.299332        -0.770861       -0.400677
H       3.813055        -2.733980       -1.618615
H       4.675356        -3.478513       -0.253920
H       2.912436        -3.286484       -0.189251
O       5.182603        0.301720        -1.050979
O       6.378674        -1.366087       -0.139358
H       2.914011        4.147616        0.394383
###
39
GlyGlyAspAla2 m062x E=-1174.88473293 au
N       -7.747443       -0.545607       -0.595209
H       -7.928290       -0.771852       0.389570
C       -6.521691       0.279148        -0.713605
H       -7.647983       -1.432477       -1.100631
H       -8.557101       -0.046987       -0.976105
C       -5.405113       -0.404860       0.052679
H       -6.279653       0.401674        -1.768717
H       -6.725298       1.255404        -0.269945
O       -5.659912       -1.284485       0.885691
N       -4.173974       0.024057        -0.219485
H       -4.015855       0.749700        -0.913346
C       -3.023554       -0.487328       0.491310
C       -1.776815       0.215671        -0.014046
H       -3.124952       -0.309748       1.567236
H       -2.923372       -1.566335       0.338098
O       -1.844372       1.136739        -0.840463
N       -0.625748       -0.231581       0.495440
H       -0.619669       -1.002664       1.156555
C       0.656458        0.335116        0.116359
H       0.648676        0.523786        -0.960438
C       0.929798        1.655133        0.853150
C       1.725916        -0.709873       0.435168
H       0.001134        2.236867        0.869024
H       1.201352        1.461892        1.896404
C       1.992714        2.557279        0.217984
O       1.482452        -1.649934       1.212524
O       2.331510        3.571856        0.887597
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O       2.438939        2.258612        -0.925255
N       2.907965        -0.521549       -0.149050
H       3.053486        0.324564        -0.700330
C       4.055557        -1.380201       0.100443
H       4.130163        -1.559276       1.178871
C       3.920828        -2.719263       -0.627866
C       5.341873        -0.661826       -0.343131
H       3.916547        -2.560879       -1.710967
H       4.755598        -3.374986       -0.371510
H       2.988789        -3.212735       -0.341820
O       5.233545        0.449114        -0.926397
O       6.420962        -1.265296       -0.095509
###
25
GlyGlyGLI1 m062x E=-700.714620127 au
N       5.447950        0.056238        0.073946
H       5.487947        0.951350        -0.426548
C       4.199568        -0.666563       -0.263738
H       5.495308        0.265257        1.076784
C       3.025878        0.268769        -0.044452
H       4.245963        -0.955425       -1.315054
H       4.128958        -1.560257       0.355599
O       3.203443        1.488714        0.064001
N       1.827141        -0.312216       -0.012654
H       1.735107        -1.322456       -0.070564
C       0.617168        0.470087        0.111817
C       -0.580709       -0.458231       0.075696
H       0.607748        1.020065        1.059086
H       0.544805        1.201667        -0.698771
O       -0.452720       -1.689100       0.093387
N       -1.774122       0.145071        0.037135
H       -1.840918       1.158193        0.025915
C       -2.992866       -0.628854       0.053180
C       -4.181464       0.286903        -0.041761
H       -3.028355       -1.328248       -0.788568
H       -3.081702       -1.216223       0.973553
O       -4.115594       1.497389        -0.116785
O       -5.325353       -0.396049       -0.034443
H       6.268775        -0.501716       -0.178952
H       -6.074071       0.223840        -0.095203
###
24
GlyGlyGLI2 m062x E=-700.263576605 au
N       5.381412        0.089051        0.082136
H       5.408944        0.989334        -0.409802
C       4.143342        -0.647715       -0.263901
H       5.424967        0.289614        1.086858
C       2.957220        0.271511        -0.042086
H       4.196687        -0.928269       -1.317137
H       4.082723        -1.546704       0.348744
O       3.120447        1.493133        0.074640
N       1.765847        -0.323527       -0.018305
H       1.685914        -1.334762       -0.077239
C       0.545366        0.441845        0.112007
C       -0.644403       -0.499666       0.066565
H       0.529358        0.981195        1.065364
H       0.467526        1.181754        -0.690180
O       -0.496635       -1.731711       0.107740
N       -1.836464       0.091415        -0.000445
H       -1.914366       1.103593        -0.033850
C       -3.077553       -0.655000       0.023968
C       -4.283075       0.287037        -0.036865
H       -3.131033       -1.342524       -0.826154
H       -3.147522       -1.254249       0.937551
O       -4.065350       1.525164        -0.107994
O       -5.412741       -0.270423       -0.013234
H       6.210085        -0.454938       -0.175207
###
23
GlyGlyGLI3 m062x E=-699.805393284 au
N       -5.513167       0.012425        -0.163944
H       -5.629923       0.684522        0.590829
C       -4.230511       -0.648981       -0.011424
H       -5.505123       0.559181        -1.022309
C       -3.026900       0.282646        0.036701
H       -4.227873       -1.226576       0.918327
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H       -4.084546       -1.363889       -0.825408
O       -3.145790       1.512451        0.154636
N       -1.827148       -0.311232       -0.037083
H       -1.755336       -1.321799       -0.100027
C       -0.600408       0.442414        0.083183
C       0.587083        -0.501240       0.036888
H       -0.515262       1.180570        -0.720384
H       -0.573619       0.987584        1.033697
O       0.441332        -1.733892       0.075593
N       1.780977        0.088657        -0.028648
H       1.859100        1.100909        -0.053766
C       3.021861        -0.657343       0.001993
C       4.227594        0.285719        -0.034673
H       3.082047        -1.265805       0.910260
H       3.086284        -1.336589       -0.854026
O       4.010411        1.524728        -0.090406
O       5.357461        -0.271581       -0.008008
###
43
GlyGlyGluAla1 m062x E=-1214.63332749 au
N       -7.874055       -0.611498       -0.338820
H       -8.019878       -0.515956       0.672049
C       -6.610284       0.045022        -0.747551
H       -7.854003       -1.614203       -0.552937
H       -8.671466       -0.192747       -0.827205
C       -5.479140       -0.531002       0.083949
H       -6.456473       -0.127685       -1.812669
H       -6.706431       1.115897        -0.562267
O       -5.719240       -1.246342       1.064937
N       -4.249036       -0.196921       -0.304330
H       -4.096297       0.377062        -1.128648
C       -3.087161       -0.654845       0.423056
C       -1.834835       -0.120793       -0.247451
H       -3.117519       -0.304099       1.459778
H       -3.051246       -1.749009       0.441503
O       -1.889780       0.567594        -1.273712
N       -0.686885       -0.461506       0.354722
H       -0.714906       -0.955542       1.242287
C       0.599588        0.061373        -0.073123
H       0.647261        0.026476        -1.165333
C       0.786482        1.511197        0.403489
C       1.677040        -0.830465       0.532075
H       -0.025834       2.105202        -0.026878
H       0.691058        1.541943        1.493924
C       2.145995        2.090755        -0.018038
O       1.567990        -1.225464       1.704746
H       2.962782        1.606491        0.520803
H       2.299328        1.954492        -1.094672
C       2.191946        3.557127        0.319426
O       2.686204        4.008662        1.335002
O       1.611668        4.406249        -0.545480
N       2.718834        -1.110059       -0.250569
H       2.787525        -0.688759       -1.172740
C       3.913083        -1.783056       0.239679
H       4.136984        -1.398480       1.240727
C       3.717073        -3.298782       0.309068
C       5.102024        -1.438207       -0.674747
H       3.566444        -3.708158       -0.694737
H       4.595233        -3.771187       0.754440
H       2.843863        -3.538426       0.921007
O       4.868682        -0.800933       -1.736816
O       6.228515        -1.846900       -0.287606
H       1.258399        3.943720        -1.323005
###
42
GlyGlyGluAla2 m062x E=-1214.17869809 au
N       7.811596        -0.654679       0.368283
H       7.958104        -0.565069       -0.643109
C       6.548492        0.006300        0.771911
H       7.790025        -1.656013       0.588495
H       8.609247        -0.234272       0.854857
C       5.418622        -0.560783       -0.067558
H       6.388716        -0.166509       1.836071
H       6.650222        1.076969        0.588052
O       5.660363        -1.253381       -1.064528
N       4.188419        -0.239174       0.330001
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H       4.036317        0.301145        1.176826
C       3.024610        -0.682893       -0.403775
C       1.776215        -0.140430       0.268401
H       3.066868        -0.333614       -1.439834
H       2.973646        -1.777013       -0.421063
O       1.829122        0.433329        1.363807
N       0.637035        -0.353143       -0.402956
H       0.682262        -0.732514       -1.344142
C       -0.636296       0.204595        0.033742
H       -0.695054       0.108770        1.121403
C       -0.755012       1.681626        -0.367663
C       -1.734073       -0.620396       -0.625164
H       0.075449        2.214878        0.104280
H       -0.622278       1.757505        -1.452893
C       -2.082290       2.299965        0.049432
O       -1.699377       -0.827448       -1.850852
H       -2.915439       1.851253        -0.503199
H       -2.277851       2.104858        1.112316
C       -2.174320       3.815473        -0.149164
O       -3.316567       4.335669        0.020738
O       -1.132021       4.460026        -0.451570
N       -2.703037       -1.070754       0.171340
H       -2.710701       -0.825231       1.156817
C       -3.873290       -1.777293       -0.328776
H       -4.230538       -1.262012       -1.226606
C       -3.549141       -3.233957       -0.670936
C       -4.988408       -1.726937       0.729430
H       -3.256835       -3.779392       0.231843
H       -4.424426       -3.719903       -1.107602
H       -2.728130       -3.280395       -1.390347
O       -4.690329       -1.324781       1.885934
O       -6.120984       -2.129767       0.352956
###
45
GlyGlyHisAla1 m062x E=-1212.23973415 au
N       -8.205807       0.206968        -0.240818
H       -8.352260       -0.795385       -0.075374
C       -6.878373       0.438579        -0.857546
H       -8.953394       0.556773        -0.847342
H       -8.277733       0.680036        0.666100
C       -5.830817       -0.293431       -0.038991
H       -6.897091       0.036212        -1.871555
H       -6.691714       1.511282        -0.896235
O       -6.160677       -1.178227       0.760840
N       -4.569223       0.065150        -0.272807
H       -4.350737       0.802733        -0.937051
C       -3.457192       -0.614080       0.353882
C       -2.166766       0.031713        -0.116852
H       -3.526406       -0.547320       1.444053
H       -3.446288       -1.675346       0.083388
O       -2.166273       0.929181        -0.967998
N       -1.046608       -0.450818       0.439164
H       -1.097434       -1.161109       1.163816
C       0.260963        0.054861        0.077948
H       0.272658        0.275368        -0.992670
C       0.587989        1.352008        0.863796
C       1.302299        -1.003654       0.411516
H       -0.165588       2.099360        0.605609
H       0.516692        1.144886        1.936044
C       1.940503        1.894652        0.548773
O       1.174165        -1.713859       1.420678
N       3.083646        1.500441        1.223652
C       2.359633        2.766904        -0.411241
H       3.119592        0.824544        1.983668
C       4.151788        2.092676        0.699704
N       3.727806        2.875158        -0.285843
H       1.804437        3.314722        -1.155840
H       5.173867        1.968356        1.023862
N       2.362490        -1.041980       -0.398635
H       2.440432        -0.358627       -1.148445
C       3.604371        -1.708430       -0.028333
H       3.722897        -1.626944       1.058195
C       3.606868        -3.184068       -0.428574
C       4.786094        -0.970427       -0.685448
H       3.544794        -3.283087       -1.516730
H       4.524205        -3.665078       -0.082400
```

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H       2.751754        -3.696241       0.020061
O       4.529910        -0.101977       -1.561179
O       5.932957        -1.320487       -0.300379
H       4.336375        3.449548        -0.861651
###
44
GlyGlyHisAla2 m062x E=-1211.78502963 au
N       -8.169922       0.175840        -0.317090
H       -8.336378       -0.812370       -0.095980
C       -6.838424       0.344771        -0.944223
H       -8.909688       0.505378        -0.944277
H       -8.232189       0.701174        0.561675
C       -5.798609       -0.312490       -0.055366
H       -6.853852       -0.147881       -1.917525
H       -6.646618       1.408890        -1.079354
O       -6.136521       -1.123099       0.816609
N       -4.535245       0.026062        -0.308039
H       -4.314257       0.721664        -1.015274
C       -3.430037       -0.556703       0.419353
C       -2.138904       0.082398        -0.060507
H       -3.543148       -0.383174       1.494435
H       -3.382025       -1.638333       0.257271
O       -2.140197       0.966208        -0.927699
N       -1.021253       -0.387098       0.507237
H       -1.076257       -1.093725       1.234924
C       0.291003        0.114927        0.144271
H       0.298620        0.321929        -0.929360
C       0.636345        1.415970        0.909668
C       1.323517        -0.950138       0.477597
H       -0.120623       2.159310        0.643878
H       0.560430        1.216767        1.983420
C       2.006977        1.920777        0.590805
O       1.211013        -1.634310       1.507967
N       3.114313        1.521961        1.314125
C       2.395312        2.738217        -0.440811
C       4.146449        2.092013        0.722653
N       3.760652        2.842291        -0.334862
H       1.834961        3.244118        -1.212390
H       5.180652        2.003631        1.023243
N       2.348000        -1.047174       -0.373344
H       2.427998        -0.357403       -1.116516
C       3.593447        -1.711550       -0.014475
H       3.744852        -1.597807       1.064163
C       3.573934        -3.199594       -0.367377
C       4.760371        -1.011545       -0.734331
H       3.477327        -3.333403       -1.449378
H       4.497700        -3.677611       -0.033649
H       2.729728        -3.690976       0.123433
O       4.484414        -0.217091       -1.673007
O       5.916880        -1.322423       -0.342498
H       4.373951        3.370040        -0.943434
###
48
GlyGlyLysAla1 m062x E=-1160.04497457 au
N       8.200753        0.321719        0.331734
H       8.433724        -0.642139       0.103300
C       6.851286        0.362192        0.863478
H       8.222719        0.828444        -0.550579
C       5.784251        -0.227175       -0.049968
H       6.813116        -0.194171       1.805264
H       6.576304        1.394233        1.097132
O       6.067955        -0.867259       -1.074544
N       4.515901        -0.023666       0.333359
H       4.312525        0.494232        1.182134
C       3.400047        -0.568930       -0.403793
C       2.101129        -0.143361       0.256152
H       3.412870        -0.217430       -1.440391
H       3.441360        -1.663913       -0.425882
O       2.087484        0.465356        1.334482
N       0.990164        -0.498076       -0.402577
H       1.067724        -0.926414       -1.320189
C       -0.338156       -0.113967       0.046187
H       -0.367531       -0.182394       1.137271
C       -0.680659       1.318364        -0.397119
C       -1.332758       -1.089810       -0.565515
H       0.068483        1.984439        0.046060
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H       -0.570950       1.375258        -1.486941
C       -2.082318       1.764739        0.010913
O       -1.215790       -1.437514       -1.753190
H       -2.835398       1.152614        -0.501722
H       -2.223073       1.609577        1.089024
C       -2.319454       3.233849        -0.333193
H       -1.590675       3.862165        0.192971
H       -2.173786       3.387363        -1.409699
C       -3.724478       3.658068        0.049864
H       -4.480380       3.076587        -0.479633
H       -3.895511       3.572376        1.123746
N       -3.953218       5.092476        -0.311276
H       -3.822188       5.239843        -1.317247
H       -4.902936       5.389753        -0.069483
H       -3.293350       5.702800        0.181286
N       -2.327275       -1.490168       0.227440
H       -2.415827       -1.097960       1.160519
C       -3.479571       -2.228928       -0.268487
H       -3.740494       -1.832448       -1.255898
C       -3.185988       -3.725896       -0.385216
C       -4.679577       -1.989596       0.665435
H       -2.977277       -4.150298       0.601694
H       -4.044271       -4.244216       -0.818213
H       -2.317951       -3.890155       -1.028517
O       -4.475618       -1.384639       1.752187
O       -5.784533       -2.443622       0.266167
###
47
GlyGlyLysAla2 m062x E=-1159.57926124 au
N       8.203427        0.325163        0.317491
H       8.437088        -0.638009       0.086928
C       6.856355        0.362163        0.855978
H       8.220137        0.832929        -0.564341
C       5.787215        -0.233374       -0.050827
H       6.824781        -0.194286       1.798018
H       6.579452        1.393363        1.090866
O       6.069588        -0.899432       -1.059233
N       4.519284        -0.009790       0.321903
H       4.314573        0.547058        1.145394
C       3.401329        -0.553180       -0.413022
C       2.103697        -0.115609       0.242563
H       3.412744        -0.202604       -1.450547
H       3.440678        -1.647730       -0.434562
O       2.093683        0.582822        1.265198
N       0.991898        -0.550884       -0.363368
H       1.064725        -1.063350       -1.237376
C       -0.339078       -0.152647       0.062650
H       -0.370094       -0.154975       1.156217
C       -0.699543       1.250240        -0.460198
C       -1.321764       -1.177782       -0.483305
H       0.059974        1.940162        -0.074477
H       -0.613028       1.243896        -1.553811
C       -2.089964       1.726464        -0.043042
O       -1.143477       -1.686329       -1.603160
H       -2.859081       1.111880        -0.529725
H       -2.216089       1.586880        1.040321
C       -2.326096       3.193299        -0.396550
H       -1.570937       3.818415        0.099140
H       -2.201022       3.336843        -1.478693
C       -3.715477       3.670810        0.013489
H       -4.472800       3.049086        -0.476112
H       -3.843361       3.527922        1.092080
N       -4.007837       5.074111        -0.297788
H       -3.891150       5.215113        -1.299640
H       -3.300175       5.658360        0.144142
N       -2.376053       -1.445622       0.289627
H       -2.520151       -0.900943       1.135521
C       -3.533972       -2.181945       -0.195321
H       -3.669634       -1.941880       -1.255918
C       -3.346171       -3.691618       -0.042999
C       -4.794027       -1.698874       0.546975
H       -3.264717       -3.961849       1.014314
H       -4.193308       -4.225007       -0.479132
H       -2.433880       -4.007228       -0.555952
O       -4.655082       -0.849663       1.468092
O       -5.882809       -2.205221       0.165847
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###
47
GlyGlyTyrAla1 m062x E=-1292.53803773 au
N       8.632027        -0.746006       -0.179861
H       8.951529        0.218943        -0.135096
C       7.303443        -0.770365       -0.764307
H       8.573521        -1.062676       0.785473
C       6.275176        0.097059        -0.050366
H       7.354621        -0.417184       -1.799242
H       6.933069        -1.798031       -0.800098
O       6.603876        0.987145        0.749642
N       4.993264        -0.144820       -0.358422
H       4.749967        -0.883877       -1.010196
C       3.913592        0.624221        0.215002
C       2.587001        0.023114        -0.209085
H       3.982590        0.628421        1.307219
H       3.948460        1.666745        -0.121707
O       2.523062        -0.876125       -1.057832
N       1.508028        0.555705        0.379784
H       1.622042        1.249726        1.112524
C       0.161821        0.107151        0.080378
H       0.105648        -0.144435       -0.982248
C       -0.222525       -1.135762       0.923960
C       -0.807685       1.232835        0.407316
H       0.473901        -1.936489       0.656888
H       -0.069874       -0.885259       1.979073
C       -1.651063       -1.558902       0.689840
O       -0.651634       1.916208        1.432312
C       -2.678260       -1.075638       1.507287
C       -1.996804       -2.360999       -0.403284
H       -2.432084       -0.444604       2.359033
C       -4.014613       -1.369599       1.243173
C       -3.326465       -2.670549       -0.679067
H       -1.214297       -2.746043       -1.053089
H       -4.806682       -0.981227       1.878300
C       -4.334347       -2.164953       0.142386
H       -3.592814       -3.290975       -1.529190
O       -5.632460       -2.477886       -0.181271
H       -6.240798       -2.053950       0.441815
N       -1.840203       1.370365        -0.429122
H       -1.955124       0.683535        -1.170416
C       -3.061689       2.067640        -0.048240
H       -3.202954       1.945656        1.031705
C       -3.007649       3.557620        -0.386831
C       -4.256054       1.403321        -0.758777
H       -2.921557       3.699363        -1.468658
H       -3.915136       4.054992        -0.036938
H       -2.145358       4.022503        0.098161
O       -4.013672       0.619815        -1.715117
O       -5.398393       1.729720        -0.338516
###
46
GlyGlyTyrAla2 m062x E=-1292.06107269 au
N       8.650183        -0.482951       -0.454170
H       8.781636        0.456971        -0.821358
C       7.264878        -0.871421       -0.643747
H       8.838430        -0.418472       0.543744
C       6.245326        0.051272        0.011618
H       7.040263        -0.935072       -1.711783
H       7.106739        -1.872151       -0.229567
O       6.575238        0.932241        0.820946
N       4.965821        -0.163523       -0.325306
H       4.724257        -0.884679       -0.997588
C       3.883115        0.587819        0.265385
C       2.558743        -0.007391       -0.175772
H       3.950505        0.566010        1.357606
H       3.915490        1.638146        -0.046052
O       2.502517        -0.900900       -1.031923
N       1.475382        0.523321        0.404789
H       1.583860        1.214384        1.141115
C       0.129841        0.076372        0.093070
H       0.082225        -0.168728       -0.971452
C       -0.265029       -1.171356       0.925258
C       -0.837810       1.203589        0.416166
H       0.437679        -1.967733       0.658201
H       -0.111887       -0.925582       1.982262
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C       -1.692199       -1.595233       0.688560
O       -0.684225       1.886771        1.442554
C       -2.729339       -1.114238       1.499780
C       -2.051062       -2.389782       -0.407972
H       -2.482816       -0.485690       2.355747
C       -4.063753       -1.402443       1.232243
C       -3.381002       -2.692891       -0.686938
H       -1.269013       -2.776974       -1.060388
H       -4.846721       -1.008907       1.877259
C       -4.446878       -2.200682       0.117610
H       -3.629392       -3.313819       -1.544934
O       -5.702314       -2.464146       -0.148933
N       -1.863768       1.350585        -0.427006
H       -1.985115       0.657137        -1.160997
C       -3.078190       2.063205        -0.053353
H       -3.230705       1.938869        1.024835
C       -2.998375       3.553906        -0.384321
C       -4.277174       1.421185        -0.776142
H       -2.905658       3.699958        -1.465075
H       -3.898973       4.064373        -0.035539
H       -2.130625       4.002170        0.106587
O       -4.040398       0.628917        -1.726585
O       -5.417075       1.774153        -0.370988
###
35
GlyHisGly2 m062x E=-964.987356358 au
N       -5.844831       -0.156881       -0.623358
H       -5.792645       0.840509        -0.859891
C       -4.773322       -0.514652       0.335186
H       -6.767185       -0.353757       -0.223853
H       -5.750999       -0.683882       -1.498300
C       -3.447212       -0.031072       -0.218912
H       -4.979831       -0.010534       1.281074
H       -4.784542       -1.593041       0.489943
O       -3.414061       0.798701        -1.133341
N       -2.360479       -0.547830       0.365866
H       -2.455938       -1.210218       1.130914
C       -1.025702       -0.104551       0.019994
H       -0.987283       0.099526        -1.053117
C       -0.659040       1.185775        0.798526
C       -0.037849       -1.200981       0.388995
H       -1.371708       1.963634        0.515200
H       -0.764407       0.993235        1.870849
C       0.724021        1.663708        0.510752
O       -0.208124       -1.883228       1.410395
N       1.834318        1.213966        1.205827
C       1.202027        2.519024        -0.436776
H       1.822519        0.536024        1.964886
C       2.938993        1.757462        0.705421
N       2.571041        2.562525        -0.284558
H       0.687872        3.096304        -1.188493
H       3.947824        1.583841        1.047982
N       1.028904        -1.302850       -0.406626
H       1.141931        -0.635255       -1.166524
C       2.245369        -1.977745       0.005478
C       3.466880        -1.355076       -0.680948
H       2.366143        -1.894233       1.089953
H       2.214945        -3.043367       -0.243904
O       3.268376        -0.474520       -1.558211
O       4.584888        -1.795049       -0.303533
H       3.217013        3.110115        -0.845556
###
34
GlyHisGly3 m062x E=-964.533062076 au
N       -5.823581       -0.210446       -0.619094
H       -5.783948       0.786497        -0.859343
C       -4.743563       -0.552425       0.335831
H       -6.741691       -0.417354       -0.215103
H       -5.726357       -0.738897       -1.492650
C       -3.423906       -0.062599       -0.230252
H       -4.949984       -0.044766       1.279705
H       -4.744649       -1.630074       0.496746
O       -3.405721       0.735908        -1.174174
N       -2.331688       -0.539953       0.373291
H       -2.422796       -1.169649       1.165863
C       -0.999860       -0.072396       0.033850
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H       -0.953672       0.094343        -1.045575
C       -0.667475       1.249256        0.769476
C       0.000160        -1.142593       0.440455
H       -1.388298       1.999009        0.430619
H       -0.816368       1.091003        1.842285
C       0.732818        1.709811        0.520313
O       -0.170266       -1.803804       1.477586
N       1.779738        1.328027        1.337460
C       1.208755        2.461011        -0.524732
C       2.862463        1.842788        0.786672
N       2.565963        2.541714        -0.333197
H       0.712316        2.936769        -1.356891
H       3.872122        1.748948        1.160226
N       1.062013        -1.274286       -0.356855
H       1.188630        -0.604177       -1.111627
C       2.271275        -1.948303       0.073467
C       3.495393        -1.392738       -0.662160
H       2.412382        -1.810818       1.149564
H       2.214607        -3.025104       -0.117226
O       3.306422        -0.549334       -1.577586
O       4.608859        -1.845882       -0.284359
H       3.229873        3.022885        -0.927079
###
50
GlyHisLys3 m062x E=-1177.97378381 au
N       -6.089871       -3.129042       -0.484390
H       -6.687807       -2.296940       -0.440850
C       -4.862812       -2.940898       0.324317
H       -6.624208       -3.933938       -0.143819
H       -5.858333       -3.285710       -1.471163
C       -4.110011       -1.737975       -0.214008
H       -5.154151       -2.778495       1.362753
H       -4.259701       -3.846335       0.254238
O       -4.572648       -1.069039       -1.143447
N       -2.939831       -1.479504       0.382507
H       -2.634865       -2.032750       1.178801
C       -2.142178       -0.327284       0.017710
H       -2.170243       -0.204655       -1.068299
C       -2.698056       0.955507        0.690587
C       -0.714753       -0.558315       0.493570
H       -3.739550       1.068678        0.380957
H       -2.674267       0.823496        1.776699
C       -1.947858       2.188118        0.314373
O       -0.496329       -1.176059       1.546622
N       -0.842998       2.644998        1.013801
C       -2.113467       3.055992        -0.723603
C       -0.349723       3.732976        0.430797
N       -1.115932       4.001718        -0.620039
H       -2.851909       3.080582        -1.509183
H       0.509521        4.298300        0.758707
H       -0.970372       4.786469        -1.248058
N       0.232159        0.013398        -0.253319
H       -0.041202       0.539734        -1.079361
C       1.595907        0.231607        0.215284
H       1.588221        0.191431        1.308026
C       2.549081        -0.839450       -0.332485
C       2.030334        1.641786        -0.229268
H       2.188170        -1.813250       0.020494
H       2.482721        -0.842075       -1.427503
C       3.999064        -0.635782       0.098777
O       1.626673        2.029592        -1.359417
O       2.768282        2.290496        0.557224
H       4.397712        0.277816        -0.358623
H       4.045556        -0.493965       1.186238
C       4.878196        -1.821242       -0.295473
H       4.537198        -2.725105       0.224119
H       4.795347        -2.007311       -1.373520
C       6.328203        -1.551895       0.057631
H       6.730435        -0.709406       -0.506246
H       6.454799        -1.360511       1.124191
N       7.179000        -2.738213       -0.270662
H       7.122020        -2.962828       -1.269238
H       8.161913        -2.565292       -0.040426
H       6.870001        -3.562383       0.254120
H       -0.434082       2.202167        1.834568
###
```

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49
GlyHisLys4 m062x E=-1177.51982502 au
N       6.011133        -3.208588       0.502067
H       6.560432        -2.376792       0.745812
C       4.901228        -2.847591       -0.411570
H       6.629673        -3.898267       0.065291
H       5.652385        -3.607189       1.376474
C       4.130768        -1.692025       0.202430
H       5.330837        -2.536810       -1.365363
H       4.271872        -3.723856       -0.563854
O       4.608362        -1.053479       1.147381
N       2.946699        -1.429558       -0.358470
H       2.637638        -1.963586       -1.166080
C       2.166090        -0.261563       0.007074
H       2.207175        -0.135401       1.092378
C       2.722882        1.011141        -0.680314
C       0.731581        -0.488520       -0.443671
H       3.748647        1.146949        -0.325660
H       2.755736        0.827761        -1.759044
C       1.904753        2.231845        -0.405728
O       0.493966        -1.100450       -1.498005
N       0.877238        2.623132        -1.242749
C       1.973609        3.077791        0.672702
C       0.341121        3.684136        -0.670970
N       0.974922        4.001004        0.481481
H       2.630957        3.105141        1.528603
H       -0.487751       4.262218        -1.053292
H       0.744755        4.775190        1.092194
N       -0.207803       0.058168        0.330717
H       0.083826        0.618670        1.127076
C       -1.573118       0.284457        -0.126740
H       -1.568596       0.308734        -1.220218
C       -2.510949       -0.834278       0.351221
C       -2.034390       1.657333        0.396557
H       -2.123420       -1.779637       -0.047979
H       -2.457639       -0.895410       1.445411
C       -3.959402       -0.641372       -0.089893
O       -1.598793       2.014886        1.525549
O       -2.836522       2.305304        -0.325607
H       -4.383384       0.240053        0.405612
H       -3.993196       -0.445937       -1.169630
C       -4.822614       -1.859897       0.231093
H       -4.449481       -2.736797       -0.312093
H       -4.768391       -2.085297       1.303544
C       -6.266311       -1.601655       -0.155215
H       -6.690973       -0.771566       0.410587
H       -6.368295       -1.395526       -1.221636
N       -7.113264       -2.800609       0.134750
H       -7.074218       -3.041110       1.130437
H       -8.092722       -2.632122       -0.112588
H       -6.785927       -3.613135       -0.396943
###
48
GlyHisLys5 m062x E=-1177.06234424 au
N       6.051732        -3.405168       0.353772
H       6.700956        -2.621618       0.360923
C       4.838871        -3.006457       -0.334539
H       5.831557        -3.591034       1.329696
C       4.134814        -1.787862       0.251295
H       5.067050        -2.779977       -1.380616
H       4.127943        -3.837497       -0.342312
O       4.614132        -1.131005       1.186688
N       2.955621        -1.483114       -0.317605
H       2.641098        -2.011662       -1.125495
C       2.198959        -0.297991       0.031150
H       2.236933        -0.159098       1.115390
C       2.777927        0.960896        -0.664650
C       0.760867        -0.498938       -0.420246
H       3.802438        1.085964        -0.302617
H       2.817896        0.765336        -1.741071
C       1.973631        2.195604        -0.411566
O       0.510200        -1.111921       -1.471502
N       0.962441        2.593259        -1.265641
C       2.035298        3.047255        0.662997
C       0.429175        3.663148        -0.707779
N       1.049268        3.979960        0.452017
```

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H       2.679571        3.072324        1.528863
H       -0.387212       4.248240        -1.106004
H       0.817907        4.759756        1.055045
N       -0.171437       0.069006        0.348636
H       0.127302        0.630638        1.141265
C       -1.532759       0.307596        -0.113279
H       -1.524442       0.329280        -1.206873
C       -2.481258       -0.802749       0.363337
C       -1.984678       1.685421        0.404065
H       -2.094309       -1.752461       -0.026019
H       -2.437972       -0.857097       1.458369
C       -3.924809       -0.607264       -0.092319
O       -1.546995       2.045813        1.531333
O       -2.782123       2.335850        -0.321491
H       -4.351250       0.277466        0.395159
H       -3.947873       -0.416785       -1.173235
C       -4.793204       -1.822796       0.226038
H       -4.416263       -2.702534       -0.309906
H       -4.748759       -2.043763       1.299881
C       -6.233356       -1.565280       -0.173952
H       -6.662398       -0.732393       0.384372
H       -6.326364       -1.364322       -1.242175
N       -7.083112       -2.762624       0.114937
H       -7.049832       -2.999841       1.111632
H       -8.061012       -2.594387       -0.138542
H       -6.753134       -3.577155       -0.412075
###
47
GlyHisLys6 m062x E=-1176.59638547 au
N       6.165868        -3.176910       0.157229
H       6.656516        -2.408122       -0.294599
C       4.751081        -3.079985       -0.153812
H       6.291107        -3.034719       1.156879
C       4.084060        -1.788431       0.301945
H       4.598029        -3.200351       -1.229167
H       4.214909        -3.899544       0.335885
O       4.576959        -1.074857       1.188611
N       2.909150        -1.502124       -0.283793
H       2.584666        -2.065888       -1.063076
C       2.145831        -0.314308       0.041661
H       2.189589        -0.150055       1.122273
C       2.714587        0.931785        -0.684996
C       0.706278        -0.531160       -0.397402
H       3.746700        1.057864        -0.346179
H       2.731454        0.720796        -1.759195
C       1.921116        2.172840        -0.429547
O       0.452717        -1.170795       -1.432061
N       0.894842        2.568540        -1.266183
C       2.009605        3.033583        0.635852
C       0.379145        3.646488        -0.707220
N       1.024504        3.969856        0.436986
H       2.671912        3.062317        1.487900
H       -0.442789       4.232046        -1.093182
H       0.809175        4.755148        1.038864
N       -0.223591       0.053878        0.361406
H       0.078289        0.635212        1.138415
C       -1.586490       0.282879        -0.102988
H       -1.579222       0.279065        -1.196895
C       -2.536862       -0.814368       0.399675
C       -2.034554       1.672547        0.383978
H       -2.135207       -1.774978       0.053647
H       -2.510236       -0.827212       1.496887
C       -3.974696       -0.655374       -0.088354
O       -1.596135       2.055224        1.503940
O       -2.829619       2.311122        -0.354755
H       -4.416726       0.250196        0.345654
H       -3.975586       -0.513348       -1.177900
C       -4.846415       -1.858831       0.264964
H       -4.422835       -2.767383       -0.184877
H       -4.845746       -2.011826       1.353260
C       -6.285293       -1.691795       -0.213564
H       -6.716810       -0.793756       0.241415
H       -6.289620       -1.526470       -1.296452
N       -7.173061       -2.822871       0.078028
H       -7.160791       -2.991906       1.082331
H       -6.776494       -3.660433       -0.344626
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###
29
GlySerGly1 m062x E=-815.203847956 au
N       5.027556        -1.150442       -0.220644
H       5.202369        -0.907911       0.760534
C       4.014393        -0.248970       -0.816799
H       5.912026        -1.087391       -0.734264
H       4.706795        -2.124460       -0.239951
C       2.724011        -0.386224       -0.029516
H       4.390926        0.773398        -0.776400
H       3.861852        -0.538361       -1.857291
O       2.629379        -1.206713       0.888279
N       1.734364        0.425609        -0.419281
H       1.890750        1.104675        -1.158868
C       0.440528        0.429765        0.236734
H       0.219104        -0.586911       0.568230
C       0.476057        1.370274        1.446126
C       -0.585274       0.932462        -0.774245
H       1.261989        1.025084        2.126981
H       0.717308        2.383524        1.103165
O       -0.798350       1.329621        2.066797
O       -0.267270       1.841207        -1.555178
H       -0.805665       1.962566        2.797420
N       -1.809947       0.391593        -0.773534
H       -2.460022       0.774491        -1.453411
C       -2.263843       -0.701877       0.069179
C       -3.741256       -0.967979       -0.061570
H       -1.758360       -1.640115       -0.183444
H       -2.080206       -0.487837       1.125121
O       -4.368068       -0.186941       -0.938163
O       -4.295364       -1.834629       0.584333
H       -5.312988       -0.423138       -0.971598
###
28
GlySerGly2 m062x E=-814.756140192 au
N       4.944896        -1.257424       -0.149415
H       5.085188        -1.045399       0.844283
C       3.983195        -0.309070       -0.757666
H       5.849984        -1.206795       -0.627020
H       4.599595        -2.221143       -0.208751
C       2.682613        -0.373826       0.022097
H       4.407485        0.694349        -0.701803
H       3.836349        -0.582874       -1.802487
O       2.603456        -1.040659       1.058629
N       1.671593        0.331513        -0.498130
H       1.816864        0.894053        -1.331920
C       0.393610        0.451158        0.181048
H       0.156331        -0.507325       0.647190
C       0.483865        1.537964        1.256945
C       -0.647695       0.843881        -0.861683
H       1.286513        1.268297        1.952255
H       0.729368        2.494014        0.779206
O       -0.768539       1.606174        1.918939
O       -0.334546       1.667409        -1.740669
H       -0.721281       2.298970        2.591578
N       -1.863914       0.306470        -0.780969
H       -2.555865       0.620260        -1.458029
C       -2.342561       -0.671706       0.183803
C       -3.830071       -0.966420       -0.040577
H       -1.796542       -1.615301       0.090692
H       -2.222506       -0.305170       1.206150
O       -4.427393       -0.358092       -0.965779
O       -4.332632       -1.815049       0.743185
###
27
GlySerGly3 m062x E=-814.298332072 au
N       5.081859        -1.260887       -0.242659
H       4.740522        -2.219087       -0.269703
C       4.042659        -0.376788       -0.734765
H       5.251628        -1.055609       0.739463
C       2.730203        -0.433936       0.038373
H       4.395050        0.658657        -0.698588
H       3.833859        -0.600314       -1.784552
O       2.604903        -1.088287       1.081901
N       1.719131        0.279453        -0.493440
H       1.885943        0.848837        -1.317282
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C       0.442822        0.432145        0.178359
H       0.186219        -0.515013       0.657026
C       0.544891        1.531042        1.240470
C       -0.594254       0.828789        -0.866203
H       1.334485        1.254182        1.947634
H       0.816373        2.474728        0.751803
O       -0.712379       1.638317        1.889973
O       -0.277440       1.647132        -1.749321
H       -0.651814       2.331510        2.560954
N       -1.815788       0.301405        -0.784924
H       -2.503931       0.616769        -1.464901
C       -2.304525       -0.664047       0.187217
C       -3.795444       -0.944217       -0.032702
H       -1.769222       -1.614446       0.101037
H       -2.179452       -0.291516       1.206878
O       -4.386802       -0.340286       -0.964724
O       -4.307555       -1.777678       0.761282
###
58
PheAlaArg1 m062x E=-1332.77041638 au
N       6.362228        -1.107450       -0.172194
H       6.560942        -0.801947       0.789421
H       6.815385        -0.447252       -0.813372
H       6.778495        -2.033730       -0.315727
C       4.888922        -1.144911       -0.387926
H       4.711306        -1.295716       -1.454123
C       4.287829        -2.294759       0.439407
C       4.330445        0.186694        0.094429
H       4.725053        -3.229877       0.075942
H       4.582283        -2.157639       1.485911
C       2.783212        -2.330771       0.319650
O       4.822026        0.735949        1.088663
C       1.980095        -1.691365       1.271025
C       2.176603        -2.948972       -0.777348
H       2.448134        -1.198441       2.120816
C       0.592403        -1.678105       1.132884
C       0.788021        -2.942344       -0.915400
H       2.795688        -3.441666       -1.523338
H       -0.020466       -1.176887       1.877013
C       -0.006342       -2.310518       0.041500
H       0.327511        -3.433330       -1.767263
H       -1.087527       -2.308217       -0.064237
N       3.272544        0.647779        -0.574672
H       2.869318        0.084875        -1.320472
C       2.439185        1.704264        -0.025541
H       2.423633        1.596371        1.064989
C       2.958636        3.096750        -0.393586
C       1.025259        1.490866        -0.558405
H       2.916610        3.246141        -1.476032
H       2.363147        3.869514        0.098595
H       3.994615        3.193461        -0.060711
O       0.803710        0.766010        -1.536335
N       0.066678        2.175701        0.082091
H       0.310090        2.710959        0.909272
C       -1.324084       2.116814        -0.340631
H       -1.355585       2.103884        -1.432863
C       -2.025005       0.860100        0.205380
C       -2.068211       3.357049        0.105901
H       -1.450603       0.004927        -0.165560
H       -1.954189       0.860718        1.299170
C       -3.481288       0.733510        -0.232261
O       -1.672864       3.800875        1.300380
O       -2.970222       3.860224        -0.532288
H       -4.095249       1.502117        0.250478
H       -3.562043       0.875930        -1.316475
C       -4.013836       -0.641301       0.141294
H       -3.460047       -1.414637       -0.403683
H       -3.880149       -0.814788       1.215849
N       -5.434214       -0.736282       -0.190753
H       -5.888892       0.064784        -0.614935
C       -6.169541       -1.823671       0.024506
N       -5.626010       -2.908822       0.574110
N       -7.458656       -1.839619       -0.326288
H       -4.650044       -2.938032       0.833436
H       -6.192360       -3.732127       0.730734
H       -7.899801       -0.998109       -0.672616
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H       -8.039495       -2.631269       -0.085585
H       -2.198764       4.580368        1.556670
###
57
PheAlaArg2 m062x E=-1332.32183645 au
N       6.316053        -1.161770       -0.254164
H       6.543161        -0.879257       0.708111
H       6.763902        -0.495814       -0.893111
H       6.713638        -2.091303       -0.426667
C       4.837473        -1.173866       -0.435339
H       4.632608        -1.318972       -1.497505
C       4.237896        -2.316167       0.403492
C       4.311620        0.165310        0.062377
H       4.644104        -3.258008       0.022057
H       4.568222        -2.191349       1.440776
C       2.729502        -2.322872       0.335473
O       4.827310        0.699060        1.053277
C       1.974376        -1.656695       1.307787
C       2.070323        -2.944952       -0.728313
H       2.483199        -1.160889       2.132140
C       0.582878        -1.621750       1.223757
C       0.677401        -2.917354       -0.811687
H       2.650858        -3.458923       -1.490758
H       0.008366        -1.100045       1.984121
C       -0.068674       -2.259854       0.166396
H       0.176144        -3.412420       -1.637812
H       -1.153166       -2.241061       0.104544
N       3.254976        0.647878        -0.591624
H       2.833594        0.094688        -1.334771
C       2.436697        1.710958        -0.031827
H       2.428090        1.598497        1.058362
C       2.969682        3.098138        -0.398731
C       1.015195        1.509488        -0.556256
H       2.918715        3.252612        -1.480216
H       2.388542        3.876436        0.101815
H       4.010212        3.182149        -0.076349
O       0.788334        0.763961        -1.523210
N       0.070642        2.213963        0.068833
H       0.312215        2.795178        0.866150
C       -1.330868       2.200537        -0.328546
H       -1.385232       2.249430        -1.420015
C       -2.011141       0.912020        0.159565
C       -2.025426       3.439229        0.261063
H       -1.446600       0.071704        -0.258527
H       -1.918319       0.858977        1.251616
C       -3.477212       0.789013        -0.244103
O       -1.585258       3.876099        1.359217
O       -3.004235       3.900094        -0.382491
H       -4.081581       1.537801        0.278854
H       -3.587844       0.967656        -1.320610
C       -3.992849       -0.601291       0.095094
H       -3.441793       -1.355794       -0.478678
H       -3.842864       -0.804396       1.162352
N       -5.417974       -0.699418       -0.217855
H       -5.876747       0.098492        -0.643549
C       -6.145174       -1.792465       -0.007820
N       -5.593097       -2.877775       0.532901
N       -7.435118       -1.816421       -0.358788
H       -4.615395       -2.902785       0.786142
H       -6.154036       -3.704925       0.688264
H       -7.886344       -0.967834       -0.673686
H       -8.013432       -2.603320       -0.096811
###
56
PheAlaArg3 m062x E=-1331.86529835 au
N       6.317733        -1.341141       -0.514217
H       6.708640        -0.621300       -1.118755
H       6.641397        -1.125765       0.428151
C       4.864894        -1.242555       -0.531304
H       4.513142        -1.386494       -1.557720
C       4.263946        -2.348952       0.359667
C       4.346355        0.096125        -0.014273
H       4.607049        -3.308815       -0.037162
H       4.676610        -2.231291       1.368855
C       2.755999        -2.310413       0.408640
O       4.847412        0.634733        0.986043
```

```
C       2.088780        -1.603664       1.416780
C       1.999245        -2.925797       -0.594017
H       2.668103        -1.112952       2.196477
C       0.696317        -1.519690       1.427402
C       0.605653        -2.852498       -0.582804
H       2.507880        -3.471186       -1.385816
H       0.193578        -0.966290       2.215883
C       -0.049276       -2.153153       0.431277
H       0.032602        -3.344574       -1.363072
H       -1.134218       -2.101514       0.445901
N       3.293492        0.613018        -0.664935
H       2.855010        0.060581        -1.396792
C       2.486462        1.672910        -0.087456
H       2.499770        1.560822        1.002984
C       3.010852        3.062219        -0.461372
C       1.052392        1.482479        -0.579766
H       2.932420        3.220468        -1.540938
H       2.446306        3.841930        0.056047
H       4.060272        3.141666        -0.167568
O       0.798005        0.755726        -1.554498
N       0.123506        2.180002        0.078457
H       0.385868        2.742260        0.882482
C       -1.282905       2.199256        -0.301688
H       -1.350502       2.302482        -1.388868
C       -1.973278       0.896437        0.130362
C       -1.957138       3.415527        0.354082
H       -1.419858       0.071323        -0.329595
H       -1.874423       0.790491        1.218277
C       -3.442531       0.802396        -0.269688
O       -1.497583       3.800214        1.463850
O       -2.941697       3.913091        -0.252615
H       -4.038132       1.539707        0.278802
H       -3.555979       1.015070        -1.339794
C       -3.967335       -0.593743       0.029183
H       -3.416292       -1.335853       -0.560677
H       -3.824810       -0.824534       1.091701
N       -5.391378       -0.679077       -0.292508
H       -5.843441       0.124836        -0.714075
C       -6.124852       -1.771299       -0.099541
N       -5.580281       -2.866209       0.429503
N       -7.414215       -1.784426       -0.453696
H       -4.600384       -2.904107       0.672304
H       -6.145170       -3.693557       0.568799
H       -7.862259       -0.928796       -0.753734
H       -7.995750       -2.573396       -0.205462
###
55
PheAlaArg4 m062x E=-1331.38758814 au
N       6.236546        -1.391798       -0.590580
H       6.614480        -0.701411       -1.236188
H       6.590199        -1.140593       0.331868
C       4.784585        -1.282502       -0.568468
H       4.400939        -1.465574       -1.577125
C       4.203843        -2.346231       0.385889
C       4.290129        0.080338        -0.093452
H       4.523646        -3.324687       0.015720
H       4.652042        -2.194085       1.375119
C       2.699119        -2.287234       0.485045
O       4.824495        0.657135        0.867670
C       2.075365        -1.544781       1.495151
C       1.901417        -2.917466       -0.475964
H       2.686567        -1.043177       2.242907
C       0.685213        -1.438470       1.547640
C       0.510327        -2.821292       -0.422912
H       2.376451        -3.490832       -1.268871
H       0.216384        -0.857280       2.336979
C       -0.101226       -2.084820       0.592143
H       -0.095309       -3.324044       -1.171119
H       -1.184182       -2.015041       0.638676
N       3.220761        0.577260        -0.732761
H       2.759006        0.001827        -1.431701
C       2.441033        1.667366        -0.172744
H       2.479316        1.590977        0.920073
C       2.973088        3.037207        -0.604306
C       0.993961        1.483905        -0.627897
H       2.850948        3.171011        -1.683183
```

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H       2.443634        3.839010        -0.083923
H       4.035296        3.105114        -0.357275
O       0.714217        0.763926        -1.601021
N       0.084999        2.181880        0.056736
H       0.369776        2.729814        0.862967
C       -1.333099       2.206876        -0.279761
H       -1.435823       2.333070        -1.361871
C       -2.008646       0.894233        0.146563
C       -1.984911       3.410786        0.420346
H       -1.489587       0.082790        -0.374183
H       -1.841749       0.748784        1.221786
C       -3.501274       0.818439        -0.160520
O       -1.489322       3.775643        1.521763
O       -2.987706       3.920866        -0.144230
H       -4.057640       1.515555        0.475370
H       -3.686460       1.109190        -1.202854
C       -4.013715       -0.597002       0.066197
H       -3.497552       -1.287728       -0.614757
H       -3.775014       -0.901565       1.091807
N       -5.462508       -0.649257       -0.136376
H       -5.808743       0.022350        -0.813253
C       -6.131806       -1.848704       -0.236215
N       -5.530560       -2.914267       0.400145
N       -7.235187       -1.913841       -0.911881
H       -4.940814       -2.703288       1.195945
H       -6.136224       -3.711911       0.548083
H       -7.641840       -2.842556       -0.811844
###
# AMINO ACIDS optimized with pm6
# opt freq pm6 scf=(xqc,tight) scrf(smd,solvent=water)
###
14
Ala1 pm6 E=-0.289447988066E-01 au
N       -1.560691       -0.968457       -0.138075
H       -1.548359       -1.249979       0.862074
H       -1.313280       -1.796581       -0.714102
H       -2.536483       -0.690923       -0.376941
C       -0.611858       0.190053        -0.399767
H       -0.634964       0.421576        -1.516264
C       -1.043459       1.405414        0.398971
C       0.810495        -0.218588       -0.029786
H       -1.034939       1.231665        1.487432
H       -0.387529       2.270107        0.206030
H       -2.065793       1.728247        0.136046
O       1.182499        -1.284516       0.427756
O       1.676633        0.789975        -0.287953
H       2.642053        0.560140        -0.052682
###
12
Ala3 pm6 E=-0.350675522431 au
N       -1.434994       -1.111137       -0.339899
H       -0.901954       -1.898155       -0.714755
H       -1.637823       -1.339701       0.634869
C       -0.628570       0.134560        -0.423988
H       -0.657625       0.469812        -1.498435
C       -1.213517       1.222399        0.471091
C       0.849025        -0.051461       -0.039685
H       -1.180276       0.960265        1.537530
H       -0.688139       2.179216        0.355845
H       -2.269102       1.417536        0.233803
O       1.226489        -1.044249       0.646371
O       1.690791        0.813749        -0.423131
###
13
AlaZW pm6 E=-0.208900430763 au
N       -1.414493       -1.051307       -0.146510
H       -1.078054       -1.858006       -0.701932
H       -1.386857       -1.315482       0.855409
C       -0.570640       0.183043        -0.409645
H       -0.624806       0.412142        -1.517708
C       -1.108834       1.353078        0.393607
C       0.904189        -0.079402       -0.049477
H       -1.065351       1.184086        1.480727
H       -0.547715       2.277173        0.189202
H       -2.162046       1.571395        0.151167
O       1.239408        -1.180714       0.453597
```

```
O       1.738654        0.833346        -0.283236
H       -2.406501       -0.873535       -0.401084
###
28
Arg1 pm6 E=0.118786721404 au
N       3.640099        -1.446201       -0.373734
H       3.722673        -1.759033       0.613832
H       4.559077        -1.062835       -0.674760
H       3.435097        -2.284777       -0.958170
C       2.539661        -0.414057       -0.538407
H       2.493599        -0.116918       -1.636895
C       1.190435        -1.002819       -0.095868
C       2.868315        0.817091        0.301571
H       1.091356        -2.045546       -0.482501
H       1.160164        -1.112814       1.012412
C       0.017481        -0.157513       -0.598051
O       3.521661        0.868627        1.327481
H       0.195606        0.923681        -0.404865
H       -0.069033       -0.239232       -1.704175
C       -1.274940       -0.614983       0.085394
H       -1.450410       -1.706765       -0.080028
H       -1.200499       -0.474037       1.191826
N       -2.423107       0.165016        -0.452334
H       -2.241515       0.791216        -1.256295
C       -3.689280       0.071699        0.058193
N       -3.964728       -0.641466       1.215257
N       -4.727425       0.727401        -0.603271
H       -3.360949       -1.428477       1.471442
H       -4.950007       -0.803330       1.455329
H       -4.484525       1.528490        -1.198334
H       -5.599744       0.874880        -0.083018
O       2.309409        1.921367        -0.246167
H       2.466655        2.765789        0.305270
###
27
Arg2 pm6 E=-0.603171275466E-01 au
N       3.644181        -1.387554       -0.414908
H       3.739710        -1.696812       0.569615
H       4.557615        -1.007281       -0.726764
H       3.429891        -2.224844       -0.993409
C       2.549865        -0.347265       -0.557697
H       2.493051        -0.046538       -1.646196
C       1.207885        -0.941306       -0.109019
C       2.894884        0.901246        0.284857
H       1.074243        -1.950577       -0.565001
H       1.211858        -1.126413       0.987960
C       0.033066        -0.041107       -0.501127
O       3.555907        0.769331        1.343912
H       0.157461        0.974555        -0.070495
H       0.011917        0.107600        -1.603396
C       -1.279754       -0.665798       -0.016019
H       -1.404376       -1.701486       -0.417449
H       -1.275069       -0.760940       1.096548
N       -2.420281       0.180476        -0.463003
H       -2.249707       0.823235        -1.256726
C       -3.681630       0.078251        0.059778
N       -3.951780       -0.676272       1.190698
N       -4.719082       0.773321        -0.560333
H       -3.360508       -1.483926       1.406913
H       -4.935359       -0.821780       1.447582
H       -5.579816       0.921033        -0.020694
O       2.492401        2.015117        -0.131389
H       -4.474544       1.584675        -1.140484
###
26
Arg3 pm6 E=-0.205468049127 au
N       -3.715077       1.392495        -0.293860
H       -3.625672       1.850509        0.617094
H       -3.660523       2.143232        -0.988531
C       -2.585311       0.443167        -0.505573
H       -2.562531       0.161977        -1.594706
C       -1.213435       1.010762        -0.114233
C       -2.959319       -0.811510       0.298019
H       -1.076140       2.000674        -0.601942
H       -1.177583       1.227507        0.973121
C       -0.071261       0.072872        -0.515431
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```
O       -2.615512       -0.972449       1.499976
H       -0.217412       -0.934296       -0.073769
H       -0.075688       -0.092655       -1.614619
C       1.268355        0.666045        -0.065853
H       1.430457        1.675246        -0.517412
H       1.276358        0.814238        1.040586
N       2.373445        -0.244799       -0.474497
H       2.176299        -0.912480       -1.241237
C       3.649601        -0.140640       0.012668
N       3.958727        0.663490        1.098058
N       4.658185        -0.891354       -0.587821
H       3.388205        1.491915        1.287794
H       4.949220        0.795991        1.333527
H       4.385581        -1.713934       -1.138272
H       5.522964        -1.039952       -0.055682
O       -3.658521       -1.696422       -0.284563
###
25
Arg4 pm6 E=-0.343745713425 au
N       -3.566705       1.544995        0.177422
H       -3.502246       1.641754        1.194093
H       -3.416481       2.485640        -0.198988
C       -2.496767       0.636545        -0.323028
H       -2.461600       0.725557        -1.443937
C       -1.099106       0.936074        0.238669
C       -2.970188       -0.779385       0.030751
H       -0.849586       1.999678        0.031371
H       -1.095777       0.859923        1.344439
C       -0.032965       0.017272        -0.365420
O       -2.787200       -1.282931       1.173373
H       -0.170929       -1.022801       -0.004246
H       -0.151517       -0.040682       -1.467301
C       1.368986        0.528283        -0.011385
H       1.546845        1.520972        -0.485977
H       1.457698        0.686660        1.086818
N       2.402318        -0.431132       -0.523173
H       2.076695        -1.410132       -0.428998
C       3.733023        -0.256332       -0.014855
N       4.199820        1.083402        0.100008
N       4.421398        -1.328006       0.308773
H       3.729092        1.784264        -0.474613
H       5.214358        1.190804        0.020356
H       5.412533        -1.201528       0.529350
O       -3.588399       -1.442027       -0.857368
###
18
Asn1 pm6 E=-0.108505849994 au
N       -1.802373       1.656896        -0.309247
H       -2.677061       1.377524        -0.799759
H       -1.462043       2.545250        -0.738869
H       -2.031452       1.851716        0.687250
C       -0.741445       0.580092        -0.436742
H       -0.537216       0.417060        -1.546478
C       0.538667        1.014003        0.276558
C       -1.255012       -0.725522       0.178441
H       0.793807        2.080431        0.009472
H       0.379981        1.075262        1.385604
C       1.726382        0.156251        -0.077778
O       -1.879505       -0.875120       1.208762
O       1.836041        -0.409509       -1.187223
N       2.707471        0.009646        0.855569
H       3.550359        -0.524112       0.655307
H       2.678861        0.471123        1.764113
O       -0.891310       -1.769344       -0.604371
H       -1.164283       -2.677205       -0.221108
###
16
Asn3 pm6 E=-0.438352859507 au
N       -1.799696       1.664246        -0.362646
H       -2.688948       1.337683        -0.748488
H       -1.976016       1.900466        0.616229
C       -0.780662       0.589682        -0.464735
H       -0.551924       0.455172        -1.558161
C       0.491082        1.010485        0.285786
C       -1.260622       -0.771178       0.085348
H       0.739054        2.078105        0.047908
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H       0.311499        1.038528        1.387680
C       1.683433        0.167436        -0.065926
O       -2.132493       -0.819798       0.994336
O       1.803514        -0.394871       -1.182663
N       2.663566        0.001343        0.864779
H       3.506617        -0.530028       0.658172
H       2.635380        0.448136        1.780813
O       -0.773788       -1.831048       -0.404413
###
17
AsnZW pm6 E=-0.292554529674 au
N       -1.882650       1.534149        -0.263867
H       -2.732549       1.244555        -0.784593
H       -1.594700       2.472504        -0.612008
H       -2.132999       1.630744        0.738977
C       -0.767758       0.525848        -0.455770
H       -0.568820       0.434092        -1.566058
C       0.489693        1.004921        0.268615
C       -1.207091       -0.859908       0.083454
H       0.710434        2.077656        0.002524
H       0.316158        1.057275        1.374494
C       1.709143        0.190419        -0.068060
O       -2.085252       -0.918241       0.973633
O       1.852456        -0.382135       -1.174315
N       2.683482        0.071502        0.875291
H       3.545868        -0.434726       0.685403
H       2.634479        0.538998        1.780485
O       -0.658157       -1.878165       -0.407896
###
17
Asp1 pm6 E=-0.172468991456 au
N       1.672244        1.717745        0.212775
H       2.495227        1.544391        0.826557
H       1.239357        2.623686        0.499516
H       2.011098        1.822111        -0.765842
C       0.659165        0.594765        0.332848
H       0.308525        0.552778        1.419995
C       -0.524252       0.851053        -0.598835
C       1.331616        -0.737311       -0.012100
H       -0.756533       1.958019        -0.659849
H       -0.267651       0.607297        -1.665976
C       -1.785851       0.152950        -0.207375
O       2.392954        -0.903198       -0.579497
O       -1.939123       0.052490        1.140227
O       -2.644718       -0.281851       -0.960225
O       0.566315        -1.766290       0.417336
H       0.967874        -2.683529       0.205735
H       -2.791109       -0.426920       1.420478
###
16
Asp2 pm6 E=-0.355904043573 au
N       1.864042        1.532703        -0.007820
H       2.685487        1.319387        0.589709
H       1.582110        2.519668        0.167107
H       2.159127        1.457671        -1.000544
C       0.721850        0.586418        0.297254
H       0.446013        0.709245        1.391720
C       -0.476436       0.924153        -0.588173
C       1.169324        -0.883081       0.088060
H       -0.690640       2.031926        -0.567697
H       -0.249141       0.731164        -1.669425
C       -1.718139       0.196445        -0.189934
O       2.375099        -1.120977       -0.146687
O       -1.992205       0.313721        1.138373
O       -2.466191       -0.448659       -0.912248
O       0.292070        -1.776566       0.179476
H       -2.831026       -0.181733       1.429328
###
15
Asp3 pm6 E=-0.537575847722 au
N       1.987179        -1.398411       -0.045075
H       2.807571        -1.085499       -0.598188
H       1.831534        -2.409153       -0.239254
H       2.221213        -1.301377       0.961557
C       0.756766        -0.590431       -0.405521
H       0.573069        -0.713608       -1.516348
```

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C       -0.441806       -1.103148       0.388712
C       0.991118        0.913094        -0.124113
H       -0.650857       -2.173537       0.136772
H       -0.216796       -1.133677       1.481211
C       -1.686654       -0.283665       0.131221
O       1.982014        1.271973        0.549919
O       -2.197417       -0.238417       -1.023049
O       -2.209247       0.363921        1.084330
O       0.150585        1.726352        -0.592702
###
14
Asp4 pm6 E=-0.683583788931 au
N       1.938983        -1.539674       -0.159541
H       2.798021        -1.099653       -0.499835
H       2.063571        -1.674883       0.846467
C       0.778099        -0.655345       -0.429296
H       0.560599        -0.725653       -1.531523
C       -0.441282       -1.127215       0.373591
C       1.035067        0.830112        -0.101702
H       -0.688439       -2.182376       0.109198
H       -0.207640       -1.181341       1.460136
C       -1.648870       -0.257375       0.131910
O       1.849968        1.165464        0.797776
O       -2.133960       -0.136225       -1.030928
O       -2.165671       0.375608        1.098770
O       0.395028        1.707724        -0.754953
###
15
Cys1 pm6 E=-0.226588862801E-01 au
N       2.152562        -0.853982       0.003628
H       2.870738        -0.146205       -0.251888
H       2.427595        -1.762612       -0.430414
H       2.166205        -0.980492       1.035303
C       0.780705        -0.443840       -0.493415
H       0.831361        -0.389248       -1.632414
C       -0.288475       -1.440855       -0.063737
C       0.392239        0.937221        0.050499
H       -0.432401       -2.244807       -0.818756
H       -0.028093       -1.986359       0.877769
S       -1.786498       -0.480491       0.255649
O       0.616642        1.411811        1.148335
H       -2.105432       -0.097663       -1.006730
O       -0.236234       1.638572        -0.926173
H       -0.564014       2.554903        -0.626020
###
14
Cys2 pm6 E=-0.203458069673 au
N       1.847780        -1.327787       0.002950
H       1.942649        -1.325090       1.035736
H       2.705502        -0.908488       -0.404810
H       1.796960        -2.320900       -0.306939
C       0.610116        -0.573764       -0.444988
H       0.585390        -0.603746       -1.577478
C       -0.642471       -1.229194       0.114231
C       0.686198        0.907276        0.009420
H       -0.891270       -2.163897       -0.440409
H       -0.528044       -1.550693       1.172492
S       -1.994788       -0.040036       -0.092321
O       0.749547        1.189694        1.229593
H       -2.150450       0.375658        1.189021
O       0.700246        1.786097        -0.889981
###
13
Cys3 pm6 E=-0.356534607019 au
N       1.976477        -1.046361       0.049246
H       1.978917        -1.105061       1.083467
H       2.762827        -0.436826       -0.241550
H       2.158737        -2.002799       -0.317563
C       0.649275        -0.526390       -0.476679
H       0.705203        -0.537059       -1.603729
C       -0.514252       -1.386346       -0.005682
C       0.413161        0.929615        -0.008673
H       -0.726585       -2.216705       -0.699433
H       -0.350359       -1.833712       0.990864
S       -1.898391       -0.200030       0.062493
O       0.553726        1.252915        1.202742
```

```
O       0.286408        1.816573        -0.904049
###
12
Cys4 pm6 E=-0.501268781469 au
N       -1.765745       1.417011        -0.064036
H       -1.793193       1.552202        0.949523
H       -1.726286       2.359693        -0.462551
C       -0.534455       0.668926        -0.450039
H       -0.471713       0.683670        -1.571718
C       0.766621        1.207548        0.134238
C       -0.728171       -0.781098       0.005238
H       1.122933        2.093106        -0.415922
H       0.667601        1.504678        1.191074
S       1.975673        -0.154606       -0.004763
O       -0.907605       -1.091434       1.220963
O       -0.851627       -1.684939       -0.883783
###
21
Gln1 pm6 E=-0.120600899622 au
N       2.267071        -1.682736       -0.328341
H       2.341393        -1.938323       0.676765
H       3.221634        -1.468229       -0.681871
H       1.913274        -2.516537       -0.844581
C       1.330106        -0.507679       -0.535095
H       1.271055        -0.295135       -1.654101
C       -0.069063       -0.842559       0.010458
C       1.889326        0.721845        0.175190
H       -0.344261       -1.883231       -0.283955
H       -0.061501       -0.848000       1.124245
C       -1.113037       0.137185        -0.519993
O       2.667171        0.749937        1.111199
H       -0.789645       1.194239        -0.341379
H       -1.184625       0.066826        -1.635260
C       -2.471693       -0.098174       0.079052
O       -2.761794       -1.110796       0.755976
N       -3.433030       0.850572        -0.129675
H       -4.371621       0.743726        0.243638
H       -3.269301       1.687716        -0.684935
O       1.387333        1.850598        -0.375582
H       1.699793        2.700480        0.097132
###
19
Gln3 pm6 E=-0.446841044087 au
N       -2.367839       1.631053        -0.127677
H       -2.286573       1.876683        0.862521
H       -2.148274       2.487387        -0.645598
C       -1.381304       0.572745        -0.480586
H       -1.398836       0.441054        -1.597448
C       0.058944        0.876845        -0.038264
C       -1.905814       -0.717124       0.169298
H       0.337663        1.899610        -0.371322
H       0.124122        0.906055        1.068701
C       1.047441        -0.141516       -0.607349
O       -1.594402       -1.033406       1.348803
H       0.678958        -1.183361       -0.456007
H       1.107887        -0.045156       -1.719829
C       2.422236        0.014380        -0.021020
O       2.761262        0.998469        0.678107
N       3.340072        -0.970034       -0.256634
H       4.286836        -0.911015       0.107501
H       3.138194        -1.784524       -0.833187
O       -2.678688       -1.458293       -0.509112
###
20
GlnZW pm6 E=-0.300149013784 au
N       -2.226337       1.635709        -0.494847
H       -2.335380       1.937754        0.490796
H       -3.168472       1.423804        -0.875958
H       -1.837812       2.437478        -1.032321
C       -1.315041       0.429217        -0.605633
H       -1.247861       0.142089        -1.698052
C       0.082415        0.782609        -0.079506
C       -1.913933       -0.758185       0.184529
H       0.460728        1.682278        -0.620008
H       0.031551        1.081762        0.990702
C       1.060283        -0.377836       -0.262679
```

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O       -2.409348       -0.563850       1.319905
H       0.758787        -1.259418       0.354318
H       1.028680        -0.750465       -1.315055
C       2.458963        0.013809        0.131519
O       2.701233        0.890090        0.993504
N       3.503554        -0.629819       -0.467533
H       4.466219        -0.422615       -0.214433
H       3.377206        -1.356311       -1.169422
O       -1.880670       -1.888148       -0.361320
###
20
Glu1 pm6 E=-0.184997031505 au
N       -2.022781       1.877597        0.031392
H       -2.969436       1.879292        -0.400107
H       -1.533206       2.749451        -0.264454
H       -2.134234       1.911017        1.064250
C       -1.229610       0.661919        -0.407080
H       -1.167558       0.674355        -1.545874
C       0.184324        0.709597        0.193901
C       -1.944615       -0.609361       0.044972
H       0.614742        1.729522        0.036612
H       0.147296        0.582684        1.302260
C       1.087136        -0.349563       -0.436890
O       -2.529259       -0.803201       1.094049
H       0.781427        -1.378702       -0.116657
H       0.969343        -0.364569       -1.550112
C       2.519426        -0.109308       -0.086435
O       2.955261        -0.408076       1.177135
O       3.390424        0.331872        -0.827338
O       -1.841530       -1.561126       -0.910959
H       -2.281422       -2.445565       -0.651203
H       2.233373        -0.776134       1.791642
###
19
Glu2 pm6 E=-0.364766201658 au
N       -2.079243       1.773444        -0.287733
H       -2.171551       1.969931        0.726639
H       -3.031806       1.678237        -0.688775
H       -1.629343       2.601193        -0.730674
C       -1.255480       0.526040        -0.536485
H       -1.197700       0.362860        -1.655020
C       0.157271        0.718384        0.029350
C       -1.949735       -0.698996       0.108721
H       0.607173        1.639135        -0.414813
H       0.118062        0.918307        1.125297
C       1.044402        -0.492886       -0.260144
O       -2.251329       -0.677009       1.324591
H       0.771667        -1.356778       0.398318
H       0.874096        -0.871951       -1.298767
C       2.491806        -0.174135       -0.080629
O       2.953157        0.240643        1.140731
O       3.364489        -0.247479       -0.939269
O       -2.186312       -1.683216       -0.635687
H       2.244479        0.310998        1.864119
###
18
Glu3 pm6 E=-0.545112454208 au
N       -2.077967       1.767764        0.175789
H       -2.226273       1.655505        1.195702
H       -3.008229       1.794673        -0.285002
H       -1.615884       2.686249        0.021410
C       -1.230970       0.643448        -0.385491
H       -1.174892       0.776927        -1.507113
C       0.180887        0.700656        0.216276
C       -1.886124       -0.721138       -0.076402
H       0.603556        1.720902        0.063463
H       0.138720        0.571683        1.320650
C       1.093960        -0.352057       -0.410150
O       -2.414030       -0.915666       1.045345
H       0.767606        -1.377240       -0.133347
H       1.028637        -0.327697       -1.521617
C       2.527202        -0.127973       0.012021
O       3.060474        -0.887944       0.872532
O       3.199182        0.810444        -0.508297
O       -1.855276       -1.598455       -0.974855
###
```

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17
Glu4 pm6 E=-0.691027174615 au
N       2.224524        1.636976        -0.516049
H       2.050596        1.524129        -1.518535
H       2.014599        2.619102        -0.310956
C       1.306784        0.763983        0.266633
H       1.426636        1.022525        1.354623
C       -0.175121       0.906588        -0.114526
C       1.805454        -0.673100       0.052383
H       -0.477192       1.971367        -0.014703
H       -0.314749       0.676048        -1.191250
C       -1.072944       0.023295        0.754150
O       1.479882        -1.339202       -0.971249
H       -0.611597       -0.966179       0.955055
H       -1.199975       0.465781        1.766240
C       -2.411438       -0.157605       0.083935
O       -2.647030       -1.214785       -0.575886
O       -3.293991       0.745839        0.160701
O       2.564089        -1.185672       0.925987
###
11
Gly1 pm6 E=-0.205903340032E-01 au
N       1.904467        0.102428        0.000000
H       1.951465        0.706321        -0.842834
C       0.652546        -0.726823       -0.000002
H       2.738861        -0.518919       -0.000035
H       1.951495        0.706270        0.842868
C       -0.592279       0.111604        0.000002
H       0.647159        -1.430924       -0.887240
H       0.647161        -1.430928       0.887233
O       -0.691094       1.325767        0.000000
O       -1.692024       -0.687842       0.000001
H       -2.564069       -0.160906       0.000001
###
Gly3 pm6 E=-0.341479358210 au
###
10
GlyZW pm6 E=-0.199136603960 au
N       1.812641        0.119002        -0.146228
C       0.615032        -0.710193       0.211702
C       -0.702738       0.032430        0.027597
O       -1.737022       -0.660889       -0.164267
O       -0.736478       1.285943        0.088685
H       1.809721        0.353441        -1.155831
H       0.687584        -1.059865       1.279512
H       0.615926        -1.661934       -0.382684
H       1.827119        1.004640        0.389491
H       2.685395        -0.403146       0.061969
###
22
His1 pm6 E=0.169198004511 au
N       2.654229        -1.439670       -0.078037
H       3.400054        -1.161895       -0.749090
H       2.449857        -2.452866       -0.223448
H       3.021873        -1.327037       0.887449
C       1.396180        -0.621802       -0.296501
H       1.022982        -0.830389       -1.355310
C       0.319070        -1.017006       0.727499
C       1.714373        0.868017        -0.166090
H       0.288181        -2.137679       0.838211
H       0.594253        -0.661412       1.755024
C       -1.021196       -0.538513       0.325467
O       2.534256        1.396559        0.559565
N       -1.771059       0.383944        1.080135
C       -1.794146       -0.882031       -0.785065
H       -1.473324       0.822199        1.960421
C       -2.971108       0.600219        0.440015
N       -2.993574       -0.169077       -0.702909
H       -1.565956       -1.566802       -1.598077
H       -3.771578       1.268603        0.783198
O       0.922384        1.577097        -1.003208
H       1.056589        2.586801        -0.934099
H       -3.762257       -0.208451       -1.381411
###
21
His2 pm6 E=-0.837459662080E-02 au
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```
N       -2.370447       1.620136        -0.381410
H       -3.091128       1.396808        -1.093991
H       -1.958749       2.546484        -0.616162
H       -2.842609       1.704263        0.538505
C       -1.297262       0.550232        -0.350346
H       -0.850556       0.475940        -1.390406
C       -0.212476       0.929017        0.667632
C       -1.931505       -0.820590       -0.016132
H       -0.167513       2.044084        0.803620
H       -0.479206       0.560995        1.691295
C       1.131928        0.440956        0.285676
O       -3.174769       -0.891967       0.138551
N       1.428210        -0.914261       0.040649
C       2.322828        1.150835        0.135425
H       0.734634        -1.683388       0.056445
C       2.767840        -1.023744       -0.262048
N       3.324857        0.233301        -0.202134
H       2.509903        2.214772        0.246577
H       3.296130        -1.952477       -0.510375
O       -1.178567       -1.820643       0.073061
H       4.309324        0.458928        -0.379377
###
20
His3 pm6 E=-0.167526328350 au
N       -2.859605       -1.034559       -0.010744
H       -3.099203       -0.768311       -0.983824
H       -3.570423       -0.621990       0.623055
H       -2.929579       -2.070684       0.060789
C       -1.467723       -0.571403       0.363253
H       -1.270789       -0.886629       1.431772
C       -0.423586       -1.219282       -0.563846
C       -1.362426       0.967431        0.268022
H       -0.413534       -2.325152       -0.400793
H       -0.717100       -1.099317       -1.633214
C       0.925227        -0.655055       -0.313175
O       -1.870759       1.568935        -0.709185
N       1.513765        0.297801        -1.157260
C       1.780571        -0.928316       0.760659
C       2.717368        0.599862        -0.594634
N       2.912614        -0.130309       0.576299
H       1.664484        -1.607841       1.589838
H       3.440700        1.306158        -0.989671
O       -0.730958       1.566688        1.176130
H       3.725168        -0.101168       1.186758
###
19
His4 pm6 E=-0.313814202459 au
N       -2.913049       -1.008996       0.038840
H       -3.020931       -2.018222       0.181947
H       -3.108988       -0.848554       -0.952349
C       -1.518831       -0.612903       0.358532
H       -1.309380       -0.920131       1.420077
C       -0.449443       -1.244013       -0.560708
C       -1.414412       0.914719        0.261376
H       -0.425439       -2.345458       -0.390371
H       -0.739629       -1.136074       -1.628666
C       0.890746        -0.661180       -0.308887
O       -1.832169       1.540975        -0.752510
N       1.481453        0.274072        -1.170472
C       1.734242        -0.893491       0.783972
C       2.675543        0.604690        -0.600674
N       2.861843        -0.089072       0.591936
H       1.615564        -1.549738       1.630330
H       3.396477        1.306433        -1.007549
O       -0.866593       1.542202        1.216093
H       3.663622        -0.032632       1.214119
###
23
Ile1 pm6 E=-0.514292298651E-01 au
N       1.397070        -1.710863       -0.721662
H       1.623868        -2.033449       0.239362
H       2.288027        -1.598585       -1.246516
H       0.841404        -2.459994       -1.187381
C       0.611800        -0.414598       -0.701540
H       0.467712        -0.079350       -1.781732
C       -0.792505       -0.625441       -0.053684
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C       1.405703        0.650733        0.036932
H       -1.223687       -1.561455       -0.504438
C       -0.689052       -0.810300       1.455438
C       -1.705364       0.558661        -0.429777
O       2.269238        0.486648        0.881150
H       -0.319526       0.082291        1.975159
H       -1.675861       -1.029875       1.891665
H       -0.041424       -1.651732       1.735471
H       -1.601700       0.786913        -1.511880
H       -1.375916       1.477467        0.097169
C       -3.167439       0.273594        -0.112949
H       -3.332181       0.084448        0.955928
H       -3.805549       1.123261        -0.388313
H       -3.544897       -0.601846       -0.655736
O       1.033190        1.889258        -0.364432
H       1.521964        2.634802        0.132605
###
22
Ile2 pm6 E=-0.230487034413 au
N       1.441390        -1.624980       -0.715324
H       1.687244        -1.918243       0.247838
H       2.322759        -1.495408       -1.246779
H       0.908291        -2.400344       -1.158534
C       0.623504        -0.349846       -0.710700
H       0.469002        -0.039726       -1.788367
C       -0.765978       -0.595868       -0.057108
C       1.394371        0.772839        0.007168
H       -1.175130       -1.548115       -0.491898
C       -0.655644       -0.764316       1.455604
C       -1.721510       0.553479        -0.438239
O       2.279170        0.473768        0.849326
H       -0.309006       0.142907        1.963448
H       -1.634857       -1.005457       1.896014
H       0.015547        -1.585207       1.738274
H       -1.628148       0.777013        -1.521656
H       -1.425798       1.484639        0.084126
C       -3.173853       0.224184        -0.117469
H       -3.330166       0.033655        0.952347
H       -3.839006       1.052215        -0.394136
H       -3.524753       -0.664806       -0.655884
O       1.116949        1.963596        -0.280959
###
21
Ile3 pm6 E=-0.372870076557 au
N       -1.502102       1.537679        -0.929542
H       -1.584712       2.023789        -0.032497
H       -1.028012       2.195230        -1.556075
C       -0.656806       0.322744        -0.768787
H       -0.534481       -0.126201       -1.794841
C       0.765515        0.591507        -0.198237
C       -1.421789       -0.684329       0.093303
H       1.223020        1.386545        -0.843773
C       0.724127        1.111313        1.237170
C       1.629187        -0.681006       -0.321175
O       -2.093848       -0.331020       1.104329
H       0.410991        0.344711        1.954243
H       1.716471        1.451728        1.564506
H       0.049086        1.968608        1.350395
H       1.513595        -1.112257       -1.336824
H       1.262176        -1.459600       0.375890
C       3.105754        -0.412478       -0.056395
H       3.282540        -0.043030       0.961698
H       3.703220        -1.325450       -0.172978
H       3.521365        0.332473        -0.745488
O       -1.393211       -1.904831       -0.245923
###
23
Leu1 pm6 E=-0.531110843465E-01 au
N       1.663630        1.822190        0.167040
H       1.929373        1.946002        -0.829850
H       2.534789        1.728608        0.727782
H       1.173834        2.688246        0.476455
C       0.758907        0.618214        0.355121
H       0.483732        0.552379        1.459982
C       -0.514849       0.766858        -0.488669
C       1.498253        -0.651947       -0.054816
```

```
H       -0.913953       1.801578        -0.384178
H       -0.277955       0.667814        -1.570214
C       -1.605931       -0.249998       -0.084071
O       2.300915        -0.794964       -0.959033
H       -1.151111       -1.274491       -0.064653
C       -2.156389       0.060086        1.309014
C       -2.722518       -0.239096       -1.130305
H       -2.659523       1.033092        1.352540
H       -2.887280       -0.692458       1.628850
H       -1.364570       0.078599        2.069929
H       -2.360115       -0.541323       -2.120557
H       -3.529182       -0.933408       -0.864647
H       -3.177311       0.751885        -1.245952
O       1.128217        -1.682589       0.742027
H       1.575967        -2.566135       0.493639
###
21
Leu3 pm6 E=-0.374309277788 au
N       -1.737727       1.690067        -0.679149
H       -2.654768       1.382506        -1.009419
H       -1.885700       2.122421        0.233889
C       -0.817953       0.527104        -0.564864
H       -0.621070       0.156791        -1.608618
C       0.505741        0.964703        0.079918
C       -1.436859       -0.631511       0.237338
H       0.940353        1.791646        -0.518215
H       0.315821        1.408991        1.078261
C       1.537715        -0.175885       0.213172
O       -1.957422       -0.433335       1.371786
H       1.104734        -0.970517       0.872256
C       1.876765        -0.805698       -1.139994
C       2.804590        0.362767        0.886030
H       2.250959        -0.068203       -1.859332
H       2.654397        -1.573634       -1.042401
H       1.010589        -1.291308       -1.602647
H       2.592198        0.813144        1.862983
H       3.540265        -0.432154       1.056963
H       3.301022        1.131355        0.282192
O       -1.443166       -1.785465       -0.279470
###
22
LeuZW pm6 E=-0.232588018784 au
N       1.753863        1.698627        0.286580
H       2.038744        1.835963        -0.700383
H       2.609310        1.540391        0.851646
H       1.309862        2.579892        0.615545
C       0.789284        0.536116        0.423400
H       0.527553        0.428817        1.519680
C       -0.481646       0.816555        -0.386937
C       1.455422        -0.770813       -0.053307
H       -0.863089       1.832928        -0.142710
H       -0.244731       0.858691        -1.471380
C       -1.594936       -0.224869       -0.133825
O       2.308897        -0.737222       -0.975090
H       -1.180259       -1.245010       -0.336997
C       -2.083394       -0.183234       1.315569
C       -2.752881       0.021975        -1.104219
H       -2.498069       0.794636        1.587055
H       -2.870824       -0.925229       1.496286
H       -1.278160       -0.394049       2.030348
H       -2.429331       -0.022781       -2.151157
H       -3.544581       -0.727758       -0.985202
H       -3.218003       1.003953        -0.957130
O       1.112783        -1.840930       0.509373
###
26
Lys1 pm6 E=0.824413532402E-01 au
N       2.726353        -1.666491       -0.181609
H       2.874026        -1.801174       0.837801
H       3.643421        -1.447350       -0.619740
H       2.390490        -2.570916       -0.577685
C       1.712715        -0.572509       -0.459164
H       1.605861        -0.466385       -1.588057
C       0.355379        -0.945175       0.159202
C       2.204317        0.747542        0.126672
H       0.085216        -1.982756       -0.150832
```

```
H       0.429470        -0.991801       1.268363
C       -0.745903       0.029531        -0.267011
O       2.818970        0.924310        1.162678
H       -0.552312       1.039016        0.152789
H       -0.739035       0.163082        -1.369942
C       -2.117018       -0.479308       0.189754
H       -2.328131       -1.471061       -0.266465
H       -2.117547       -0.658328       1.287007
C       -3.209702       0.522658        -0.185355
H       -3.046966       1.506169        0.319788
H       -3.201808       0.738761        -1.282338
N       -4.574756       -0.010570       0.201317
H       -4.622024       -0.213621       1.215749
H       -5.314746       0.677851        -0.023709
H       -4.787885       -0.887246       -0.306258
O       1.845621        1.775623        -0.677128
H       2.105335        2.689275        -0.303408
###
25
Lys2 pm6 E=-0.971595878454E-01 au
N       -2.754418       1.601730        -0.174916
H       -2.906399       1.702238        0.845190
H       -3.664890       1.378950        -0.619078
H       -2.436690       2.522638        -0.540740
C       -1.727166       0.528711        -0.477110
H       -1.611930       0.464728        -1.600244
C       -0.381935       0.902997        0.159700
C       -2.211211       -0.839061       0.050705
H       -0.103893       1.937251        -0.149779
H       -0.473709       0.955261        1.265907
C       0.727456        -0.075939       -0.238696
O       -2.814824       -0.907599       1.149628
H       0.547476        -1.070543       0.218079
H       0.718607        -0.246036       -1.335882
C       2.097000        0.459964        0.192335
H       2.294650        1.437850        -0.298930
H       2.102878        0.676333        1.282485
C       3.198905        -0.541966       -0.155321
H       3.071572        -1.495640       0.412952
H       3.165525        -0.823098       -1.236798
N       4.563637        0.039014        0.158878
H       4.639721        0.290529        1.160672
H       5.311321        -0.643797       -0.058540
H       4.739870        0.895164        -0.395787
O       -1.969794       -1.851810       -0.652993
###
23
Lys3 pm6 E=-0.371171799741 au
N       -2.681725       1.681072        -0.191799
H       -3.624643       1.383590        -0.452050
H       -2.709949       1.895510        0.806639
C       -1.703819       0.594522        -0.467462
H       -1.614518       0.502813        -1.584434
C       -0.333318       0.956671        0.126331
C       -2.182876       -0.758603       0.086421
H       -0.052960       1.978058        -0.208635
H       -0.395047       1.032428        1.230564
C       0.755538        -0.042101       -0.280163
O       -2.371977       -0.924448       1.324139
H       0.562999        -1.030975       0.180845
H       0.728536        -0.219580       -1.374346
C       2.140592        0.470245        0.131346
H       2.343039        1.444442        -0.357124
H       2.162847        0.684920        1.219255
C       3.237117        -0.539431       -0.229205
H       3.038714        -1.512591       0.269431
H       3.226005        -0.756022       -1.319963
N       4.589496        0.009967        0.107915
H       4.572013        0.416378        1.045418
H       5.257634        -0.761927       0.158762
O       -2.419082       -1.698320       -0.727987
###
24
LysZW pm6 E=-0.241983178307 au
N       -2.822476       1.591270        -0.071810
H       -2.802766       1.808026        0.928021
```

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H       -2.644405       2.478621        -0.551387
C       -1.743124       0.621574        -0.410894
H       -1.633462       0.600267        -1.530229
C       -0.376426       0.949040        0.208317
C       -2.272570       -0.745392       0.043861
H       -0.083392       1.977554        -0.093827
H       -0.445197       0.991662        1.313357
C       0.699835        -0.053004       -0.221710
O       -2.231727       -1.112954       1.250447
H       0.508774        -1.043287       0.238393
H       0.650676        -0.227060       -1.316800
C       2.097820        0.445572        0.160975
H       2.317630        1.397956        -0.368666
H       2.138949        0.697912        1.241894
C       3.154062        -0.607899       -0.176535
H       3.030834        -1.519125       0.457942
H       3.057157        -0.957242       -1.233923
N       4.548153        -0.048322       0.028842
H       4.682913        0.260847        1.007692
H       5.265295        -0.764371       -0.183723
H       4.715742        0.766209        -0.588129
O       -2.792782       -1.503039       -0.830939
###
21
Met1 pm6 E=-0.306438461135E-01 au
N       -2.475005       -1.625186       0.258401
H       -2.626003       -1.788382       -0.756576
H       -3.390338       -1.391119       0.692670
H       -2.139898       -2.518608       0.679677
C       -1.458034       -0.526782       0.501122
H       -1.340155       -0.395880       1.627631
C       -0.103476       -0.909532       -0.127491
C       -1.964128       0.780261        -0.100192
H       0.096850        -1.993973       0.057938
H       -0.160587       -0.823585       -1.237260
C       1.016744        -0.063183       0.451477
O       -2.781434       0.920937        -0.992074
H       0.800760        1.023171        0.384245
H       1.173513        -0.270671       1.529474
S       2.519436        -0.459851       -0.499218
C       3.733364        0.633894        0.252687
H       3.843290        0.466086        1.331638
H       4.712661        0.447865        -0.214138
H       3.497221        1.695274        0.104394
O       -1.363234       1.836696        0.494163
H       -1.642733       2.734731        0.096661
###
19
Met3 pm6 E=-0.357068950170 au
N       -2.745200       -1.299126       -0.173211
H       -2.615061       -1.452541       -1.176928
H       -2.807118       -2.233709       0.241959
C       -1.569039       -0.582738       0.395337
H       -1.655381       -0.605876       1.516831
C       -0.208133       -1.180282       -0.004659
C       -1.719060       0.875332        -0.065572
H       -0.207395       -2.270672       0.215789
H       -0.092969       -1.132075       -1.108912
C       0.939426        -0.498251       0.725325
O       -1.188615       1.301872        -1.130787
H       0.683310        0.520506        1.075787
H       1.226189        -1.053497       1.639340
S       2.351519        -0.416713       -0.427963
C       3.384659        0.862652        0.306629
H       3.625027        0.659418        1.357530
H       4.332855        0.908997        -0.250872
H       2.927283        1.857926        0.255586
O       -2.410356       1.660945        0.649715
###
20
MetZW pm6 E=-0.210457794376 au
N       2.583668        -1.486924       -0.163541
H       2.706017        -1.569005       0.862494
H       3.493665        -1.211206       -0.578560
H       2.336217        -2.429255       -0.528781
C       1.504444        -0.481645       -0.511499
```

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H       1.452374        -0.402427       -1.638418
C       0.146803        -0.948110       0.040855
C       1.858408        0.904439        0.071816
H       0.000922        -2.030057       -0.193715
H       0.156281        -0.903740       1.153277
C       -0.987287       -0.126016       -0.549314
O       2.419175        0.982325        1.192546
H       -0.790392       0.963102        -0.505080
H       -1.149061       -0.357857       -1.620826
S       -2.478361       -0.522541       0.421389
C       -3.639632       0.734730        -0.134706
H       -3.770769       0.738504        -1.224439
H       -4.622099       0.530086        0.317756
H       -3.345496       1.747084        0.168294
O       1.556327        1.916863        -0.606590
###
24
Phe1 pm6 E=0.151768894846E-01 au
N       -2.996050       -1.249952       -0.120092
H       -3.385272       -0.863630       -1.002573
H       -3.682213       -1.075757       0.643414
H       -2.901294       -2.281956       -0.239926
C       -1.647504       -0.641217       0.214298
H       -1.311230       -1.072987       1.214068
C       -0.618709       -0.979729       -0.875763
C       -1.775213       0.876967        0.335281
H       -0.623533       -2.082973       -1.065882
H       -0.923502       -0.539324       -1.854057
C       0.764167        -0.540109       -0.483799
O       -2.411614       1.633872        -0.373187
C       1.374277        0.534987        -1.145806
C       1.450884        -1.207677       0.542194
H       0.846526        1.059956        -1.943642
C       2.664407        0.934050        -0.786159
C       2.737804        -0.800702       0.900140
H       0.980690        -2.045053       1.060858
H       3.138306        1.768482        -1.305850
C       3.347330        0.268356        0.235549
H       3.268909        -1.319662       1.699889
H       4.354201        0.581759        0.514019
O       -1.030574       1.318499        1.375630
H       -1.036397       2.332293        1.485170
###
22
Phe3 pm6 E=-0.308769424168 au
N       2.811898        1.546097        0.079238
H       3.554364        1.251290        0.718709
H       3.185979        1.427496        -0.864164
C       1.609907        0.694238        0.273290
H       1.144225        1.004909        1.249159
C       0.601877        0.913682        -0.871083
C       1.934887        -0.807763       0.357077
H       0.583554        1.992189        -1.149902
H       0.942540        0.405014        -1.798046
C       -0.777356       0.461389        -0.480423
O       2.789204        -1.328334       -0.415129
C       -1.230439       -0.821626       -0.821639
C       -1.619034       1.324987        0.238231
H       -0.588692       -1.497585       -1.386599
C       -2.511406       -1.234642       -0.445383
C       -2.898777       0.907521        0.609751
H       -1.276816       2.325824        0.504135
H       -2.860224       -2.233917       -0.711958
C       -3.347256       -0.372738       0.270266
H       -3.550741       1.584004        1.165339
H       -4.346961       -0.696032       0.561770
O       1.330179        -1.518686       1.212175
###
23
PheZW pm6 E=-0.166020708009 au
N       -2.884827       1.366435        0.051338
H       -3.334498       1.006610        0.912969
H       -3.558784       1.264425        -0.731552
H       -2.700760       2.381817        0.185994
C       -1.595303       0.626662        -0.243952
H       -1.176042       1.030595        -1.213509
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C       -0.589336       0.850230        0.894783
C       -1.874329       -0.883590       -0.412341
H       -0.591381       1.926572        1.199123
H       -0.912240       0.311560        1.814226
C       0.801212        0.448407        0.487922
O       -2.808755       -1.413970       0.236871
C       1.348971        -0.762217       0.936827
C       1.557658        1.287794        -0.344576
H       0.771584        -1.417494       1.589814
C       2.642618        -1.128224       0.554956
C       2.849744        0.916335        -0.722296
H       1.138969        2.232577        -0.694734
H       3.066690        -2.070402       0.906643
C       3.394632        -0.291327       -0.274372
H       3.436525        1.572788        -1.367456
H       4.404728        -0.577304       -0.569795
O       -1.137022       -1.537431       -1.193470
###
18
Pro1 pm6 E=-0.211812152301E-01 au
N       0.860222        -0.908000       0.874854
H       0.410474        -1.844853       0.757021
H       1.280367        -0.885515       1.837116
C       1.942681        -0.679831       -0.179275
C       -0.152405       0.227746        0.747002
H       1.882913        -1.471749       -0.960815
H       2.945303        -0.794529       0.295161
C       1.726728        0.721442        -0.756199
C       0.604249        1.376089        0.059084
H       -0.508857       0.524888        1.781405
C       -1.344152       -0.201884       -0.095126
H       1.465095        0.671560        -1.832133
H       2.656942        1.322484        -0.713539
H       -0.059647       1.997971        -0.574130
H       1.012490        2.072856        0.821707
O       -1.380553       -1.060098       -0.959373
O       -2.433989       0.533974        0.228065
H       -3.252896       0.310512        -0.338228
###
16
Pro3 pm6 E=-0.349417697954 au
N       0.768207        -0.998307       0.829998
H       1.265855        -0.977318       1.734380
C       1.765964        -0.806972       -0.278520
C       -0.149021       0.182946        0.776725
H       1.469565        -1.452367       -1.129421
H       2.770385        -1.154186       0.030022
C       1.766059        0.678431        -0.684505
C       0.622994        1.339719        0.101056
H       -0.472488       0.462515        1.812626
C       -1.414087       -0.124074       -0.027227
H       1.626595        0.793701        -1.773980
H       2.735298        1.158324        -0.463660
H       -0.017609       1.957263        -0.550515
H       1.015411        2.035172        0.865838
O       -1.600668       -1.202604       -0.660486
O       -2.314570       0.770697        -0.047071
###
17
ProZW pm6 E=-0.201418556022 au
N       0.770496        -1.050788       0.659533
H       0.263243        -1.896590       0.310368
H       1.159282        -1.280734       1.604134
C       1.898720        -0.672051       -0.299575
C       -0.178171       0.138322        0.770105
H       1.885355        -1.348718       -1.183889
H       2.879704        -0.838524       0.201678
C       1.687327        0.792634        -0.688360
C       0.609892        1.349601        0.251296
H       -0.470904       0.272058        1.851359
C       -1.459449       -0.092583       -0.046538
H       1.379019        0.881467        -1.748772
H       2.629420        1.369914        -0.611501
H       -0.038723       2.084245        -0.261466
H       1.065879        1.903037        1.097715
O       -1.613883       -1.181453       -0.656940
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O       -2.323075       0.820681        -0.067801
###
15
Ser1 pm6 E=-0.924517886867E-01 au
N       0.012576        1.952652        -0.369169
H       -0.168685       2.301430        0.594041
H       -0.796754       2.210562        -0.971654
H       0.855712        2.444725        -0.737787
C       0.237704        0.457404        -0.379257
H       0.493450        0.138555        -1.447394
C       1.414690        0.074082        0.540811
C       -1.029612       -0.268368       0.061854
H       2.194878        0.866379        0.569932
H       1.100835        -0.153110       1.579430
O       1.979477        -1.101547       -0.070082
O       -1.809389       0.042055        0.939206
H       2.661226        -1.490353       0.550299
O       -1.190629       -1.392618       -0.680346
H       -2.001054       -1.948583       -0.403350
###
13
Ser3 pm6 E=-0.422276818579 au
N       -0.210625       1.970691        -0.109594
H       -0.215257       2.135113        0.901146
H       0.499706        2.603450        -0.492473
C       0.178177        0.566835        -0.398935
H       0.324390        0.462876        -1.510291
C       1.472433        0.124503        0.301814
C       -0.998367       -0.325659       0.021297
H       2.311381        0.816567        0.093182
H       1.366145        0.020444        1.396453
O       1.789551        -1.166770       -0.269038
O       -1.238499       -0.558627       1.236398
H       2.599936        -1.530712       0.180966
O       -1.716726       -0.836684       -0.885720
###
14
SerZW pm6 E=-0.275552993583 au
N       -0.486381       1.877416        -0.294242
H       -0.816799       2.065858        0.671126
H       -1.293472       1.980906        -0.940362
H       0.218700        2.603347        -0.539767
C       0.110359        0.495812        -0.407297
H       0.425081        0.329504        -1.483684
C       1.350619        0.368961        0.495943
C       -0.924430       -0.587428       -0.028549
H       1.987491        1.278409        0.455196
H       1.097772        0.158431        1.552528
O       2.116351        -0.714742       -0.066072
O       -1.811527       -0.330520       0.816124
H       2.598297        -1.193594       0.663284
O       -0.808786       -1.708345       -0.584952
###
18
Thr1 pm6 E=-0.106536493988 au
N       0.285806        1.791654        -0.053203
H       -0.489225       2.447987        -0.281418
H       1.154835        2.155807        -0.501724
H       0.429671        1.796726        0.974685
C       -0.016012       0.399756        -0.555813
H       -0.011535       0.423286        -1.701712
C       1.053304        -0.641242       -0.111369
C       -1.401329       -0.038125       -0.103533
H       0.781033        -1.636995       -0.547436
C       2.466077        -0.242902       -0.465154
O       0.891192        -0.733948       1.322380
O       -2.142177       0.515963        0.685581
H       2.829350        0.634374        0.090695
H       3.174737        -1.058037       -0.244533
H       2.579708        -0.011307       -1.536061
H       1.593293        -1.331229       1.702905
O       -1.748369       -1.191892       -0.724736
H       -2.659928       -1.548098       -0.433566
###
16
Thr3 pm6 E=-0.435910103670 au
```

```
N       -0.022454       -0.555555       1.681103
H       -0.885188       -1.032728       1.964237
H       -0.135732       0.416144        1.979384
C       0.094358        -0.611366       0.201638
H       0.076958        -1.698309       -0.101336
C       -1.035279       0.093165        -0.591646
C       1.465351        -0.036839       -0.186315
H       -0.723283       0.280122        -1.646480
C       -2.345589       -0.666133       -0.532752
O       -1.197240       1.397170        0.034042
O       1.782745        1.155364        0.079112
H       -2.685552       -0.860602       0.493406
H       -3.154700       -0.115275       -1.035716
H       -2.277257       -1.642390       -1.034767
H       -2.001586       1.848478        -0.333846
O       2.273304        -0.799974       -0.787924
###
17
ThrZW pm6 E=-0.289194822060 au
N       0.161170        1.754272        -0.013293
H       -0.642572       2.372696        -0.232390
H       1.019668        2.181348        -0.419370
H       0.274781        1.721427        1.015150
C       -0.058343       0.372277        -0.575863
H       -0.034327       0.442311        -1.709701
C       1.046307        -0.622589       -0.143408
C       -1.442818       -0.174515       -0.165129
H       0.833515        -1.622417       -0.599279
C       2.449208        -0.158680       -0.461709
O       0.873647        -0.762162       1.290038
O       -2.073761       0.380939        0.764920
H       2.765346        0.718382        0.121946
H       3.189407        -0.946773       -0.251515
H       2.568468        0.107469        -1.523400
H       1.592695        -1.343941       1.659367
O       -1.882548       -1.169947       -0.791346
###
28
Trp1 pm6 E=0.341179783486E-01 au
N       3.287629        1.539340        -0.551676
H       3.954021        0.909144        -1.038067
H       3.777642        1.974442        0.257242
H       3.026201        2.301462        -1.214650
C       2.045157        0.796644        -0.097971
H       1.376973        1.531648        0.457023
C       1.290812        0.227783        -1.317843
C       2.438500        -0.338524       0.841840
H       1.083467        1.058199        -2.038313
H       1.943311        -0.478749       -1.883537
C       0.023237        -0.422367       -0.915041
O       3.425948        -1.046591       0.786402
C       -0.250146       -1.787492       -0.961079
C       -1.150101       0.234825        -0.399713
H       0.384485        -2.596997       -1.297102
N       -1.549574       -2.023202       -0.496121
C       -2.121093       -0.793067       -0.141880
C       -1.485314       1.578114        -0.132266
H       -1.997828       -2.928968       -0.421772
C       -3.400105       -0.493769       0.375816
C       -2.739567       1.861282        0.371636
H       -0.758125       2.367362        -0.325184
H       -4.119011       -1.289060       0.565620
C       -3.688905       0.832278        0.625407
H       -3.023535       2.892251        0.585725
H       -4.665528       1.112509        1.024732
O       1.495982        -0.500744       1.803445
H       1.701265        -1.261774       2.450656
###
26
Trp3 pm6 E=-0.290332934398 au
N       -3.225621       -1.653021       -0.546688
H       -3.727171       -2.038296       0.256531
H       -3.888655       -1.061664       -1.049677
C       -2.064313       -0.852479       -0.084202
H       -1.369991       -1.548288       0.461209
C       -1.330796       -0.242059       -1.298703
```

```
C       -2.451035       0.285644        0.875553
H       -1.115475       -1.046224       -2.037780
H       -1.998013       0.462421        -1.840992
C       -0.068686       0.424505        -0.896223
O       -3.544642       0.901665        0.729253
C       0.172983        1.795088        -0.885522
C       1.117623        -0.223759       -0.398124
H       -0.472744       2.603864        -1.196680
N       1.465108        2.043340        -0.397536
C       2.062863        0.815272        -0.092203
C       1.486209        -1.568913       -0.186478
H       1.890774        2.956000        -0.286358
C       3.347658        0.525053        0.419466
C       2.744028        -1.842944       0.311788
H       0.782293        -2.367414       -0.419659
H       4.046330        1.328773        0.645768
C       3.667850        -0.802269       0.612921
H       3.053696        -2.874618       0.482294
H       4.649816        -1.076342       1.003866
O       -1.659554       0.604675        1.810922
###
27
TrpZW pm6 E=-0.147202258153 au
N       3.257440        1.564493        -0.478937
H       3.945652        0.952761        -0.952918
H       3.723325        2.007319        0.336421
H       2.989565        2.319295        -1.143969
C       2.034610        0.783339        -0.042049
H       1.354226        1.488433        0.521285
C       1.298246        0.222922        -1.274137
C       2.443564        -0.372532       0.893802
H       1.097991        1.050626        -1.997469
H       1.955705        -0.482165       -1.832715
C       0.024418        -0.428954       -0.887885
O       3.558443        -0.928364       0.739043
C       -0.243704       -1.795150       -0.915766
C       -1.151728       0.229654        -0.380867
H       0.390432        -2.607183       -1.244215
N       -1.542417       -2.030178       -0.443663
C       -2.118752       -0.798376       -0.108725
C       -1.495106       1.576194        -0.138824
H       -1.986396       -2.937049       -0.356749
C       -3.401479       -0.496243       0.400161
C       -2.752347       1.861899        0.354732
H       -0.772577       2.365787        -0.345889
H       -4.117282       -1.291627       0.601102
C       -3.697728       0.832192        0.623908
H       -3.043731       2.895130        0.547036
H       -4.677669       1.115290        1.013424
O       1.628511        -0.734948       1.781801
###
25
Tyr1 pm6 E=-0.643561748518E-01 au
N       3.429624        -1.152893       -0.030800
H       4.057247        -0.945302       -0.835329
H       3.378964        -2.188950       0.079828
H       3.862000        -0.763716       0.830017
C       2.042737        -0.587682       -0.267584
H       1.664278        -0.998143       -1.260710
C       1.086644        -1.003419       0.864706
C       2.105882        0.936715        -0.340920
H       1.161144        -2.107754       1.028795
H       1.412611        -0.563680       1.835864
C       -0.329957       -0.628338       0.540969
O       2.741289        1.696324        0.365396
C       -0.937989       0.458490        1.188646
C       -1.050140       -1.370076       -0.412324
H       -0.380485       1.036129        1.931370
C       -2.254510       0.811004        0.892622
C       -2.364235       -1.033643       -0.726885
H       -0.576435       -2.219384       -0.913594
H       -2.738013       1.651660        1.391903
C       -2.945922       0.058315        -0.064408
H       -2.930646       -1.598669       -1.465973
O       -4.250121       0.344744        -0.425395
H       -4.616167       1.127819        0.092971
```

```
O       1.299617        1.383014        -1.333211
H       1.256794        2.399386        -1.402805
###
23
Tyr3 pm6 E=-0.388132164745 au
N       -3.304170       1.394696        -0.173385
H       -3.992776       1.046127        -0.845517
H       -3.711456       1.248206        0.752368
C       -2.036209       0.632137        -0.310088
H       -1.555477       0.966915        -1.270678
C       -1.091835       0.936473        0.869711
C       -2.245036       -0.889944       -0.388519
H       -1.151589       2.018760        1.125585
H       -1.438919       0.422985        1.791699
C       0.326859        0.565965        0.544780
O       -3.104459       -1.462293       0.339910
C       0.856825        -0.662077       0.969176
C       1.128189        1.454203        -0.195255
H       0.241892        -1.352922       1.550804
C       2.170121        -1.013779       0.656074
C       2.441743        1.125311        -0.519957
H       0.719663        2.415697        -0.517635
H       2.592000        -1.965515       0.981608
C       2.941631        -0.112134       -0.086233
H       3.069731        1.805709        -1.093684
O       4.248091        -0.387690       -0.450805
H       4.565344        -1.261284       -0.061000
O       -1.539001       -1.565576       -1.193853
###
22
Tyr4 pm6 E=-0.547414339175 au
N       3.515663        -0.909616       0.011017
H       4.131645        -0.413693       -0.638962
H       3.758069        -0.566861       0.942948
C       2.097829        -0.594891       -0.303084
H       1.849717        -1.105185       -1.273149
C       1.162899        -1.127378       0.803892
C       1.840757        0.912699        -0.475078
H       1.251930        -2.233733       0.857087
H       1.501588        -0.773188       1.800050
C       -0.259758       -0.726467       0.542510
O       2.322550        1.746362        0.342990
C       -0.843473       0.338609        1.248474
C       -1.009186       -1.387495       -0.446765
H       -0.276417       0.839793        2.035957
C       -2.130585       0.768028        0.956956
C       -2.297184       -0.978391       -0.755559
H       -0.568354       -2.231693       -0.982128
H       -2.575588       1.592163        1.502356
C       -2.879309       0.121710        -0.065249
H       -2.871262       -1.487256       -1.521513
O       -4.067230       0.536370        -0.376089
O       1.131816        1.315821        -1.446445
###
24
TyrZW pm6 E=-0.245457327795 au
N       3.405747        -1.156322       -0.030344
H       3.848097        -0.727256       0.802907
H       4.027080        -0.995064       -0.846351
H       3.345589        -2.182291       0.134238
C       2.028313        -0.576458       -0.281654
H       1.631451        -1.030484       -1.238725
C       1.087822        -0.918167       0.885517
C       2.118538        0.955024        -0.452103
H       1.164867        -2.007012       1.125989
H       1.421233        -0.408184       1.817479
C       -0.334969       -0.571868       0.554519
O       2.976824        1.599914        0.199062
C       -0.939472       0.558129        1.126514
C       -1.063554       -1.382069       -0.335237
H       -0.379566       1.186198        1.824172
C       -2.258103       0.889430        0.814467
C       -2.379532       -1.068545       -0.664477
H       -0.595132       -2.267934       -0.773635
H       -2.739026       1.763322        1.255788
C       -2.956413       0.070074        -0.080584
```

```
H       -2.952231       -1.686991       -1.354644
O       -4.261669       0.333122        -0.455704
H       -4.628524       1.144448        0.016999
O       1.309865        1.513489        -1.237556
###
20
Val1 pm6 E=-0.454265071099E-01 au
N       -0.278496       1.920464        -0.732588
H       -0.260779       2.324723        0.223621
H       -1.182475       2.177033        -1.179301
H       0.488259        2.365772        -1.281336
C       -0.093245       0.417595        -0.711946
H       -0.202792       0.041716        -1.782604
C       1.335850        0.032974        -0.209649
C       -1.165169       -0.230319       0.149300
H       2.062249        0.624491        -0.832805
C       1.542123        0.384556        1.258753
C       1.574364        -1.452313       -0.463886
O       -1.639994       0.167315        1.197030
H       0.889558        -0.185453       1.932001
H       2.573407        0.164299        1.572740
H       1.382959        1.450535        1.468482
H       1.426817        -1.724520       -1.517641
H       2.606875        -1.733834       -0.211270
H       0.920916        -2.097029       0.137666
O       -1.568656       -1.400192       -0.408906
H       -2.249856       -1.902917       0.158144
###
18
Val3 pm6 E=-0.367163371122 au
N       -0.512300       1.788261        -0.889868
H       -0.389159       2.257692        0.010996
H       0.152190        2.240742        -1.525971
C       -0.151848       0.349129        -0.761424
H       -0.226914       -0.098166       -1.792657
C       1.291906        0.084864        -0.245459
C       -1.200348       -0.334309       0.118322
H       1.981492        0.648689        -0.929131
C       1.516850        0.594736        1.176651
C       1.627336        -1.403120       -0.351648
O       -1.642907       0.191586        1.178011
H       0.939134        0.037947        1.922053
H       2.571519        0.500561        1.468896
H       1.260576        1.656053        1.284868
H       1.499457        -1.783046       -1.372692
H       2.673986        -1.594966       -0.079283
H       1.014771        -2.022980       0.312178
O       -1.656384       -1.455106       -0.264115
###
19
ValZW pm6 E=-0.224447692726 au
N       -0.736027       1.761564        -0.690171
H       -1.651657       1.799039        -1.176416
H       -0.871517       2.097672        0.279996
C       -0.172635       0.355847        -0.711127
H       -0.122851       0.021954        -1.791292
C       1.269016        0.338700        -0.126206
C       -1.110851       -0.601292       0.044115
H       1.824622        1.195406        -0.598398
C       1.278673        0.533074        1.387771
C       1.973833        -0.958033       -0.519893
O       -1.850569       -0.154278       0.957556
H       0.796490        -0.290229       1.927670
H       2.308934        0.586488        1.768935
H       0.789292        1.465750        1.696491
H       1.963068        -1.125587       -1.604752
H       3.030477        -0.940466       -0.217929
H       1.534438        -1.842539       -0.044531
O       -1.122860       -1.811880       -0.293524
H       -0.089901       2.421050        -1.168803
###
# PEPTIDES optimized with pm6
# opt freq pm6 scf=(xqc,tight) scrf(smd,solvent=water)
###
24
AlaAla1 pm6 E=-0.120732927471 au
```

```
N       -3.541913       -0.540606       0.313450
H       -3.503848       -0.314124       1.325246
H       -3.531461       -1.573528       0.210512
H       -4.447627       -0.186374       -0.058549
C       -2.384343       0.096775        -0.440796
H       -2.454188       -0.238053       -1.524165
C       -2.479571       1.608496        -0.351844
C       -1.060246       -0.383883       0.173601
H       -2.354237       1.990258        0.673187
H       -1.718459       2.099434        -0.980963
H       -3.453922       1.981420        -0.712813
O       -1.013911       -0.895235       1.299619
N       0.063324        -0.225090       -0.600355
H       0.020932        0.210305        -1.536043
C       1.393669        -0.660988       -0.123498
H       1.273377        -1.278810       0.820149
C       2.121983        -1.470629       -1.186461
C       2.250685        0.569841        0.195420
H       2.262805        -0.920863       -2.129207
H       3.118798        -1.789821       -0.840379
H       1.577611        -2.393823       -1.440575
O       2.196250        1.673427        -0.321318
O       3.219675        0.434905        1.151049
H       3.291153        -0.488596       1.568598
###
23
AlaAla2 pm6 E=-0.301186232816 au
N       -3.532424       -0.511630       -0.153585
H       -3.664143       -0.674782       0.862129
H       -3.449443       -1.434123       -0.622119
H       -4.388779       -0.043250       -0.515980
C       -2.311145       0.353911        -0.422573
H       -2.211710       0.469208        -1.549144
C       -2.488063       1.714033        0.225886
C       -1.067091       -0.348339       0.144591
H       -2.562144       1.664969        1.323297
H       -1.650403       2.389468        -0.013789
H       -3.400238       2.223182        -0.130661
O       -1.164332       -1.234226       1.009584
N       0.144521        0.062196        -0.337012
H       0.217162        0.773481        -1.079431
C       1.409360        -0.556320       0.134234
H       1.265601        -0.932032       1.186926
C       1.839413        -1.707312       -0.765555
C       2.520818        0.513532        0.132777
H       2.002754        -1.402840       -1.807938
H       2.773102        -2.169859       -0.412568
H       1.087033        -2.509209       -0.790281
O       2.594967        1.351081        -0.803288
O       3.353961        0.504995        1.079652
###
22
AlaAla3 pm6 E=-0.445364745912 au
N       -3.609668       -0.486676       -0.164024
H       -3.480275       -1.458491       -0.452306
H       -3.815521       -0.502829       0.836243
C       -2.385483       0.304010        -0.437936
H       -2.272133       0.371210        -1.558553
C       -2.507796       1.704726        0.150698
C       -1.122830       -0.366421       0.143563
H       -2.567562       1.706283        1.247419
H       -1.660713       2.345303        -0.132935
H       -3.414348       2.211825        -0.211670
O       -1.191722       -1.227823       1.043890
N       0.091336        0.013535        -0.365586
H       0.157399        0.700427        -1.129093
C       1.365264        -0.576011       0.112957
H       1.216273        -0.985318       1.151194
C       1.854299        -1.685075       -0.809897
C       2.442199        0.526512        0.157837
H       2.017518        -1.346266       -1.841631
H       2.802580        -2.116931       -0.457077
H       1.137023        -2.516579       -0.865422
O       2.513855        1.382259        -0.762882
O       3.257139        0.527678        1.121214
###
```

```
21
AlaGly1 pm6 E=-0.110747718532 au
N       -3.411715       -0.436451       -0.545954
H       -3.603119       -1.028304       0.283994
H       -3.268384       -1.060474       -1.363325
H       -4.256186       0.144607        -0.725368
C       -2.199559       0.455711        -0.321563
H       -2.017298       1.036852        -1.280959
C       -2.462005       1.411738        0.826629
C       -0.985355       -0.433728       -0.011357
H       -2.612518       0.901999        1.790794
H       -1.628421       2.121358        0.962263
H       -3.359533       2.029930        0.652382
O       -1.121399       -1.621435       0.319218
N       0.245187        0.151296        -0.123103
H       0.361424        1.143865        -0.380122
C       1.463157        -0.627447       0.181650
C       2.699789        0.185254        -0.082970
H       1.458258        -0.975448       1.254216
H       1.493789        -1.574816       -0.428049
O       2.788582        1.320538        -0.519158
O       3.811015        -0.533236       0.235439
H       4.675952        -0.019593       0.079257
###
20
AlaGly2 pm6 E=-0.289637067680 au
N       -3.373771       -0.441279       -0.445328
H       -3.539840       -0.961773       0.436301
H       -3.276419       -1.132759       -1.213202
H       -4.215012       0.140587        -0.635827
C       -2.137772       0.440812        -0.341748
H       -1.987255       0.944568        -1.348971
C       -2.338855       1.482853        0.742130
C       -0.923199       -0.445749       -0.027945
H       -2.427683       1.048392        1.749944
H       -1.507083       2.205810        0.772934
H       -3.251797       2.080826        0.575922
O       -1.067675       -1.639241       0.290690
N       0.309862        0.129150        -0.121593
H       0.442683        1.118582        -0.375256
C       1.518182        -0.659246       0.189138
C       2.797873        0.129025        -0.046219
H       1.493331        -1.012678       1.253092
H       1.545144        -1.595532       -0.426123
O       2.765435        1.308473        -0.479990
O       3.886480        -0.461394       0.200237
###
19
AlaGly3 pm6 E=-0.437629236545 au
N       2.932113        1.123946        -0.503639
H       2.403891        1.938531        -0.821929
H       3.237690        1.325287        0.449920
C       2.081624        -0.090610       -0.537836
H       1.865666        -0.320634       -1.622009
C       2.804734        -1.266716       0.108020
C       0.727633        0.128943        0.170591
H       2.971142        -1.127752       1.184982
H       2.258414        -2.211817       -0.022129
H       3.796297        -1.425640       -0.341291
O       0.478205        1.189819        0.783978
N       -0.199279       -0.876188       0.100092
H       -0.010954       -1.744531       -0.422350
C       -1.516060       -0.784762       0.751734
C       -2.477053       0.054066        -0.094788
H       -1.928469       -1.812778       0.906934
H       -1.436714       -0.355352       1.779866
O       -3.268807       -0.531407       -0.880482
O       -2.460906       1.310945        0.014818
###
32
AlaHis1 pm6 E=0.771793221207E-01 au
N       -4.752546       -1.136549       0.337241
H       -4.858429       -0.607269       1.223519
H       -4.488605       -2.112947       0.572040
H       -5.680472       -1.156071       -0.134154
C       -3.716141       -0.490910       -0.570750
```

```
H       -3.626427       -1.131103       -1.505255
C       -4.155129       0.914831        -0.935762
C       -2.364768       -0.459535       0.161112
H       -4.157396       1.604227        -0.077425
H       -3.508040       1.354912        -1.713013
H       -5.176960       0.933343        -1.354316
O       -2.269823       -0.703605       1.368532
N       -1.267941       -0.146524       -0.608243
H       -1.360969       0.101607        -1.608594
C       0.087820        -0.091645       -0.024205
H       0.177574        -0.873835       0.793940
C       1.134171        -0.353234       -1.122699
C       0.316827        1.301519        0.583111
H       0.876153        -1.304305       -1.663387
H       1.072323        0.430085        -1.922795
C       2.506965        -0.463961       -0.583471
O       -0.111060       2.364730        0.168743
O       1.073391        1.393191        1.715856
N       3.577475        0.318385        -1.057974
C       3.024938        -1.311910       0.397619
H       3.518504        1.034122        -1.791878
C       4.719420        -0.046369       -0.380824
N       4.391054        -1.040920       0.513908
H       2.517652        -2.061843       0.999950
H       5.719322        0.381989        -0.528387
H       1.435483        0.518668        2.082247
H       5.039312        -1.499576       1.163146
###
31
AlaHis2 pm6 E=-0.104984889671 au
N       -4.397170       -1.600218       0.166715
H       -4.585396       -1.404110       1.167869
H       -3.827342       -2.467413       0.103203
H       -5.311649       -1.783142       -0.296324
C       -3.698154       -0.431809       -0.511644
H       -3.557365       -0.707494       -1.605087
C       -4.545628       0.822557        -0.408508
C       -2.343633       -0.188346       0.177165
H       -4.766586       1.113245        0.629906
H       -4.054467       1.681067        -0.895016
H       -5.518716       0.703565        -0.915536
O       -2.269889       0.094214        1.384543
N       -1.229140       -0.273980       -0.611376
H       -1.291960       -0.500526       -1.619309
C       0.127440        -0.109312       -0.033636
H       0.185799        -0.683420       0.937053
C       1.184293        -0.649349       -1.009363
C       0.359963        1.393752        0.268428
H       0.943416        -1.711103       -1.283351
H       1.139486        -0.104355       -1.984312
C       2.541360        -0.600405       -0.420847
O       0.559638        2.210065        -0.664227
O       0.322064        1.764556        1.473668
N       3.613439        0.107946        -0.997966
C       3.032009        -1.209744       0.734745
H       3.577727        0.653034        -1.867402
C       4.729821        -0.066467       -0.207806
N       4.383117        -0.868674       0.854893
H       2.521159        -1.851127       1.447688
H       5.723302        0.361098        -0.396193
H       5.011549        -1.170777       1.607877
###
30
AlaHis3 pm6 E=-0.259148378593 au
N       4.561636        -0.267168       -0.207954
C       3.440695        0.128494        -0.942275
C       2.373421        -0.658034       -0.489598
N       2.820741        -1.532018       0.509754
C       4.149924        -1.274049       0.663302
C       0.959560        -0.594512       -0.935154
C       0.098412        0.171435        0.090493
C       0.725717        1.562366        0.338616
O       1.312953        1.749709        1.440323
N       -1.288035       0.336090        -0.395986
C       -2.317289       -0.406911       0.119856
O       -2.139100       -1.235702       1.024801
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C       -3.716566       -0.130496       -0.455098
C       -4.346083       1.027881        0.296833
N       -4.573435       -1.377994       -0.303780
O       0.682711        2.451161        -0.547004
H       -4.648877       -1.666058       0.690120
H       -4.177729       -2.171557       -0.843600
H       -5.536727       -1.195896       -0.654534
H       -3.652669       0.108053        -1.563950
H       -4.398894       0.860525        1.384246
H       -3.789598       1.965707        0.139213
H       -5.378011       1.226419        -0.040639
H       -1.432134       0.984003        -1.185775
H       0.088907        -0.397053       1.063245
H       0.542827        -1.617178       -1.082501
H       0.890964        -0.120119       -1.940753
H       3.474353        0.888015        -1.705623
H       4.814163        -1.773530       1.361096
H       5.497831        0.117915        -0.301580
###
29
AlaHis4 pm6 E=-0.405614840291 au
N       -4.454341       0.253439        -0.686897
C       -3.225983       -0.136082       -1.227937
C       -2.520997       -0.768345       -0.195648
N       -3.295546       -0.771097       0.972021
C       -4.463634       -0.147988       0.646614
C       -1.146465       -1.327351       -0.241796
C       -0.114465       -0.210632       -0.490964
C       -0.352255       0.938208        0.514687
O       -0.870505       1.999257        0.066119
N       1.264660        -0.745454       -0.386432
C       2.358574        0.072728        -0.314411
O       2.222620        1.314886        -0.265947
C       3.753926        -0.583489       -0.296411
C       4.086447        -0.948645       1.145792
N       4.788994        0.308657        -0.873363
O       -0.075536       0.809345        1.735152
H       4.460096        0.718091        -1.750945
H       4.988707        1.089530        -0.246004
H       3.727873        -1.515935       -0.930350
H       4.082630        -0.082111       1.820427
H       3.383853        -1.690655       1.551628
H       5.088543        -1.396350       1.225898
H       1.362882        -1.772998       -0.353775
H       -0.255781       0.198829        -1.533070
H       -1.072560       -2.092736       -1.051974
H       -0.907995       -1.889183       0.689583
H       -2.953192       0.036113        -2.256247
H       -5.298882       0.019201        1.318950
H       -5.196068       0.741050        -1.183566
###
34
AlaLys3 pm6 E=-0.339075518937 au
N       -4.445838       -1.966747       0.419214
H       -4.909465       -1.480188       1.187390
H       -3.789744       -2.631057       0.836297
C       -3.732837       -1.014427       -0.465210
H       -3.368966       -1.597905       -1.359492
C       -4.652926       0.108781        -0.929841
C       -2.531799       -0.359928       0.251136
H       -5.063262       0.701565        -0.101874
H       -4.141089       0.801219        -1.613033
H       -5.516882       -0.284082       -1.486598
O       -2.651147       0.173801        1.376383
N       -1.325422       -0.365376       -0.394887
H       -1.220017       -0.797335       -1.327557
C       -0.098992       0.209741        0.213833
H       -0.114918       0.026171        1.325962
C       1.143933        -0.454088       -0.392131
C       -0.133498       1.738157        -0.018533
H       1.047928        -1.560095       -0.319945
H       1.204228        -0.250912       -1.481981
C       2.426458        0.003885        0.309952
O       0.375144        2.265059        -1.038466
O       -0.722616       2.448834        0.850838
H       2.549642        1.102078        0.221620
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H       2.360015        -0.191196       1.400777
C       3.646403        -0.713710       -0.278515
H       3.531438        -1.814653       -0.175131
H       3.711669        -0.533295       -1.373185
C       4.926819        -0.245596       0.413280
H       5.079945        0.853525        0.283023
H       4.876514        -0.416962       1.516807
N       6.130848        -0.980432       -0.143151
H       6.219460        -0.830508       -1.163584
H       7.002124        -0.647345       0.306514
H       6.051853        -1.999590       0.021897
###
33
AlaLys4 pm6 E=-0.470080849881 au
N       4.750318        -1.472792       -0.544394
H       5.160347        -0.691847       -1.057636
H       4.338747        -2.101938       -1.236844
C       3.719080        -1.001661       0.409316
H       3.380244        -1.896709       1.005805
C       4.283151        0.064212        1.343228
C       2.501965        -0.382893       -0.309700
H       4.569258        0.987162        0.821468
H       3.569185        0.335387        2.133650
H       5.188784        -0.288248       1.858952
O       2.614261        0.174101        -1.424233
N       1.289731        -0.440500       0.323884
H       1.195009        -0.880487       1.253956
C       0.053088        0.122576        -0.275007
H       0.086062        -0.012383       -1.393461
C       -1.177402       -0.598536       0.289046
C       0.032343        1.640286        0.021464
H       -1.046163       -1.698545       0.201674
H       -1.264241       -0.414586       1.380670
C       -2.460900       -0.171282       -0.432190
O       -0.582094       2.115129        1.008848
O       0.672464        2.398777        -0.767718
H       -2.528567       0.932999        -0.496330
H       -2.438831       -0.516003       -1.486072
C       -3.695524       -0.732791       0.282402
H       -3.646658       -1.840484       0.317355
H       -3.700427       -0.414686       1.344115
C       -4.985990       -0.282273       -0.412034
H       -5.036018       0.827674        -0.463319
H       -4.990649       -0.628958       -1.467977
N       -6.193575       -0.747523       0.343063
H       -6.978200       -0.829289       -0.306364
H       -6.039124       -1.693224       0.698168
###
25
AsnGly1 pm6 E=-0.193244563947 au
N       2.328209        -2.297961       -0.078473
H       2.005699        -3.100854       0.498527
H       3.355258        -2.188140       0.065690
H       2.170614        -2.531099       -1.078226
C       1.600876        -1.025020       0.319114
H       1.807645        -0.844442       1.423931
C       2.125018        0.151958        -0.505917
C       0.093727        -1.218025       0.057865
H       3.241113        0.067016        -0.625910
H       1.768805        0.103493        -1.569129
C       1.752671        1.490745        0.077500
O       -0.307072       -1.829282       -0.939434
O       0.675491        1.680977        0.684146
N       2.628049        2.521450        -0.083522
H       2.415149        3.453831        0.263472
H       3.512438        2.422804        -0.581080
N       -0.761765       -0.700908       0.999811
H       -0.414582       -0.078234       1.748934
C       -2.210907       -0.676192       0.765158
C       -2.624826       0.429300        -0.173778
H       -2.579846       -1.664598       0.366639
H       -2.746357       -0.564450       1.753757
O       -1.883408       1.171014        -0.812242
O       -3.953134       0.643163        -0.372667
H       -4.571758       0.023034        0.150602
###
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24
AsnGly2 pm6 E=-0.379505527115 au
N       -2.095357       -2.424880       -0.203931
H       -1.521899       -3.182486       -0.628015
H       -3.039552       -2.450554       -0.646638
H       -2.214151       -2.631218       0.807150
C       -1.452345       -1.069508       -0.428745
H       -1.356524       -0.915067       -1.553487
C       -2.344153       0.031614        0.148434
C       -0.064278       -1.030009       0.241419
H       -3.390555       -0.085509       -0.248377
H       -2.490571       -0.095857       1.254638
C       -1.819409       1.415890        -0.124379
O       0.060205        -0.827827       1.463209
O       -0.603052       1.650500        -0.329316
N       -2.703919       2.448049        -0.122937
H       -2.400133       3.407472        -0.275931
H       -3.701297       2.321230        0.049724
N       1.016034        -1.171406       -0.578824
H       0.916840        -1.344772       -1.593601
C       2.389744        -1.020174       -0.070562
C       2.794938        0.452525        0.028285
H       2.517580        -1.508202       0.929343
H       3.093147        -1.577534       -0.740790
O       2.153219        1.236913        0.790359
O       3.769982        0.867680        -0.646863
###
23
AsnGly3 pm6 E=-0.526204546988 au
N       1.779278        2.626416        -0.120463
H       1.046130        3.279346        -0.412030
H       1.937399        2.779049        0.878039
C       1.356255        1.230124        -0.385451
H       1.312835        1.094142        -1.505853
C       2.392950        0.255439        0.188632
C       -0.038389       0.938355        0.212934
H       3.405176        0.525719        -0.211278
H       2.514060        0.403848        1.291694
C       2.098688        -1.190656       -0.092503
O       -0.191292       0.469190        1.360977
O       0.994042        -1.593512       -0.539655
N       3.069858        -2.107728       0.168532
H       2.915827        -3.102202       0.016460
H       3.982355        -1.854940       0.547238
N       -1.120572       1.202355        -0.579213
H       -1.023996       1.606383        -1.522821
C       -2.488468       0.886500        -0.139535
C       -2.758357       -0.609666       -0.059543
H       -2.712614       1.366077        0.846967
H       -3.224159       1.350326        -0.850268
O       -1.987635       -1.442958       -0.618717
O       -3.768743       -1.002175       0.583977
###
24
AspGly1 pm6 E=-0.261951705022 au
N       -2.244232       -2.344747       -0.089858
H       -1.726999       -3.107944       -0.574820
H       -3.227159       -2.347681       -0.440701
H       -2.271115       -2.561613       0.926438
C       -1.595526       -1.000437       -0.362530
H       -1.611065       -0.833265       -1.491774
C       -2.401722       0.109124        0.315950
C       -0.146950       -1.022672       0.173248
H       -3.481610       0.043972        0.001117
H       -2.462397       -0.039654       1.429939
C       -1.852484       1.472451        0.036340
O       0.091024        -1.008953       1.388528
O       -2.731003       2.229224        -0.664701
O       -0.772126       1.932908        0.385693
N       0.845133        -1.023219       -0.767239
H       0.642506        -0.998548       -1.782669
C       2.263521        -1.037859       -0.388052
C       2.759043        0.333066        0.009529
H       2.464006        -1.748148       0.465831
H       2.872780        -1.453011       -1.241719
O       2.152585        1.219708        0.598285
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O       4.055067        0.496980        -0.343895
H       -2.386871       3.164655        -0.878616
H       4.461941        1.376031        -0.031530
###
23
AspGly2 pm6 E=-0.443634588242 au
N       -2.168855       -2.357984       -0.178534
H       -1.624412       -3.118815       -0.636133
H       -3.129446       -2.360030       -0.585949
H       -2.253546       -2.580026       0.833136
C       -1.507416       -1.012833       -0.406719
H       -1.448548       -0.841923       -1.533851
C       -2.359465       0.095415        0.216495
C       -0.095594       -1.017312       0.214467
H       -3.407005       0.048458        -0.195406
H       -2.525646       -0.073786       1.317356
C       -1.772552       1.456948        0.019961
O       0.069491        -0.853295       1.437765
O       -2.629272       2.277005        -0.630522
O       -0.678115       1.870127        0.393312
N       0.952238        -1.143847       -0.644324
H       0.818773        -1.264785       -1.663587
C       2.342459        -1.072304       -0.165428
C       2.818176        0.375879        -0.033565
H       2.469644        -1.596533       0.816404
H       3.003825        -1.641874       -0.867696
O       2.215766        1.169294        0.748395
O       3.812636        0.758069        -0.700524
H       -2.265013       3.217772        -0.782940
###
22
AspGly3 pm6 E=-0.624232706989 au
N       -2.832529       -1.696623       -0.139326
H       -2.513528       -2.656733       -0.385210
H       -3.711064       -1.504099       -0.668170
H       -3.064086       -1.678634       0.873629
C       -1.777035       -0.667153       -0.492970
H       -1.632767       -0.704522       -1.622327
C       -2.250232       0.732279        -0.092356
C       -0.452708       -0.986867       0.231213
H       -3.064942       1.072046        -0.780293
H       -2.746008       0.724976        0.907831
C       -1.119717       1.741206        -0.101190
O       -0.334319       -0.839601       1.462838
O       -0.613014       2.108338        1.003397
O       -0.660400       2.189683        -1.183025
N       0.595895        -1.350582       -0.556042
H       0.494403        -1.497714       -1.575978
C       1.964768        -1.439583       -0.022308
C       2.624549        -0.059796       0.006342
H       1.990570        -1.892581       1.000946
H       2.561166        -2.151223       -0.649710
O       2.069902        0.891601        0.634340
O       3.713448        0.112278        -0.593241
###
21
AspGly4 pm6 E=-0.773634001373 au
N       -2.492822       -2.083266       0.058386
H       -3.396268       -2.134292       -0.425356
H       -2.712144       -2.044468       1.057936
C       -1.770289       -0.861278       -0.367448
H       -1.785634       -0.820645       -1.495134
C       -2.358728       0.450608        0.183016
C       -0.325155       -1.008898       0.143484
H       -3.342095       0.649834        -0.304066
H       -2.619159       0.349675        1.260228
C       -1.432050       1.621106        -0.023248
O       -0.042201       -0.869516       1.354512
O       -0.760432       2.061762        0.965161
O       -1.276231       2.142451        -1.159474
N       0.648219        -1.255905       -0.779826
H       0.437776        -1.357222       -1.784467
C       2.072472        -1.250835       -0.410174
C       2.602383        0.134467        -0.061978
H       2.267201        -1.947454       0.445676
H       2.674815        -1.676018       -1.257027
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O       1.871033        1.165009        -0.157249
O       3.789823        0.230765        0.343348
###
35
AspHis0 pm6 E=-0.728567266312E-01 au
N       3.210772        2.706136        -0.025225
H       2.439357        3.325289        -0.351288
H       4.084051        2.999118        -0.515665
H       3.348865        2.860615        0.993237
C       2.901432        1.253337        -0.333946
H       2.820502        1.152085        -1.468030
C       4.040180        0.363175        0.166466
C       1.570271        0.860742        0.344241
H       5.031929        0.772898        -0.177409
H       4.140173        0.402113        1.287634
C       3.886722        -1.060430       -0.260354
O       1.490970        0.636869        1.556295
O       5.059119        -1.566063       -0.716466
O       2.881311        -1.758927       -0.216526
N       0.494154        0.716107        -0.493708
H       0.570292        0.909825        -1.511344
C       -0.845087       0.350150        0.022294
H       -1.145212       1.080776        0.838654
C       -1.869108       0.383017        -1.126578
C       -0.802677       -1.059742       0.630613
H       -1.741665       1.329908        -1.721435
H       -1.655882       -0.424668       -1.873765
C       -3.261708       0.312246        -0.633529
O       -0.047321       -1.982600       0.370834
O       -1.760402       -1.187916       1.577304
N       -4.171118       -0.681687       -1.042947
C       -3.945684       1.153134        0.246442
H       -3.969946       -1.447126       -1.698797
C       -5.379604       -0.450459       -0.423858
N       -5.251529       0.668967        0.367752
H       -3.593111       2.038429        0.769386
H       -6.288645       -1.054163       -0.543871
H       -5.988948       1.075154        0.954153
H       5.005943        -2.541537       -1.001570
H       -1.791487       -2.107317       2.016749
###
34
AspHis2 pm6 E=-0.256557991619 au
N       3.100373        2.774651        0.081360
H       2.314277        3.370615        -0.253642
H       3.973026        3.109430        -0.383539
H       3.210130        2.918198        1.104706
C       2.850921        1.318378        -0.257480
H       2.781550        1.236081        -1.394000
C       4.023611        0.462467        0.226897
C       1.534365        0.849483        0.397961
H       4.989875        0.874325        -0.181882
H       4.175560        0.553818        1.339627
C       3.878783        -0.983204       -0.123934
O       1.496638        0.478461        1.582795
O       5.031789        -1.488011       -0.619701
O       2.894130        -1.704016       0.015581
N       0.440897        0.782430        -0.416790
H       0.469317        1.121682        -1.397124
C       -0.844499       0.211681        0.061617
H       -0.962182       0.409835        1.168034
C       -2.004482       0.866815        -0.695266
C       -0.752945       -1.324389       -0.144195
H       -1.915309       1.984791        -0.627977
H       -1.920568       0.670708        -1.795507
C       -3.336181       0.450430        -0.199716
O       -0.031535       -1.975085       0.670385
O       -1.344796       -1.899960       -1.085400
N       -4.520216       0.865019        -0.840405
C       -3.718212       -0.357066       0.872562
H       -4.576277       1.472138        -1.667955
C       -5.595746       0.318726        -0.171528
N       -5.115968       -0.431583       0.874641
H       -3.109067       -0.856490       1.619797
H       -6.652473       0.464725        -0.431962
H       -5.684266       -0.955334       1.549855
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H       4.987310        -2.479188       -0.850861
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33
AspHis3 pm6 E=-0.438902445957 au
N       3.759307        2.422909        -0.125911
H       3.218616        3.235650        -0.487818
H       4.715028        2.459427        -0.542093
H       3.858893        2.526552        0.902783
C       3.080753        1.119458        -0.496093
H       2.988247        1.093592        -1.629752
C       3.919263        -0.071604       -0.019065
C       1.694833        1.034257        0.172781
H       4.840255        -0.167775       -0.647267
H       4.325051        0.101360        1.007436
C       3.134579        -1.366755       -0.053370
O       1.574073        1.038518        1.407002
O       2.660903        -1.835336       1.026306
O       2.902468        -1.953749       -1.143610
N       0.626206        0.823570        -0.654530
H       0.702235        0.899793        -1.684150
C       -0.674100       0.385008        -0.088342
H       -0.928572       1.039317        0.796983
C       -1.785905       0.479955        -1.140715
C       -0.498449       -1.075582       0.407026
H       -1.702779       1.449123        -1.703633
H       -1.658528       -0.294070       -1.936704
C       -3.125461       0.405195        -0.514791
O       -0.087600       -1.972632       -0.379512
O       -0.708867       -1.318097       1.621650
N       -4.093807       -0.554458       -0.866429
C       -3.697715       1.220957        0.463133
H       -3.984440       -1.290177       -1.574491
C       -5.228690       -0.326430       -0.117371
N       -4.994609       0.754787        0.700974
H       -3.277666       2.079328        0.980401
H       -6.158595       -0.907639       -0.168554
H       -5.659896       1.151480        1.374281
###
32
AspHis4 pm6 E=-0.595460472499 au
N       -3.959409       -2.190741       0.001934
H       -3.481882       -3.081426       -0.247853
H       -4.890138       -2.180413       -0.469100
H       -4.126347       -2.184167       1.027503
C       -3.138779       -0.997902       -0.442794
H       -3.039789       -1.057579       -1.575062
C       -3.839470       0.310136        -0.056889
C       -1.753257       -1.019166       0.231613
H       -4.719965       0.485172        -0.724669
H       -4.298636       0.243845        0.959313
C       -2.897886       1.494605        -0.124179
O       -1.633230       -0.945917       1.465227
O       -2.412283       1.969604        0.947374
O       -2.545835       1.977719        -1.233718
N       -0.669089       -0.974882       -0.599410
H       -0.749449       -1.128642       -1.620355
C       0.671162        -0.636494       -0.057703
H       0.880381        -1.275492       0.848052
C       1.767911        -0.867155       -1.107272
C       0.637700        0.850594        0.374728
H       1.761867        -1.935834       -1.433275
H       1.560150        -0.295451       -2.039770
C       3.095507        -0.516135       -0.544494
O       0.386359        1.757258        -0.467354
O       0.821059        1.124922        1.588650
N       3.709111        0.725670        -0.761029
C       3.912139        -1.311343       0.268440
C       4.889826        0.681334        -0.081895
N       5.045456        -0.547256       0.557182
H       3.767716        -2.316207       0.631604
H       5.624324        1.479052        -0.037414
H       5.831615        -0.841915       1.131518
###
31
AspHis5 pm6 E=-0.746348533458 au
N       5.034724        -0.487905       0.618695
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C       3.892659        -1.257282       0.382309
C       3.090676        -0.516233       -0.493762
N       3.724084        0.695524        -0.804295
C       4.899444        0.689437        -0.114695
C       1.768690        -0.899459       -1.046759
C       0.652258        -0.634138       -0.028194
C       0.539024        0.866746        0.336075
O       0.407829        1.187510        1.550345
N       -0.672631       -1.004204       -0.591166
C       -1.783321       -1.080834       0.211590
O       -1.669225       -1.062759       1.451908
C       -3.153168       -1.052190       -0.487560
C       -3.845650       0.266009        -0.079846
C       -2.906998       1.444743        -0.098207
O       -2.478668       1.924974        -1.185904
N       -3.875976       -2.282693       -0.097355
O       -2.489571       1.934571        0.998072
O       0.470603        1.745798        -0.565981
H       -4.733297       -2.369927       -0.654624
H       -4.179357       -2.232031       0.879461
H       -3.025273       -1.065916       -1.608642
H       -4.708287       0.456241        -0.761393
H       -4.324106       0.168589        0.920801
H       -0.734138       -1.117644       -1.616899
H       0.849338        -1.227119       0.908914
H       1.774748        -1.982384       -1.323443
H       1.566574        -0.375217       -2.008184
H       3.733381        -2.229496       0.820277
H       5.644240        1.478709        -0.126299
H       5.815341        -0.750393       1.215646
###
34
AspHis pm6 E=-0.254086527608 au
N       3.410278        2.630343        0.041980
H       2.666544        3.313349        -0.212401
H       4.283906        2.908477        -0.455442
H       3.589731        2.705611        1.062588
C       3.012153        1.220036        -0.354982
H       2.920282        1.198094        -1.489856
C       4.089359        0.232009        0.088598
C       1.665927        0.865826        0.308884
H       5.071174        0.506819        -0.372907
H       4.290138        0.310856        1.184715
C       3.740576        -1.201191       -0.265151
O       1.570545        0.652265        1.524525
O       2.988688        -1.862233       0.512933
O       4.210780        -1.731528       -1.303666
N       0.594835        0.713218        -0.532958
H       0.670444        0.903723        -1.550891
C       -0.742926       0.350932        -0.011382
H       -1.006024       1.041012        0.852651
C       -1.794182       0.473367        -1.128112
C       -0.723128       -1.091154       0.519731
H       -1.666762       1.454903        -1.663768
H       -1.614898       -0.286184       -1.932443
C       -3.174096       0.389997        -0.601007
O       0.027851        -2.007822       0.219503
O       -1.687955       -1.258461       1.449136
N       -4.132160       -0.515233       -1.096004
C       -3.797642       1.136238        0.401106
H       -3.982404       -1.198028       -1.849334
C       -5.311061       -0.322140       -0.409602
N       -5.115014       0.682615        0.510877
H       -3.396783       1.938773        1.015020
H       -6.245332       -0.876420       -0.569945
H       -5.818811       1.040270        1.166074
H       -1.735916       -2.199132       1.840734
###
29
CysAsn1 pm6 E=-0.198477776275 au
N       -3.349822       -2.271372       0.062166
H       -2.780680       -3.127013       -0.094674
H       -4.269435       -2.405273       -0.409861
H       -3.528189       -2.177627       1.080481
C       -2.653488       -1.045344       -0.497867
H       -2.471250       -1.239476       -1.606170
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C       -3.518595       0.199483        -0.328684
C       -1.320865       -0.810895       0.243925
H       -4.167985       0.363051        -1.218036
H       -4.221158       0.134244        0.530455
S       -2.340548       1.570635        -0.140479
O       -1.236953       -0.891352       1.475123
H       -2.742155       2.075030        1.051524
N       -0.211987       -0.602917       -0.550976
H       -0.297256       -0.526599       -1.580744
C       1.056324        -0.129863       0.035988
H       1.087273        -0.371521       1.145104
C       2.235636        -0.803131       -0.670806
C       1.145700        1.404408        -0.094048
H       2.005674        -1.888209       -0.851165
H       2.365887        -0.408788       -1.710579
C       3.518721        -0.692094       0.108564
O       0.066850        2.015175        0.437752
O       2.063687        2.048747        -0.581985
O       3.589598        -0.096284       1.207700
N       4.638203        -1.260639       -0.419766
H       5.529753        -1.222823       0.069225
H       4.634692        -1.773308       -1.300662
H       0.122790        3.036980        0.411642
###
28
CysAsn2 pm6 E=-0.379388715463 au
N       2.821916        -1.816956       1.452119
H       2.112849        -1.997121       2.192040
H       3.762681        -1.816643       1.903026
H       2.797293        -2.602187       0.774859
C       2.573388        -0.482650       0.771204
H       2.640765        0.322660        1.573981
C       3.629573        -0.223447       -0.296263
C       1.175996        -0.480413       0.117383
H       4.599827        0.080168        0.168232
H       3.876798        -1.130956       -0.889493
S       3.049581        1.135908        -1.341078
O       0.952254        -1.074285       -0.944644
H       2.283251        0.452835        -2.227683
N       0.211279        0.258303        0.751702
H       0.369340        0.679617        1.680801
C       -1.138520       0.416289        0.165271
H       -1.052993       0.373056        -0.960438
C       -2.097828       -0.681226       0.649912
C       -1.685276       1.808031        0.563736
H       -1.517286       -1.570043       1.010011
H       -2.646367       -0.374126       1.576050
C       -3.100653       -1.080335       -0.398720
O       -1.310254       2.356979        1.625478
O       -2.510138       2.361427        -0.217750
O       -3.622637       -0.244406       -1.179376
N       -3.459377       -2.389409       -0.492440
H       -4.164966       -2.702529       -1.155554
H       -3.085093       -3.108037       0.126947
###
27
CysAsn3 pm6 E=-0.534895102499 au
N       -3.716664       -1.557238       -0.804772
H       -3.384552       -2.234886       -1.517130
H       -4.678935       -1.259127       -1.069052
H       -3.777001       -2.049496       0.106023
C       -2.790666       -0.348714       -0.724005
H       -2.755829       0.114223        -1.760075
C       -3.334838       0.655993        0.289073
C       -1.387029       -0.832010       -0.336868
H       -4.397186       0.895522        0.082384
H       -3.301730       0.265994        1.323154
S       -2.331500       2.162662        0.149603
O       -1.195380       -1.998188       0.055158
N       -0.352981       0.051098        -0.489822
H       -0.548596       1.074912        -0.638290
C       1.029810        -0.331246       -0.130892
H       1.219477        -1.384800       -0.490178
C       2.015358        0.634008        -0.797387
C       1.244764        -0.306305       1.403463
H       1.726536        0.804694        -1.870584
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H       1.935945        1.658265        -0.355266
C       3.434459        0.135585        -0.769587
O       0.688138        0.551109        2.135635
O       2.003196        -1.187459       1.897657
O       3.725797        -1.068264       -0.566277
N       4.434314        1.037720        -0.965297
H       5.409583        0.747858        -0.998269
H       4.258439        2.021738        -1.167291
###
26
CysAsn4 pm6 E=-0.672645977360 au
N       4.241247        -2.143400       -0.398380
H       3.868695        -2.768398       -1.114482
H       5.078846        -2.468067       0.080282
C       3.694075        -0.929481       -0.129289
C       2.479807        -0.488035       -0.902624
O       4.218647        -0.191375       0.744183
H       2.809272        0.182488        -1.736955
H       2.027025        -1.343983       -1.472126
C       1.437150        0.186127        -0.001910
C       1.543848        1.723217        -0.152851
O       2.574531        2.282608        0.323100
O       0.639596        2.396181        -0.705998
H       1.642832        -0.053823       1.084101
N       0.081698        -0.305931       -0.336775
H       -0.020578       -0.799200       -1.238765
C       -0.995862       -0.083821       0.485605
O       -0.854165       0.531408        1.560815
C       -2.355904       -0.620467       0.011057
H       -2.277387       -0.951845       -1.062446
N       -2.636340       -1.827127       0.837965
H       -3.469683       -2.292656       0.462458
H       -2.893550       -1.546546       1.788360
C       -3.399847       0.491164        0.122302
H       -3.078470       1.405597        -0.404631
H       -3.596193       0.774117        1.170316
S       -4.934095       -0.126581       -0.640395
###
42
DLeuTyr3 pm6 E=-0.504897586496 au
C       1.540457        -1.617440       0.782477
C       2.708305        -2.131129       -0.079351
C       0.764710        -0.542681       0.009757
H       3.253212        -2.912363       0.491482
H       2.288916        -2.678960       -0.949981
C       3.701407        -1.059279       -0.577697
O       0.237310        -0.844771       -1.083386
H       3.128646        -0.152212       -0.894491
C       4.689869        -0.641314       0.513684
C       4.456232        -1.591382       -1.801748
H       5.257328        -1.489752       0.911933
H       5.422822        0.083795        0.138936
H       4.186184        -0.160294       1.365818
H       3.779350        -1.831996       -2.629712
H       5.175196        -0.856504       -2.183419
H       5.022760        -2.502664       -1.577982
N       0.645849        0.732859        0.499311
H       0.995597        0.980208        1.434247
C       -0.158859       1.768474        -0.191752
H       -0.305865       1.469863        -1.268068
C       -1.532199       1.973259        0.472137
C       0.633956        3.093239        -0.154590
H       -1.412061       2.169054        1.560318
H       -1.999307       2.902465        0.070631
C       -2.441364       0.802039        0.235304
O       1.044946        3.564480        0.937824
O       0.859246        3.678308        -1.248846
C       -2.745257       -0.080320       1.283619
C       -2.989632       0.584029        -1.041409
H       -2.326492       0.086187        2.279615
C       -3.589203       -1.171014       1.071206
C       -3.832144       -0.499109       -1.277901
H       -2.759008       1.272023        -1.859243
H       -3.833460       -1.857833       1.882379
C       -4.119984       -1.362254       -0.209379
H       -4.262571       -0.676185       -2.262981
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O       -4.971734       -2.411279       -0.508298
H       -5.151505       -2.988692       0.297388
N       1.913537        -1.151709       2.142461
H       2.199114        -1.957168       2.706972
H       2.740765        -0.538387       2.094615
H       0.808783        -2.473247       0.914643
###
41
DLeuTyr4 pm6 E=-0.664634718264 au
C       1.513340        -1.878098       0.439055
C       2.813792        -2.060688       -0.364233
C       0.685236        -0.727273       -0.148107
H       3.421678        -2.850274       0.127014
H       2.555291        -2.496212       -1.353632
C       3.680303        -0.802828       -0.582780
O       -0.009933       -0.946183       -1.166163
H       3.027991        0.022955        -0.960463
C       4.358976        -0.331667       0.704988
C       4.733126        -1.093852       -1.659422
H       5.011429        -1.099284       1.137134
H       4.983980        0.552816        0.530977
H       3.631744        -0.054243       1.482272
H       4.276636        -1.379150       -2.614508
H       5.360414        -0.216432       -1.857199
H       5.408036        -1.908745       -1.373625
N       0.720886        0.525264        0.407000
H       1.235119        0.706135        1.280228
C       -0.136010       1.629331        -0.089633
H       -0.427013       1.422927        -1.157450
C       -1.412139       1.800521        0.759468
C       0.702591        2.924190        -0.053551
H       -1.164331       1.773906        1.841672
H       -1.829916       2.818146        0.590260
C       -2.433743       0.756703        0.416947
O       1.164997        3.358537        1.033404
O       0.912789        3.523884        -1.143414
C       -2.521841       -0.429972       1.163634
C       -3.294638       0.943792        -0.679135
H       -1.867853       -0.577104       2.025649
C       -3.431887       -1.420711       0.823055
C       -4.213852       -0.030328       -1.036749
H       -3.236254       1.868237        -1.258468
H       -3.496650       -2.334420       1.402839
C       -4.296300       -1.240503       -0.291499
H       -4.875419       0.117278        -1.882842
O       -5.139669       -2.165349       -0.632468
N       1.674224        -1.716329       1.907114
H       2.015663        -2.596915       2.305389
H       2.406629        -1.019723       2.110889
H       0.889874        -2.811264       0.281963
###
41
GluHisOMe2 pm6 E=-0.731680170913E-01 au
N       3.102968        3.282572        -0.086715
H       3.178252        3.379232        0.944370
H       2.505784        4.055002        -0.444142
H       4.056880        3.401667        -0.487992
C       2.531026        1.933329        -0.480721
H       2.435095        1.918521        -1.615415
C       3.479171        0.809417        -0.030167
C       1.157936        1.755779        0.189370
H       4.500082        1.008409        -0.438791
H       3.602358        0.823430        1.077197
C       2.991529        -0.559136       -0.498039
O       0.949788        2.102469        1.355201
H       2.005812        -0.828238       -0.033920
H       2.764701        -0.545406       -1.599130
C       3.975037        -1.637139       -0.204383
O       5.064103        -1.549764       0.347659
O       3.647632        -2.917316       -0.582793
N       0.184563        1.173118        -0.589564
H       0.388754        0.839224        -1.550384
C       -1.123303       0.795699        -0.020723
H       -1.442471       1.567602        0.748755
C       -2.176352       0.703367        -1.139089
C       -1.031981       -0.557239       0.710218
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H       -2.250290       1.693969        -1.663442
H       -1.839001       0.000152        -1.944963
C       -3.507369       0.324323        -0.616351
O       -1.667459       -0.861222       1.706008
N       -4.251069       -0.754258       -1.131260
C       -4.271156       0.896733        0.402517
C       -5.440948       -0.833299       -0.441394
N       -5.462087       0.170434        0.500112
H       -4.048481       1.751473        1.035610
H       -6.236074       -1.570372       -0.616150
H       -6.223142       0.352764        1.164383
O       -0.150483       -1.397790       0.116443
C       0.039064        -2.717846       0.714730
H       0.553527        -2.613140       1.675019
H       -0.923471       -3.227859       0.823052
H       0.675240        -3.224348       -0.027051
H       -3.960253       -1.373085       -1.898650
H       2.751510        -3.007003       -1.052309
###
40
GluHisOMe3 pm6 E=-0.252165546643 au
N       3.179635        3.193064        0.124799
H       3.295990        3.165629        1.156171
H       2.591377        4.015586        -0.115377
H       4.121084        3.336039        -0.297411
C       2.559207        1.910630        -0.399295
H       2.478798        2.005868        -1.530197
C       3.450617        0.709064        -0.038057
C       1.170394        1.728985        0.234126
H       4.508490        0.941359        -0.309945
H       3.467518        0.557439        1.064352
C       2.996766        -0.557678       -0.757575
O       0.937021        2.062968        1.399368
H       1.948168        -0.831843       -0.496852
H       2.965689        -0.391491       -1.857908
C       3.893991        -1.725072       -0.420805
O       3.867452        -2.237217       0.735235
O       4.652381        -2.211594       -1.311452
N       0.213363        1.148723        -0.566761
H       0.433334        0.833956        -1.530484
C       -1.104186       0.762326        -0.024885
H       -1.472945       1.572276        0.682081
C       -2.102574       0.572333        -1.179964
C       -1.016485       -0.536699       0.797130
H       -2.140582       1.511371        -1.796783
H       -1.730566       -0.200820       -1.902791
C       -3.465288       0.250030        -0.702748
O       -1.773931       -0.851709       1.698203
N       -4.206982       -0.838512       -1.200194
C       -4.269505       0.893813        0.239549
C       -5.435292       -0.852921       -0.576311
N       -5.481936       0.200263        0.308577
H       -4.061162       1.777151        0.837293
H       -6.238532       -1.579500       -0.757268
H       -6.274008       0.436835        0.916649
O       0.028443        -1.319044       0.418142
C       0.234674        -2.575129       1.135902
H       0.627225        -2.357941       2.134288
H       -0.697900       -3.147429       1.189107
H       0.974576        -3.091074       0.508815
H       -3.889928       -1.503503       -1.917065
###
39
GluHisOMe4 pm6 E=-0.406871280793 au
N       3.185379        3.192937        0.138758
H       3.300801        3.164556        1.170147
H       2.587853        4.009168        -0.101076
H       4.125828        3.348061        -0.281852
C       2.581137        1.904927        -0.388638
H       2.494604        2.003122        -1.518495
C       3.485893        0.710191        -0.037135
C       1.203239        1.692045        0.258448
H       4.544829        0.959112        -0.287874
H       3.491025        0.542600        1.063302
C       3.062058        -0.549375       -0.787466
O       1.017999        1.867032        1.467719
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H       1.959747        -0.709192       -0.759893
H       3.283588        -0.446949       -1.873190
C       3.740262        -1.772146       -0.214424
O       3.340079        -2.252556       0.886187
O       4.677467        -2.333161       -0.852244
N       0.201051        1.254101        -0.573961
H       0.374450        1.065835        -1.578419
C       -1.110050       0.844182        -0.033774
H       -1.415122       1.554293        0.797497
C       -2.171637       0.857701        -1.150791
C       -1.040358       -0.561331       0.586455
H       -2.271060       1.899140        -1.546953
H       -1.826432       0.261529        -2.029301
C       -3.484900       0.375931        -0.658743
O       -1.742263       -0.968314       1.497861
N       -4.094380       -0.782158       -1.159194
C       -4.288900       0.939767        0.340642
C       -5.258292       -0.920205       -0.464834
N       -5.407700       0.112249        0.459783
H       -4.145750       1.828587        0.933647
H       -5.982933       -1.716844       -0.600083
H       -6.182124       0.248590        1.104730
O       -0.089203       -1.341078       0.006196
C       0.043502        -2.712300       0.493825
H       0.379304        -2.705844       1.535096
H       -0.910665       -3.241503       0.391416
H       0.797254        -3.135872       -0.183538
###
21
GlyAla1 pm6 E=-0.115236611121 au
N       -3.739207       -0.350723       0.052865
H       -3.632939       -1.365651       0.232886
C       -2.557540       0.417721        0.576279
H       -3.850670       -0.211240       -0.967991
H       -4.608144       -0.025990       0.522954
C       -1.273773       0.026395        -0.123126
H       -2.748339       1.526925        0.473887
H       -2.463977       0.266686        1.692440
O       -1.220378       -0.885469       -0.958319
N       -0.157588       0.758837        0.218060
H       -0.194589       1.504442        0.933059
C       1.134277        0.548408        -0.469728
H       0.948739        0.161522        -1.517894
C       1.938200        1.836692        -0.521778
C       1.950628        -0.498299       0.305512
H       2.111265        2.282779        0.469823
H       2.925489        1.684150        -0.986974
H       1.432793        2.605673        -1.128362
O       2.241750        -0.531671       1.487128
O       2.384162        -1.469723       -0.544287
H       2.962917        -2.176706       -0.099434
###
20
GlyAla2 pm6 E=-0.294473135422 au
N       -3.602622       -0.359457       0.027224
H       -3.651658       -0.575995       -0.985490
C       -2.499118       0.618782        0.319031
H       -4.517094       0.040907        0.320052
H       -3.458844       -1.246977       0.542538
C       -1.153300       0.117794        -0.159445
H       -2.738177       1.616491        -0.154529
H       -2.473605       0.848778        1.425034
O       -1.021400       -0.979095       -0.731222
N       -0.085676       0.947578        0.057126
H       -0.183996       1.831818        0.582349
C       1.270647        0.609674        -0.445099
H       1.208835        0.457641        -1.561477
C       2.243190        1.734310        -0.129221
C       1.796978        -0.699249       0.186308
H       2.345810        1.929419        0.948086
H       3.250790        1.518840        -0.515877
H       1.936852        2.686235        -0.591022
O       1.614302        -0.969410       1.400467
O       2.425697        -1.490480       -0.572940
###
19
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```
GlyAla3 pm6 E=-0.439148981406 au
N       -3.704142       -0.251404       0.182437
H       -3.839313       -0.324918       -0.828080
C       -2.536023       0.604106        0.478048
H       -3.538191       -1.201404       0.518703
C       -1.229321       0.115063        -0.118110
H       -2.746463       1.644564        0.118399
H       -2.428070       0.706390        1.588768
O       -1.158119       -0.946565       -0.775066
N       -0.111784       0.883777        0.089459
H       -0.152743       1.747531        0.653537
C       1.201986        0.546299        -0.515953
H       1.049386        0.295850        -1.604326
C       2.160120        1.718286        -0.395628
C       1.780100        -0.704201       0.187691
H       2.305587        2.055648        0.640579
H       3.152719        1.469405        -0.800283
H       1.808689        2.596095        -0.959879
O       2.281167        -0.640938       1.338418
O       1.731790        -1.799133       -0.444224
###
24
GlyAsp1 pm6 E=-0.258675276396 au
N       4.525632        -0.560858       -0.398662
H       4.402563        -1.086070       -1.284177
C       3.338533        -0.745311       0.506151
H       4.665065        0.439827        -0.631080
C       2.062025        -0.256492       -0.140997
H       3.248901        -1.832359       0.804405
H       3.517584        -0.215831       1.488043
O       2.039378        0.285801        -1.252282
N       0.905524        -0.437230       0.590018
H       0.909407        -0.893252       1.518674
C       -0.399085       -0.024439       0.037215
H       -0.389075       -0.172942       -1.092700
C       -1.521412       -0.856364       0.666250
C       -0.631771       1.472363        0.308855
H       -1.189546       -1.924949       0.797236
H       -1.725424       -0.547252       1.730336
C       -2.793684       -0.807741       -0.111560
O       -0.028843       2.191053        1.086596
O       -1.605642       2.091586        -0.415416
O       -3.201633       0.096877        -0.836973
O       -3.531766       -1.929437       0.066026
H       5.385568        -0.912416       0.068669
H       -4.414640       -1.923901       -0.445167
H       -2.128078       1.476633        -1.072824
###
23
GlyAsp2 pm6 E=-0.443879806911 au
N       -4.509602       -0.607919       0.169620
H       -4.362785       -1.613567       0.375549
C       -3.363530       -0.049616       -0.627140
H       -4.616616       -0.105456       1.069705
C       -2.053477       -0.164811       0.123175
H       -3.294437       -0.576286       -1.624395
H       -3.576284       1.024714        -0.906391
O       -1.967001       -0.723570       1.224681
N       -0.961314       0.418458        -0.480013
H       -1.024857       0.831432        -1.423711
C       0.389668        0.283490        0.098847
H       0.307705        -0.023138       1.182195
C       1.203153        -0.771924       -0.664313
C       1.099092        1.659322        0.019876
H       0.596856        -1.709226       -0.787766
H       1.386873        -0.460667       -1.726561
C       2.502842        -1.086115       -0.007767
O       1.239132        2.243281        -1.079868
O       1.550194        2.140017        1.095574
O       3.110561        -0.445566       0.843687
O       3.028882        -2.245453       -0.486344
H       -5.396108       -0.511349       -0.365149
H       3.915438        -2.501984       -0.058633
###
22
GlyAsp3 pm6 E=-0.627220674411 au
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```
N       -4.483223       -0.439033       0.152000
H       -4.460819       -1.151808       0.904352
C       -3.261847       -0.541913       -0.719186
H       -5.339510       -0.592748       -0.417976
H       -4.549685       0.496573        0.593000
C       -1.998799       -0.233627       0.052887
H       -3.211248       -1.568742       -1.189004
H       -3.359838       0.153244        -1.604922
O       -2.025911       0.158431        1.231759
N       -0.816761       -0.380652       -0.629044
H       -0.795951       -0.713575       -1.608458
C       0.488951        -0.130586       0.029711
H       0.421001        -0.424675       1.118910
C       1.578439        -0.957456       -0.649058
C       0.752765        1.397369        -0.028313
H       1.264559        -2.026895       -0.717768
H       1.709969        -0.663974       -1.715394
C       2.900579        -0.863563       0.083624
O       1.434050        1.912176        -0.955453
O       0.264803        2.107083        0.891677
O       3.230081        -1.760980       0.904107
O       3.679586        0.109422        -0.152268
###
21
GlyAsp4 pm6 E=-0.767927061748 au
N       -4.628035       -0.447910       -0.053080
H       -4.519029       -1.457848       -0.165335
C       -3.433784       0.252002        -0.570064
H       -4.726749       -0.280847       0.950064
C       -2.131967       -0.136522       0.105711
H       -3.351401       0.067703        -1.673059
H       -3.591589       1.357843        -0.481033
O       -2.072329       -0.987945       1.012378
N       -0.994542       0.520226        -0.313109
H       -1.020904       1.173287        -1.109411
C       0.338768        0.175378        0.218602
H       0.227592        -0.219005       1.268287
C       1.027899        -0.880715       -0.655897
C       1.227268        1.439510        0.257169
H       0.462116        -1.842645       -0.612975
H       0.978478        -0.601675       -1.731664
C       2.456307        -1.138662       -0.239034
O       1.203444        2.275369        -0.676940
O       2.012576        1.565386        1.240331
O       2.745479        -1.362670       0.972221
O       3.359902        -1.111261       -1.120550
###
18
GlyGly1 pm6 E=-0.106171882381 au
N       3.479738        -0.384900       -0.102487
H       3.275506        -1.400547       -0.131352
C       2.322447        0.412544        -0.636265
H       3.688449        -0.124713       0.879150
C       1.062604        0.182735        0.170501
H       2.596142        1.508289        -0.670377
H       2.140282        0.154037        -1.721818
O       0.983998        -0.705085       1.033482
N       0.005666        1.014375        -0.110514
H       0.060181        1.735693        -0.848734
C       -1.291683       0.860450        0.558483
C       -2.111996       -0.236924       -0.082618
H       -1.177351       0.629621        1.655516
H       -1.843412       1.841606        0.534779
O       -1.736632       -1.330857       -0.476758
H       4.328851        -0.207294       -0.676234
O       -3.415219       0.128104        -0.182909
H       -4.011878       -0.593155       -0.581057
###
17
GlyGly2 pm6 E=-0.284018351471 au
N       -3.425236       -0.362260       -0.177733
H       -3.238168       -1.375042       -0.291499
C       -2.318228       0.308524        0.587494
H       -3.530144       0.056098        -1.120216
C       -0.974578       0.107750        -0.083883
H       -2.562764       1.401315        0.731089
```

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H       -2.276035       -0.089737       1.643695
O       -0.766146       -0.858310       -0.841481
N       -0.009131       1.038963        0.181551
H       -0.159390       1.804533        0.856425
C       1.324861        0.953345        -0.431425
C       2.221389        -0.146914       0.124896
H       1.238779        0.817943        -1.541281
H       1.843827        1.941394        -0.309110
O       1.842643        -0.915500       1.049607
O       3.364731        -0.273185       -0.396614
H       -4.326018       -0.253679       0.329590
###
16
GlyGly3 pm6 E=-0.424923054968 au
N       -3.745778       0.232081        0.208802
H       -3.773586       -0.345730       1.052370
C       -2.407267       0.844923        0.064157
H       -3.926430       -0.403494       -0.571021
C       -1.281475       -0.164218       -0.070812
H       -2.405596       1.519814        -0.830061
H       -2.219173       1.524553        0.933596
O       -1.504759       -1.385254       -0.214657
N       0.004670        0.304139        -0.037236
H       0.221885        1.301891        0.073713
C       1.145628        -0.620349       -0.184703
C       2.479893        0.080138        0.019869
H       1.048856        -1.475807       0.529244
H       1.146400        -1.091239       -1.202955
O       2.613743        1.307467        -0.220561
O       3.450357        -0.625525       0.415605
###
27
GlyHis2 pm6 E=-0.250892782842 au
N       -5.001466       -0.919640       0.061827
H       -4.726533       -1.914077       -0.039032
C       -3.957188       -0.009352       -0.522174
H       -5.142727       -0.724034       1.069927
C       -2.590893       -0.267226       0.078629
H       -3.923894       -0.133280       -1.644948
H       -4.265052       1.067885        -0.381554
O       -2.399688       -1.153872       0.924243
N       -1.576892       0.558132        -0.346072
H       -1.725804       1.248422        -1.097911
C       -0.182315       0.339883        0.094969
H       -0.176788       -0.299065       1.023181
C       0.646325        -0.355612       -1.004948
C       0.461641        1.704794        0.426054
H       0.149635        -1.309387       -1.300752
H       0.652762        0.253440        -1.936169
C       2.025504        -0.628564       -0.531650
O       0.481770        2.620705        -0.434536
O       1.002042        1.841959        1.557229
N       3.095315        0.247259        -0.766524
C       2.472380        -1.734214       0.201747
C       4.181302        -0.325404       -0.174414
N       3.836785        -1.534842       0.425877
H       1.937937        -2.601883       0.552802
H       5.186423        0.083105        -0.165976
H       4.451712        -2.161672       0.938423
H       -5.907400       -0.781986       -0.428506
###
28
GlyHis3 pm6 E=-0.945420500525E-01 au
N       -4.939158       -1.109592       -0.118788
H       -4.971535       -1.294040       0.901097
C       -3.991198       0.013930        -0.433988
H       -4.648490       -1.981823       -0.597133
H       -5.899467       -0.868228       -0.435306
C       -2.602689       -0.266153       0.104982
H       -3.970782       0.196723        -1.548457
H       -4.386256       0.983320        -0.010342
O       -2.371072       -1.224432       0.856012
N       -1.621981       0.629143        -0.252005
H       -1.800869       1.377578        -0.938826
C       -0.219741       0.426163        0.168385
H       -0.198829       -0.179509       1.120108
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C       0.583406        -0.310369       -0.922936
C       0.427502        1.805509        0.440669
H       0.053321        -1.254212       -1.209956
H       0.604134        0.282968        -1.868963
C       1.949102        -0.637735       -0.457614
O       0.374478        2.708278        -0.429957
O       1.020843        1.965135        1.540201
N       3.115334        -0.168416       -1.091761
C       2.360833        -1.426991       0.617701
H       3.150324        0.429092        -1.926327
C       4.210560        -0.662068       -0.414797
N       3.759163        -1.432150       0.631885
H       1.763531        -1.971509       1.343277
H       5.261374        -0.473450       -0.670245
H       4.349404        -1.925366       1.311308
###
26
GlyHis4 pm6 E=-0.395736776147 au
N       -5.230406       -0.606219       -0.064625
H       -5.111932       -1.613963       -0.186769
C       -4.054235       0.110302        -0.600904
H       -5.308364       -0.448602       0.941901
C       -2.736663       -0.261965       0.053820
H       -3.991962       -0.063908       -1.706119
H       -4.221545       1.213844        -0.498492
O       -2.664187       -1.060484       1.007400
N       -1.604996       0.343226        -0.443583
H       -1.652417       0.970995        -1.259366
C       -0.257059       0.065011        0.093148
H       -0.336818       -0.595027       1.001671
C       0.629939        -0.633485       -0.959499
C       0.400657        1.401958        0.504337
H       0.267960        -1.675845       -1.118170
H       0.515807        -0.146908       -1.953884
C       2.049895        -0.647212       -0.527749
O       0.495694        2.345510        -0.323212
O       0.876119        1.494863        1.668834
N       3.016858        0.202215        -1.085022
C       2.633191        -1.433772       0.473119
C       4.176515        -0.067803       -0.422091
N       3.977731        -1.059460       0.536557
H       2.203607        -2.197437       1.100777
H       5.134324        0.409504        -0.602994
H       4.672585        -1.448301       1.168894
###
33
GlyLys1 pm6 E=-0.166891931826E-02 au
N       5.228890        -1.015508       -0.274531
C       3.919832        -1.273406       0.417530
H       5.981838        -1.580550       0.166712
H       5.492927        -0.014959       -0.211357
C       2.796824        -0.456850       -0.184289
H       3.674538        -2.376238       0.381520
H       4.022371        -1.064992       1.523250
O       2.965694        0.300738        -1.148937
N       1.562729        -0.598664       0.409041
H       1.421285        -1.218486       1.224896
C       0.376819        0.114160        -0.115464
H       0.385387        0.076818        -1.249107
C       -0.906794       -0.538721       0.424707
C       0.440031        1.579661        0.329437
H       -0.828819       -1.645479       0.317537
H       -0.997942       -0.374024       1.520927
C       -2.157149       -0.035799       -0.301191
O       0.901898        2.018385        1.371522
O       -0.047937       2.533635        -0.515579
H       -2.262923       1.063459        -0.182396
H       -2.059119       -0.196114       -1.395934
C       -3.409299       -0.742820       0.227710
H       -3.319055       -1.842320       0.091920
H       -3.502511       -0.594472       1.325413
C       -4.655234       -0.218290       -0.486585
H       -4.775264       0.882491        -0.334703
H       -4.580763       -0.367063       -1.591940
N       -5.896765       -0.924178       0.022159
H       -6.007645       -0.792368       1.042811
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H       -6.744033       -0.552626       -0.442868
H       -5.847444       -1.941672       -0.163093
H       -0.479895       2.190459        -1.370347
H       5.175677        -1.273092       -1.277086
###
32
GlyLys2 pm6 E=-0.184764258298 au
N       5.188718        -1.088868       -0.225707
C       3.928794        -1.130276       0.594272
H       5.969999        -1.529197       0.301306
H       5.456404        -0.112485       -0.448037
C       2.782566        -0.439913       -0.111953
H       3.669525        -2.201652       0.842823
H       4.112375        -0.658999       1.604496
O       2.944508        0.149050        -1.196989
N       1.562999        -0.477118       0.510398
H       1.431684        -0.962884       1.413442
C       0.364996        0.145544        -0.108521
H       0.417961        0.019427        -1.228541
C       -0.909054       -0.528471       0.414887
C       0.404439        1.661522        0.201185
H       -0.823618       -1.631734       0.303839
H       -1.017624       -0.366198       1.507680
C       -2.148800       -0.021085       -0.330001
O       -0.120858       2.140637        1.236020
O       1.007306        2.406851        -0.626875
H       -2.243635       1.079036        -0.226006
H       -2.041858       -0.197925       -1.420791
C       -3.412835       -0.711716       0.192331
H       -3.328796       -1.813077       0.066612
H       -3.516292       -0.554370       1.287588
C       -4.649608       -0.186328       -0.537495
H       -4.768935       0.915129        -0.391934
H       -4.563947       -0.340324       -1.641360
N       -5.898071       -0.887592       -0.039426
H       -6.019325       -0.752739       0.979703
H       -6.739711       -0.515695       -0.514358
H       -5.848927       -1.905857       -0.221394
H       5.068551        -1.603375       -1.117396
###
31
GlyLys3 pm6 E=-0.327912735627 au
N       -4.787634       -0.459414       -0.885757
C       -4.000030       -1.420151       -0.065203
H       -5.785335       -0.609810       -0.723405
H       -4.627213       -0.645659       -1.877923
C       -2.838515       -0.616709       0.492551
H       -4.595984       -1.833311       0.783789
H       -3.656403       -2.320637       -0.626293
O       -2.987987       0.128551        1.488122
N       -1.631579       -0.693166       -0.152335
H       -1.503922       -1.309680       -0.971800
C       -0.435037       0.057099        0.307710
H       -0.425040       0.089586        1.434405
C       0.838723        -0.636939       -0.189051
C       -0.567470       1.511569        -0.206443
H       0.832040        -1.701460       0.133441
H       0.851150        -0.682582       -1.298751
C       2.101606        0.056827        0.332284
O       -0.129983       1.870048        -1.326342
O       -1.168200       2.335415        0.549704
H       2.118356        1.122075        0.025696
H       2.101267        0.076592        1.442018
C       3.355108        -0.659632       -0.182316
H       3.346903        -1.723315       0.141337
H       3.352111        -0.696995       -1.293111
C       4.619020        0.038119        0.320712
H       4.668129        1.095614        -0.036729
H       4.634685        0.092868        1.437141
N       5.856478        -0.699713       -0.151501
H       5.909099        -0.719327       -1.185127
H       6.713482        -0.241346       0.205415
H       5.854755        -1.679763       0.183723
###
30
GlyLys4 pm6 E=-0.453863706307 au
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N       -4.962379       -1.138502       0.274369
C       -3.831419       -1.199951       -0.694303
H       -5.771365       -1.612746       -0.136213
H       -5.242476       -0.163536       0.406257
C       -2.555115       -0.847963       0.041297
H       -3.730842       -2.239356       -1.100704
H       -3.979891       -0.562890       -1.599595
O       -2.225250       -1.376927       1.121440
N       -1.741990       0.109983        -0.524782
H       -1.928896       0.487043        -1.465056
C       -0.457569       0.491326        0.112365
H       -0.484856       0.194879        1.201796
C       0.735952        -0.210273       -0.551213
C       -0.368478       2.032346        0.057292
H       0.528138        -1.298471       -0.630922
H       0.860050        0.127620        -1.598849
C       2.019255        0.023140        0.253136
O       0.206359        2.632534        -0.887001
O       -0.909552       2.677594        1.001704
H       2.238949        1.107282        0.324259
H       1.876213        -0.308807       1.302444
C       3.209185        -0.714718       -0.369559
H       2.978088        -1.794059       -0.478528
H       3.385184        -0.354303       -1.402137
C       4.469505        -0.528489       0.484576
H       4.706512        0.552017        0.599523
H       4.287286        -0.901395       1.515764
N       5.657485        -1.181402       -0.153227
H       6.327454        -1.434764       0.576583
H       5.378287        -2.067176       -0.579831
###
31
GlyPhe1 pm6 E=-0.715627131251E-01 au
N       -5.290029       -0.705295       0.289675
H       -5.168444       -1.624849       0.752020
C       -4.168776       -0.435048       -0.675047
H       -6.199391       -0.712638       -0.214423
H       -5.332990       0.024078        1.024444
C       -2.835963       -0.332805       0.033536
H       -4.138094       -1.243518       -1.465173
H       -4.386405       0.505494        -1.262717
O       -2.718373       -0.498446       1.254180
N       -1.747762       -0.042918       -0.761660
H       -1.842444       0.107702        -1.780106
C       -0.386859       0.015873        -0.192066
H       -0.322275       -0.653409       0.719887
C       0.661977        -0.417343       -1.227757
C       -0.110914       1.467559        0.234180
H       0.382504        -1.415408       -1.643817
H       0.647507        0.255214        -2.115659
C       2.032689        -0.478629       -0.613046
O       0.000263        2.461104        -0.460361
C       2.910116        0.609257        -0.731655
C       2.438239        -1.627460       0.082493
H       2.603993        1.506767        -1.270543
C       4.184443        0.543326        -0.162643
C       3.714274        -1.688013       0.647552
H       1.759997        -2.476599       0.180413
H       4.865445        1.391037        -0.256840
C       4.589289        -0.604280       0.525330
H       4.028645        -2.584901       1.184178
H       5.586075        -0.654485       0.965032
O       0.017012        1.540498        1.584558
H       0.218096        2.473130        1.934914
###
30
GlyPhe2 pm6 E=-0.249767334554 au
N       -0.304216       4.085659        -0.369211
C       -0.698727       2.950956        0.533515
H       0.649287        3.945898        -0.749456
H       -0.314206       4.981321        0.159553
C       -0.649195       1.618996        -0.187554
H       -0.019149       2.916073        1.435862
H       -1.716657       3.156045        0.976766
O       -0.011797       1.470460        -1.241638
N       -1.379474       0.596897        0.369541
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H       -1.835466       0.709803        1.288226
C       -1.278890       -0.785064       -0.154936
H       -0.945212       -0.752102       -1.231133
C       -0.292999       -1.642917       0.657881
C       -2.681041       -1.431407       -0.091927
H       -0.515982       -1.568538       1.744971
H       -0.452175       -2.719702       0.415841
C       1.132164        -1.260744       0.374589
O       -3.278655       -1.554168       1.007316
C       1.843328        -0.457684       1.278179
C       1.756784        -1.701917       -0.802837
H       1.367204        -0.108397       2.195169
C       3.168945        -0.107303       1.008336
C       3.080974        -1.346893       -1.067623
H       1.210830        -2.326130       -1.511045
H       3.719865        0.514067        1.716464
C       3.790018        -0.550488       -0.162679
H       3.563542        -1.693176       -1.983154
H       4.825219        -0.277898       -0.369539
O       -3.186751       -1.846295       -1.169993
H       -0.961819       4.171666        -1.165983
###
29
GlyPhe3 pm6 E=-0.391920111263 au
N       -2.412551       3.454699        -0.458470
C       -1.542142       2.748106        0.520050
H       -1.842536       4.071344        -1.041710
H       -3.057549       4.066044        0.049885
C       -1.046965       1.480869        -0.151006
H       -0.655434       3.335757        0.862825
H       -2.110784       2.533018        1.458187
O       -0.327196       1.504392        -1.168695
N       -1.444419       0.283031        0.398132
H       -1.961973       0.256811        1.289432
C       -0.944130       -1.012900       -0.115613
H       -0.613979       -0.884300       -1.185507
C       0.231521        -1.555656       0.714918
C       -2.118310       -2.016057       -0.087188
H       0.006830        -1.485082       1.801602
H       0.346984        -2.648302       0.524509
C       1.514885        -0.847501       0.384426
O       -2.597142       -2.417202       1.004929
C       2.039821        0.117785        1.255752
C       2.193229        -1.148323       -0.807740
H       1.523483        0.359020        2.185549
C       3.235594        0.768823        0.939176
C       3.386397        -0.493608       -1.119043
H       1.792272        -1.898289       -1.490562
H       3.643732        1.515500        1.622746
C       3.910517        0.465387        -0.246259
H       3.911722        -0.733209       -2.045236
H       4.844487        0.972480        -0.489905
O       -2.574532       -2.420497       -1.191769
###
32
GlyTyr1 pm6 E=-0.149957445837 au
N       -5.604253       -0.839911       0.447598
H       -5.444821       -1.757650       0.901420
C       -4.529248       -0.541771       -0.560636
H       -6.533716       -0.863833       -0.017780
H       -5.631671       -0.113920       1.186803
C       -3.171578       -0.413443       0.093612
H       -4.510213       -1.346693       -1.354694
H       -4.793668       0.395494        -1.134349
O       -2.995485       -0.620694       1.302164
N       -2.131091       -0.049540       -0.732146
H       -2.275752       0.152174        -1.735955
C       -0.748379       0.033703        -0.218976
H       -0.605397       -0.717394       0.618780
C       0.270767        -0.244048       -1.335768
C       -0.547803       1.430610        0.394250
H       0.001410        -1.192575       -1.858562
H       0.206083        0.531042        -2.132909
C       1.661146        -0.330953       -0.774802
O       -0.338832       2.396178        -0.524794
O       -0.575757       1.688815        1.588697
```

```
C       2.460835        0.819398        -0.684941
C       2.161410        -1.566709       -0.329193
H       2.077442        1.782119        -1.036207
C       3.743533        0.749953        -0.142879
C       3.441210        -1.661229       0.212557
H       1.541913        -2.464930       -0.405628
H       4.369643        1.639475        -0.064274
C       4.211596        -0.491981       0.303363
H       3.837656        -2.614021       0.561028
O       5.463000        -0.646307       0.871552
H       5.951687        0.232096        0.942993
H       -0.187529       3.319668        -0.119309
###
31
GlyTyr2 pm6 E=-0.332011473050 au
N       -3.204021       3.331094        -0.251885
H       -2.634533       3.642667        -1.059750
C       -2.435445       2.367070        0.608419
H       -3.468744       4.169588        0.303309
H       -4.072058       2.897238        -0.615841
C       -2.147402       1.069739        -0.116722
H       -1.483568       2.856191        0.970599
H       -3.005452       2.161951        1.562471
O       -2.662967       0.799218        -1.215097
N       -1.302715       0.195971        0.518538
H       -0.859976       0.430198        1.423120
C       -0.913412       -1.091086       -0.109084
H       -0.677431       -0.919009       -1.197948
C       0.314313        -1.698251       0.584246
C       -2.118616       -2.056884       -0.017342
H       0.138183        -1.797143       1.679254
H       0.448303        -2.746713       0.226521
C       1.559373        -0.902531       0.316105
O       -2.480991       -2.539723       1.085417
O       -2.737387       -2.325496       -1.085231
C       2.045532        -0.009987       1.284514
C       2.238988        -1.047138       -0.905980
H       1.518329        0.105098        2.236289
C       3.199302        0.736308        1.044825
C       3.393650        -0.312692       -1.167283
H       1.861488        -1.741212       -1.661802
H       3.583708        1.432067        1.791379
C       3.855681        0.570534        -0.180252
H       3.928624        -0.416844       -2.110247
O       5.011542        1.264145        -0.497513
H       5.276920        1.900821        0.236798
###
30
GlyTyr3 pm6 E=-0.474043023296 au
N       -1.019684       4.154005        -0.334617
H       0.000530        4.102526        -0.367175
C       -1.564155       2.987836        0.392541
H       -1.337065       4.141626        -1.306156
C       -1.199586       1.641410        -0.206303
H       -1.213492       3.021159        1.456724
H       -2.677684       3.091190        0.459458
O       -0.387385       1.529697        -1.145938
N       -1.840216       0.536868        0.308222
H       -2.431302       0.620227        1.149362
C       -1.500505       -0.838027       -0.124000
H       -1.059684       -0.802996       -1.159998
C       -0.502366       -1.521919       0.830053
C       -2.812174       -1.651812       -0.182082
H       -0.763768       -1.308352       1.889197
H       -0.598352       -2.628504       0.739241
C       0.907643        -1.103675       0.529797
O       -3.458750       -1.902469       0.868041
O       -3.204033       -2.062386       -1.308247
C       1.498364        -0.040745       1.230420
C       1.634263        -1.770511       -0.473413
H       0.940468        0.477334        2.014487
C       2.800110        0.365355        0.934684
C       2.934895        -1.383314       -0.785302
H       1.177124        -2.602152       -1.016345
H       3.268032        1.190216        1.473511
C       3.497131        -0.314178       -0.070985
```

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H       3.506176        -1.892217       -1.560659
O       4.788607        0.027339        -0.433593
H       5.139080        0.793864        0.118566
###
29
GlyTyr4 pm6 E=-0.636945289408 au
N       5.748980        0.158054        -0.256545
H       5.729629        0.015429        -1.268136
C       4.599036        -0.522382       0.374747
H       5.685879        1.166733        -0.106931
C       3.245383        -0.117071       -0.175602
H       4.733908        -1.630457       0.273240
H       4.621895        -0.336464       1.480006
O       3.116604        0.778302        -1.038117
N       2.142699        -0.772237       0.313547
H       2.223298        -1.472204       1.068211
C       0.780591        -0.468500       -0.181371
H       0.773502        -0.550470       -1.305810
C       -0.241572       -1.459957       0.408093
C       0.380669        0.977551        0.181288
H       -0.108848       -2.455206       -0.069836
H       -0.035869       -1.644770       1.486259
C       -1.639376       -0.950045       0.214330
O       0.554209        1.454794        1.332756
O       -0.139843       1.683302        -0.733549
C       -2.321626       -0.340463       1.281446
C       -2.262581       -1.032179       -1.042417
H       -1.854244       -0.302126       2.268375
C       -3.580148       0.212739        1.100960
C       -3.521176       -0.487241       -1.247331
H       -1.745642       -1.525161       -1.869196
H       -4.102064       0.685088        1.925300
C       -4.199857       0.161858        -0.178828
H       -3.999408       -0.548271       -2.218737
O       -5.355951       0.715014        -0.370296
###
27
GlyVal1 pm6 E=-0.130183156644 au
N       4.253789        -0.272331       -0.133864
H       4.275857        -0.964949       -0.904903
C       2.981792        -0.391926       0.658893
H       5.073941        -0.445518       0.481092
H       4.348938        0.673754        -0.545437
C       1.769503        -0.050458       -0.180752
H       2.904382        -1.429182       1.099873
H       3.022925        0.283022        1.564248
O       1.860508        0.529043        -1.272093
N       0.549740        -0.419512       0.337810
H       0.465546        -0.886333       1.255808
C       -0.701072       -0.118043       -0.381556
H       -0.477641       -0.028257       -1.492022
C       -1.749752       -1.258078       -0.182703
C       -1.288586       1.225042        0.050935
H       -1.221563       -2.224043       -0.406582
C       -2.277614       -1.308889       1.247001
C       -2.884018       -1.083786       -1.189818
O       -1.964665       1.963751        -0.651080
H       -2.844153       -0.412021       1.526473
H       -2.957410       -2.162094       1.385702
H       -1.476863       -1.436515       1.987873
H       -2.520916       -1.046266       -2.225432
H       -3.588084       -1.926668       -1.141159
H       -3.474186       -0.175877       -1.017660
O       -1.001442       1.568201        1.329804
H       -1.412204       2.452712        1.619467
###
26
GlyVal2 pm6 E=-0.309661977762 au
N       4.172963        -0.089304       0.028179
H       4.247325        0.334948        -0.914190
C       2.931573        -0.929772       0.148047
H       5.016492        -0.675066       0.191108
H       4.169853        0.675387        0.727625
C       1.695285        -0.159170       -0.261373
H       3.031123        -1.859792       -0.486128
H       2.843102        -1.332517       1.199006
```

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O       1.771871        0.942130        -0.835954
N       0.485431        -0.741786       0.006460
H       0.407860        -1.614863       0.552894
C       -0.771275       -0.092009       -0.433037
H       -0.651990       0.202607        -1.518173
C       -1.965867       -1.082412       -0.330007
C       -1.039359       1.204731        0.355700
H       -1.634464       -2.048190       -0.798700
C       -2.364390       -1.364739       1.116556
C       -3.149754       -0.543224       -1.134078
O       -1.578045       2.157014        -0.280623
H       -2.784417       -0.488154       1.621470
H       -3.131192       -2.150856       1.167296
H       -1.521356       -1.726539       1.719080
H       -2.885360       -0.335620       -2.178705
H       -3.971244       -1.272628       -1.162126
H       -3.569305       0.377117        -0.713160
O       -0.717884       1.342278        1.564000
###
25
GlyVal3 pm6 E=-0.454634885737 au
N       4.261212        -0.228559       -0.107141
H       4.306146        -0.098383       -1.119873
C       2.990289        -0.889062       0.261049
H       4.302155        0.707000        0.301058
C       1.747010        -0.145008       -0.185950
H       2.985228        -1.927891       -0.158259
H       2.958441        -1.034656       1.371607
O       1.804869        0.986362        -0.715885
N       0.531682        -0.753261       -0.000130
H       0.444549        -1.653551       0.494973
C       -0.719383       -0.096819       -0.444604
H       -0.591385       0.200916        -1.527308
C       -1.921598       -1.078767       -0.354381
C       -0.980595       1.196448        0.349203
H       -1.597326       -2.039892       -0.837507
C       -2.320276       -1.381412       1.088089
C       -3.102490       -0.518694       -1.148429
O       -1.505507       2.160010        -0.282043
H       -2.688143       -0.499798       1.623364
H       -3.127464       -2.126922       1.125629
H       -1.490378       -1.805526       1.668190
H       -2.838477       -0.297627       -2.190263
H       -3.929944       -1.240878       -1.186171
H       -3.514185       0.398217        -0.712528
O       -0.665265       1.325080        1.561443
###
29
HisGly1 pm6 E=0.844747442668E-01 au
N       2.948226        -2.118121       0.036184
H       2.774013        -2.991349       0.573893
H       3.914241        -1.792514       0.255345
H       2.914095        -2.345774       -0.977085
C       1.933330        -1.050954       0.402134
H       1.986435        -0.902239       1.531432
C       2.294380        0.267673        -0.299935
C       0.532403        -1.523083       -0.028115
H       3.318028        0.597226        0.034681
H       2.422770        0.110293        -1.403915
C       1.322627        1.346670        -0.021018
O       0.343828        -2.063268       -1.125341
N       0.839488        2.207898        -1.024747
C       0.726480        1.743813        1.177376
H       1.102797        2.180482        -2.018003
C       -0.041915       3.097937        -0.450014
N       -0.114272       2.824593        0.896773
H       0.850463        1.333686        2.178609
H       -0.580764       3.897811        -0.974769
H       -0.695048       3.325895        1.578961
N       -0.480195       -1.318444       0.871847
H       -0.330592       -0.817346       1.765243
C       -1.869330       -1.669636       0.550386
C       -2.576815       -0.555668       -0.183669
H       -1.933988       -2.610241       -0.068300
H       -2.415991       -1.935161       1.501592
O       -2.062935       0.303808        -0.886154
```

```
O       -3.935891       -0.486462       -0.091098
H       -4.366169       -1.195381       0.499808
###
28
HisGly2 pm6 E=-0.974226205204E-01 au
N       3.161856        -1.823050       -0.666615
C       2.406217        -0.717240       -1.069712
C       2.340230        0.167546        0.007259
N       3.067703        -0.417088       1.062875
C       3.564480        -1.628790       0.634697
C       1.718925        1.504884        0.125202
C       0.356468        1.593955        -0.577865
C       -0.700195       0.779380        0.188055
N       -1.025559       -0.443913       -0.321811
C       -1.966005       -1.339868       0.370871
C       -3.418752       -0.997770       0.031264
O       -4.071813       -1.777029       -0.711479
N       -0.093058       3.042586        -0.639738
O       -1.239408       1.227508        1.214914
O       -3.950475       0.040600        0.516271
H       -1.001670       3.125112        -1.138196
H       0.608461        3.614399        -1.159429
H       -0.197692       3.450523        0.308652
H       0.456154        1.224492        -1.652092
H       2.420999        2.268397        -0.315560
H       1.633295        1.821010        1.198282
H       3.210563        -0.005769       1.992473
H       1.972194        -0.630472       -2.063900
H       4.177796        -2.317381       1.230414
H       3.383669        -2.640515       -1.245478
H       -0.591586       -0.809111       -1.186997
H       -1.823709       -1.311490       1.480978
H       -1.739720       -2.400152       0.091602
###
27
HisGly3 pm6 E=-0.250893149340 au
N       -2.973368       -1.908090       0.695003
C       -2.411373       -0.690390       1.083832
C       -2.280808       0.075301        -0.081978
N       -2.749189       -0.655875       -1.182835
C       -3.167137       -1.852734       -0.684058
C       -1.792586       1.468667        -0.219811
C       -0.460020       1.704846        0.511589
C       0.678093        0.957001        -0.197077
N       0.839465        -0.359094       0.131107
C       1.820350        -1.221156       -0.548927
C       3.221294        -1.074473       0.049174
O       3.722203        -2.039498       0.683509
N       -0.150541       3.190430        0.532835
O       1.411648        1.528504        -1.023861
O       3.866268        -0.001974       -0.122709
H       0.721610        3.380773        1.063633
H       -0.928467       3.711535        0.993235
H       -0.038484       3.569027        -0.426589
H       -0.547310       1.358165        1.592881
H       -2.569844       2.166846        0.188962
H       -1.704177       1.761272        -1.293793
H       -2.151543       -0.458944       2.105503
H       -3.595091       -2.664667       -1.262254
H       0.253747        -0.813182       0.850983
H       1.479312        -2.285490       -0.481890
H       1.863812        -1.011760       -1.648023
H       -3.195970       -2.683813       1.312615
###
26
HisGly4 pm6 E=-0.399924443639 au
N       3.427107        -1.240808       0.149304
H       3.373512        -2.212555       0.464368
H       3.600229        -1.263027       -0.857520
C       2.168531        -0.525323       0.460554
H       2.108352        -0.423075       1.583272
C       2.186953        0.880949        -0.171451
C       0.928931        -1.274866       -0.065820
H       2.999370        1.479209        0.307273
H       2.488785        0.826986        -1.242065
C       0.892269        1.587322        -0.014421
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O       0.859658        -1.678277       -1.246401
N       0.218644        2.155498        -1.103981
C       0.167925        1.821992        1.161418
C       -0.900890       2.738611        -0.589131
N       -0.959725       2.559288        0.791219
H       0.376441        1.532169        2.179537
H       -1.647175       3.284620        -1.156357
N       -0.096722       -1.498966       0.811935
H       -0.084554       -1.104172       1.765879
C       -1.350455       -2.147298       0.396533
C       -2.346021       -1.129079       -0.157866
H       -1.171346       -2.944582       -0.367009
H       -1.791085       -2.691749       1.269779
O       -2.024262       -0.389448       -1.131073
O       -3.482933       -1.047784       0.374116
H       -1.680814       2.901321        1.421467
###
44
HisLys0 pm6 E=0.188140288283 au
N       -3.497207       -2.849001       -0.883016
H       -2.886116       -3.570118       -1.316162
H       -3.715723       -3.144966       0.088545
C       -2.825282       -1.488510       -0.909070
H       -2.546833       -1.262293       -1.990675
C       -3.804909       -0.423143       -0.394945
C       -1.574296       -1.538736       -0.013250
H       -4.733212       -0.433684       -1.033249
H       -4.188865       -0.695672       0.624371
C       -3.232285       0.940741        -0.398704
O       -1.594433       -2.082187       1.096502
N       -3.514595       1.873100        0.619037
C       -2.396564       1.581206        -1.315565
C       -2.852990       3.046964        0.332896
N       -2.169287       2.879378        -0.850111
H       -1.969220       1.204231        -2.243713
H       -2.877189       3.961871        0.939290
H       -1.581581       3.585840        -1.307433
N       -0.449136       -0.927227       -0.505061
H       -0.446614       -0.447103       -1.423929
C       0.805688        -0.880501       0.281675
H       1.061526        -1.926168       0.637250
C       1.943853        -0.319025       -0.587585
C       0.606365        0.027181        1.501525
H       1.955635        -0.851297       -1.566756
H       1.745995        0.744260        -0.849273
C       3.308185        -0.460210       0.092295
O       -0.101383       1.019381        1.573843
O       1.272585        -0.280947       2.650969
H       3.310404        0.053601        1.076871
H       3.516091        -1.526775       0.322226
C       4.414603        0.117089        -0.796891
H       4.437683        -0.409562       -1.775098
H       4.196236        1.179308        -1.043335
C       5.770220        0.002291        -0.099020
H       5.756759        0.514375        0.894230
H       6.027474        -1.064922       0.110660
N       6.861424        0.615369        -0.955026
H       6.668810        1.615575        -1.141754
H       7.779868        0.548639        -0.482438
H       6.933088        0.131916        -1.867434
H       -4.392376       -2.821717       -1.418021
H       -4.116764       1.705722        1.435219
H       1.856845        -1.114452       2.619182
###
43
HisLys1 pm6 E=0.394783268484E-02 au
N       1.757213        3.219900        -0.299614
H       0.863188        3.409943        -0.798259
H       1.648635        3.504666        0.693950
C       2.150895        1.757983        -0.419179
H       2.184030        1.497304        -1.529678
C       3.545407        1.561592        0.191656
C       1.100439        0.871461        0.278068
H       4.256404        2.321343        -0.240668
H       3.532960        1.809024        1.285695
C       4.095273        0.206699        -0.038357
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O       1.334896        0.293029        1.351150
N       5.094213        -0.338389       0.793801
C       3.830110        -0.740309       -1.027774
C       5.426912        -1.588595       0.318200
N       4.659399        -1.843556       -0.793799
H       3.134090        -0.695673       -1.861311
H       6.176990        -2.261774       0.754982
H       4.689286        -2.700890       -1.357051
N       -0.093950       0.716928        -0.369257
H       -0.286977       1.192060        -1.270230
C       -1.218944       -0.035705       0.244667
H       -1.216355       0.129429        1.360532
C       -2.548990       0.454625        -0.339376
C       -0.978973       -1.542136       -0.018177
H       -2.596799       1.565369        -0.285992
H       -2.605959       0.231236        -1.425372
C       -3.746848       -0.149635       0.400533
O       -1.423890       -2.107008       -1.047245
O       -0.304426       -2.187688       0.838499
H       -3.686683       -1.256503       0.412434
H       -3.728568       0.150355        1.469105
C       -5.058760       0.299645        -0.252431
H       -5.107948       1.409559        -0.292505
H       -5.093092       -0.028956       -1.313690
C       -6.259711       -0.255715       0.514095
H       -6.215438       -1.369817       0.588233
H       -6.276710       0.118648        1.566889
N       -7.552072       0.142806        -0.170954
H       -7.578613       -0.206420       -1.145535
H       -8.369461       -0.247038       0.330417
H       -7.654354       1.172887        -0.202178
H       2.491374        3.825761        -0.725404
H       5.512880        0.119550        1.613602
###
42
HisLys2 pm6 E=-0.149960966557 au
N       -3.358521       -3.067263       -0.384100
H       -2.655457       -3.789955       -0.640336
H       -3.635443       -3.215950       0.605226
C       -2.804700       -1.674245       -0.605834
H       -2.520606       -1.589698       -1.703691
C       -3.872040       -0.609993       -0.280954
C       -1.587350       -1.438229       0.304683
H       -4.728211       -0.712889       -0.994487
H       -4.323808       -0.797161       0.722139
C       -3.300923       0.756684        -0.365257
O       -1.686962       -1.484072       1.542267
N       -3.134249       1.572670        0.762490
C       -2.846683       1.430189        -1.506574
C       -2.570797       2.726648        0.307559
N       -2.391724       2.677067        -1.074906
H       -2.827863       1.116220        -2.539072
H       -2.317586       3.589289        0.915148
H       -2.000364       3.406608        -1.666067
N       -0.414589       -1.107176       -0.312970
H       -0.330520       -1.095234       -1.344723
C       0.772438        -0.664689       0.465295
H       0.853014        -1.269951       1.411737
C       2.044995        -0.849457       -0.369065
C       0.512160        0.815322        0.848259
H       2.155848        -1.920759       -0.646700
H       1.953628        -0.313593       -1.338242
C       3.292136        -0.375668       0.385504
O       0.784826        1.749618        0.057458
O       -0.040733       1.040811        1.964977
H       3.150322        0.652451        0.776528
H       3.459580        -1.006337       1.282989
C       4.521819        -0.421963       -0.528475
H       4.717332        -1.467450       -0.852158
H       4.328517        0.141064        -1.466948
C       5.744846        0.152116        0.187582
H       5.581055        1.219642        0.476121
H       5.949512        -0.393854       1.140827
N       6.969882        0.066503        -0.701694
H       6.831196        0.599886        -1.578368
H       7.800042        0.454800        -0.219777
```

```
H       7.175071        -0.915546       -0.958297
H       -4.203308       -3.215345       -0.977524
###
41
HisLys3 pm6 E=-0.297845494101 au
N       -3.856577       -2.671854       -0.730630
H       -3.301581       -3.485990       -1.005792
H       -4.170209       -2.835712       0.227793
C       -3.035342       -1.443010       -0.817462
H       -2.765372       -1.287723       -1.901015
C       -3.844801       -0.231429       -0.304131
C       -1.754036       -1.540981       0.033990
H       -4.766923       -0.124132       -0.924629
H       -4.230661       -0.426803       0.721559
C       -3.060361       1.026108        -0.356720
O       -1.748938       -2.149225       1.124759
N       -2.806602       1.808487        0.778113
C       -2.459369       1.613997        -1.478077
C       -2.046269       2.855826        0.346207
N       -1.819374       2.768692        -1.025333
H       -2.450980       1.298887        -2.509967
H       -1.680487       3.668218        0.964434
H       -1.286854       3.417977        -1.599947
N       -0.627703       -0.912247       -0.428918
H       -0.639555       -0.390716       -1.321766
C       0.621760        -0.818895       0.369705
H       0.758799        -1.761397       0.970853
C       1.820317        -0.627387       -0.567743
C       0.441323        0.359811        1.361407
H       1.790548        -1.387905       -1.378164
H       1.744292        0.347493        -1.094190
C       3.151838        -0.733854       0.184952
O       0.930107        1.492432        1.141665
O       -0.251597       0.144075        2.403176
H       3.103066        -0.197189       1.154072
H       3.353929        -1.791553       0.453241
C       4.297356        -0.172499       -0.664910
H       4.339824        -0.694480       -1.645057
H       4.108260        0.894578        -0.912851
C       5.630649        -0.315056       0.069956
H       5.600260        0.190534        1.065925
H       5.863514        -1.388066       0.279179
N       6.756306        0.282967        -0.751476
H       6.587791        1.287692        -0.937823
H       7.659836        0.196638        -0.253560
H       6.845190        -0.196705       -1.664426
###
40
HisLys4 pm6 E=-0.428190868246 au
N       -3.459188       -3.019206       -0.473643
H       -2.773331       -3.759154       -0.645334
H       -3.780556       -3.130134       0.489885
C       -2.838571       -1.690352       -0.677581
H       -2.571469       -1.602578       -1.769010
C       -3.834296       -0.572485       -0.297775
C       -1.578813       -1.505124       0.192055
H       -4.723741       -0.634875       -0.968722
H       -4.246905       -0.746244       0.721551
C       -3.213347       0.770361        -0.404685
O       -1.556961       -1.874175       1.384999
N       -2.978020       1.584797        0.711776
C       -2.760433       1.415725        -1.562810
C       -2.374400       2.709767        0.231895
N       -2.232116       2.641224        -1.152432
H       -2.780688       1.094974        -2.592359
H       -2.066036       3.563676        0.825029
H       -1.819621       3.344533        -1.760177
N       -0.488516       -0.896604       -0.371787
H       -0.512403       -0.550101       -1.344309
C       0.747709        -0.622149       0.404683
H       0.905032        -1.443555       1.160119
C       1.959386        -0.561046       -0.532697
C       0.513965        0.700082        1.177096
H       2.014371        -1.496479       -1.130559
H       1.833889        0.250886        -1.278804
C       3.261673        -0.366803       0.253145
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O       0.849359        1.810546        0.703677
O       -0.074501       0.617794        2.298130
H       3.208809        0.554088        0.867857
H       3.396745        -1.194975       0.978541
C       4.467229        -0.298416       -0.691036
H       4.587099        -1.264265       -1.222937
H       4.292695        0.452033        -1.487368
C       5.747149        0.045789        0.081388
H       5.675642        1.067012        0.516016
H       5.868199        -0.641750       0.946430
N       6.928729        0.023417        -0.837710
H       7.781500        0.104312        -0.279720
H       6.987861        -0.888221       -1.296073
###
44
LeuTyr1 pm6 E=-0.182477964784 au
N       -4.095243       2.618608        0.162930
H       -4.106324       2.880056        -0.841341
H       -3.567616       3.346824        0.683638
H       -5.079710       2.627223        0.503259
C       -3.479659       1.246737        0.375432
H       -3.467237       1.049020        1.495391
C       -4.326461       0.175648        -0.325547
C       -2.056205       1.242572        -0.202782
H       -5.382571       0.262136        0.018040
H       -4.368819       0.374311        -1.418809
C       -3.819342       -1.262274       -0.074769
O       -1.804173       1.697006        -1.324329
H       -2.752411       -1.334198       -0.412134
C       -3.883124       -1.631183       1.407909
C       -4.648002       -2.239365       -0.913710
H       -4.896612       -1.539706       1.815820
H       -3.563332       -2.666403       1.579631
H       -3.232185       -0.997394       2.024838
H       -4.605260       -2.003656       -1.984069
H       -4.288318       -3.269549       -0.802705
H       -5.707229       -2.237699       -0.630557
N       -1.078795       0.699643        0.598477
H       -1.307758       0.268692        1.512305
C       0.290114        0.481031        0.090356
H       0.537924        1.272541        -0.684155
C       1.303835        0.543677        1.248448
C       0.401731        -0.880549       -0.610677
H       1.211857        1.530022        1.762976
H       1.041810        -0.200890       2.035590
C       2.711637        0.348972        0.765348
O       -0.508637       -1.781217       -0.178052
O       1.206670        -1.170978       -1.483613
C       3.411242        -0.821396       1.100368
C       3.332450        1.333913        -0.022873
H       2.935381        -1.586112       1.720835
C       4.713393        -1.022303       0.644047
C       4.630792        1.152736        -0.493618
H       2.793763        2.252618        -0.272698
H       5.264138        -1.928952       0.898602
C       5.301240        -0.031920       -0.152098
H       5.118597        1.906646        -1.110085
O       6.578069        -0.163820       -0.667113
H       7.016660        -1.018586       -0.360081
H       -0.453768       -2.680402       -0.654299
###
43
LeuTyr2 pm6 E=-0.364742318519 au
N       1.583665        -3.019352       -0.937669
H       1.825772        -2.960865       -1.945229
H       0.559337        -3.176096       -0.855228
H       2.066996        -3.853732       -0.543566
C       2.007567        -1.769383       -0.187578
H       1.754070        -1.928369       0.910060
C       3.521086        -1.553614       -0.323926
C       1.260920        -0.547477       -0.748560
H       4.056560        -2.470770       0.010542
H       3.798978        -1.440563       -1.393862
C       4.021516        -0.336271       0.485913
O       1.452281        -0.137103       -1.905617
H       3.422086        0.563235        0.192470
```

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C       3.852418        -0.558680       1.989632
C       5.486951        -0.062889       0.137985
H       4.397972        -1.442425       2.341974
H       4.225484        0.295904        2.566795
H       2.801786        -0.703386       2.272711
H       5.628826        0.132670        -0.931725
H       5.869899        0.813711        0.674933
H       6.140570        -0.904432       0.397058
N       0.400479        0.086911        0.106041
H       0.228597        -0.264225       1.064454
C       -0.283735       1.346660        -0.278908
H       -0.678604       1.250548        -1.329716
C       -1.437961       1.667951        0.679640
C       0.770232        2.482364        -0.249656
H       -1.092483       1.619454        1.737496
H       -1.741857       2.732226        0.535275
C       -2.621930       0.769725        0.466949
O       1.189109        2.949187        0.838965
O       1.211549        2.902502        -1.356154
C       -2.879129       -0.279719       1.363026
C       -3.481947       0.985560        -0.624209
H       -2.208323       -0.454244       2.209182
C       -3.990330       -1.104499       1.186538
C       -4.595705       0.172759        -0.822281
H       -3.280031       1.800036        -1.325144
H       -4.203048       -1.917891       1.881287
C       -4.832856       -0.861349       0.095745
H       -5.269270       0.331293        -1.663217
O       -5.963891       -1.622621       -0.147120
H       -6.087296       -2.337540       0.552393
###
42
LeuTyr3 pm6 E=-0.507429210818 au
N       -0.616260       -2.780889       -0.976422
H       -0.297278       -3.223025       -0.113069
H       0.217626        -2.455154       -1.472364
C       -1.524615       -1.642579       -0.687658
H       -1.893574       -1.249890       -1.678474
C       -2.724095       -2.113270       0.149258
C       -0.773276       -0.533523       0.077000
H       -3.221871       -2.953263       -0.378631
H       -2.376986       -2.551579       1.107318
C       -3.751429       -0.995856       0.431928
O       -0.171536       -0.772960       1.143838
H       -3.231586       -0.158946       0.963157
C       -4.358995       -0.442819       -0.858843
C       -4.847515       -1.534915       1.356394
H       -4.871538       -1.215679       -1.442374
H       -5.097176       0.341540        -0.651592
H       -3.601098       0.004970        -1.514657
H       -4.440406       -1.898692       2.307346
H       -5.583456       -0.760130       1.602618
H       -5.400440       -2.368033       0.907671
N       -0.771829       0.726697        -0.463530
H       -1.226542       0.915389        -1.369040
C       0.017962        1.832532        0.125793
H       0.231318        1.601730        1.207775
C       1.351212        2.041914        -0.618103
C       -0.824919       3.122986        0.057384
H       1.176446        2.144727        -1.711178
H       1.793479        3.017276        -0.310885
C       2.309063        0.921556        -0.331613
O       -1.254719       3.550926        -1.044803
O       -1.068976       3.726354        1.138028
C       2.437915        -0.148973       -1.230893
C       3.062348        0.931296        0.855908
H       1.856758        -0.162738       -2.156544
C       3.311593        -1.202275       -0.958436
C       3.941246        -0.108488       1.148492
H       2.962451        1.763218        1.558239
H       3.419389        -2.035936       -1.653434
C       4.053223        -1.162008       0.228018
H       4.531074        -0.109590       2.064320
O       4.954622        -2.153677       0.573339
H       5.016596        -2.865455       -0.137546
###
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41
LeuTyr4 pm6 E=-0.667107810452 au
N       -0.645847       -2.796578       -0.970899
H       -0.336033       -3.243759       -0.107134
H       0.193173        -2.498087       -1.473956
C       -1.522003       -1.632610       -0.685485
H       -1.882875       -1.234667       -1.677239
C       -2.731462       -2.067740       0.156124
C       -0.738630       -0.540776       0.071953
H       -3.251900       -2.896555       -0.367829
H       -2.394423       -2.511605       1.115178
C       -3.730404       -0.924435       0.437099
O       -0.125014       -0.800943       1.129104
H       -3.191189       -0.102006       0.971384
C       -4.320625       -0.354354       -0.854306
C       -4.842190       -1.436830       1.358033
H       -4.847581       -1.113892       -1.442416
H       -5.042203       0.445480        -0.647528
H       -3.550633       0.079209        -1.505635
H       -4.447166       -1.810725       2.310153
H       -5.559641       -0.644257       1.602435
H       -5.413927       -2.255964       0.907213
N       -0.722844       0.721530        -0.460228
H       -1.183912       0.920869        -1.360509
C       0.091669        1.813939        0.122600
H       0.307294        1.580583        1.202720
C       1.426775        1.999564        -0.627935
C       -0.729572       3.117319        0.058824
H       1.247318        2.098782        -1.719330
H       1.881190        2.969064        -0.324536
C       2.367164        0.866749        -0.340360
O       -1.159604       3.552562        -1.040880
O       -0.957130       3.726246        1.140402
C       2.443438        -0.236648       -1.207574
C       3.157202        0.880890        0.822115
H       1.844111        -0.251517       -2.120721
C       3.274312        -1.310579       -0.922274
C       3.998620        -0.179064       1.124876
H       3.106559        1.737625        1.498183
H       3.325429        -2.160930       -1.593123
C       4.071675        -1.302314       0.255034
H       4.606456        -0.162347       2.022499
O       4.851122        -2.300193       0.535843
###
36
LysAla1 pm6 E=-0.107397386743E-01 au
N       0.143175        3.621041        -0.124540
H       0.304267        3.669099        -1.148652
H       0.967168        4.037927        0.352151
H       -0.688665       4.208001        0.094367
C       -0.086368       2.191914        0.334872
H       -0.208651       2.212096        1.465723
C       -1.361143       1.628936        -0.314530
C       1.126417        1.342470        -0.071281
H       -2.167630       2.399915        -0.274991
H       -1.203153       1.451122        -1.400603
C       -1.838805       0.352239        0.382431
O       1.718300        1.525093        -1.142695
H       -1.074048       -0.446563       0.309347
H       -1.963058       0.533382        1.472182
C       -3.157550       -0.131902       -0.229871
H       -3.918725       0.678090        -0.196332
H       -3.023815       -0.352845       -1.310886
C       -3.667434       -1.368665       0.510164
H       -2.925273       -2.202660       0.471700
H       -3.823768       -1.153888       1.596464
N       -4.975836       -1.844438       -0.090223
H       -4.858491       -2.101187       -1.086581
H       -5.329448       -2.675908       0.415725
H       -5.699608       -1.106548       -0.038518
N       1.513781        0.362129        0.809158
H       0.990658        0.182664        1.684270
C       2.628711        -0.559871       0.492785
H       3.488812        0.030637        0.047063
C       3.082460        -1.288838       1.746920
C       2.178975        -1.592196       -0.549334
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H       2.280909        -1.874069       2.223492
H       3.911677        -1.985302       1.535019
H       3.460846        -0.591198       2.511480
O       1.040073        -1.826678       -0.923623
O       3.140076        -2.343116       -1.164101
H       4.092991        -2.170806       -0.852759
###
35
LysAla2 pm6 E=-0.193976222918 au
N       -0.371208       3.386079        0.015782
H       -0.289634       3.545397        1.038451
H       -1.349847       3.591327        -0.270537
H       0.251404        4.071152        -0.461474
C       0.023938        1.969932        -0.363388
H       -0.061019       1.876459        -1.493902
C       1.479009        1.707421        0.053723
C       -0.925433       0.969365        0.321550
H       2.124488        2.543897        -0.302527
H       1.573601        1.730001        1.161320
C       1.998663        0.381406        -0.509780
O       -0.682033       0.503047        1.447778
H       1.291168        -0.444090       -0.292447
H       2.050122        0.430288        -1.618135
C       3.378287        0.059698        0.074486
H       4.091121        0.882407        -0.151889
H       3.328949        0.020133        1.184464
C       3.903278        -1.264011       -0.481210
H       3.201327        -2.105278       -0.263881
H       3.995197        -1.226821       -1.594774
N       5.258958        -1.588900       0.114945
H       5.195176        -1.704789       1.141906
H       5.634646        -2.468017       -0.284441
H       5.940772        -0.833755       -0.077983
N       -2.034362       0.579165        -0.379587
H       -2.254676       0.975270        -1.308825
C       -2.996432       -0.400577       0.193170
H       -3.172948       -0.149863       1.278263
C       -4.314998       -0.371719       -0.556466
C       -2.349306       -1.805608       0.115471
H       -4.208983       -0.566199       -1.632997
H       -5.015664       -1.121631       -0.157532
H       -4.820418       0.602563        -0.466802
O       -2.268872       -2.423553       -0.975838
O       -1.881662       -2.299281       1.181861
###
34
LysAla3 pm6 E=-0.339242105940 au
N       0.307279        3.501822        0.115219
H       1.225976        3.762858        0.480576
H       0.352481        3.615278        -0.898942
C       -0.015811       2.099489        0.478213
H       -0.200056       2.079609        1.591112
C       -1.280529       1.635938        -0.266306
C       1.152808        1.156223        0.132537
H       -2.008190       2.476993        -0.303057
H       -1.056351       1.425082        -1.331836
C       -1.934310       0.422716        0.400343
O       1.865854        1.357958        -0.875460
H       -1.237556       -0.437367       0.426094
H       -2.152428       0.642245        1.467026
C       -3.222538       0.028365        -0.331067
H       -3.938190       0.878678        -0.336590
H       -3.012637       -0.175733       -1.403047
C       -3.856675       -1.195656       0.330088
H       -3.157938       -2.067277       0.328154
H       -4.089668       -0.998516       1.405660
N       -5.133708       -1.587335       -0.386497
H       -4.949334       -1.814601       -1.379732
H       -5.562766       -2.419159       0.058220
H       -5.825769       -0.818123       -0.362401
N       1.411452        0.105250        0.969209
H       0.790427        -0.101574       1.770559
C       2.547319        -0.832375       0.760049
H       3.503992        -0.286859       1.003955
C       2.409496        -2.043408       1.667451
C       2.617899        -1.292378       -0.712914
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H       1.479010        -2.605139       1.507412
H       3.243633        -2.748066       1.524491
H       2.423098        -1.764835       2.733179
O       1.658647        -1.905357       -1.254436
O       3.671893        -1.034493       -1.359695
###
33
LysAla4 pm6 E=-0.471854044696 au
N       -0.349981       3.560238        0.022220
H       -1.333125       3.768455        -0.168993
H       -0.209145       3.687760        1.025749
C       -0.024909       2.172699        -0.390139
H       -0.099309       2.125921        -1.513612
C       1.406138        1.807066        0.042713
C       -1.002234       1.163499        0.243657
H       2.106251        2.585364        -0.328730
H       1.499899        1.850866        1.147163
C       1.834103        0.431544        -0.479507
O       -1.028158       0.966495        1.476801
H       1.092549        -0.342100       -0.199380
H       1.846740        0.433338        -1.588737
C       3.212439        0.042726        0.065868
H       3.954124        0.832023        -0.170121
H       3.186775        -0.003209       1.172890
C       3.678321        -1.302753       -0.509906
H       2.913483        -2.087973       -0.328729
H       3.777597        -1.229842       -1.615218
N       4.979779        -1.778111       0.040697
H       4.882269        -1.964996       1.041028
H       5.674559        -1.031055       -0.024487
N       -1.858378       0.481226        -0.581529
H       -1.873265       0.642943        -1.599886
C       -2.796318       -0.540395       -0.045246
H       -3.301593       -0.129068       0.873632
C       -3.844337       -0.913796       -1.076757
C       -1.962501       -1.778018       0.369166
H       -3.417275       -1.298914       -2.012982
H       -4.527949       -1.686002       -0.691004
H       -4.475994       -0.055543       -1.354269
O       -1.461956       -2.540714       -0.497883
O       -1.772480       -1.980389       1.601941
###
34
LysDAla3 pm6 E=-0.339249895560 au
N       0.187268        3.388725        0.380043
H       1.122850        3.591953        0.738438
H       0.175196        3.688960        -0.596194
C       -0.100870       1.937871        0.488329
H       -0.124554       1.683425        1.587424
C       -1.460799       1.612038        -0.158406
C       0.992863        1.094444        -0.195401
H       -2.130485       2.496213        -0.079648
H       -1.348715       1.453511        -1.250942
C       -2.133879       0.403474        0.498649
O       1.758153        1.594203        -1.050573
H       -1.455666       -0.474973       0.503496
H       -2.331654       0.613577        1.570957
C       -3.440213       0.042742        -0.217481
H       -4.143412       0.902519        -0.196122
H       -3.250150       -0.147804       -1.295823
C       -4.078004       -1.184037       0.435791
H       -3.381745       -2.058138       0.423537
H       -4.305752       -0.994621       1.513782
N       -5.358668       -1.565890       -0.278932
H       -5.177756       -1.789999       -1.273505
H       -5.790432       -2.397540       0.163531
H       -6.046802       -0.793582       -0.249822
N       1.124720        -0.219291       0.169546
H       0.492350        -0.640245       0.872624
C       2.069020        -1.146104       -0.507619
C       3.458267        -0.992880       0.156265
O       4.173371        -0.007286       -0.197977
O       3.877498        -1.812388       1.010869
C       1.551863        -2.571501       -0.429413
H       1.384218        -2.915027       0.601132
H       0.591446        -2.688293       -0.955119
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H       2.175529        -0.851052       -1.591266
H       2.250631        -3.276203       -0.903910
###
33
LysDAla4 pm6 E=-0.472226353909 au
N       -0.149896       3.173348        -0.530562
H       -1.088585       3.314868        -0.909927
H       -0.168967       3.504133        0.435372
C       0.218067        1.736886        -0.587790
H       0.281775        1.449785        -1.676185
C       1.581096        1.510039        0.091436
C       -0.841877       0.867117        0.115620
H       2.246376        2.372583        -0.130554
H       1.478092        1.519307        1.195271
C       2.248209        0.214202        -0.379628
O       -1.458247       1.290329        1.118210
H       1.599741        -0.658655       -0.168076
H       2.362793        0.225753        -1.483481
C       3.612562        0.019223        0.289881
H       4.242755        0.920478        0.150968
H       3.489144        -0.077106       1.386908
C       4.332034        -1.214577       -0.275500
H       3.679005        -2.110948       -0.203416
H       4.532903        -1.074820       -1.360186
N       5.625501        -1.518993       0.400719
H       5.453581        -1.744347       1.382800
H       6.210145        -0.680705       0.416707
N       -1.124397       -0.369173       -0.401823
H       -0.614093       -0.735208       -1.221879
C       -2.100308       -1.286991       0.244733
C       -3.510264       -0.659483       0.147830
O       -4.101780       -0.549278       -0.956005
O       -4.042091       -0.235087       1.215020
C       -2.085453       -2.650905       -0.422585
H       -2.301080       -2.610248       -1.499507
H       -1.109448       -3.150647       -0.321438
H       -1.833158       -1.395378       1.334289
H       -2.826889       -3.325893       0.032217
###
42
LysGlu1 pm6 E=-0.166666079748 au
N       1.446542        3.556572        0.066877
H       1.622206        3.712660        1.077812
H       0.490932        3.899820        -0.156273
H       2.128559        4.135460        -0.466489
C       1.602054        2.093142        -0.306060
H       1.436385        2.005337        -1.428016
C       3.020357        1.606185        0.029186
C       0.565246        1.260292        0.470361
H       3.767538        2.326504        -0.377269
H       3.185050        1.615118        1.128727
C       3.278937        0.211362        -0.548253
O       0.711893        0.968465        1.662557
H       2.509800        -0.506377       -0.196001
H       3.175285        0.231121        -1.654291
C       4.675269        -0.283041       -0.156069
H       5.448242        0.438220        -0.499729
H       4.779973        -0.312770       0.950206
C       4.936634        -1.666880       -0.751338
H       4.199045        -2.415773       -0.372957
H       4.819845        -1.658334       -1.863311
N       6.335310        -2.138340       -0.406639
H       6.477309        -2.166141       0.618806
H       6.501415        -3.090159       -0.780134
H       7.049520        -1.506477       -0.807749
N       -0.531078       0.828477        -0.238864
H       -0.658706       1.064300        -1.238833
C       -1.598400       0.040582        0.418346
H       -1.833405       0.502539        1.429026
C       -2.860167       0.032460        -0.459319
C       -1.098300       -1.394492       0.630309
H       -3.078550       1.077321        -0.794659
H       -2.682726       -0.537115       -1.400051
C       -4.065047       -0.532925       0.291637
O       -0.370337       -2.035124       -0.111993
O       -1.474481       -2.049762       1.764112
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H       -3.903152       -1.602973       0.571111
H       -4.200418       -0.017497       1.279012
C       -5.309881       -0.405739       -0.522668
O       -5.933765       -1.312225       -1.062798
O       -5.859925       0.836520        -0.708993
H       -5.345781       1.593205        -0.265782
H       -2.111082       -1.543602       2.377369
###
41
LysGlu2 pm6 E=-0.352666858159 au
N       1.148579        3.186009        -0.259027
H       1.068932        3.438272        0.745254
H       0.234751        3.371162        -0.719463
H       1.854073        3.821585        -0.687708
C       1.573754        1.739290        -0.441057
H       1.562351        1.512845        -1.557638
C       2.999381        1.538861        0.095849
C       0.578929        0.804037        0.269115
H       3.636876        2.408874        -0.186506
H       3.003028        1.540549        1.206816
C       3.619389        0.249684        -0.451996
O       0.877146        0.192565        1.308729
H       2.954694        -0.616715       -0.260532
H       3.702498        0.307815        -1.558545
C       4.997121        0.004131        0.171151
H       5.649812        0.892228        0.023145
H       4.911147        -0.108360       1.273394
C       5.645476        -1.237401       -0.441756
H       5.022430        -2.148697       -0.271086
H       5.738627        -1.138250       -1.551582
N       7.022932        -1.462710       0.149548
H       6.966998        -1.620153       1.171279
H       7.473318        -2.291808       -0.278789
H       7.634227        -0.643612       -0.013496
N       -0.644435       0.634381        -0.323539
H       -0.898102       1.134862        -1.195317
C       -1.703208       -0.188718       0.312719
H       -1.644736       -0.074621       1.434766
C       -3.083229       0.271009        -0.171906
C       -1.429204       -1.673165       -0.033379
H       -3.184074       1.374030        -0.040138
H       -3.188150       0.105167        -1.266946
C       -4.195269       -0.446399       0.597637
O       -1.936487       -2.210637       -1.047721
O       -0.670943       -2.324531       0.742603
H       -4.035559       -1.550687       0.622614
H       -4.181064       -0.151874       1.678011
C       -5.522961       -0.141321       -0.010712
O       -6.157557       -0.851114       -0.783687
O       -6.141351       1.041189        0.298891
H       -5.619153       1.633803        0.939087
###
40
LysGlu3 pm6 E=-0.535623097264 au
N       1.183918        3.061070        -0.426744
H       1.015675        3.326100        0.563351
H       0.322153        3.260006        -0.974620
H       1.936412        3.681361        -0.794218
C       1.605680        1.605266        -0.550576
H       1.647695        1.346909        -1.659538
C       3.004255        1.434724        0.063681
C       0.580829        0.673741        0.119904
H       3.635326        2.322419        -0.178143
H       2.942140        1.432924        1.173192
C       3.700421        0.168899        -0.445310
O       0.893521        -0.096973       1.043575
H       3.058478        -0.721218       -0.288168
H       3.846505        0.226769        -1.544697
C       5.047323        -0.016976       0.261404
H       5.695363        0.870348        0.089800
H       4.906010        -0.058809       1.363161
C       5.741831        -1.285657       -0.232884
H       5.130835        -2.195342       -0.015603
H       5.874710        -1.268743       -1.342886
N       7.100748        -1.435314       0.422073
H       7.009501        -1.520244       1.449849
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H       7.584320        -2.281105       0.070568
H       7.700421        -0.615295       0.223482
N       -0.699185       0.676713        -0.372439
H       -0.980134       1.272647        -1.172035
C       -1.781134       -0.087359       0.298798
H       -1.524015       -0.223472       1.391726
C       -3.099860       0.688048        0.192324
C       -1.839870       -1.497806       -0.332632
H       -2.942708       1.741375        0.516951
H       -3.405593       0.779589        -0.872493
C       -4.199138       0.047148        1.044761
O       -2.767529       -1.844771       -1.113452
O       -0.919221       -2.306264       -0.026016
H       -3.889816       -0.933497       1.466173
H       -4.395039       0.660840        1.951210
C       -5.458673       -0.112743       0.231518
O       -5.621033       -1.151992       -0.484203
O       -6.345313       0.784431        0.244694
###
39
LysGlu4 pm6 E=-0.679896298696 au
N       1.216766        3.111561        -0.351905
H       0.289817        3.283737        -0.748417
H       1.177810        3.379447        0.633023
C       1.601574        1.685591        -0.500027
H       1.597881        1.436834        -1.601604
C       3.017476        1.481491        0.064421
C       0.596314        0.746750        0.200934
H       3.648493        2.355258        -0.208211
H       3.000916        1.489004        1.173078
C       3.665861        0.196520        -0.459285
O       0.881073        0.065630        1.207115
H       3.023361        -0.680388       -0.246287
H       3.745071        0.230335        -1.566018
C       5.052344        0.001257        0.163966
H       5.694026        0.884362        -0.046882
H       4.978463        -0.041071       1.271810
C       5.709545        -1.270393       -0.372775
H       5.106351        -2.176827       -0.123117
H       5.779960        -1.249952       -1.488172
N       7.101910        -1.431823       0.205359
H       7.065550        -1.536686       1.234486
H       7.565178        -2.270769       -0.188475
H       7.691439        -0.608250       -0.007592
N       -0.669583       0.677557        -0.332109
H       -0.921234       1.211377        -1.181432
C       -1.780529       -0.021697       0.360367
H       -1.595103       -0.015451       1.474958
C       -3.102366       0.703199        0.074847
C       -1.780928       -1.497785       -0.093995
H       -2.981802       1.790964        0.280400
H       -3.334897       0.660467        -1.011198
C       -4.253469       0.149452        0.920584
O       -2.657131       -1.957558       -0.875652
O       -0.870651       -2.250537       0.357233
H       -3.965792       -0.768916       1.475997
H       -4.519272       0.863668        1.729945
C       -5.448008       -0.126736       0.041727
O       -5.542230       -1.236958       -0.570698
O       -6.343154       0.751411        -0.106786
###
38
LysGlu5 pm6 E=-0.813145387513 au
N       1.289426        3.123927        -0.388181
H       0.369734        3.307085        -0.796403
H       1.242932        3.395660        0.595303
C       1.657668        1.693101        -0.527417
H       1.642771        1.434794        -1.626709
C       3.076425        1.480393        0.028224
C       0.652918        0.762176        0.184868
H       3.710475        2.350623        -0.246528
H       3.064090        1.487431        1.136712
C       3.717960        0.192325        -0.498505
O       0.956747        0.048629        1.163330
H       3.052339        -0.674776       -0.322643
H       3.831505        0.245011        -1.600504
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C       5.079139        -0.046336       0.162991
H       5.746279        0.821324        -0.013482
H       4.965931        -0.098016       1.264378
C       5.739260        -1.330110       -0.360765
H       5.054026        -2.196458       -0.239435
H       5.927554        -1.246476       -1.453229
N       7.031086        -1.655355       0.309289
H       6.865679        -1.838881       1.301241
H       7.645269        -0.838448       0.287099
N       -0.632122       0.730108        -0.303317
H       -0.910369       1.295548        -1.122858
C       -1.715002       -0.015108       0.385981
H       -1.496811       -0.062964       1.493260
C       -3.054610       0.702574        0.178416
C       -1.700179       -1.465104       -0.148826
H       -2.959230       1.765524        0.494913
H       -3.290100       0.765889        -0.906385
C       -4.187856       0.032335        0.961112
O       -2.520732       -1.870037       -1.015938
O       -0.821498       -2.245965       0.316957
H       -3.883482       -0.943787       1.396561
H       -4.451650       0.634992        1.857309
C       -5.389436       -0.152413       0.067543
O       -5.416343       -1.112946       -0.765291
O       -6.348598       0.665590        0.122831
###
48
PheArg1 pm6 E=0.656981051020E-01 au
N       3.389507        3.539783        -0.090244
H       2.563266        4.136140        -0.297889
H       3.645301        3.669449        0.907737
C       3.101455        2.085518        -0.406867
H       2.891125        2.012822        -1.522427
C       4.321384        1.210678        -0.067052
C       1.897535        1.602056        0.421297
H       5.183634        1.509189        -0.711391
H       4.673077        1.414738        0.971674
C       4.005621        -0.247084       -0.255726
O       1.882876        1.652001        1.654858
C       3.782093        -1.067310       0.860468
C       3.911783        -0.787965       -1.546639
H       3.862873        -0.657449       1.868611
C       3.461592        -2.415730       0.684433
C       3.591348        -2.136837       -1.716042
H       4.085504        -0.154869       -2.419002
H       3.286111        -3.050272       1.555515
C       3.363771        -2.951903       -0.602850
H       3.518677        -2.554553       -2.721989
H       3.116530        -4.005485       -0.738605
N       0.851980        1.064190        -0.293559
H       0.852225        1.050229        -1.328862
C       -0.286921       0.409839        0.386952
H       -0.429449       0.854882        1.418777
C       -1.571633       0.573929        -0.434271
C       0.081710        -1.076904       0.530394
H       -1.750485       1.661202        -0.609287
H       -1.451211       0.145819        -1.453837
C       -2.776018       -0.053250       0.272698
O       0.107663        -1.941028       -0.328021
O       0.444294        -1.348415       1.808990
H       -2.703509       -1.162585       0.258136
H       -2.786397       0.217649        1.351095
C       -4.067330       0.417479        -0.403974
H       -4.194745       1.519698        -0.268589
H       -4.030163       0.239351        -1.507398
N       -5.230338       -0.305228       0.179732
H       -5.034878       -1.064669       0.855330
C       -6.524257       -0.015792       -0.159331
N       -6.848639       1.094231        -0.928362
N       -7.540297       -0.853384       0.293752
H       -6.149865       1.462647        -1.581952
H       -7.802589       1.149177        -1.305862
H       -7.357727       -1.424416       1.127205
H       -8.502373       -0.499350       0.258315
H       4.185586        3.880568        -0.669792
H       0.742521        -2.307876       1.967673
```

```
###
47
PheArg2 pm6 E=-0.114988408808 au
N       -3.329763       3.544072        0.017261
H       -2.488164       4.131931        0.185089
H       -3.590483       3.623072        -0.984420
C       -3.070989       2.104877        0.416561
H       -2.820738       2.100586        1.526320
C       -4.327292       1.246347        0.184502
C       -1.910039       1.528579        -0.412689
H       -5.111252       1.529265        0.928994
H       -4.788112       1.487468        -0.802797
C       -4.025308       -0.222708       0.291896
O       -2.001535       1.360954        -1.640245
C       -4.192551       -1.052014       -0.827406
C       -3.567322       -0.770802       1.499969
H       -4.558275       -0.636785       -1.768552
C       -3.905135       -2.416250       -0.737928
C       -3.275359       -2.134132       1.581749
H       -3.442031       -0.132831       2.377825
H       -4.047567       -3.058969       -1.608730
C       -3.440891       -2.958287       0.463841
H       -2.925481       -2.557917       2.525006
H       -3.221441       -4.024578       0.533259
N       -0.796639       1.145120        0.282157
H       -0.707989       1.308675        1.300410
C       0.310799        0.413092        -0.384512
H       0.433617        0.793293        -1.439266
C       1.617780        0.623379        0.385891
C       -0.122811       -1.073186       -0.452343
H       1.807465        1.715086        0.501032
H       1.529376        0.245452        1.426716
C       2.800015        -0.042512       -0.325770
O       0.136977        -1.875217       0.477169
O       -0.785118       -1.442046       -1.466414
H       2.702628        -1.148322       -0.297488
H       2.804625        0.216099        -1.406705
C       4.108006        0.406705        0.332692
H       4.249464        1.507259        0.197514
H       4.084281        0.227292        1.436081
N       5.253965        -0.328990       -0.268954
H       5.040927        -1.090042       -0.936956
C       6.554895        -0.060511       0.061848
N       6.900010        1.045931        0.827179
N       7.555644        -0.911404       -0.399064
H       6.213523        1.421729        1.489411
H       7.859337        1.091232        1.192571
H       7.359254        -1.481881       -1.229734
H       8.522970        -0.571127       -0.370692
H       -4.113831       3.935922        0.581190
###
46
PheArg3 pm6 E=-0.261314511154 au
N       -3.394300       3.566065        0.017603
H       -2.546861       4.137687        0.071259
H       -3.717619       3.599320        -0.950876
C       -3.099659       2.175779        0.434791
H       -2.822968       2.202495        1.528189
C       -4.342502       1.280943        0.251424
C       -1.942297       1.568686        -0.385694
H       -5.092411       1.542480        1.033391
H       -4.854831       1.523399        -0.706688
C       -4.017875       -0.184544       0.326541
O       -2.012913       1.428826        -1.624451
C       -4.192557       -0.997237       -0.804411
C       -3.531870       -0.750620       1.515481
H       -4.579541       -0.570516       -1.731337
C       -3.888958       -2.359606       -0.745210
C       -3.223149       -2.111779       1.567640
H       -3.398964       -0.128449       2.402609
H       -4.039401       -2.987993       -1.624978
C       -3.398156       -2.918264       0.438301
H       -2.853590       -2.548491       2.497344
H       -3.167013       -3.983010       0.485281
N       -0.827754       1.162298        0.300429
H       -0.751291       1.285290        1.323218
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C       0.279951        0.436796        -0.371112
H       0.422242        0.848493        -1.410924
C       1.581720        0.597880        0.419969
C       -0.178171       -1.036247       -0.491502
H       1.787018        1.681651        0.575243
H       1.477076        0.186268        1.446109
C       2.761518        -0.061126       -0.302321
O       0.007858        -1.863856       0.434054
O       -0.800396       -1.369503       -1.543755
H       2.666106        -1.167200       -0.281031
H       2.761020        0.204880        -1.381385
C       4.072033        0.386486        0.352612
H       4.207420        1.489145        0.228473
H       4.056012        0.195343        1.454116
N       5.217728        -0.337039       -0.264137
H       5.004036        -1.099265       -0.930438
C       6.519549        -0.060594       0.057000
N       6.863546        1.047324        0.820305
N       7.522604        -0.904550       -0.412065
H       6.180482        1.418929        1.488286
H       7.826086        1.100241        1.176070
H       7.323203        -1.476919       -1.240733
H       8.487166        -0.555520       -0.393983
###
45
PheArg4 pm6 E=-0.403630237776 au
N       3.117406        3.630891        -0.150346
H       2.262728        4.165511        -0.327621
H       3.351697        3.761642        0.835645
C       2.901006        2.198626        -0.460863
H       2.761150        2.111174        -1.576784
C       4.125512        1.363223        -0.035848
C       1.664205        1.638721        0.270696
H       4.986572        1.624448        -0.693201
H       4.464205        1.662808        0.981356
C       3.862690        -0.115397       -0.097399
O       1.569514        1.654923        1.514386
C       3.755722        -0.858094       1.088843
C       3.721940        -0.764725       -1.333604
H       3.874473        -0.365910       2.055480
C       3.519551        -2.234058       1.037651
C       3.484191        -2.140164       -1.378830
H       3.803505        -0.196398       -2.262051
H       3.454137        -2.808037       1.963789
C       3.383879        -2.877895       -0.194858
H       3.383817        -2.641891       -2.343348
H       3.211570        -3.954141       -0.233798
N       0.660453        1.103146        -0.496051
H       0.715970        1.097082        -1.526522
C       -0.484064       0.387308        0.121188
H       -0.807796       0.931072        1.052100
C       -1.663018       0.296808        -0.854109
C       0.043753        -1.013801       0.519417
H       -1.874199       1.299921        -1.286386
H       -1.400961       -0.335917       -1.727894
C       -2.913232       -0.242147       -0.153630
O       0.178604        -1.916574       -0.344755
O       0.385882        -1.199247       1.721616
H       -2.687228       -1.179613       0.394863
H       -3.250954       0.472034        0.625746
C       -4.035760       -0.490929       -1.171203
H       -4.180224       0.397988        -1.826883
H       -3.758822       -1.323639       -1.859678
N       -5.325226       -0.867978       -0.528323
H       -5.218524       -1.719182       0.050992
C       -6.062301       0.192506        0.103420
N       -6.133254       1.440026        -0.301485
N       -6.952646       -0.246763       1.121627
H       -5.567674       1.704491        -1.112367
H       -6.590401       -0.971316       1.745321
H       -7.396619       0.499921        1.658076
###
22
SerGly1 pm6 E=-0.179871571106 au
N       2.887462        -1.333070       -0.231752
H       2.770024        -2.204423       0.323083
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H       3.881917        -1.031523       -0.156140
H       2.697218        -1.556614       -1.228695
C       1.963541        -0.245076       0.271829
H       2.216001        -0.049549       1.366719
C       2.168465        1.065222        -0.524881
C       0.511725        -0.730207       0.148107
H       3.137680        1.080891        -1.074400
H       1.347795        1.246770        -1.248769
O       2.276098        2.174414        0.363927
O       0.200667        -1.607817       -0.668376
H       1.440837        2.294115        0.897547
N       -0.401986       -0.155125       0.991654
H       -0.148165       0.616651        1.632798
C       -1.826162       -0.501311       0.913293
C       -2.542366       0.248747        -0.182458
H       -1.976153       -1.609345       0.764577
H       -2.315689       -0.291019       1.909403
O       -2.043836       0.929333        -1.068306
O       -3.904851       0.167134        -0.222908
H       -4.325630       -0.407338       0.504526
###
21
SerGly2 pm6 E=-0.359579032830 au
N       2.434628        1.653107        -0.441295
H       1.862894        2.319433        -0.996053
H       3.371265        1.580309        -0.891802
H       2.565328        2.051406        0.509276
C       1.771436        0.293723        -0.373931
H       1.677617        -0.105693       -1.440867
C       2.638736        -0.695608       0.441055
C       0.357691        0.453933        0.198272
H       3.649785        -0.289147       0.672649
H       2.158425        -0.994172       1.393765
O       2.918625        -1.848025       -0.350111
O       -0.054226       1.561712        0.580625
H       2.086059        -2.363515       -0.543282
N       -0.419372       -0.668478       0.253779
H       -0.101912       -1.577947       -0.116996
C       -1.754140       -0.641419       0.874357
C       -2.806556       -0.143758       -0.118719
H       -2.015374       -1.668409       1.235364
H       -1.766892       -0.006548       1.794914
O       -3.477789       -0.988115       -0.771248
O       -2.991233       1.094509        -0.263086
###
20
SerGly3 pm6 E=-0.502065447767 au
N       -3.333153       -0.821472       -0.325429
H       -3.221185       -1.700981       -0.836573
H       -3.522108       -1.073864       0.648362
C       -2.092607       -0.018013       -0.422982
H       -1.968971       0.295967        -1.502963
C       -2.239994       1.240954        0.449817
C       -0.832680       -0.809392       -0.030505
H       -3.213421       1.742954        0.286919
H       -2.118526       1.038202        1.529721
O       -1.204065       2.143702        -0.002581
O       -0.891413       -2.015364       0.283096
H       -0.967422       2.767877        0.734779
N       0.361684        -0.148386       -0.075452
H       0.405431        0.864587        -0.285323
C       1.630279        -0.816636       0.272096
C       2.825878        0.074074        -0.035939
H       1.653220        -1.092186       1.358329
H       1.726047        -1.786799       -0.275770
O       2.664116        1.298877        -0.273480
O       3.966609        -0.463800       -0.037815
###
34
SerLeu1 pm6 E=-0.210263488580 au
N       -4.087692       -0.677959       -0.883962
H       -3.841028       -1.254155       -1.713086
H       -4.983257       -0.186364       -1.087379
H       -4.245804       -1.318749       -0.081247
C       -2.995902       0.325688        -0.578463
H       -2.951795       1.079675        -1.434696
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C       -3.343717       1.087277        0.722275
C       -1.645309       -0.396372       -0.530014
H       -4.420813       1.371768        0.738282
H       -3.111195       0.503835        1.633489
O       -2.630615       2.325297        0.696780
O       -1.544795       -1.586899       -0.849780
H       -1.902247       2.328821        1.380633
N       -0.557602       0.349605        -0.150876
H       -0.662159       1.323545        0.187017
C       0.813381        -0.212264       -0.167539
H       1.001128        -0.700978       -1.175763
C       1.833895        0.910332        0.077216
C       0.959560        -1.274590       0.927151
H       1.579450        1.786269        -0.561146
H       1.747404        1.290985        1.118408
C       3.290394        0.481566        -0.206833
O       0.342245        -1.359703       1.976296
O       1.888676        -2.258769       0.738508
H       3.527253        -0.425838       0.406630
C       3.489045        0.133192        -1.682646
C       4.237012        1.605013        0.222863
H       3.248153        0.972113        -2.345565
H       4.527782        -0.149687       -1.893602
H       2.863348        -0.715497       -1.992522
H       4.150937        1.827466        1.293623
H       5.285566        1.342356        0.036676
H       4.046177        2.541249        -0.315013
H       2.383920        -2.236799       -0.149358
###
33
SerLeu2 pm6 E=-0.397508122701 au
N       -3.960887       -1.170605       -0.871684
H       -3.667870       -1.923832       -1.526638
H       -4.874114       -0.791930       -1.204518
H       -4.108121       -1.590678       0.065496
C       -2.924234       -0.072009       -0.827034
H       -2.770878       0.310867        -1.889923
C       -3.428252       1.095958        0.057912
C       -1.608361       -0.608534       -0.254389
H       -4.341453       1.551477        -0.381241
H       -3.641314       0.779949        1.101407
O       -2.414003       2.089306        0.195170
O       -1.599062       -1.505086       0.606707
H       -2.139707       2.443227        -0.700563
N       -0.461806       -0.022194       -0.708443
H       -0.487944       0.739794        -1.410590
C       0.857120        -0.345739       -0.107095
H       1.085248        -1.432696       -0.310761
C       1.945613        0.542111        -0.723407
C       0.812655        -0.133150       1.421774
H       1.859129        0.529486        -1.832061
H       1.782984        1.604290        -0.446035
C       3.369627        0.104210        -0.311789
O       0.177839        0.833434        1.926532
O       1.419740        -0.963285       2.150889
H       3.413570        0.023542        0.803795
C       3.725494        -1.257694       -0.911776
C       4.376545        1.170639        -0.749899
H       3.731326        -1.239545       -2.008119
H       4.720621        -1.591384       -0.593526
H       3.017334        -2.040209       -0.612906
H       4.173466        2.143777        -0.286711
H       5.401413        0.896893        -0.471062
H       4.371823        1.326871        -1.835328
###
32
SerLeu3 pm6 E=-0.545185268005 au
N       -4.050902       -1.099407       -0.916407
H       -3.746742       -1.883905       -1.498545
H       -4.253747       -1.480358       0.010308
C       -2.983110       -0.078195       -0.842863
H       -2.836709       0.342407        -1.881950
C       -3.438826       1.053014        0.105559
C       -1.647078       -0.635082       -0.331136
H       -4.387324       1.502710        -0.248628
H       -3.567852       0.716043        1.153399
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O       -2.441740       2.078853        0.201999
O       -1.595672       -1.637164       0.410573
H       -2.208900       2.434247        -0.700351
N       -0.503522       0.020731        -0.708125
H       -0.550657       0.892416        -1.263138
C       0.814536        -0.332969       -0.124831
H       1.034749        -1.413541       -0.362458
C       1.911457        0.566869        -0.706796
C       0.760306        -0.175298       1.409789
H       1.838527        0.579811        -1.815858
H       1.746554        1.622461        -0.406466
C       3.329735        0.118908        -0.286343
O       0.135681        0.783973        1.942205
O       1.334572        -1.046683       2.117688
H       3.352626        -0.007467       0.825725
C       3.703192        -1.215995       -0.934172
C       4.340066        1.206554        -0.660253
H       3.712026        -1.158016       -2.029174
H       4.701340        -1.549638       -0.625484
H       3.003405        -2.016786       -0.666464
H       4.124142        2.158427        -0.160145
H       5.360872        0.925022        -0.374445
H       4.354266        1.408231        -1.738050
###
49
TyrArg1 pm6 E=-0.135595530546E-01 au
N       3.161991        3.844882        -0.282446
H       2.337033        4.420120        -0.545707
H       3.390264        4.034924        0.712359
C       2.893874        2.371437        -0.518322
H       2.672919        2.235023        -1.625847
C       4.133811        1.536723        -0.143597
C       1.703945        1.920957        0.346303
H       4.981611        1.814174        -0.815543
H       4.492505        1.807706        0.877257
C       3.845368        0.066946        -0.242110
O       1.659004        2.122563        1.563583
C       3.672765        -0.694478       0.926360
C       3.731325        -0.546825       -1.500481
H       3.776149        -0.221567       1.907476
C       3.367687        -2.052187       0.851887
C       3.426844        -1.903440       -1.599329
H       3.874798        0.042793        -2.410956
H       3.224465        -2.648283       1.752538
C       3.244620        -2.634269       -0.418361
H       3.331339        -2.388875       -2.571568
O       2.902143        -3.973846       -0.427408
N       0.706811        1.239613        -0.313316
H       0.743153        1.084357        -1.336621
C       -0.427185       0.628481        0.414490
H       -0.635646       1.205977        1.365898
C       -1.682006       0.603427        -0.468377
C       0.000827        -0.803157       0.778275
H       -1.912543       1.643211        -0.799843
H       -1.493439       0.044869        -1.411592
C       -2.883154       0.012537        0.274555
O       0.101840        -1.774009       0.049006
O       0.320281        -0.881624       2.094487
H       -2.725964       -1.068273       0.481637
H       -2.994297       0.484290        1.275137
C       -4.152069       0.221534        -0.559601
H       -4.315418       1.311617        -0.748114
H       -4.052539       -0.259675       -1.563146
N       -5.318984       -0.362843       0.155593
H       -5.121338       -1.005747       0.942350
C       -6.616223       -0.095668       -0.188480
N       -6.945891       0.594099        -1.347312
N       -7.635907       -0.541594       0.650382
H       -6.261189       1.241851        -1.749315
H       -7.909548       0.939100        -1.437295
H       -7.438337       -1.340804       1.263847
H       -8.588607       -0.561555       0.270271
H       2.811363        -4.331211       -1.365237
H       3.969789        4.159369        -0.860520
H       0.638617        -1.799265       2.395613
###
```

```
48
TyrArg2 pm6 E=-0.196012067677 au
N       3.528551        -3.622041       0.237826
H       2.742783        -4.285971       0.393402
H       3.841480        -3.710698       -0.747758
C       3.107160        -2.203566       0.567196
H       2.758607        -2.195807       1.650155
C       4.297741        -1.233354       0.425493
C       1.971125        -1.767635       -0.376460
H       5.015548        -1.408638       1.262826
H       4.884703        -1.464609       -0.494279
C       3.834368        0.195442        0.421111
O       2.147188        -1.629748       -1.597852
C       3.981528        0.973634        -0.739623
C       3.224394        0.747927        1.560276
H       4.494531        0.560367        -1.613601
C       3.468096        2.268392        -0.798024
C       2.696040        2.037642        1.522651
H       3.149570        0.159278        2.480233
H       3.576376        2.878077        -1.694317
C       2.806219        2.768202        0.332338
H       2.210973        2.472790        2.397621
O       2.234181        4.018367        0.181287
N       0.768268        -1.490374       0.213080
H       0.617298        -1.633399       1.227370
C       -0.353952       -0.891353       -0.553873
H       -0.400363       -1.352466       -1.580858
C       -1.677924       -1.136890       0.176821
C       -0.032333       0.616797        -0.703599
H       -1.836122       -2.231678       0.305161
H       -1.630336       -0.739972       1.214416
C       -2.861598       -0.523220       -0.578004
O       -0.307651       1.435728        0.208109
O       0.556032        0.990313        -1.759372
H       -2.680367       0.551985        -0.791528
H       -2.973778       -0.995666       -1.577230
C       -4.140315       -0.701444       0.246536
H       -4.437100       -1.778428       0.288152
H       -3.975028       -0.383157       1.305559
N       -5.240731       0.104598        -0.350708
H       -5.017398       0.682427        -1.179052
C       -6.502972       0.140794        0.178546
N       -6.811349       -0.474516       1.382480
N       -7.499930       0.823648        -0.515576
H       -6.253420       -1.277730       1.687938
H       -7.802682       -0.556385       1.638753
H       -7.208544       1.561613        -1.167877
H       -8.355389       1.065050        -0.003103
H       1.801259        4.341678        1.033037
H       4.320260        -3.913344       0.849576
###
47
TyrArg3 pm6 E=-0.342366507417 au
N       3.690382        -3.582116       0.281884
H       2.926315        -4.262992       0.273611
H       4.101948        -3.584865       -0.653514
C       3.177839        -2.237634       0.633382
H       2.792579        -2.285301       1.692055
C       4.314116        -1.194514       0.556064
C       2.042509        -1.801303       -0.317605
H       4.980937        -1.323973       1.438821
H       4.972103        -1.404226       -0.316833
C       3.790289        0.211576        0.501901
O       2.205141        -1.757924       -1.554229
C       3.936973        0.966535        -0.673743
C       3.128808        0.767705        1.610466
H       4.478085        0.548470        -1.527733
C       3.391006        2.245811        -0.772314
C       2.573713        2.044353        1.535249
H       3.040020        0.193608        2.537610
H       3.501601        2.837771        -1.679999
C       2.700461        2.756057        0.335371
H       2.055575        2.484224        2.388609
O       2.113450        3.995604        0.149349
N       0.842638        -1.452252       0.244758
H       0.707254        -1.472874       1.269238
```

```
C       -0.293316       -0.943203       -0.565285
H       -0.336409       -1.496862       -1.545004
C       -1.609356       -1.150354       0.193744
C       0.004092        0.547578        -0.859321
H       -1.754358       -2.235225       0.396906
H       -1.554542       -0.681309       1.200477
C       -2.808361       -0.601105       -0.585965
O       -0.316809       1.453511        -0.050431
O       0.628392        0.821291        -1.926379
H       -2.645607       0.462306        -0.863575
H       -2.919279       -1.133158       -1.554741
C       -4.080123       -0.751214       0.255149
H       -4.390488       -1.823259       0.315512
H       -3.899910       -0.419270       1.307572
N       -5.176612       0.059137        -0.343607
H       -4.952969       0.626491        -1.179209
C       -6.427637       0.133044        0.208318
N       -6.725845       -0.452442       1.429289
N       -7.424873       0.818009        -0.483209
H       -6.173925       -1.256171       1.744111
H       -7.714129       -0.514996       1.702350
H       -7.132580       1.539077        -1.153639
H       -8.267912       1.083084        0.038516
H       1.658385        4.327262        0.986110
###
46
TyrArg4 pm6 E=-0.508599676894 au
N       -3.281631       3.740932        -0.015165
H       -2.414328       4.279039        -0.088298
H       -3.701825       3.725305        -0.946536
C       -3.000087       2.367522        0.464111
H       -2.642979       2.449044        1.531114
C       -4.286855       1.510531        0.435537
C       -1.908454       1.691170        -0.393345
H       -4.921716       1.792356        1.303941
H       -4.902623       1.767959        -0.453737
C       -3.973476       0.044150        0.459118
O       -2.033887       1.526454        -1.624713
C       -4.232653       -0.751179       -0.668440
C       -3.361492       -0.537636       1.584278
H       -4.782065       -0.329512       -1.513972
C       -3.768270       -2.058350       -0.738659
C       -2.888280       -1.840728       1.537991
H       -3.237789       0.052341        2.496059
H       -3.961320       -2.667578       -1.614197
C       -3.019806       -2.596603       0.340538
H       -2.404394       -2.285733       2.399932
O       -2.382359       -3.722638       0.202959
N       -0.769887       1.271049        0.247454
H       -0.657405       1.393315        1.267503
C       0.341272        0.594409        -0.468143
H       0.451264        1.038035        -1.498781
C       1.649412        0.779820        0.309094
C       -0.056787       -0.890380       -0.622321
H       1.822558        1.865274        0.490553
H       1.568035        0.339141        1.325925
C       2.843640        0.182003        -0.440735
O       0.193448        -1.741866       0.270558
O       -0.695301       -1.230247       -1.663705
H       2.681903        -0.895711       -0.653906
H       2.951856        0.658002        -1.439120
C       4.114634        0.381446        0.391595
H       4.286926        1.469285        0.588593
H       4.013526        -0.106158       1.391883
N       5.283102        -0.194579       -0.328745
H       5.094466        -0.770264       -1.166899
C       6.570621        -0.034610       0.107601
N       6.861510        0.537934        1.338848
N       7.614739        -0.460046       -0.709582
H       6.201948        1.213371        1.737788
H       7.839900        0.791096        1.524797
H       7.419473        -1.196302       -1.397979
H       8.544034        -0.552335       -0.284448
###
45
TyrArg5 pm6 E=-0.647061331344 au
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```
N       3.486026        -3.613364       0.151200
H       2.670124        -4.230381       0.121629
H       3.890071        -3.606547       -0.787255
C       3.089066        -2.249142       0.571106
H       2.731652        -2.313627       1.638519
C       4.300698        -1.289639       0.506884
C       1.956539        -1.696500       -0.320114
H       4.957031        -1.486162       1.382718
H       4.934438        -1.528497       -0.374929
C       3.871033        0.147196        0.477755
O       2.101183        -1.527842       -1.549369
C       4.066146        0.919190        -0.679004
C       3.222369        0.722054        1.585162
H       4.632856        0.504373        -1.516577
C       3.522716        2.192695        -0.786685
C       2.670727        1.992433        1.502289
H       3.136112        0.152935        2.514505
H       3.670151        2.783727        -1.683239
C       2.755640        2.721444        0.284465
H       2.162720        2.431805        2.353243
O       2.069951        3.815449        0.125718
N       0.760623        -1.389494       0.279808
H       0.616718        -1.525271       1.293203
C       -0.366979       -0.799581       -0.484624
H       -0.389781       -1.248464       -1.518767
C       -1.704139       -1.073348       0.212367
C       -0.078951       0.711956        -0.618107
H       -1.849250       -2.171416       0.320516
H       -1.694339       -0.688726       1.253797
C       -2.867685       -0.462242       -0.575541
O       -0.378377       1.528289        0.292723
O       0.517655        1.112563        -1.661367
H       -2.771866       0.642570        -0.622817
H       -2.834162       -0.798651       -1.633665
C       -4.206101       -0.852212       0.062231
H       -4.364336       -1.953908       -0.006666
H       -4.195277       -0.614870       1.150425
N       -5.343803       -0.187283       -0.650959
H       -5.017902       0.551534        -1.298520
C       -6.450122       0.244405        0.151044
N       -6.983017       -0.717031       1.051115
N       -7.012798       1.397588        -0.137995
H       -6.350646       -1.427134       1.418622
H       -7.571627       -0.337569       1.796067
H       -7.880951       1.631428        0.349985
###
32
TyrGly1 pm6 E=-0.149642974623 au
N       3.523600        -1.756583       -0.142909
H       4.208359        -1.119593       -0.596942
H       3.676888        -2.715293       -0.520725
H       3.727713        -1.782551       0.874958
C       2.100012        -1.309115       -0.417298
H       1.948431        -1.312001       -1.544903
C       1.100260        -2.294379       0.216552
C       1.891802        0.103312        0.159155
H       1.194103        -3.287408       -0.286271
H       1.375861        -2.499679       1.277788
C       -0.310823       -1.790988       0.115979
O       1.826233        0.312600        1.378312
C       -1.001831       -1.405727       1.275472
C       -0.942238       -1.696163       -1.137136
H       -0.525654       -1.501598       2.255470
C       -2.297336       -0.894572       1.193298
C       -2.234312       -1.187913       -1.243946
H       -0.412273       -2.017038       -2.039464
H       -2.838431       -0.586623       2.088607
C       -2.889297       -0.783418       -0.070239
H       -2.728655       -1.103374       -2.211240
O       -4.154785       -0.254667       -0.246645
H       -4.550189       0.071976        0.620721
N       1.760524        1.116670        -0.754185
H       1.795322        0.948536        -1.773358
C       1.459951        2.489171        -0.329836
C       -0.007673       2.701919        -0.056183
H       2.051956        2.779970        0.585972
```

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H       1.815284        3.213938        -1.119920
O       -0.879157       1.847475        0.052239
O       -0.444554       3.982104        0.114396
H       0.279422        4.697268        0.047631
###
31
TyrGly2 pm6 E=-0.332474970848 au
N       3.772037        -1.139236       -0.167715
H       4.359977        -0.318756       -0.417301
H       4.120869        -1.959350       -0.708043
H       3.906856        -1.344456       0.841178
C       2.312970        -0.882987       -0.494408
H       2.233756        -0.751034       -1.621990
C       1.453132        -2.090746       -0.073600
C       1.836935        0.388512        0.230335
H       1.667457        -2.948218       -0.756640
H       1.764130        -2.458170       0.933004
C       -0.013312       -1.768171       -0.094388
O       1.681128        0.424587        1.463352
C       -0.754810       -1.813253       1.097263
C       -0.647025       -1.409261       -1.297100
H       -0.275202       -2.125479       2.029837
C       -2.101501       -1.450921       1.109543
C       -1.989927       -1.039249       -1.308315
H       -0.079757       -1.410361       -2.233399
H       -2.682424       -1.478671       2.032538
C       -2.693827       -1.052344       -0.094387
H       -2.485868       -0.747356       -2.233496
O       -4.000139       -0.602553       -0.157145
H       -4.471794       -0.697446       0.729135
N       1.557322        1.468259        -0.557472
H       1.668084        1.439314        -1.584347
C       0.994471        2.706796        0.003810
C       -0.530123       2.643291        0.094198
H       1.415230        2.932391        1.017043
H       1.314593        3.574872        -0.627190
O       -1.090250       1.712172        0.741168
O       -1.211155       3.540740        -0.467593
###
30
TyrGly3 pm6 E=-0.478528488408 au
N       -3.849493       -1.036712       0.130881
H       -4.396637       -0.182287       0.266953
H       -3.922838       -1.283864       -0.857736
C       -2.437426       -0.809028       0.519207
H       -2.416916       -0.644904       1.635529
C       -1.578948       -2.044895       0.177317
C       -1.852087       0.424956        -0.199541
H       -1.801213       -2.851444       0.912985
H       -1.895686       -2.474013       -0.800078
C       -0.107246       -1.746268       0.173847
O       -1.726842       0.467988        -1.442432
C       0.641047        -1.956061       -0.995944
C       0.523747        -1.237568       1.322839
H       0.161393        -2.374663       -1.885529
C       1.995511        -1.628344       -1.041462
C       1.873379        -0.892259       1.297968
H       -0.049301       -1.102424       2.245210
H       2.582979        -1.787891       -1.946952
C       2.587747        -1.089523       0.106796
H       2.367928        -0.487391       2.180048
O       3.903551        -0.660337       0.121626
H       4.377609        -0.881672       -0.740837
N       -1.480622       1.487709        0.578838
H       -1.523737       1.439366        1.608735
C       -0.858032       2.697562        0.017269
C       0.647212        2.511285        -0.170264
H       -1.321552       2.984697        -0.959878
H       -1.064876       3.567035        0.690813
O       1.085866        1.622374        -0.957642
O       1.437954        3.262892        0.457763
###
29
TyrGly4 pm6 E=-0.644178018691 au
N       3.935336        -0.403800       -0.064963
H       4.330114        0.527266        -0.221066
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H       4.028632        -0.605215       0.931987
C       2.516600        -0.442828       -0.489557
H       2.499555        -0.332264       -1.612408
C       1.875003        -1.798476       -0.114975
C       1.704078        0.702638        0.150520
H       2.231293        -2.570413       -0.831788
H       2.252615        -2.143954       0.872088
C       0.376685        -1.725300       -0.115631
O       1.597771        0.838382        1.387307
C       -0.338608       -1.864969       1.084846
C       -0.326384       -1.468267       -1.306139
H       0.190032        -2.145607       1.999543
C       -1.705461       -1.623089       1.133270
C       -1.691583       -1.223528       -1.284160
H       0.213879        -1.441223       -2.255940
H       -2.252856       -1.723889       2.063424
C       -2.389047       -1.224480       -0.045133
H       -2.232676       -1.017558       -2.200574
O       -3.605188       -0.767012       0.017522
N       1.112066        1.601785        -0.701406
H       1.148129        1.472780        -1.724255
C       0.234214        2.680839        -0.214911
C       -1.143149       2.107578        0.114363
H       0.669461        3.192242        0.677281
H       0.153952        3.482552        -0.991366
O       -2.028313       2.046888        -0.781049
O       -1.369026       1.656579        1.274058
###
46
TyrHisOMe3 pm6 E=0.447946576114E-01 au
N       -2.706367       -3.857255       -0.001157
H       -2.784213       -4.012829       1.022297
H       -1.951324       -4.470166       -0.369286
H       -3.603452       -4.157439       -0.438630
C       -2.428594       -2.402054       -0.326355
H       -2.401236       -2.302441       -1.459182
C       -3.553632       -1.506592       0.226938
C       -1.088427       -1.977356       0.300527
H       -4.513230       -1.763771       -0.283489
H       -3.744842       -1.739493       1.301200
C       -3.237021       -0.050746       0.042554
O       -0.901329       -1.970570       1.520215
C       -2.803071       0.715520        1.136390
C       -3.368958       0.548088        -1.222375
H       -2.713945       0.257769        2.125727
C       -2.480478       2.062489        0.975426
C       -3.053590       1.892591        -1.406716
H       -3.717171       -0.046026       -2.072771
H       -2.140039       2.664194        1.819657
C       -2.606304       2.628642        -0.299112
H       -3.151575       2.365154        -2.383506
O       -2.282491       3.949768        -0.550850
H       -1.893642       4.399951        0.262937
N       -0.116410       -1.557235       -0.581257
H       -0.257333       -1.594392       -1.606333
C       1.141266        -0.956410       -0.097445
H       1.421734        -1.406526       0.905343
C       2.279411        -1.183906       -1.106025
C       0.904319        0.556352        0.074346
H       2.380174        -2.283540       -1.312431
H       2.025904        -0.750065       -2.107879
C       3.565616        -0.657193       -0.598282
O       0.367507        1.327479        -0.699139
O       1.392352        0.944664        1.282282
N       4.307117        0.333756        -1.269605
C       4.281862        -0.993810       0.551402
H       4.042948        0.783481        -2.154401
C       5.448362        0.594792        -0.543597
N       5.440662        -0.211068       0.573089
H       4.044670        -1.719372       1.324699
H       6.227899        1.320338        -0.809834
H       6.164664        -0.231788       1.299882
C       1.278925        2.352060        1.653735
H       1.887210        2.961538        0.977766
H       0.227363        2.659950        1.648042
H       1.687998        2.362541        2.674183
```

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###
45
TyrHisOMe4 pm6 E=-0.110502092750 au
N       -3.100422       -3.622020       -0.003442
H       -3.281131       -3.723607       1.014056
H       -2.385070       -4.323731       -0.281089
H       -3.984305       -3.847313       -0.507257
C       -2.648707       -2.217804       -0.351464
H       -2.565289       -2.152944       -1.484165
C       -3.684774       -1.184305       0.131344
C       -1.293444       -1.924775       0.316353
H       -4.629443       -1.310465       -0.450096
H       -3.982183       -1.392249       1.186373
C       -3.157769       0.214324        -0.013887
O       -1.148554       -1.902266       1.541999
C       -2.729088       0.921278        1.121178
C       -3.072460       0.811360        -1.283595
H       -2.813363       0.467917        2.113081
C       -2.189258       2.200908        0.997842
C       -2.536910       2.089096        -1.431274
H       -3.420294       0.266529        -2.166650
H       -1.848134       2.754570        1.873919
C       -2.093758       2.760991        -0.281915
H       -2.462073       2.558946        -2.411390
O       -1.540980       4.010390        -0.497549
H       -1.159729       4.402211        0.350204
N       -0.252569       -1.637008       -0.538442
H       -0.353517       -1.713370       -1.565760
C       1.039996        -1.146454       -0.022911
H       1.210295        -1.534046       1.028071
C       2.205308        -1.584564       -0.928052
C       0.983022        0.392811        0.011327
H       2.326953        -2.693897       -0.858538
H       1.965160        -1.405620       -2.002499
C       3.465998        -0.910545       -0.533098
O       0.716374        1.160586        -0.895933
O       1.296117        0.816906        1.263817
N       4.127568        0.003821        -1.364247
C       4.171059        -1.054139       0.668524
C       5.226074        0.410324        -0.669006
N       5.282487        -0.214155       0.576354
H       3.966587        -1.672123       1.528358
H       5.966835        1.122897        -1.017458
H       5.997953        -0.092949       1.288513
C       1.365210        2.251571        1.524002
H       2.315166        2.631201        1.132280
H       0.510570        2.777453        1.085813
H       1.338918        2.300742        2.621808
###
44
TyrHisOMe5 pm6 E=-0.256466384156 au
N       -3.012955       -3.729316       0.035839
H       -2.254437       -4.390659       -0.150373
H       -3.212540       -3.778939       1.037115
C       -2.608296       -2.359757       -0.357758
H       -2.534732       -2.338692       -1.483022
C       -3.664302       -1.333316       0.102714
C       -1.250201       -1.972284       0.265335
H       -4.594065       -1.480609       -0.492013
H       -3.977248       -1.542757       1.150523
C       -3.172362       0.078447        -0.035167
O       -1.025831       -2.063706       1.482359
C       -2.789313       0.799366        1.107250
C       -3.073647       0.676462        -1.303477
H       -2.883806       0.346375        2.097975
C       -2.283700       2.094102        0.994236
C       -2.572148       1.969225        -1.441393
H       -3.385630       0.121891        -2.193205
H       -1.979074       2.658253        1.877029
C       -2.174564       2.654687        -0.283723
H       -2.488873       2.439846        -2.420383
O       -1.650769       3.919395        -0.489059
H       -1.295239       4.319898        0.365512
N       -0.273180       -1.514020       -0.595210
H       -0.446222       -1.436125       -1.611020
C       1.030596        -1.034465       -0.103375
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H       1.250168        -1.485613       0.911554
C       2.170540        -1.386737       -1.077011
C       0.949404        0.497492        0.029786
H       2.255105        -2.497525       -1.162211
H       1.932117        -1.050738       -2.112917
C       3.453202        -0.812869       -0.601909
O       0.751831        1.322370        -0.844852
O       1.143246        0.841043        1.330331
N       4.076109        0.269947        -1.236935
C       4.210899        -1.210980       0.506403
C       5.202236        0.527809        -0.515278
N       5.314894        -0.356713       0.556946
H       4.044566        -2.005255       1.216386
H       5.924915        1.308502        -0.729320
H       6.055522        -0.384370       1.253291
C       1.167556        2.255222        1.692860
H       2.171294        2.642676        1.485207
H       0.399313        2.821246        1.156060
H       0.961587        2.236064        2.772138
###
43
TyrHisOMe6 pm6 E=-0.417792836139 au
N       -3.260046       -3.513893       -0.056833
H       -2.552099       -4.234048       -0.222736
H       -3.484794       -3.543911       0.939753
C       -2.737961       -2.181759       -0.442510
H       -2.639535       -2.170166       -1.565566
C       -3.713106       -1.068280       -0.003322
C       -1.366414       -1.904031       0.205454
H       -4.646034       -1.151352       -0.603336
H       -4.043754       -1.237841       1.044974
C       -3.111296       0.296833        -0.160465
O       -1.154535       -2.079691       1.416224
C       -2.786636       1.062573        0.971101
C       -2.850157       0.818776        -1.439292
H       -3.003320       0.672181        1.968524
C       -2.189734       2.309218        0.842715
C       -2.247415       2.058901        -1.592264
H       -3.118554       0.235706        -2.324002
H       -1.944253       2.897988        1.720311
C       -1.893141       2.823791        -0.447703
H       -2.042043       2.454924        -2.580614
O       -1.263398       3.953342        -0.578267
N       -0.359178       -1.447394       -0.621103
H       -0.532246       -1.264224       -1.623487
C       0.983587        -1.120587       -0.104605
H       1.232743        -1.796029       0.770221
C       2.055476        -1.278377       -1.196609
C       0.956392        0.339677        0.386312
H       2.150182        -2.360235       -1.463295
H       1.734375        -0.790474       -2.146871
C       3.364636        -0.752430       -0.738895
O       0.881185        1.364317        -0.272103
O       1.028652        0.349054        1.741179
N       4.028023        0.287599        -1.404433
C       4.118694        -1.163907       0.367028
C       5.174797        0.507136        -0.702698
N       5.260446        -0.359378       0.386382
H       3.927068        -1.935790       1.095327
H       5.931016        1.247432        -0.942392
H       6.007541        -0.405466       1.075091
C       0.985779        1.624575        2.448306
H       1.752302        2.303306        2.062504
H       -0.022187       2.047122        2.371575
H       1.212639        1.333509        3.484341
###
27
ValGly1 pm6 E=-0.128588036258 au
N       2.787535        -1.427850       -0.269944
H       2.581461        -1.447565       -1.287038
H       2.724354        -2.400313       0.089725
H       3.769545        -1.102406       -0.150039
C       1.831065        -0.513442       0.472425
H       2.020569        -0.656293       1.584830
C       2.114965        0.978192        0.112012
C       0.395948        -0.917815       0.125419
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H       3.233100        1.112449        0.141765
C       1.622520        1.333214        -1.287025
C       1.503852        1.894574        1.167832
O       0.138508        -1.523088       -0.926491
H       0.530601        1.305056        -1.381557
H       1.923382        2.356149        -1.559512
H       2.044742        0.678986        -2.061327
H       1.746085        1.575582        2.191396
H       1.884156        2.920826        1.063978
H       0.411303        1.964567        1.104922
N       -0.577893       -0.605907       1.040537
H       -0.375455       -0.044902       1.884563
C       -1.997406       -0.840304       0.747954
C       -2.578370       0.206615        -0.171047
H       -2.165013       -1.858485       0.292658
H       -2.574368       -0.877416       1.717322
O       -1.968084       0.962292        -0.915227
O       -3.937142       0.330563        -0.213580
H       -4.443663       -0.294267       0.411120
###
26
ValGly2 pm6 E=-0.309819174981 au
N       -2.776845       -1.391502       0.029927
H       -2.739835       -1.370804       1.066132
H       -2.635906       -2.373634       -0.278281
H       -3.732843       -1.096371       -0.260133
C       -1.732795       -0.477761       -0.581464
H       -1.784127       -0.616208       -1.709394
C       -2.053914       1.015839        -0.264171
C       -0.351058       -0.878935       -0.059503
H       -3.115892       1.189883        -0.595655
C       -1.953944       1.328462        1.225143
C       -1.139967       1.923829        -1.082031
O       -0.199056       -1.326890       1.091814
H       -0.942387       1.197648        1.625025
H       -2.227772       2.375519        1.424623
H       -2.636087       0.719704        1.833836
H       -1.107117       1.641059        -2.143554
H       -1.489328       2.965791        -1.047557
H       -0.105781       1.936904        -0.719226
N       0.700707        -0.748995       -0.922807
H       0.590949        -0.311890       -1.852440
C       2.081146        -1.034706       -0.497918
C       2.721908        0.163900        0.202635
H       2.127650        -1.924153       0.181313
H       2.680780        -1.335443       -1.394296
O       3.821512        0.599071        -0.231122
O       2.155345        0.695531        1.197260
###
25
ValGly3 pm6 E=-0.454530318632 au
N       -2.565408       -1.676516       -0.080730
H       -2.801670       -1.492228       0.898825
H       -3.457290       -1.663876       -0.586200
C       -1.690953       -0.593702       -0.608369
H       -1.608133       -0.752145       -1.723871
C       -2.216771       0.855745        -0.389009
C       -0.318881       -0.781747       0.041884
H       -3.185037       0.923540        -0.953826
C       -2.501569       1.172501        1.077419
C       -1.237301       1.863237        -0.990389
O       -0.160309       -0.902257       1.275008
H       -1.605521       1.115865        1.704672
H       -2.898354       2.190612        1.192546
H       -3.252720       0.499934        1.511034
H       -0.953727       1.601905        -2.018561
H       -1.674686       2.869445        -1.032767
H       -0.312217       1.953344        -0.410024
N       0.763510        -0.864396       -0.800146
H       0.676094        -0.681881       -1.810763
C       2.128131        -1.090074       -0.295295
C       2.771392        0.218070        0.169734
H       2.133625        -1.829762       0.543115
H       2.744536        -1.569620       -1.095750
O       3.687594        0.732700        -0.524294
O       2.373227        0.764192        1.238266
```

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###
28
AlaGlyGly1 pm6 E=-0.200883568733 au
N       -4.782843       0.105921        0.029439
H       -4.783685       -0.096782       1.046479
H       -5.046166       -0.762735       -0.475998
H       -5.518364       0.820427        -0.151832
C       -3.430394       0.619941        -0.438437
H       -3.487804       0.745506        -1.566506
C       -3.123634       1.956760        0.212969
C       -2.336815       -0.387576       -0.046621
H       -3.085903       1.908075        1.311864
H       -2.160453       2.366094        -0.131522
H       -3.882133       2.717968        -0.039959
O       -2.341046       -0.942906       1.064002
N       -1.360221       -0.635341       -0.973812
H       -1.326170       -0.136844       -1.878054
C       -0.228817       -1.525447       -0.674847
C       0.860878        -0.805861       0.106359
H       -0.555294       -2.428457       -0.089072
H       0.160552        -1.951543       -1.641840
O       0.612123        0.117433        0.905472
N       2.147566        -1.237783       -0.093983
H       2.373433        -1.985414       -0.771841
C       3.285951        -0.638447       0.614313
C       3.700004        0.667855        -0.027235
H       3.058219        -0.447197       1.701043
H       4.143193        -1.367727       0.635204
O       2.975859        1.583048        -0.396170
O       5.045615        0.747749        -0.149465
H       5.375627        1.623114        -0.549187
###
27
AlaGlyGly2 pm6 E=-0.370299609416 au
N       5.120353        0.506907        -0.539973
H       5.291523        1.153896        0.251989
H       4.959704        1.074959        -1.394274
H       5.983005        -0.057636       -0.683240
C       3.936444        -0.407666       -0.262753
H       3.796662        -1.070287       -1.174547
C       4.209257        -1.253632       0.966696
C       2.684874        0.458334        -0.045394
H       4.293109        -0.659581       1.889952
H       3.413397        -1.998776       1.131588
H       5.146428        -1.829118       0.874324
O       2.777517        1.663577        0.239241
N       1.478496        -0.163791       -0.184675
H       1.398454        -1.167205       -0.413303
C       0.219898        0.589213        0.005080
C       -0.968117       -0.347579       -0.103177
H       0.220288        1.115982        0.997668
H       0.139775        1.409109        -0.760370
O       -0.824309       -1.565644       -0.323896
N       -2.210676       0.204691        0.039538
H       -2.354065       1.202898        0.244179
C       -3.414416       -0.641893       -0.075781
C       -4.698199       0.164034        0.051852
H       -3.413773       -1.191954       -1.051586
H       -3.409265       -1.443420       0.708160
O       -4.670371       1.382343        0.361017
O       -5.782948       -0.447574       -0.156851
###
26
AlaGlyGly3 pm6 E=-0.520283238886 au
N       -4.971062       0.108483        0.061964
H       -4.960295       0.358461        1.051972
H       -5.131386       -0.900258       0.014918
C       -3.686551       0.464506        -0.586959
H       -3.814591       0.303161        -1.695696
C       -3.323751       1.920379        -0.314942
C       -2.522568       -0.410095       -0.079283
H       -3.178684       2.135083        0.752393
H       -2.406054       2.219117        -0.841827
H       -4.115065       2.600924        -0.662893
O       -2.553827       -0.951976       1.045105
N       -1.447821       -0.596460       -0.910978
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H       -1.370972       -0.103217       -1.813350
C       -0.268150       -1.367583       -0.488856
C       0.691927        -0.518489       0.336706
H       -0.560622       -2.266018       0.117501
H       0.229468        -1.800164       -1.399530
O       0.296363        0.198713        1.279351
N       2.016288        -0.593662       0.008814
H       2.351198        -1.199367       -0.754596
C       3.036773        0.179059        0.742819
C       4.279736        0.384640        -0.116396
H       2.627114        1.162574        1.078797
H       3.334907        -0.347139       1.687039
O       4.764433        -0.585445       -0.758267
O       4.814113        1.525434        -0.142671
###
46
AlaLysAla1 pm6 E=-0.100056712265 au
N       3.713985        -3.147753       -1.143789
H       4.033443        -2.462030       -1.851830
H       2.974731        -3.740547       -1.570029
C       3.204630        -2.457843       0.112260
H       2.834159        -3.268053       0.817711
C       4.321730        -1.667380       0.768420
C       2.066735        -1.493976       -0.266115
H       4.750678        -0.893590       0.112878
H       3.976543        -1.161623       1.685028
H       5.159434        -2.317181       1.075435
O       2.151778        -0.740858       -1.247023
N       0.969487        -1.491008       0.554800
H       0.887857        -2.137406       1.358170
C       -0.178032       -0.585049       0.315956
H       -0.098215       -0.136738       -0.721811
C       -1.506693       -1.351082       0.428152
C       -0.124996       0.513573        1.395280
H       -1.447671       -2.286311       -0.171411
H       -1.676856       -1.694453       1.470642
C       -2.681622       -0.497824       -0.060122
O       -0.204325       0.243062        2.603028
H       -2.780360       0.419433        0.556375
C       -3.984749       -1.303159       -0.014526
H       -3.863146       -2.262868       -0.562540
H       -4.220089       -1.592871       1.032262
C       -5.135754       -0.495694       -0.615714
H       -5.293108       0.461330        -0.061198
H       -4.917258       -0.205083       -1.673014
N       -6.420240       -1.301086       -0.584384
H       -6.683966       -1.544250       0.386974
H       -7.199164       -0.763909       -1.004482
H       -6.319249       -2.184797       -1.114681
N       0.039943        1.837990        1.050160
H       0.046017        2.550658        1.801895
C       0.093456        2.366859        -0.327475
H       -0.195055       1.560229        -1.073850
C       -0.824534       3.564395        -0.496681
C       1.547781        2.772553        -0.626744
H       -0.656457       4.358045        0.248785
H       -0.711369       4.028489        -1.490412
H       -1.884554       3.273769        -0.412505
O       2.146675        3.777105        0.067414
O       2.253058        2.244385        -1.475651
H       1.565114        4.229584        0.770161
H       4.522429        -3.762068       -0.911309
H       -2.491306       -0.136557       -1.093051
###
45
AlaLysAla2 pm6 E=-0.283812182672 au
N       4.395639        -2.161788       -1.316406
H       4.729937        -1.194735       -1.482633
H       3.930197        -2.502132       -2.180413
C       3.453363        -2.228110       -0.124939
H       3.061315        -3.292877       -0.057942
C       4.194894        -1.867598       1.149433
C       2.301215        -1.231845       -0.333743
H       4.608068        -0.847364       1.138357
H       3.541616        -1.945602       2.033790
H       5.041193        -2.551304       1.337899
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O       2.485715        -0.127584       -0.869952
N       1.066946        -1.621195       0.113992
H       0.929738        -2.525742       0.597922
C       -0.105422       -0.718072       0.036327
H       -0.043998       -0.113636       -0.921577
C       -1.411330       -1.529162       0.036170
C       -0.081104       0.209622        1.268162
H       -1.349631       -2.335351       -0.728360
H       -1.540937       -2.062641       1.002338
C       -2.620499       -0.633161       -0.253204
O       -0.065553       -0.244221       2.425875
H       -2.667992       0.207998        0.468879
C       -3.920419       -1.442143       -0.187848
H       -3.883054       -2.289520       -0.905977
H       -4.031711       -1.910389       0.814490
C       -5.122073       -0.545508       -0.489210
H       -5.169414       0.319569        0.216704
H       -5.050879       -0.104839       -1.513965
N       -6.410765       -1.337431       -0.382888
H       -6.511587       -1.758658       0.557262
H       -7.230720       -0.728724       -0.553613
H       -6.433101       -2.104760       -1.077215
N       -0.056195       1.574105        1.115189
H       -0.090830       2.166668        1.958852
C       -0.121226       2.296363        -0.177441
H       -0.291947       1.562531        -1.021084
C       -1.238323       3.326270        -0.170568
C       1.240245        2.995393        -0.398947
H       -1.154290       4.053703        0.648685
H       -1.265609       3.900188        -1.109723
H       -2.227450       2.852517        -0.069159
O       1.715180        3.780515        0.461278
O       1.864780        2.735899        -1.466121
H       5.230739        -2.760723       -1.144571
H       -2.515912       -0.159179       -1.251944
###
44
AlaLysAla3 pm6 E=-0.429463666135 au
N       4.197544        -2.677288       -1.243972
H       4.630275        -1.865907       -1.686739
H       3.553600        -3.086508       -1.924582
C       3.473492        -2.288610       -0.011503
H       3.069702        -3.231789       0.455248
C       4.401772        -1.583357       0.971703
C       2.312542        -1.315289       -0.310515
H       4.864612        -0.679075       0.553777
H       3.879269        -1.288305       1.892512
H       5.228220        -2.239710       1.282361
O       2.471707        -0.316483       -1.041131
N       1.094195        -1.579915       0.260690
H       0.957863        -2.396214       0.879669
C       -0.069709       -0.675279       0.105367
H       0.017360        -0.113669       -0.870846
C       -1.377867       -1.483497       0.108759
C       -0.059437       0.292298        1.305299
H       -1.306313       -2.306097       -0.636892
H       -1.517461       -1.995661       1.085155
C       -2.588543       -0.601747       -0.213302
O       -0.037966       -0.131960       2.475118
H       -2.662013       0.241917        0.503317
C       -3.877256       -1.430744       -0.174197
H       -3.814391       -2.272909       -0.896824
H       -3.996239       -1.907384       0.823471
C       -5.089785       -0.554029       -0.488756
H       -5.158170       0.310684        0.215691
H       -5.015525       -0.113100       -1.513126
N       -6.366124       -1.367556       -0.394778
H       -6.464208       -1.798731       0.541238
H       -7.194906       -0.770634       -0.564009
H       -6.372721       -2.129095       -1.095945
N       -0.040692       1.653283        1.124416
H       -0.047614       2.259773        1.959891
C       -0.131129       2.359455        -0.175949
H       -0.483846       1.649217        -0.979159
C       -1.092395       3.533501        -0.083960
C       1.282605        2.871747        -0.543167
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H       -0.839399       4.240687        0.718128
H       -1.120897       4.107095        -1.023502
H       -2.125458       3.201685        0.103413
O       1.913084        3.640310        0.227267
O       1.788933        2.479223        -1.632968
H       -2.468008       -0.131347       -1.211701
###
43
AlaLysAla4 pm6 E=-0.564063056356 au
N       4.665385        -1.733522       -1.128750
H       5.052762        -0.904667       -0.674450
H       4.399127        -1.447512       -2.073746
C       3.481670        -2.235050       -0.388826
H       3.140986        -3.183304       -0.895465
C       3.833123        -2.519189       1.066991
C       2.320610        -1.219472       -0.420824
H       4.090074        -1.612995       1.631431
H       3.011053        -3.021462       1.597561
H       4.699409        -3.192926       1.147584
O       2.503043        -0.037098       -0.774227
N       1.068560        -1.650712       -0.060279
H       0.914687        -2.610303       0.289462
C       -0.103735       -0.744435       -0.067128
H       -0.052506       -0.085659       -0.988327
C       -1.409859       -1.554791       -0.100365
C       -0.069493       0.116336        1.211735
H       -1.368073       -2.290161       -0.934124
H       -1.511955       -2.170203       0.818641
C       -2.628841       -0.642048       -0.274441
O       -0.036475       -0.396859       2.344939
H       -2.674158       0.106291        0.542715
C       -3.927148       -1.455105       -0.296645
H       -3.900454       -2.198875       -1.117719
H       -4.020102       -2.050823       0.633712
C       -5.147003       -0.534711       -0.458156
H       -5.132814       0.259784        0.319805
H       -5.099260       -0.004733       -1.434241
N       -6.455691       -1.243195       -0.374820
H       -6.529063       -1.725565       0.523616
H       -6.490624       -1.983739       -1.078609
N       -0.054037       1.487999        1.133694
H       -0.074421       2.033350        2.009135
C       -0.143653       2.280221        -0.115941
H       -0.311541       1.591593        -0.997548
C       -1.275923       3.290916        -0.044190
C       1.205977        3.010838        -0.307371
H       -1.187909       3.983804        0.803971
H       -1.328860       3.903907        -0.957369
H       -2.255979       2.798137        0.053475
O       1.666541        3.771091        0.581284
O       1.839443        2.797150        -1.380379
H       -2.534668       -0.053272       -1.210392
###
29
CysGlyGly1 pm6 E=-0.191328559959 au
N       -4.272433       -1.365614       -0.291893
H       -3.960700       -2.277608       -0.681644
H       -5.169875       -1.112295       -0.757607
H       -4.465400       -1.488268       0.721328
C       -3.235549       -0.282390       -0.536160
H       -3.053087       -0.232556       -1.660190
C       -3.763260       1.060621        -0.051409
C       -1.924883       -0.632996       0.197400
H       -4.570308       1.436535        -0.725305
H       -4.235391       0.993453        0.954083
S       -2.402848       2.254555        -0.070265
O       -1.668176       -0.193220       1.325112
H       -1.919140       2.081337        1.184889
N       -1.051571       -1.443367       -0.480529
H       -1.252205       -1.794393       -1.430840
C       0.236168        -1.836474       0.110489
C       1.241285        -0.694715       0.117241
H       0.090554        -2.243114       1.148964
H       0.657026        -2.707234       -0.468424
O       1.068605        0.372653        -0.497250
N       2.377572        -0.901428       0.863222
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H       2.550325        -1.788852       1.362370
C       3.420256        0.124850        0.984275
C       4.254288        0.266240        -0.265314
H       2.982451        1.126747        1.254272
H       4.090539        -0.122471       1.858379
O       4.156043        -0.315103       -1.334796
O       5.212897        1.214869        -0.082305
H       5.801023        1.364282        -0.896857
###
28
CysGlyGly2 pm6 E=-0.362701935934 au
N       -3.992010       -2.014993       0.228077
H       -3.317948       -2.804588       0.196236
H       -4.844046       -2.298281       -0.301671
H       -4.270471       -1.862122       1.216537
C       -3.391055       -0.762090       -0.383973
H       -3.111157       -1.014108       -1.459043
C       -4.401306       0.379362        -0.380524
C       -2.142514       -0.340172       0.421605
H       -5.011846       0.376284        -1.313228
H       -5.146083       0.303495        0.443035
S       -3.438814       1.911771        -0.276606
O       -2.190239       -0.164995       1.648327
H       -3.833747       2.359891        0.939802
N       -0.979642       -0.223503       -0.288427
H       -0.941037       -0.382972       -1.306587
C       0.259976        0.258802        0.353158
C       1.476013        -0.337280       -0.331867
H       0.302930        1.383196        0.313586
H       0.270518        0.008315        1.448454
O       1.389891        -1.186184       -1.238318
N       2.699259        0.103185        0.102163
H       2.795227        0.816705        0.837362
C       3.931901        -0.402347       -0.535977
C       5.178220        0.167094        0.138256
H       3.971274        -1.521290       -0.494662
H       3.934978        -0.159135       -1.627335
O       5.423627        -0.099536       1.342233
O       5.959442        0.872372        -0.557684
###
27
CysGlyGly3 pm6 E=-0.520044900368 au
N       4.576919        -1.086502       -0.383248
H       4.614877        -2.010482       0.088157
H       5.514771        -0.643310       -0.303941
H       4.388777        -1.246279       -1.390881
C       3.514901        -0.191110       0.244456
H       3.758358        -0.107680       1.348355
C       3.539202        1.188129        -0.408487
C       2.137200        -0.837042       0.048359
H       4.530544        1.667462        -0.296411
H       3.335781        1.143826        -1.494195
S       2.269872        2.170227        0.435986
O       1.932576        -1.615334       -0.902611
N       1.176428        -0.584989       0.991878
H       1.269068        0.229373        1.630573
C       -0.161225       -1.190486       0.896098
C       -1.083028       -0.454400       -0.066211
H       -0.097172       -2.263753       0.566001
H       -0.595184       -1.247113       1.932580
O       -0.670094       0.036197        -1.141038
N       -2.398662       -0.360930       0.282363
H       -2.766566       -0.767687       1.155869
C       -3.381101       0.275334        -0.616927
C       -4.797146       0.181429        -0.068837
H       -3.117931       1.350482        -0.788373
H       -3.354384       -0.195634       -1.633828
O       -5.046982       -0.510345       0.952414
O       -5.702314       0.809854        -0.683431
###
26
CysGlyGly4 pm6 E=-0.664404002775 au
N       -4.737189       -0.813435       0.123235
H       -4.710301       -1.776243       -0.220103
H       -4.766235       -0.870241       1.142824
C       -3.536560       -0.066128       -0.332770
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H       -3.656770       0.091620        -1.442191
C       -3.443716       1.282711        0.381586
C       -2.234817       -0.844267       -0.078080
H       -4.374369       1.862270        0.253219
H       -3.292308       1.173836        1.469195
S       -2.049683       2.191942        -0.354245
O       -2.156642       -1.692545       0.839361
N       -1.183858       -0.651133       -0.939468
H       -1.154754       0.200629        -1.533096
C       0.092478        -1.364627       -0.778153
C       1.025047        -0.667330       0.202618
H       -0.064632       -2.419407       -0.426856
H       0.560856        -1.484085       -1.793849
O       0.620220        -0.223545       1.301047
N       2.331997        -0.541467       -0.167230
H       2.682956        -0.922871       -1.058917
C       3.326351        0.094592        0.719359
C       4.658055        0.276817        0.000682
H       2.948534        1.077620        1.093561
H       3.498923        -0.523108       1.639110
O       5.077165        -0.617596       -0.781282
O       5.324925        1.320003        0.233100
###
31
GlyAlaAla1 pm6 E=-0.207178356544 au
N       4.592947        -1.586222       -0.166146
H       5.124275        -0.992037       0.496524
C       3.565972        -0.779306       -0.912177
H       5.266648        -2.010680       -0.835080
H       4.145863        -2.350294       0.372350
C       2.627274        -0.066936       0.038069
H       4.081110        -0.047587       -1.601633
H       2.989067        -1.443945       -1.619833
O       2.648364        -0.285746       1.259195
N       1.741349        0.821067        -0.522495
H       1.733176        1.007706        -1.540257
C       0.828199        1.641195        0.314226
H       1.314444        1.850103        1.315975
C       0.519710        2.958311        -0.369467
C       -0.422782       0.784043        0.614576
H       0.127747        2.847638        -1.393554
H       -0.217903       3.548025        0.198257
H       1.417103        3.592599        -0.453326
O       -0.380972       -0.054696       1.536676
N       -1.556417       0.926269        -0.139045
H       -1.616445       1.601245        -0.919189
C       -2.788445       0.166328        0.185433
H       -2.967193       0.206646        1.306227
C       -3.983661       0.742382        -0.555244
C       -2.618844       -1.304114       -0.210454
H       -3.878350       0.699351        -1.650473
H       -4.915049       0.211795        -0.294609
H       -4.154074       1.801616        -0.301444
O       -1.734519       -1.793474       -0.899318
O       -3.532154       -2.201933       0.257792
H       -4.265872       -1.814602       0.849330
###
30
GlyAlaAla2 pm6 E=-0.390530954260 au
N       4.539349        -1.454557       -0.311563
H       5.167017        -0.808822       0.202090
C       3.432023        -0.697824       -0.991622
H       5.105289        -1.966704       -1.018561
H       4.161907        -2.144948       0.361899
C       2.508624        -0.044312       0.014226
H       3.870310        0.056245        -1.709144
H       2.846381        -1.388717       -1.667041
O       2.523370        -0.361358       1.214096
N       1.634127        0.894964        -0.474697
H       1.627046        1.159296        -1.475569
C       0.715176        1.643221        0.421061
H       1.200058        1.775960        1.435569
C       0.398934        3.007364        -0.159868
C       -0.534379       0.761367        0.645327
H       0.034972        2.975494        -1.199788
H       -0.364100       3.534754        0.434844
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H       1.286085        3.661217        -0.167885
O       -0.509610       -0.104424       1.549668
N       -1.632426       0.908271        -0.147613
H       -1.670245       1.608697        -0.905718
C       -2.860274       0.096272        0.073700
H       -3.228772       0.283518        1.123126
C       -3.938978       0.475327        -0.924760
C       -2.528410       -1.407972       -0.061990
H       -3.625389       0.358311        -1.971784
H       -4.844525       -0.136066       -0.789970
H       -4.254009       1.525476        -0.813926
O       -2.027870       -1.874154       -1.118619
O       -2.767849       -2.151954       0.930168
###
29
GlyAlaAla3 pm6 E=-0.536651721414 au
N       -3.614863       -2.291759       0.306241
H       -4.098359       -2.155771       -0.583971
C       -3.172776       -0.989842       0.847546
H       -2.807226       -2.883065       0.107205
C       -2.149473       -0.272020       -0.012767
H       -4.069014       -0.338386       1.014291
H       -2.742886       -1.142538       1.872087
O       -1.561377       -0.851335       -0.955444
N       -1.855851       1.030972        0.295053
H       -2.296385       1.497725        1.108438
C       -0.904832       1.854479        -0.498825
H       -1.300310       1.947245        -1.554720
C       -0.755391       3.235391        0.110685
C       0.458022        1.136265        -0.595460
H       -0.452604       3.219152        1.169695
H       -0.001145       3.833079        -0.426093
H       -1.695327       3.808463        0.062024
O       0.856025        0.729038        -1.709857
N       1.187912        0.911526        0.532907
H       0.869632        1.248079        1.456664
C       2.447659        0.122163        0.508495
H       3.243941        0.736060        -0.002456
C       2.881296        -0.217647       1.924888
C       2.270014        -1.191202       -0.285418
H       2.142062        -0.815817       2.475897
H       3.823961        -0.786636       1.934450
H       3.063455        0.686669        2.527886
O       1.198557        -1.858020       -0.229288
O       3.238383        -1.579055       -0.992369
###
40
GlyGlyAspAla1 pm6 E=-0.625177590728 au
N       -7.130539       -0.898412       -0.459776
H       -7.402900       -0.856448       0.540920
C       -6.013548       0.062680        -0.753513
H       -6.858786       -1.872793       -0.682228
H       -7.963283       -0.657559       -1.034179
C       -4.733049       -0.308768       -0.029146
H       -5.804348       0.095223        -1.864399
H       -6.351871       1.115097        -0.527410
O       -4.285693       -1.467664       -0.046193
N       -4.086104       0.710582        0.619897
H       -4.430242       1.684440        0.583416
C       -2.817918       0.499677        1.332584
C       -1.624437       0.535714        0.387972
H       -2.735016       1.268353        2.151847
H       -2.806481       -0.483507       1.878806
O       -1.637530       0.007476        -0.734356
N       -0.486303       1.156925        0.857562
H       -0.458179       1.615321        1.784205
C       0.752034        1.194796        0.051154
H       0.487459        1.133191        -1.049716
C       1.508730        2.502937        0.307836
C       1.622443        -0.017670       0.463618
H       0.830319        3.381668        0.131087
H       1.775520        2.627145        1.393938
C       2.746668        2.623091        -0.514610
O       2.243013        -0.041660       1.543583
O       2.981531        3.906182        -0.879116
O       3.522770        1.733307        -0.853172
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N       1.692817        -1.057088       -0.418860
H       1.187760        -1.038816       -1.321297
C       2.483150        -2.283681       -0.133045
H       1.994680        -2.826581       0.727527
C       2.518201        -3.181562       -1.358954
C       3.934876        -1.952523       0.274864
H       3.012069        -2.719890       -2.225372
H       3.049274        -4.124360       -1.155355
H       1.506716        -3.467315       -1.691316
O       4.577001        -1.008190       -0.265227
O       4.466668        -2.672065       1.161579
H       3.833231        4.035553        -1.421573
###
39
GlyGlyAspAla2 pm6 E=-0.811894515437 au
N       6.917952        1.386066        -0.561816
H       7.163556        1.579691        0.426868
C       6.129834        0.111450        -0.678907
H       6.380278        2.191163        -0.928562
H       7.801001        1.310043        -1.106996
C       4.849985        0.161923        0.129857
H       5.891395        -0.098181       -1.764439
H       6.777108        -0.763339       -0.377346
O       4.411123        1.221475        0.605698
N       4.203540        -1.036139       0.304407
H       4.535138        -1.901575       -0.151737
C       2.948305        -1.139622       1.061534
C       1.744012        -0.772781       0.208109
H       2.867108        -2.181240       1.481148
H       2.954579        -0.473912       1.968523
O       1.764210        0.146754        -0.625814
N       0.590504        -1.502272       0.409552
H       0.535652        -2.259505       1.110592
C       -0.654649       -1.143771       -0.301196
H       -0.390159       -0.783855       -1.341731
C       -1.600923       -2.349310       -0.406232
C       -1.391723       -0.030376       0.483055
H       -1.248018       -3.036189       -1.213840
H       -1.553755       -2.983155       0.511518
C       -3.030047       -1.929984       -0.674985
O       -1.779776       -0.207514       1.652983
O       -3.867986       -1.931286       0.279616
O       -3.392465       -1.528676       -1.813813
N       -1.709196       1.108557        -0.206922
H       -1.326755       1.297652        -1.149095
C       -2.719447       2.073129        0.313597
H       -2.486690       2.323214        1.386412
C       -2.744081       3.338511        -0.517719
C       -4.073288       1.326194        0.250053
H       -2.905882       3.157446        -1.590140
H       -3.541306       4.021386        -0.183113
H       -1.800554       3.901854        -0.438807
O       -4.619996       1.062132        -0.855466
O       -4.567632       0.878719        1.324446
###
43
GlyGlyGluAla1 pm6 E=-0.631035103693 au
N       -7.372272       -0.261117       -0.943793
H       -7.763559       -0.688739       -0.083408
C       -6.222511       0.650163        -0.616993
H       -7.075076       -1.022601       -1.579872
H       -8.129704       0.277081        -1.411681
C       -5.065759       -0.112437       -0.001513
H       -5.864700       1.181069        -1.549059
H       -6.582406       1.494563        0.040210
O       -4.878899       -1.316651       -0.244219
N       -4.230253       0.605919        0.813806
H       -4.371241       1.616144        0.981681
C       -3.066833       -0.002174       1.475117
C       -1.866886       -0.047911       0.535660
H       -2.849335       0.567696        2.421141
H       -3.281116       -1.046337       1.829546
O       -1.913077       -0.620775       -0.566055
N       -0.713041       0.563424        0.965328
H       -0.663308       1.046438        1.877810
C       0.511497        0.572633        0.134379
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H       0.228478        0.439418        -0.953906
C       1.252994        1.910376        0.303580
C       1.425203        -0.582777       0.597307
H       0.567420        2.747830        0.032723
H       1.508393        2.087138        1.372602
C       2.509225        1.961195        -0.566762
O       1.940290        -0.593006       1.732076
H       3.222928        1.144119        -0.308641
H       2.253743        1.770965        -1.641816
C       3.197151        3.279537        -0.429476
O       4.219019        3.513890        0.203987
O       2.668431        4.371232        -1.067114
N       1.681874        -1.582103       -0.301518
H       1.257034        -1.585525       -1.242745
C       2.617837        -2.694276       0.015564
H       2.462154        -3.016015       1.084178
C       2.387561        -3.871156       -0.913268
C       4.056277        -2.135211       -0.122039
H       2.478880        -3.609742       -1.977313
H       3.105109        -4.682329       -0.716199
H       1.383588        -4.305647       -0.787926
O       4.627790        -2.068219       -1.237442
O       4.625433        -1.717112       0.929307
H       1.822130        4.178964        -1.597735
###
42
GlyGlyGluAla2 pm6 E=-0.810747293298 au
C       3.855251        -3.377164       -1.152252
C       3.624786        -2.277612       -0.133726
C       4.763871        -1.228691       -0.175064
O       5.207669        -0.798173       0.928966
N       2.348321        -1.563518       -0.404631
C       1.770085        -0.753149       0.534400
O       2.259018        -0.632505       1.673533
C       0.518181        0.033764        0.108840
C       0.747050        1.534042        0.381225
C       1.891118        2.079441        -0.470464
C       2.014112        3.572028        -0.282729
O       1.225071        4.352123        -0.891770
N       -0.640330       -0.476931       0.879736
C       -1.922378       -0.313857       0.406186
O       -2.126615       0.187252        -0.712971
C       -3.048866       -0.755342       1.329808
N       -4.212073       -1.257779       0.585386
C       -5.171105       -0.411501       0.089109
O       -5.106868       0.818265        0.246820
C       -6.313969       -1.064183       -0.660711
N       -7.423360       -0.089823       -0.942676
O       2.909254        4.044082        0.479278
O       5.215952        -0.794868       -1.264606
H       -7.079929       0.713321        -1.499725
H       -7.830042       0.276977        -0.062181
H       -8.180581       -0.557434       -1.481450
H       -6.720850       -1.954612       -0.097968
H       -5.939650       -1.514644       -1.627304
H       -4.233932       -2.273328       0.399852
H       -3.322393       0.112060        1.991922
H       -2.713094       -1.553497       2.049788
H       -0.461268       -0.826286       1.834236
H       0.313300        -0.114084       -0.994770
H       -0.194451       2.087869        0.172057
H       0.941658        1.710416        1.460641
H       2.852659        1.581752        -0.224194
H       1.732724        1.845757        -1.547828
H       1.946168        -1.672473       -1.350049
H       3.586309        -2.721230       0.901378
H       3.847515        -3.016881       -2.190726
H       4.822462        -3.877958       -0.988868
H       3.088821        -4.165428       -1.091258
###
25
GlyGlyGly1 pm6 E=-0.191789015494 au
N       4.747407        1.027535        0.184322
H       4.506885        1.299064        1.154839
C       3.511948        0.906818        -0.665030
H       5.263638        0.128703        0.218087
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C       2.541331        -0.101283       -0.086191
H       3.007145        1.913319        -0.764728
H       3.802401        0.653655        -1.725891
O       2.615497        -0.469896       1.097078
N       1.569947        -0.571119       -0.933273
H       1.485399        -0.236600       -1.906947
C       0.583854        -1.572943       -0.501125
C       -0.600546       -0.923429       0.204761
H       0.267253        -2.178183       -1.395765
H       1.034611        -2.329804       0.196739
O       -0.448550       -0.204975       1.213060
N       -1.844606       -1.174775       -0.310495
H       -1.975666       -1.741252       -1.166462
C       -3.072068       -0.695590       0.339258
C       -3.336270       0.759039        0.018042
H       -3.939228       -1.341656       0.025662
H       -3.033063       -0.813623       1.459269
O       -2.555682       1.698402        0.103466
O       -4.614800       0.947570        -0.381801
H       5.379511        1.753382        -0.208118
H       -4.849341       1.917029        -0.583284
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24
GlyGlyGly2 pm6 E=-0.369926387290 au
N       5.009364        0.356433        -0.457416
H       4.791375        1.311867        -0.792733
C       3.822540        -0.555540       -0.601175
H       5.306382        0.420488        0.534826
C       2.611161        -0.012159       0.128119
H       3.568111        -0.700741       -1.693478
H       4.100747        -1.594811       -0.260638
O       2.464234        1.205712        0.328454
N       1.681902        -0.930273       0.544488
H       1.775049        -1.937935       0.336865
C       0.457597        -0.518895       1.249354
C       -0.605900       -0.058690       0.258186
H       0.098246        -1.370531       1.890564
H       0.658391        0.311952        1.976085
O       -0.542540       1.069505        -0.276144
N       -1.624433       -0.919652       -0.034693
H       -1.699141       -1.846294       0.413442
C       -2.717153       -0.544221       -0.948524
C       -3.822107       0.202716        -0.197540
H       -2.350635       0.085625        -1.796684
H       -3.124177       -1.464559       -1.437533
O       -3.581818       1.338280        0.299206
O       -4.949515       -0.342521       -0.083228
H       5.808101        -0.007697       -1.014196
###
23
GlyGlyGly3 pm6 E=-0.517162123464 au
N       4.583777        1.301096        0.071150
H       4.209163        1.823712        0.865057
C       3.481037        0.834146        -0.794905
H       5.083436        0.500805        0.464025
C       2.511183        -0.113123       -0.113671
H       2.919697        1.719261        -1.191724
H       3.914552        0.345233        -1.705307
O       2.581803        -0.370086       1.105541
N       1.537229        -0.688536       -0.894175
H       1.436544        -0.457312       -1.894294
C       0.572912        -1.659063       -0.354754
C       -0.616740       -0.950281       0.285633
H       0.259517        -2.360804       -1.175519
H       1.042433        -2.325823       0.416311
O       -0.456333       -0.213487       1.287632
N       -1.842896       -1.160491       -0.271501
H       -1.951815       -1.746229       -1.117664
C       -3.089982       -0.629319       0.304112
C       -3.298336       0.842836        -0.057626
H       -3.952682       -1.244675       -0.058277
H       -3.113299       -0.750246       1.416185
O       -4.141609       1.152121        -0.937405
O       -2.628207       1.729004        0.548001
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45
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GlyGlyHisAla1 pm6 E=-0.275267433416 au
N 7.610810 0.114053 1.063788
H 8.013336 0.563711 0.220475
C 6.499913 -0.828297 0.693276
H 8.370762 -0.405213 1.548460
H 7.270632 0.858077 1.698739
C 5.359031 -0.103862 0.007649
H 6.908814 -1.665882 0.056188
H 6.117015 -1.362197 1.612771
O 5.231482 1.129219 0.080838
N 4.475775 -0.885161 -0.692259
H 4.555568 -1.914354 -0.708674
C 3.333188 -0.306532 -1.412304
C 2.155210 -0.010535 -0.493834
H 3.619339 0.645165 -1.940548
H 3.045233 -1.006454 -2.246241
O 2.283007 0.278614 0.705845
N 0.908954 -0.059082 -1.080257
H 0.797080 -0.252501 -2.088516
C -0.312300 0.326073 -0.341095
H -0.053414 0.488784 0.750567
C -0.899141 1.622801 -0.927043
C -1.335921 -0.818413 -0.492966
H -0.092111 2.404413 -0.970801
H -1.170583 1.483409 -2.004836
C -2.043311 2.161913 -0.159048
O -1.666641 -1.259488 -1.607960
N -2.950796 3.073932 -0.737342
C -2.442852 1.982921 1.165269
H -2.923462 3.418327 -1.705740
C -3.879873 3.436283 0.215712
N -3.578871 2.773364 1.380826
H -1.995378 1.382294 1.954216
H -4.714505 4.134334 0.064508
N -1.875587 -1.323581 0.658480
H -1.648352 -0.917673 1.582736
C -2.917525 -2.381952 0.637121
H -2.469664 -3.313780 0.187467
C -3.409790 -2.671370 2.045802
C -4.120898 -1.952778 -0.232632
H -3.816454 -1.785823 2.554950
H -4.201878 -3.436354 2.046905
H -2.607101 -3.061608 2.691198
O -4.602791 -0.791775 -0.164770
O -4.614709 -2.818769 -1.008650
H -4.094038 2.848729 2.265652
###
44
GlyGlyHisAla2 pm6 E=-0.432776989564 au
N 7.490554 0.291191 1.200093
H 7.849594 0.918643 0.457903
C 6.505926 -0.696980 0.639210
H 8.298516 -0.210841 1.620553
H 7.053578 0.873654 1.937348
C 5.311941 -0.003385 0.014661
H 7.026056 -1.376574 -0.097231
H 6.159501 -1.404141 1.449230
O 5.059075 1.191380 0.237830
N 4.529677 -0.770315 -0.810826
H 4.711596 -1.775654 -0.956882
C 3.346501 -0.213825 -1.480722
C 2.144451 -0.098753 -0.555590
H 3.576108 0.790673 -1.932009
H 3.094465 -0.861449 -2.368116
O 2.175483 -0.366188 0.655238
N 0.983195 0.357456 -1.142329
H 0.936701 0.581580 -2.149251
C -0.247691 0.571339 -0.352134
H 0.030773 0.742087 0.731956
C -1.011158 1.798628 -0.884445
C -1.157569 -0.666915 -0.482749
H -0.354289 2.701671 -0.808983
H -1.193543 1.700039 -1.981358
C -2.277346 2.060905 -0.156395
O -1.397926 -1.204469 -1.579081
N -3.408380 2.557188 -0.820705

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C       -2.551772       1.941063        1.211471
C       -4.357237       2.740119        0.140575
N       -3.867427       2.377514        1.392559
H       -1.928011       1.606774        2.026750
H       -5.359768       3.122806        -0.025446
N       -1.729729       -1.133874       0.670842
H       -1.579389       -0.659211       1.577239
C       -2.754530       -2.208938       0.651170
H       -2.283643       -3.148351       0.244106
C       -3.288752       -2.459092       2.051560
C       -3.929698       -1.814492       -0.272151
H       -3.719727       -1.562361       2.519996
H       -4.073688       -3.231381       2.052827
H       -2.503321       -2.819910       2.734265
O       -4.399928       -0.644666       -0.275192
O       -4.406988       -2.707791       -1.024776
H       -4.362872       2.413643        2.280749
###
48
GlyGlyLysAla1 pm6 E=-0.506570632170 au
N       -7.454618       0.574110        -1.348408
H       -7.830220       1.263043        -0.693871
C       -6.511391       -0.325864       -0.652064
H       -6.965611       1.104014        -2.072116
C       -5.301146       0.372223        -0.057511
H       -7.064723       -0.889972       0.141574
H       -6.162068       -1.115348       -1.366964
O       -5.023119       1.558517        -0.326586
N       -4.515708       -0.357075       0.802627
H       -4.703289       -1.352934       0.991779
C       -3.315006       0.204627        1.437044
C       -2.105509       0.175238        0.513317
H       -3.487036       1.262503        1.775521
H       -3.112101       -0.357941       2.390394
O       -2.197364       0.082998        -0.722085
N       -0.873385       0.273411        1.120647
H       -0.786101       0.418150        2.138614
C       0.375680        0.358843        0.330272
H       0.127075        0.355366        -0.773306
C       1.152394        1.642362        0.668063
C       1.229538        -0.875769       0.687492
H       0.468134        2.516968        0.609623
H       1.491648        1.631800        1.725022
C       2.335880        1.838268        -0.284005
O       1.823741        -0.965535       1.779669
H       2.999526        0.949968        -0.270848
H       1.976361        1.910401        -1.332344
C       3.131692        3.093257        0.089320
H       2.463272        3.980925        0.117559
H       3.531843        3.003319        1.122415
C       4.270002        3.319582        -0.906205
H       4.925147        2.418602        -0.988903
H       3.874959        3.501310        -1.936263
N       5.115842        4.505414        -0.487361
H       5.597590        4.321024        0.410237
H       5.837487        4.711054        -1.202302
H       4.535040        5.353872        -0.364882
N       1.317324        -1.867730       -0.252024
H       0.828638        -1.796501       -1.159083
C       2.109803        -3.106363       -0.024154
H       1.985160        -3.431177       1.048247
C       1.645277        -4.216281       -0.948277
C       3.602971        -2.763904       -0.251416
H       1.673545        -3.936487       -2.011269
H       2.265637        -5.118130       -0.833685
H       0.609106        -4.522429       -0.736897
O       4.120850        -2.785977       -1.394810
O       4.285103        -2.436956       0.765328
###
47
GlyGlyLysAla2 pm6 E=-0.639564531461 au
N       7.338758        -0.417776       -1.068938
H       7.014093        0.396518        -1.593338
C       6.207589        -1.326781       -0.787286
H       7.728055        -0.060471       -0.194082
C       5.077410        -0.689936       0.000308
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H       5.798870        -1.720109       -1.754353
H       6.593627        -2.234298       -0.256953
O       4.981927        0.545651        0.142705
N       4.148837        -1.531325       0.565591
H       4.174132        -2.549742       0.406890
C       3.009503        -1.024275       1.344599
C       1.827529        -0.679835       0.446914
H       2.738493        -1.784026       2.127824
H       3.283725        -0.108258       1.934112
O       1.952834        -0.010577       -0.593545
N       0.592076        -1.118066       0.859933
H       0.482421        -1.682933       1.719298
C       -0.642611       -0.820773       0.095469
H       -0.417121       -0.837712       -1.012136
C       -1.717423       -1.872809       0.408937
C       -1.122667       0.591952        0.500495
H       -1.290162       -2.892084       0.284850
H       -2.008968       -1.824042       1.479860
C       -2.943843       -1.708184       -0.494628
O       -1.925794       0.782918        1.433073
H       -3.302154       -0.659587       -0.478778
H       -2.668781       -1.900442       -1.552003
C       -4.070919       -2.651481       -0.062296
H       -3.728036       -3.704511       -0.102205
H       -4.329285       -2.476540       1.001683
C       -5.314247       -2.466427       -0.944994
H       -5.592105       -1.391319       -0.998217
H       -5.090503       -2.770665       -1.990705
N       -6.505878       -3.231453       -0.480346
H       -6.732942       -2.968024       0.480954
H       -6.278465       -4.227192       -0.437885
N       -0.622224       1.645230        -0.217846
H       0.042864        1.497894        -0.993415
C       -0.967476       3.054655        0.106491
H       -0.643621       3.269508        1.165075
C       -0.270386       4.005800        -0.851001
C       -2.495591       3.266170        0.015513
H       -0.516246       3.820273        -1.906295
H       -0.531792       5.054658        -0.641330
H       0.826166        3.942575        -0.771001
O       -3.148412       2.886974        -0.992953
O       -3.069863       3.834510        0.986002
###
47
GlyGlyTyrAla1 pm6 E=-0.657588288755 au
N       7.868267        0.070164        -1.452861
H       7.442133        0.759543        -2.074350
C       6.831186        -0.816271       -0.883904
H       8.324246        0.599980        -0.707291
C       5.729133        -0.087627       -0.135656
H       6.369724        -1.421636       -1.706981
H       7.322568        -1.571659       -0.218770
O       5.561300        1.144028        -0.243511
N       4.906652        -0.843390       0.664298
H       5.011871        -1.867304       0.731485
C       3.819749        -0.253261       1.460464
C       2.575215        -0.042662       0.604280
H       3.616070        -0.910038       2.350108
H       4.117663        0.730007        1.909998
O       2.529531        0.838238        -0.274037
N       1.502974        -0.866539       0.838759
H       1.530862        -1.584868       1.582994
C       0.237045        -0.734472       0.082391
H       0.474391        -0.473633       -0.992757
C       -0.542894       -2.064992       0.115269
C       -0.620804       0.379280        0.723885
H       -0.083958       -2.775831       -0.611470
H       -0.413664       -2.568938       1.102350
C       -1.999105       -1.874618       -0.197217
O       -0.972962       0.344699        1.917306
C       -2.964961       -2.186111       0.773626
C       -2.400816       -1.372266       -1.447843
H       -2.660216       -2.611491       1.734591
C       -4.317356       -1.949255       0.529032
C       -3.745501       -1.121575       -1.712305
H       -1.651975       -1.166861       -2.219238
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H       -5.074718       -2.190707       1.276468
C       -4.682319       -1.398772       -0.705188
H       -4.066757       -0.728795       -2.676311
O       -5.986833       -1.036360       -0.990405
H       -6.623838       -1.339155       -0.267970
N       -1.012432       1.403599        -0.098080
H       -0.744133       1.423635        -1.096162
C       -1.934827       2.477791        0.357726
H       -1.725439       2.721612        1.437297
C       -1.762165       3.724816        -0.488216
C       -3.371671       1.909205        0.254302
H       -1.913074       3.545644        -1.562383
H       -2.471688       4.510817        -0.187586
H       -0.754988       4.156845        -0.385198
O       -4.063328       2.074139        -0.780191
O       -3.815551       1.245351        1.237401
###
46
GlyGlyTyrAla2 pm6 E=-0.823508353006 au
N       -7.880188       0.684054        1.119034
H       -8.275963       -0.238368       0.925463
C       -6.791070       0.979450        0.164132
H       -7.508974       0.639234        2.069763
C       -5.690439       -0.065298       0.126945
H       -7.233866       1.123152        -0.854745
H       -6.336763       1.974138        0.411679
O       -5.535714       -0.902461       1.038651
N       -4.860427       -0.065703       -0.969678
H       -4.936537       0.652742        -1.704560
C       -3.762726       -1.032033       -1.115641
C       -2.511948       -0.619098       -0.354807
H       -4.072799       -2.056495       -0.772060
H       -3.540875       -1.164276       -2.211496
O       -2.514827       0.210851        0.570037
N       -1.343447       -1.244760       -0.730092
H       -1.323660       -1.935808       -1.498551
C       -0.075160       -1.010418       -0.006281
H       -0.304914       -0.731944       1.065961
C       0.795007        -2.287257       -0.011166
C       0.684830        0.143446        -0.697228
H       0.393676        -3.003147       0.740447
H       0.698186        -2.823768       -0.982088
C       2.228458        -1.954234       0.277278
O       1.085557        0.075298        -1.874406
C       3.205444        -2.106845       -0.719824
C       2.600011        -1.433193       1.529798
H       2.941596        -2.583967       -1.667442
C       4.495132        -1.627689       -0.531790
C       3.882314        -0.950900       1.742635
H       1.863018        -1.390686       2.336388
H       5.244633        -1.738429       -1.307036
C       4.831532        -0.975884       0.683436
H       4.166914        -0.541455       2.705427
O       5.952922        -0.326875       0.799707
N       0.932926        1.261934        0.058552
H       0.609058        1.334307        1.036627
C       1.724495        2.407433        -0.465976
H       1.507668        2.537487        -1.565042
C       1.383424        3.689501        0.269354
C       3.217036        2.035773        -0.307706
H       1.466984        3.601546        1.362091
H       2.041151        4.515545        -0.042053
H       0.353302        4.019628        0.064588
O       3.839184        2.212837        0.772101
O       3.798887        1.506020        -1.300719
###
35
GlyHisGly2 pm6 E=-0.180392201551 au
N       5.778952        -0.150566       0.166711
H       5.860141        0.882696        0.193191
C       4.545739        -0.574180       -0.580964
H       6.625698        -0.533652       -0.298893
H       5.761107        -0.498986       1.142740
C       3.283773        -0.099542       0.107714
H       4.592268        -0.192560       -1.643010
H       4.533532        -1.697562       -0.704309
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O       3.304543        0.500519        1.189176
N       2.101373        -0.403806       -0.531879
H       2.092917        -0.860469       -1.458033
C       0.809514        0.102323        -0.020659
H       0.957854        0.482988        1.037591
C       0.298588        1.245446        -0.916951
C       -0.198781       -1.063873       -0.037030
H       1.132787        1.978582        -1.090194
H       0.075125        0.870134        -1.947808
C       -0.859603       1.967818        -0.346686
O       -0.315597       -1.818631       -1.018755
N       -1.848855       2.550496        -1.165130
C       -1.195489       2.273582        0.972460
H       -1.881131       2.507768        -2.190551
C       -2.760858       3.198691        -0.359064
N       -2.370103       3.034752        0.948387
H       -0.689685       2.004649        1.897234
H       -3.645756       3.749181        -0.705736
N       -0.966632       -1.226009       1.083423
H       -0.900488       -0.582255       1.889018
C       -1.963451       -2.305305       1.190359
C       -2.982163       -2.291637       0.053678
H       -1.457322       -3.301080       1.244103
H       -2.505626       -2.215425       2.168825
O       -3.592755       -1.232338       -0.251504
O       -3.198949       -3.369628       -0.567858
H       -2.856112       3.412608        1.769641
###
34
GlyHisGly3 pm6 E=-0.338066794775 au
N       -5.815028       0.254737        0.397582
H       -5.947075       -0.580401       0.998213
C       -4.674882       0.049788        -0.561180
H       -6.695655       0.421896        -0.128127
H       -5.641935       1.072225        1.010676
C       -3.346351       -0.020651       0.160858
H       -4.862150       -0.870265       -1.188017
H       -4.650864       0.886863        -1.321325
O       -3.215509       0.341484        1.337207
N       -2.282569       -0.501616       -0.569297
H       -2.390069       -0.814431       -1.547227
C       -0.929751       -0.578075       0.019485
H       -1.013332       -0.566937       1.148797
C       -0.217505       -1.868940       -0.426822
C       -0.104963       0.628904        -0.474503
H       -0.743922       -2.752471       0.010547
H       -0.320772       -2.016877       -1.527731
C       1.208177        -1.881358       -0.015947
O       0.077820        0.847796        -1.687432
N       2.235088        -2.206763       -0.913262
C       1.751302        -1.621269       1.248716
C       3.390205        -2.152004       -0.193234
N       3.131486        -1.801009       1.130824
H       1.269609        -1.339150       2.172277
H       4.384195        -2.359468       -0.576486
N       0.445102        1.436597        0.482363
H       0.379902        1.208739        1.488110
C       1.344986        2.545243        0.128272
C       2.784647        2.067340        -0.064781
H       1.005533        3.069719        -0.800845
H       1.297533        3.327882        0.927625
O       3.046372        1.116435        -0.857248
O       3.701804        2.658972        0.561433
H       3.811366        -1.692300       1.879168
###
50
GlyHisLys3 pm6 E=-0.805317210018E-01 au
N       -1.059137       5.610687        0.467071
H       -1.784321       5.649914        1.206666
C       -1.363345       4.523670        -0.526483
H       -1.031957       6.533746        -0.009954
H       -0.141774       5.453255        0.922126
C       -1.502342       3.177156        0.151757
H       -2.296632       4.787618        -1.105835
H       -0.556946       4.486053        -1.317374
O       -1.240498       3.009402        1.348262
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N       -1.935326       2.141011        -0.647481
H       -2.196341       2.287931        -1.636593
C       -2.122657       0.779371        -0.099962
H       -2.076384       0.811182        1.032862
C       -3.487229       0.227581        -0.539614
C       -0.967323       -0.092692       -0.647535
H       -4.295126       0.952638        -0.251234
H       -3.561707       0.198984        -1.657321
C       -3.793746       -1.097349       0.043407
O       -1.082913       -0.755942       -1.694826
N       -4.774848       -1.942643       -0.513647
C       -3.281038       -1.753652       1.162351
C       -4.850187       -3.088915       0.248931
N       -3.941725       -2.983103       1.275038
H       -2.521568       -1.432538       1.869370
H       -5.523626       -3.937061       0.066135
H       -3.777094       -3.685444       2.004847
N       0.195093        -0.093856       0.075089
H       0.274399        0.436980        0.959058
C       1.430793        -0.761051       -0.410241
H       1.491217        -0.662466       -1.532145
C       2.662398        -0.102219       0.224662
C       1.328804        -2.265947       -0.069278
H       2.594251        1.003407        0.122476
H       2.676647        -0.279769       1.320421
C       3.958191        -0.603914       -0.421602
O       1.775455        -2.734305       1.005735
O       0.759060        -3.015782       -0.917328
H       3.997170        -1.712348       -0.415607
H       3.985540        -0.322300       -1.494954
C       5.178590        -0.030208       0.306692
H       5.135722        1.080678        0.313283
H       5.162628        -0.324799       1.378180
C       6.471361        -0.506570       -0.356085
H       6.524907        -1.622619       -0.385066
H       6.527208        -0.171415       -1.420771
N       7.680011        0.023965        0.390176
H       7.671325        -0.283352       1.379240
H       8.555489        -0.318444       -0.043883
H       7.699502        1.058717        0.381026
H       -5.343451       -1.739515       -1.345422
###
49
GlyHisLys4 pm6 E=-0.237412146954 au
N       -4.706558       -4.295812       -0.234590
H       -4.910242       -4.249768       -1.250158
C       -4.686315       -2.920024       0.369979
H       -5.446602       -4.869234       0.219212
H       -3.797707       -4.775374       -0.107607
C       -3.559769       -2.075478       -0.184619
H       -5.687391       -2.420153       0.211988
H       -4.603905       -2.993544       1.495064
O       -2.692577       -2.534765       -0.940380
N       -3.552666       -0.752166       0.194679
H       -4.236370       -0.378741       0.873383
C       -2.509615       0.173320        -0.299136
H       -2.317298       -0.038360       -1.394506
C       -2.979227       1.633067        -0.133923
C       -1.217059       -0.020323       0.521975
H       -3.853288       1.817583        -0.805779
H       -3.381182       1.805206        0.892332
C       -1.890583       2.588584        -0.452905
O       -1.234380       -0.165155       1.757836
N       -1.343808       3.454981        0.503317
C       -1.251633       2.780632        -1.685118
C       -0.371423       4.157682        -0.144164
N       -0.294927       3.776393        -1.483207
H       -1.412533       2.296675        -2.636594
H       0.247252        4.933057        0.294866
H       0.334076        4.150227        -2.189915
N       -0.031764       -0.001446       -0.164848
H       0.002684        0.177187        -1.182306
C       1.272145        -0.090337       0.544601
H       1.157717        -0.739085       1.459543
C       2.336708        -0.699311       -0.374222
C       1.617650        1.345343        1.009965
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H       1.967824        -1.664441       -0.785740
H       2.503208        -0.057281       -1.263684
C       3.653431        -0.930510       0.376270
O       2.325688        2.110043        0.311040
O       1.111578        1.745489        2.101004
H       4.035291        0.021327        0.797507
H       3.484382        -1.589448       1.253607
C       4.700136        -1.554453       -0.553359
H       4.320696        -2.514763       -0.966206
H       4.867999        -0.903528       -1.437959
C       6.014847        -1.782573       0.193782
H       6.437210        -0.820717       0.573948
H       5.860714        -2.428115       1.093129
N       7.033281        -2.442549       -0.715636
H       7.268427        -1.832195       -1.517546
H       7.907434        -2.646171       -0.199643
H       6.668481        -3.334749       -1.095695
###
48
GlyHisLys5 pm6 E=-0.382697519575 au
N       4.103979        4.800255        -0.174566
H       4.359681        4.770384        -1.163812
C       4.230240        3.452639        0.420320
H       3.130785        5.109678        -0.141401
C       3.294534        2.421321        -0.181993
H       5.292207        3.107523        0.331961
H       4.047577        3.521582        1.524134
O       2.456836        2.708672        -1.056153
N       3.401628        1.124889        0.277742
H       4.062385        0.873338        1.029544
C       2.532062        0.049580        -0.240833
H       2.311722        0.240691        -1.333398
C       3.216019        -1.325059       -0.094566
C       1.223439        0.026052        0.579845
H       4.107997        -1.368278       -0.765365
H       3.637469        -1.452712       0.929230
C       2.268401        -2.416397       -0.431220
O       1.230997        -0.002064       1.824550
N       1.728960        -3.278060       0.534049
C       1.748039        -2.735807       -1.692065
C       0.877199        -4.104166       -0.137803
N       0.870815        -3.804048       -1.499231
H       1.940650        -2.293282       -2.657265
H       0.298491        -4.909308       0.301963
H       0.336386        -4.273510       -2.226752
N       0.048408        0.004837        -0.122110
H       0.039265        -0.033851       -1.155084
C       -1.272257       -0.055941       0.557532
H       -1.223414       0.517099        1.526825
C       -2.348678       0.563773        -0.341442
C       -1.535967       -1.544182       0.892225
H       -2.014849       1.568633        -0.683437
H       -2.469342       -0.024947       -1.274329
C       -3.689851       0.691640        0.388674
O       -2.166972       -2.291794       0.106383
O       -1.053151       -1.994202       1.973727
H       -4.037194       -0.298955       0.745387
H       -3.571262       1.306257        1.305386
C       -4.740290       1.320896        -0.533700
H       -4.385760       2.309760        -0.898841
H       -4.870473       0.702441        -1.447753
C       -6.075997       1.474988        0.193983
H       -6.472392       0.484618        0.526431
H       -5.962160       2.088206        1.121309
N       -7.098768       2.135384        -0.710703
H       -7.220301       1.601084        -1.589082
H       -8.019711       2.193545        -0.240698
H       -6.805953       3.096281        -0.963025
###
47
GlyHisLys6 pm6 E=-0.516819189879 au
N       3.706676        4.920376        0.018326
H       3.640450        5.059554        -0.992170
C       4.114685        3.530009        0.310547
H       2.771582        5.095033        0.392268
C       3.148382        2.483345        -0.211792
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H       5.133116        3.342712        -0.118309
H       4.251432        3.413279        1.416366
O       2.176890        2.774497        -0.933611
N       3.387118        1.171584        0.139628
H       4.158013        0.919762        0.778858
C       2.526077        0.068866        -0.339698
H       2.302102        0.222655        -1.437143
C       3.235432        -1.287118       -0.148780
C       1.217172        0.052661        0.480343
H       4.101381        -1.353283       -0.851669
H       3.698799        -1.353159       0.863503
C       2.298881        -2.413565       -0.384577
O       1.221072        0.047120        1.725667
N       1.796585        -3.208307       0.655681
C       1.761875        -2.840210       -1.605985
C       0.951006        -4.101198       0.067419
N       0.913739        -3.909841       -1.312930
H       1.925413        -2.469100       -2.605993
H       0.399031        -4.882453       0.579111
H       0.375779        -4.447474       -1.989292
N       0.040670        0.018769        -0.219257
H       0.027021        -0.038853       -1.250997
C       -1.274819       -0.032696       0.470580
H       -1.214504       0.545129        1.436732
C       -2.363912       0.583860        -0.415155
C       -1.540509       -1.517902       0.815609
H       -2.043415       1.593018        -0.754251
H       -2.490915       -0.000864       -1.349043
C       -3.694364       0.691074        0.338457
O       -2.176238       -2.270020       0.037635
O       -1.054825       -1.959943       1.898738
H       -4.009389       -0.303380       0.712929
H       -3.567249       1.316676        1.246112
C       -4.787804       1.284557        -0.555896
H       -4.465272       2.268576        -0.952483
H       -4.941196       0.648172        -1.449682
C       -6.106159       1.435856        0.217783
H       -6.442509       0.448239        0.601051
H       -5.948617       2.072223        1.116362
N       -7.214423       2.032097        -0.580500
H       -7.412096       1.443267        -1.391995
H       -6.912339       2.929054        -0.967454
###
29
GlySerGly1 pm6 E=-0.262886176973 au
N       -5.156054       -0.433942       0.260039
H       -5.067689       -1.308362       -0.289527
C       -4.056206       0.532770        -0.081720
H       -6.080958       -0.009235       0.050058
H       -5.132897       -0.681141       1.266756
C       -2.687427       -0.067557       0.163668
H       -4.168636       0.873319        -1.153237
H       -4.178772       1.482509        0.517788
O       -2.538761       -1.159155       0.734437
N       -1.616836       0.679789        -0.261536
H       -1.740597       1.556870        -0.795260
C       -0.230448       0.195474        -0.072791
H       -0.172991       -0.358259       0.919266
C       0.187682        -0.777607       -1.200916
C       0.694731        1.415954        -0.030064
H       -0.556559       -0.828849       -2.022787
H       1.175350        -0.527488       -1.636282
O       0.218313        -2.114322       -0.687098
O       0.369224        2.492961        -0.553496
H       0.971488        -2.220531       -0.041035
N       1.895022        1.362091        0.641041
H       2.511229        2.190941        0.622783
C       2.490205        0.149160        1.209082
C       3.491897        -0.513216       0.290059
H       3.023852        0.408101        2.173624
H       1.715665        -0.604827       1.523754
O       4.150755        0.382771        -0.497008
O       3.759781        -1.700969       0.233381
H       4.829506        -0.048760       -1.118344
###
28
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GlySerGly2 pm6 E=-0.444130451034 au
N       -4.353780       -1.266181       -0.315294
H       -4.249815       -1.421908       -1.335439
C       -3.621552       -0.026087       0.116509
H       -5.367331       -1.174134       -0.100975
H       -3.991973       -2.101294       0.179602
C       -2.131263       -0.144048       -0.123595
H       -4.047777       0.874018        -0.416272
H       -3.826795       0.183789        1.208886
O       -1.592488       -1.196336       -0.488724
N       -1.399057       1.004711        0.086918
H       -1.835970       1.880631        0.419407
C       0.054830        1.028248        -0.154558
H       0.335524        0.160979        -0.830391
C       0.470403        2.327143        -0.872656
C       0.780106        0.911229        1.199636
H       -0.356621       2.773431        -1.461941
H       0.873578        3.103698        -0.196787
O       1.493740        1.905793        -1.801502
O       0.883635        1.890421        1.961449
H       2.061928        2.688990        -2.047257
N       1.329354        -0.275904       1.604486
H       1.848757        -0.311514       2.495593
C       1.332596        -1.517088       0.819131
C       2.417096        -1.566631       -0.251695
H       1.461846        -2.383362       1.520565
H       0.334296        -1.705215       0.334918
O       2.922002        -0.510937       -0.728856
O       2.782041        -2.699327       -0.667280
###
27
GlySerGly3 pm6 E=-0.589388572391 au
N       -4.770512       -1.247323       -0.317500
H       -4.433728       -2.098193       0.138144
C       -3.936483       -0.095981       0.085033
H       -4.679065       -1.409243       -1.323457
C       -2.450240       -0.268293       -0.168694
H       -4.312819       0.824213        -0.431082
H       -4.094183       0.106525        1.177434
O       -1.939700       -1.352373       -0.497480
N       -1.663003       0.858608        -0.027134
H       -2.055895       1.758078        0.289015
C       -0.202993       0.802946        -0.219978
H       0.052107        -0.092364       -0.871932
C       0.303031        2.076131        -0.931250
C       0.464241        0.673213        1.160457
H       -0.410472       2.425871        -1.704568
H       0.514511        2.913713        -0.236443
O       1.569282        1.804945        -1.545568
O       0.283625        1.522744        2.051406
H       1.458560        1.151608        -2.293200
N       1.255387        -0.407216       1.455347
H       1.711739        -0.461064       2.379200
C       1.687620        -1.418403       0.482819
C       3.026179        -1.085236       -0.168246
H       1.764030        -2.412873       0.997469
H       0.923198        -1.579789       -0.324348
O       3.528687        0.070466        -0.085107
O       3.615704        -2.003436       -0.799762
###
58
PheAlaArg1 pm6 E=-0.272349176275E-01 au
N       -5.825149       -1.640146       -1.585203
H       -5.414829       -2.018787       -2.460557
H       -6.397193       -0.804988       -1.823739
H       -6.463546       -2.365712       -1.196416
C       -4.750723       -1.292188       -0.572479
H       -5.272337       -0.903230       0.360264
C       -3.931880       -2.542332       -0.209340
C       -3.803006       -0.233283       -1.164883
H       -4.599204       -3.296772       0.274826
H       -3.567888       -3.054780       -1.130832
C       -2.787847       -2.201609       0.705117
O       -3.181973       -0.431005       -2.216263
C       -1.475390       -2.179171       0.209308
C       -3.026087       -1.903599       2.054941
```

```
H       -1.280320       -2.411735       -0.838817
C       -0.411612       -1.869407       1.060353
C       -1.958434       -1.595133       2.901179
H       -4.045624       -1.916216       2.445493
H       0.609608        -1.858999       0.673129
C       -0.650557       -1.577869       2.406633
H       -2.146596       -1.371165       3.952870
H       0.182016        -1.342942       3.070806
N       -3.668186       0.928425        -0.447724
H       -4.187422       1.085406        0.432065
C       -2.659434       1.952364        -0.812321
H       -2.429898       1.877247        -1.916214
C       -3.155576       3.349664        -0.478070
C       -1.397448       1.676281        0.035915
H       -3.431679       3.471047        0.580132
H       -2.392687       4.110904        -0.706603
H       -4.046069       3.619999        -1.067098
O       -1.458676       1.455590        1.255520
N       -0.185649       1.685033        -0.613492
H       -0.102801       1.903937        -1.620388
C       1.071004        1.425643        0.124116
H       0.858838        0.757492        1.018310
C       2.109732        0.745869        -0.776746
C       1.550277        2.771463        0.691941
H       1.660894        -0.163756       -1.237240
H       2.377143        1.397927        -1.636609
C       3.358126        0.371017        0.026913
O       2.427543        3.419259        -0.104573
O       1.177702        3.261749        1.748954
H       3.858662        1.288557        0.409462
H       3.076806        -0.202833       0.937251
C       4.323950        -0.448590       -0.834374
H       3.894168        -1.455973       -1.055442
H       4.498242        0.043606        -1.822123
N       5.621654        -0.581062       -0.114522
H       5.730039        -0.045292       0.764888
C       6.597704        -1.468770       -0.481883
N       6.588955        -2.096147       -1.718873
N       7.648612        -1.710604       0.399671
H       5.695515        -2.226101       -2.202985
H       7.234852        -2.882913       -1.859478
H       7.848423        -1.005688       1.118491
H       8.495242        -2.152265       0.024076
H       2.762428        4.298681        0.286464
###
57
PheAlaArg2 pm6 E=-0.207787577440 au
N       -5.623158       -1.803361       -1.633126
H       -5.174895       -2.176059       -2.492362
H       -6.213707       -0.988878       -1.896664
H       -6.250816       -2.545642       -1.258183
C       -4.592855       -1.413645       -0.590810
H       -5.153681       -1.047947       0.328276
C       -3.732135       -2.629263       -0.206460
C       -3.678278       -0.311067       -1.155281
H       -4.377702       -3.407696       0.268691
H       -3.331484       -3.130699       -1.118717
C       -2.619521       -2.237091       0.726299
O       -2.944783       -0.509864       -2.131955
C       -1.303062       -2.144214       0.249231
C       -2.891199       -1.957667       2.073681
H       -1.081152       -2.368020       -0.795433
C       -0.269507       -1.776408       1.114183
C       -1.854276       -1.586771       2.933123
H       -3.912884       -2.031171       2.451873
H       0.755745        -1.717179       0.742069
C       -0.543612       -1.492192       2.455287
H       -2.068253       -1.374702       3.982405
H       0.264940        -1.208873       3.130089
N       -3.704056       0.894546        -0.501732
H       -4.325581       1.060941        0.307623
C       -2.736924       1.970134        -0.831654
H       -2.499664       1.931912        -1.935791
C       -3.295824       3.335680        -0.467900
C       -1.466114       1.728337        0.014557
H       -3.614067       3.409779        0.582766
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H       -2.556475       4.132878       -0.644021
H       -4.175520       3.594491       -1.078454
O       -1.523890       1.548548        1.245805
N       -0.261409       1.716718       -0.634876
H       -0.181860       1.903445       -1.646943
C        1.001891       1.488773        0.112118
H        0.789055       0.855154        1.022816
C        2.026090       0.764553       -0.768180
C        1.489206       2.873158        0.602217
H        1.570516      -0.157541       -1.193384
H        2.295319       1.379484       -1.652366
C        3.276479       0.405047        0.040705
O        2.301773       3.557525       -0.068373
O        1.004264       3.306428        1.687331
H        3.759541       1.325434        0.434728
H        2.998395      -0.181797        0.943201
C        4.260474      -0.391043       -0.822704
H        3.851143      -1.405955       -1.047755
H        4.425251       0.108244       -1.808409
N        5.561324      -0.501150       -0.104843
H        5.663711       0.038066        0.773075
C        6.553445      -1.368500       -0.477915
N        6.551228      -1.995335       -1.715378
N        7.613178      -1.590418        0.397983
H        5.658264      -2.143853       -2.195060
H        7.211327      -2.769972       -1.858725
H        7.804595      -0.881745        1.115344
H        8.465619      -2.017122        0.017666
###
56
PheAlaArg3 pm6 E=-0.353981884674 au
N       -5.476011       -2.274803       -1.373449
H       -6.094603       -1.529807       -1.703204
H       -5.039425       -2.690440       -2.198378
C       -4.458943       -1.729038       -0.446715
H       -4.999443       -1.372838        0.477163
C       -3.446124       -2.823288       -0.054813
C       -3.668945       -0.561198       -1.075491
H       -3.978133       -3.628342        0.501954
H       -3.057298       -3.334608       -0.963446
C       -2.321248       -2.278731        0.780080
O       -2.989692       -0.704382       -2.107569
C       -1.026899       -2.190858        0.244919
C       -2.557020       -1.850244        2.095461
H       -0.829980       -2.527351       -0.773863
C        0.019351       -1.684470        1.020114
C       -1.508604       -1.339715        2.864080
H       -3.559983       -1.918700        2.520446
H        1.027998       -1.632506        0.604017
C       -0.219701       -1.253511        2.328294
H       -1.695826       -1.014087        3.888908
H        0.599123       -0.861399        2.932358
N       -3.747216        0.659241       -0.447560
H       -4.308539        0.785353        0.409494
C       -2.904320        1.807967       -0.857696
H       -2.681814        1.733398       -1.962407
C       -3.599254        3.126797       -0.561517
C       -1.602576        1.735743       -0.028009
H       -3.883090        3.242875        0.494687
H       -2.963109        3.985424       -0.827196
H       -4.526080        3.237455       -1.146442
O       -1.624126        1.616005        1.212844
N       -0.410950        1.793307       -0.697498
H       -0.358423        1.940608       -1.717468
C        0.875555        1.654982        0.032563
H        0.709738        1.043188        0.968821
C        1.909796        0.942947       -0.845926
C        1.305331        3.073212        0.473654
H        1.461666        0.018936       -1.276773
H        2.177320        1.562652       -1.726910
C        3.160629        0.587103       -0.036455
O        2.144656        3.739736       -0.181148
O        0.751179        3.553343        1.506231
H        3.670545        1.511033        0.311720
H        2.881693        0.045267        0.893927
C        4.110829       -0.271702       -0.877793
```

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H       3.661117        -1.277397       -1.064732
H       4.286518        0.184203        -1.882416
N       5.414995        -0.399515       -0.169629
H       5.572065        0.222391        0.643052
C       6.308121        -1.409963       -0.417144
N       6.250822        -2.169869       -1.574609
N       7.328306        -1.640340       0.501126
H       5.355466        -2.266912       -2.063459
H       6.826342        -3.019683       -1.621395
H       7.571882        -0.887760       1.155039
H       8.142639        -2.180918       0.189341
###
55
PheAlaArg4 pm6 E=-0.492557057378 au
N       -4.935368       -2.476971       -1.916424
H       -5.550729       -1.791496       -2.362382
H       -4.298675       -2.822185       -2.636675
C       -4.189010       -1.849838       -0.801693
H       -4.939538       -1.576948       -0.005619
C       -3.157055       -2.837568       -0.222234
C       -3.424043       -0.589236       -1.255584
H       -3.690135       -3.727987       0.183143
H       -2.519108       -3.252476       -1.034002
C       -2.320947       -2.208665       0.856502
O       -2.661657       -0.600217       -2.238081
C       -0.944054       -2.023594       0.661330
C       -2.911814       -1.793969       2.060366
H       -0.472960       -2.347983       -0.267824
C       -0.167931       -1.431999       1.661605
C       -2.132955       -1.195595       3.052864
H       -3.981630       -1.938039       2.222408
H       0.906361        -1.304658       1.511619
C       -0.760769       -1.011405       2.855427
H       -2.596514       -0.876504       3.988127
H       -0.153945       -0.551842       3.635778
N       -3.610856       0.561434        -0.526537
H       -4.226182       0.581400        0.301633
C       -2.870578       1.807782        -0.836098
H       -2.635012       1.834862        -1.941410
C       -3.683312       3.034977        -0.458471
C       -1.567512       1.790606        -0.004067
H       -4.023818       3.025533        0.587490
H       -3.109255       3.962020        -0.609041
H       -4.588356       3.129240        -1.079207
O       -1.572647       1.901349        1.236582
N       -0.387901       1.652602        -0.686512
H       -0.357180       1.584094        -1.715486
C       0.909860        1.571857        0.031285
H       0.746623        1.122139        1.054098
C       1.899380        0.700110        -0.748161
C       1.400368        3.025012        0.230296
H       1.452219        -0.303337       -0.925936
H       2.075856        1.115599        -1.762854
C       3.224144        0.557220        0.008371
O       2.155023        3.585828        -0.603130
O       0.977620        3.642060        1.251304
H       3.700398        1.550629        0.142088
H       3.045928        0.185429        1.040067
C       4.159632        -0.399553       -0.740575
H       3.766167        -1.438894       -0.674789
H       4.191960        -0.153927       -1.828285
N       5.556592        -0.285907       -0.211227
H       5.580775        0.149974        0.727316
C       6.390760        -1.445551       -0.296257
N       6.201124        -2.299621       -1.415516
N       7.269026        -1.644317       0.663883
H       5.739430        -1.905698       -2.235818
H       7.019453        -2.848174       -1.688850
H       7.957854        -2.387024       0.517900
###
# PEPTIDES optimized with pm6 from minimum energy conformers obtained with
# openbabel (see main text)
# opt freq pm6 scf=(xqc,tight) scrf(smd,solvent=water)
###
24
AlaAla1 pm6 E=-0.122003758050 au
```

```
N       -3.433323       -0.010819       -0.782767
H       -3.358133       -1.009727       -1.053549
H       -3.349296       0.563336        -1.643796
H       -4.381935       0.138715        -0.383193
C       -2.369364       0.366877        0.236697
H       -2.523389       1.461709        0.503996
C       -2.506467       -0.497862       1.475822
C       -0.978892       0.183394        -0.390969
H       -2.325089       -1.566484       1.281579
H       -1.807233       -0.185938       2.269019
H       -3.516055       -0.427548       1.916900
O       -0.811880       -0.465877       -1.432374
N       0.066425        0.783160        0.265603
H       -0.075084       1.300861        1.149882
C       1.452035        0.701274        -0.249059
H       1.440843        0.801072        -1.379781
C       2.306291        1.798148        0.365871
C       2.065187        -0.661355       0.097089
H       2.364033        1.738472        1.464132
H       3.340181        1.773870        -0.017068
H       1.915545        2.800935        0.128687
O       1.625496        -1.506116       0.861776
O       3.238582        -1.005603       -0.512839
H       3.613579        -0.317759       -1.161860
###
23
AlaAla2 pm6 E=-0.298701850952 au
N       3.068140        -0.379491       1.111127
H       3.724752        -0.686118       0.369628
H       2.803287        -1.209128       1.676838
H       3.576267        0.284062        1.732652
C       1.842635        0.299900        0.519502
H       1.168491        0.599245        1.385058
C       2.258959        1.529071        -0.267767
C       1.121291        -0.682014       -0.410751
H       2.940274        1.300510        -1.102480
H       1.388418        2.052095        -0.700438
H       2.774326        2.269676        0.367298
O       1.747394        -1.580818       -0.999654
N       -0.230451       -0.585180       -0.609577
H       -0.666762       -1.208644       -1.305424
C       -1.121388       0.442481        -0.021813
H       -0.630804       0.907088        0.882452
C       -1.460691       1.523388        -1.039138
C       -2.435988       -0.231450       0.432349
H       -1.946948       1.129553        -1.941928
H       -2.133748       2.283964        -0.616689
H       -0.560085       2.062631        -1.375217
O       -2.906782       -1.213700       -0.201160
O       -3.031886       0.254456        1.431203
###
22
AlaAla3 pm6 E=-0.445364956101 au
N       -3.609850       -0.486004       -0.163886
H       -3.480913       -1.457633       -0.452985
H       -3.815121       -0.502839       0.836499
C       -2.385541       0.304467        -0.437757
H       -2.272478       0.372214        -1.558396
C       -2.507449       1.704894        0.151674
C       -1.122933       -0.366597       0.142988
H       -2.565852       1.705925        1.248482
H       -1.660840       2.345853        -0.132596
H       -3.414509       2.212015        -0.209374
O       -1.192004       -1.229470       1.041963
N       0.091344        0.014315        -0.365040
H       0.157689        0.702963        -1.126942
C       1.365153        -0.575667       0.113353
H       1.216119        -0.984536       1.151774
C       1.853530        -1.685236       -0.809236
C       2.442563        0.526397        0.157691
H       2.018185        -1.346538       -1.840786
H       2.800878        -2.118517       -0.455648
H       1.135208        -2.515795       -0.865663
O       3.257957        0.527346        1.120671
O       2.513951        1.382020        -0.763155
###
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21
AlaGly1 pm6 E=-0.114066275156 au
N       2.808232        -1.321775       0.080721
H       2.883358        -1.442094       -0.947002
H       2.282402        -2.129521       0.465275
H       3.771488        -1.345241       0.474750
C       2.131644        -0.006364       0.436099
H       2.063193        0.051827        1.569239
C       2.947186        1.156327        -0.098603
C       0.722670        0.013947        -0.176504
H       2.997038        1.182275        -1.198339
H       2.537976        2.125063        0.232538
H       3.989552        1.128111        0.263850
O       0.401863        -0.747012       -1.099469
N       -0.155209       0.928158        0.349879
H       0.098128        1.541926        1.140638
C       -1.508252       1.079740        -0.200086
C       -2.417680       -0.047876       0.227841
H       -1.955354       2.056865        0.148536
H       -1.490813       1.168472        -1.320886
O       -2.355605       -0.755771       1.219144
O       -3.411370       -0.223851       -0.687770
H       -4.080651       -0.943942       -0.430523
###
20
AlaGly2 pm6 E=-0.287987663652 au
N       2.786971        -0.645127       -0.753056
H       3.397291        -0.352502       0.032002
H       2.983644        -0.028916       -1.566662
H       3.048835        -1.619288       -1.012969
C       1.316096        -0.584155       -0.368121
H       0.714602        -0.831968       -1.298865
C       1.024211        -1.592028       0.729539
C       0.994223        0.824732        0.146874
H       1.583144        -1.394002       1.658066
H       -0.045263       -1.616677       0.991015
H       1.284967        -2.620672       0.424620
O       1.833507        1.462329        0.808843
N       -0.217660       1.405681        -0.108686
H       -0.431677       2.320355        0.316690
C       -1.317398       0.772548        -0.845824
C       -2.199831       -0.140936       0.000689
H       -1.962075       1.576640        -1.294429
H       -0.940608       0.199565        -1.734168
O       -3.116325       -0.767792       -0.605821
O       -2.032413       -0.274209       1.239221
###
19
AlaGly3 pm6 E=-0.437629214749 au
N       2.932151        1.123915        -0.503749
H       2.403717        1.938615        -0.821321
H       3.238399        1.324910        0.449689
C       2.081673        -0.090676       -0.537819
H       1.865762        -0.320764       -1.621978
C       2.804739        -1.266803       0.108048
C       0.727696        0.128939        0.170614
H       2.971252        -1.127851       1.184994
H       2.258342        -2.211849       -0.022111
H       3.796307        -1.425766       -0.341268
O       0.478431        1.189833        0.784075
N       -0.199272       -0.876084       0.099959
H       -0.011141       -1.744196       -0.422954
C       -1.516098       -0.784834       0.751546
C       -2.477177       0.054084        -0.094757
H       -1.928364       -1.812966       0.906490
H       -1.436863       -0.355509       1.779734
O       -2.460636       1.310948        0.014727
O       -3.269365       -0.531243       -0.880119
###
32
AlaHis1 pm6 E=0.758030977970E-01 au
N       -3.151235       -2.398398       0.896335
H       -3.737679       -1.824287       1.529871
H       -2.396500       -2.836986       1.460121
H       -3.748118       -3.159775       0.511539
C       -2.572489       -1.565916       -0.237415
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H       -1.918086       -2.252410       -0.863575
C       -3.688726       -0.989223       -1.088361
C       -1.739587       -0.418844       0.358023
H       -4.349692       -0.305441       -0.533825
H       -3.291884       -0.430437       -1.951740
H       -4.334384       -1.779080       -1.510224
O       -2.030765       0.105207        1.440154
N       -0.662629       0.002755        -0.384727
H       -0.432469       -0.422265       -1.300394
C       0.220109        1.085060        0.098574
H       0.414321        0.943662        1.210082
C       1.555329        1.092095        -0.666400
C       -0.464519       2.445290        -0.091489
H       1.376456        1.151468        -1.772685
H       2.116380        2.034853        -0.423436
C       2.386602        -0.091911       -0.360583
O       -1.406856       2.705210        -0.821408
O       -0.003884       3.490311        0.651915
N       3.369302        -0.103247       0.649238
C       2.411641        -1.347865       -0.967977
H       3.595647        0.677750        1.276468
C       3.977549        -1.338744       0.652707
N       3.399236        -2.107405       -0.332938
H       1.806671        -1.727906       -1.787782
H       4.786396        -1.653883       1.324787
H       0.794506        3.278051        1.250599
H       3.652307        -3.074724       -0.562933
###
31
AlaHis2 pm6 E=-0.971828765345E-01 au
N       3.724524        -0.963796       -1.399592
H       4.486687        -1.363754       -0.821481
H       3.990688        0.004165        -1.666946
H       3.655007        -1.530672       -2.271137
C       2.397216        -0.986254       -0.658346
H       1.598952        -0.613456       -1.377883
C       2.072162        -2.400782       -0.213016
C       2.483468        -0.079956       0.576479
H       2.819060        -2.820207       0.479564
H       1.097206        -2.452853       0.299854
H       2.007388        -3.094772       -1.068468
O       3.540010        0.031518        1.218539
N       1.369945        0.588495        1.019681
H       1.442155        1.164487        1.874217
C       0.081107        0.676690        0.300188
H       0.075657        -0.033623       -0.583125
C       -1.072258       0.317728        1.256620
C       -0.091063       2.101193        -0.284056
H       -0.712702       -0.371980       2.063720
H       -1.416096       1.219457        1.820395
C       -2.211775       -0.319674       0.557876
O       0.888487        2.892052        -0.327766
O       -1.213521       2.435123        -0.748785
N       -2.887410       0.279217        -0.523761
C       -2.845933       -1.535554       0.809298
H       -2.622260       1.185213        -0.953327
C       -3.907369       -0.557067       -0.923777
N       -3.893012       -1.667575       -0.111157
H       -2.622995       -2.287349       1.560452
H       -4.606090       -0.368202       -1.748053
H       -4.544129       -2.458323       -0.167467
###
30
AlaHis3 pm6 E=-0.252907813947 au
N       -3.340500       0.711416        -1.104054
H       -3.753488       0.055676        -1.794936
H       -2.511393       1.167363        -1.538208
H       -4.050291       1.449479        -0.907220
C       -2.958078       -0.001577       0.184605
H       -2.603412       0.782678        0.924152
C       -4.165628       -0.712762       0.767943
C       -1.852619       -1.024955       -0.123962
H       -4.587393       -1.476596       0.096527
H       -3.915351       -1.217778       1.715656
H       -4.983756       -0.009329       0.998801
O       -2.100347       -2.069272       -0.750456
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N       -0.575994       -0.823903       0.329104
H       0.133081        -1.547307       0.121717
C       -0.077535       0.420638        0.958665
H       -0.799357       0.745716        1.767807
C       1.297069        0.169774        1.604894
C       0.013014        1.573661        -0.069858
H       1.591932        1.076409        2.183330
H       1.200069        -0.624671       2.384555
C       2.354219        -0.203339       0.631663
O       -0.314909       1.384652        -1.267669
O       0.417219        2.695903        0.339422
N       3.139757        0.743447        -0.041786
C       2.735338        -1.493045       0.241039
C       3.985103        0.030009        -0.838451
N       3.765652        -1.337349       -0.690396
H       2.364477        -2.456336       0.554660
H       4.734372        0.449683        -1.502122
H       4.257087        -2.090951       -1.164399
###
29
AlaHis4 pm6 E=-0.406594357063 au
N       -4.690165       -0.250878       0.132491
H       -4.798107       0.535289        0.777829
H       -4.812319       0.127932        -0.807798
C       -3.349382       -0.866623       0.286877
H       -3.324521       -1.365994       1.297968
C       -3.095577       -1.900533       -0.803961
C       -2.224549       0.185973        0.222217
H       -3.075590       -1.468617       -1.813238
H       -2.147579       -2.435217       -0.652904
H       -3.882540       -2.670013       -0.815379
O       -2.374736       1.261851        -0.398069
N       -1.044302       -0.080644       0.862021
H       -0.891471       -0.968353       1.365223
C       0.067463        0.904619        0.883619
H       -0.289124       1.815649        1.449444
C       1.294797        0.338990        1.619704
C       0.425577        1.354817        -0.551207
H       1.759970        1.162506        2.215436
H       0.969006        -0.392665       2.399510
C       2.318534        -0.268649       0.734999
O       0.688301        2.573189        -0.738582
O       0.441295        0.532487        -1.507601
N       2.285201        -1.604439       0.313922
C       3.438279        0.370914        0.185040
C       3.373204        -1.768191       -0.492552
N       4.100954        -0.585193       -0.588596
H       3.792671        1.381200        0.305596
H       3.654566        -2.689030       -0.993711
H       4.954274        -0.432723       -1.121238
###
34
AlaLys3 pm6 E=-0.336023136336 au
N       3.863131        -0.690387       1.634320
H       3.072984        -1.164855       2.077264
H       3.860080        0.275681        1.967510
C       3.757730        -0.736244       0.158132
H       4.682657        -0.244288       -0.260869
C       3.671752        -2.170773       -0.346152
C       2.553048        0.057278        -0.400519
H       2.848310        -2.737676       0.111711
H       3.531944        -2.217454       -1.435523
H       4.595993        -2.726383       -0.129763
O       2.748261        0.979055        -1.225669
N       1.291487        -0.259191       0.018905
H       1.133607        -1.023201       0.698657
C       0.079526        0.427006        -0.498435
H       0.209084        0.633077        -1.599108
C       -1.150081       -0.466734       -0.292826
C       -0.044933       1.787970        0.228314
H       -0.972059       -1.455678       -0.769748
H       -1.291328       -0.695547       0.784900
C       -2.419010       0.169395        -0.871709
O       0.523560        2.784331        -0.312279
O       -0.659279       1.905713        1.315375
H       -2.755685       1.010429        -0.233454
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H       -2.202469       0.625375        -1.861777
C       -3.549022       -0.850486       -1.044343
H       -4.370787       -0.391560       -1.638441
H       -3.195587       -1.702291       -1.668612
C       -4.094361       -1.415036       0.264838
H       -4.647851       -2.368795       0.075356
H       -3.273319       -1.682232       0.973741
N       -5.034299       -0.436825       0.943363
H       -5.816508       -0.176632       0.317181
H       -5.437979       -0.852184       1.802967
H       -4.541540       0.431980        1.208675
###
33
AlaLys4 pm6 E=-0.467608178083 au
N       4.134486        -1.960007       -0.612925
H       4.792027        -1.217401       -0.853423
H       3.719442        -2.286949       -1.488739
C       3.084014        -1.458784       0.304700
H       2.366086        -2.305940       0.497550
C       3.691166        -0.992920       1.624238
C       2.328948        -0.255034       -0.298411
H       4.422560        -0.183525       1.500753
H       2.923222        -0.636555       2.325388
H       4.215996        -1.814708       2.133499
O       2.946990        0.698327        -0.826509
N       0.962236        -0.252545       -0.240138
H       0.446919        -1.017818       0.222660
C       0.154648        0.871039        -0.775087
H       0.673180        1.289585        -1.688122
C       -1.249165       0.432675        -1.211789
C       0.136327        1.995315        0.288274
H       -1.816433       1.346377        -1.498711
H       -1.170458       -0.146963       -2.157007
C       -2.033628       -0.380569       -0.177013
O       1.089865        2.833625        0.249982
O       -0.761382       2.092242        1.157900
H       -1.643316       -1.417966       -0.125587
H       -1.879860       0.033499        0.838911
C       -3.529446       -0.400197       -0.512063
H       -3.922562       0.634918        -0.576915
H       -3.689074       -0.829422       -1.521154
C       -4.314870       -1.199704       0.534915
H       -4.015853       -2.270438       0.513169
H       -4.062349       -0.842935       1.557062
N       -5.785597       -1.135480       0.258044
H       -6.291767       -1.391120       1.108880
H       -6.057381       -0.170893       0.059350
###
25
AsnGly1 pm6 E=-0.193244563947 au
N       2.328209        -2.297961       -0.078473
H       2.005699        -3.100854       0.498527
H       3.355258        -2.188140       0.065690
H       2.170614        -2.531099       -1.078226
C       1.600876        -1.025020       0.319114
H       1.807645        -0.844442       1.423931
C       2.125018        0.151958        -0.505917
C       0.093727        -1.218025       0.057865
H       3.241113        0.067016        -0.625910
H       1.768805        0.103493        -1.569129
C       1.752671        1.490745        0.077500
O       -0.307072       -1.829282       -0.939434
O       0.675491        1.680977        0.684146
N       2.628049        2.521450        -0.083522
H       2.415149        3.453831        0.263472
H       3.512438        2.422804        -0.581080
N       -0.761765       -0.700908       0.999811
H       -0.414582       -0.078234       1.748934
C       -2.210907       -0.676192       0.765158
C       -2.624826       0.429300        -0.173778
H       -2.579846       -1.664598       0.366639
H       -2.746357       -0.564450       1.753757
O       -1.883408       1.171014        -0.812242
O       -3.953134       0.643163        -0.372667
H       -4.571758       0.023034        0.150602
###
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24
AsnGly2 pm6 E=-0.375440657175 au
N       -0.626930       2.529720        -0.261552
H       0.154076        2.923349        0.301219
H       -1.409878       3.219071        -0.245543
H       -0.306848       2.438742        -1.248910
C       -1.092343       1.199262        0.301088
H       -1.533299       1.399072        1.333176
C       -2.180168       0.612109        -0.594710
C       0.097071        0.237101        0.504966
H       -2.979918       1.386863        -0.772098
H       -1.807576       0.416235        -1.636342
C       -2.801304       -0.636860       -0.029591
O       0.416382        -0.088975       1.663229
O       -2.340551       -1.233531       0.969755
N       -3.903830       -1.133500       -0.658658
H       -4.377133       -1.966289       -0.317411
H       -4.315966       -0.692617       -1.480665
N       0.755735        -0.256529       -0.581520
H       0.513339        0.026364        -1.546844
C       1.892687        -1.180960       -0.429938
C       3.194677        -0.412931       -0.185498
H       1.724517        -1.908233       0.403142
H       1.978119        -1.814990       -1.348399
O       3.384627        0.150368        0.928136
O       4.054796        -0.366828       -1.102008
###
23
AsnGly3 pm6 E=-0.524835057209 au
N       0.910176        2.588788        -0.429106
H       0.029922        2.837263        -0.888594
H       0.846297        2.908347        0.538994
C       1.132434        1.125578        -0.498102
H       1.251016        0.847472        -1.585990
C       2.414938        0.758676        0.263688
C       -0.057602       0.359953        0.123452
H       3.262328        1.379292        -0.123371
H       2.354399        1.063252        1.335941
C       2.729655        -0.712435       0.181921
O       -0.335448       0.480848        1.336285
O       2.156744        -1.545985       0.927102
N       3.662146        -1.139819       -0.710078
H       3.923992        -2.120431       -0.780602
H       4.151769        -0.505393       -1.340423
N       -0.798140       -0.446320       -0.692654
H       -0.598190       -0.527885       -1.702013
C       -1.935243       -1.236577       -0.187458
C       -3.184140       -0.363354       -0.044910
H       -2.134384       -2.091037       -0.882174
H       -1.694907       -1.719468       0.790672
O       -4.016747       -0.307938       -0.985247
O       -3.356020       0.287948        1.025469
###
24
AspGly1 pm6 E=-0.260721851037 au
N       1.710090        -1.807279       -1.204101
H       1.170991        -2.672929       -1.425333
H       2.722475        -2.026426       -1.343121
H       1.448914        -1.073030       -1.892265
C       1.472073        -1.357689       0.225158
H       1.720444        -2.250996       0.903293
C       2.429966        -0.223696       0.583782
C       0.023682        -0.974930       0.577394
H       2.479648        -0.108141       1.706565
H       3.490528        -0.523708       0.347058
C       2.110261        1.109346        -0.010636
O       -0.181532       -0.420444       1.671380
O       3.242492        1.795269        -0.305835
O       1.010514        1.613028        -0.208672
N       -1.013791       -1.248394       -0.270939
H       -0.905851       -1.691622       -1.197794
C       -2.398074       -0.932187       0.113814
C       -2.727605       0.524512        -0.114740
H       -3.103396       -1.596833       -0.462878
H       -2.605015       -1.182695       1.194175
O       -1.989434       1.494414        0.010069
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O       -4.022242       0.677605        -0.472616
H       3.071567        2.718424        -0.700362
H       -4.304615       1.646558        -0.607304
###
23
AspGly2 pm6 E=-0.442747814890 au
C       1.959726        0.177542        1.088708
C       1.956709        1.357998        0.138803
O       0.882223        1.729322        -0.420848
C       1.530536        -1.160448       0.501096
C       0.143783        -1.066738       -0.154250
N       -0.931331       -1.130272       0.688836
C       -2.304930       -1.040204       0.179961
C       -2.751628       0.390878        -0.002922
O       -4.093539       0.492840        0.119732
N       2.538505        -1.663489       -0.518961
O       0.014157        -0.916514       -1.379598
O       3.027655        1.989422        -0.064149
O       -2.067846       1.376327        -0.258395
H       2.307453        -2.633704       -0.819794
H       3.495026        -1.676762       -0.104256
H       2.567440        -1.064100       -1.364424
H       1.502678        -1.931111       1.345586
H       1.307895        0.422909        1.968334
H       2.971010        0.071316        1.558871
H       -0.821871       -1.216865       1.714751
H       -2.426097       -1.582547       -0.802646
H       -3.000800       -1.586228       0.880464
H       -4.459318       1.428075        -0.048328
###
22
AspGly3 pm6 E=-0.624232706989 au
N       -2.832529       -1.696623       -0.139326
H       -2.513528       -2.656733       -0.385210
H       -3.711064       -1.504099       -0.668170
H       -3.064086       -1.678634       0.873629
C       -1.777035       -0.667153       -0.492970
H       -1.632767       -0.704522       -1.622327
C       -2.250232       0.732279        -0.092356
C       -0.452708       -0.986867       0.231213
H       -3.064942       1.072046        -0.780293
H       -2.746008       0.724976        0.907831
C       -1.119717       1.741206        -0.101190
O       -0.334319       -0.839601       1.462838
O       -0.613014       2.108338        1.003397
O       -0.660400       2.189683        -1.183025
N       0.595895        -1.350582       -0.556042
H       0.494403        -1.497714       -1.575978
C       1.964768        -1.439583       -0.022308
C       2.624549        -0.059796       0.006342
H       1.990570        -1.892581       1.000946
H       2.561166        -2.151223       -0.649710
O       2.069902        0.891601        0.634340
O       3.713448        0.112278        -0.593241
###
21
AspGly4 pm6 E=-0.765834640640 au
N       1.694484        1.818788        0.489496
H       2.525334        2.149892        -0.006489
H       2.007361        1.542303        1.423212
C       1.093303        0.665639        -0.227906
H       1.109579        0.881722        -1.334091
C       1.760472        -0.691642       0.026532
C       -0.355133       0.586683        0.287995
H       1.574784        -1.037693       1.067644
H       1.280418        -1.474684       -0.611155
C       3.242359        -0.699680       -0.253133
O       -0.606351       0.320401        1.482215
O       4.004761        -1.313756       0.552634
O       3.727215        -0.133378       -1.272365
N       -1.357196       0.841663        -0.606438
H       -1.165750       1.026427        -1.602989
C       -2.772247       0.896731        -0.200634
C       -3.376839       -0.504847       -0.112541
H       -2.896142       1.424137        0.777497
H       -3.342908       1.523973        -0.931030
```

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O       -3.127048       -1.230474       0.891635
O       -4.124225       -0.914861       -1.039856
###
35
AspHis0 pm6 E=-0.702450492174E-01 au
N       -1.314142       -2.944220       0.565041
H       -0.307519       -3.088712       0.340954
H       -1.851820       -3.734384       0.147202
H       -1.432440       -2.994622       1.596563
C       -1.809439       -1.620696       0.009036
H       -1.714279       -1.668365       -1.127079
C       -3.277874       -1.418743       0.384345
C       -0.946019       -0.473868       0.582322
H       -3.848436       -2.384389       0.268682
H       -3.398545       -1.193902       1.480568
C       -3.970047       -0.361715       -0.414926
O       -1.130142       -0.023213       1.716626
O       -3.254285       0.795426        -0.496116
O       -5.065890       -0.437039       -0.947372
N       0.022349        0.030602        -0.252364
H       0.196000        -0.368498       -1.194320
C       0.894580        1.145212        0.180224
H       1.184985        1.008139        1.267869
C       2.158565        1.239866        -0.688760
C       0.097986        2.453476        0.037270
H       1.894555        1.306918        -1.776753
H       2.685060        2.207643        -0.472049
C       3.064991        0.092810        -0.468378
O       -0.383918       2.944421        -0.966150
O       -0.047945       3.039251        1.252558
N       4.085985        0.084903        0.502273
C       3.118420        -1.135870       -1.127665
H       4.303912        0.848711        1.152889
C       4.742676        -1.123680       0.433777
N       4.158999        -1.877341       -0.560385
H       2.498467        -1.508913       -1.939735
H       5.589401        -1.430890       1.061928
H       4.441229        -2.824586       -0.836926
H       -3.728715       1.523766        -1.024326
H       -0.569792       3.912967        1.232745
###
34
AspHis2 pm6 E=-0.255074167928 au
N       -2.737713       -2.530590       0.938462
H       -2.163169       -2.954851       1.695631
H       -3.271426       -3.298442       0.474049
H       -3.421121       -1.883636       1.374381
C       -1.857148       -1.816743       -0.072749
H       -1.179635       -2.606474       -0.551906
C       -2.693213       -1.182668       -1.177978
C       -0.980070       -0.781090       0.650856
H       -2.034137       -0.968435       -2.072804
H       -3.407138       -1.944856       -1.606554
C       -3.417447       0.072987        -0.820997
O       -1.203873       -0.474193       1.831969
O       -4.550985       0.204470        -1.552912
O       -3.091837       0.950050        -0.026866
N       0.032117        -0.216585       -0.074938
H       0.214923        -0.486359       -1.058183
C       0.843479        0.892417        0.489421
H       1.177151        0.620248        1.532582
C       2.059597        1.193237        -0.389214
C       -0.075603       2.141960        0.577604
H       1.753886        1.321438        -1.460656
H       2.476845        2.198106        -0.107042
C       3.136999        0.183099        -0.284003
O       -0.491871       2.487011        1.716067
O       -0.434855       2.747163        -0.462908
N       4.166155        0.100316        -1.243776
C       3.403996        -0.788996       0.679898
H       4.253172        0.684964        -2.083996
C       5.038378        -0.900004       -0.867007
N       4.580250        -1.449695       0.305925
H       2.855395        -1.044088       1.581637
H       5.941404        -1.202770       -1.413682
H       5.021442        -2.219014       0.821867
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H       -5.069702       1.058848        -1.362841
###
33
AspHis3 pm6 E=-0.426682316146 au
N       -3.066217       -1.897894       0.571465
H       -2.437270       -2.629549       0.180667
H       -4.053144       -2.166403       0.354514
H       -2.961018       -1.891377       1.605408
C       -2.765987       -0.535867       -0.032460
H       -2.756346       -0.651136       -1.165507
C       -3.839326       0.473871        0.363070
C       -1.387934       -0.040289       0.451923
H       -3.985929       0.505366        1.471793
H       -3.494714       1.505313        0.110888
C       -5.177713       0.202295        -0.293560
O       -1.281440       0.748700        1.404074
O       -5.657078       -0.963019       -0.293833
O       -5.806842       1.166584        -0.817214
N       -0.294347       -0.484847       -0.237707
H       -0.381487       -1.143459       -1.033692
C       1.075139        -0.079230       0.162808
H       1.147894        -0.084539       1.290762
C       2.098859        -1.066235       -0.412703
C       1.316485        1.374587        -0.326772
H       1.903460        -2.095231       -0.008353
H       1.954503        -1.194050       -1.516372
C       3.492980        -0.677291       -0.101923
O       1.594375        1.623823        -1.523574
O       1.208079        2.288048        0.538156
N       4.561207        -0.948376       -0.978779
C       4.036309        -0.036324       1.012669
H       4.488771        -1.426124       -1.885583
C       5.726308        -0.479707       -0.409038
N       5.414989        0.083084        0.806240
H       3.547265        0.316568        1.915691
H       6.729477        -0.551523       -0.849192
H       6.081647        0.514433        1.455498
###
32
AspHis4 pm6 E=-0.593289385252 au
N       -3.911390       -2.072071       -0.325882
H       -3.476532       -2.859032       -0.850604
H       -4.897998       -1.974985       -0.650143
H       -3.937989       -2.327402       0.681037
C       -3.148007       -0.779186       -0.557229
H       -3.144942       -0.581271       -1.677478
C       -3.841561       0.368587        0.174379
C       -1.714207       -0.941080       -0.018948
H       -4.892266       0.478647        -0.197962
H       -3.984741       0.137161        1.257510
C       -3.108706       1.686567        0.018882
O       -1.513689       -1.219230       1.178621
O       -2.211727       2.002915        0.860226
O       -3.402194       2.461126        -0.925011
N       -0.686793       -0.710994       -0.882291
H       -0.848608       -0.461840       -1.875739
C       0.728246        -0.805731       -0.442883
H       1.022400        -1.896987       -0.440417
C       1.647790        -0.038841       -1.412544
C       0.919024        -0.256324       0.988405
H       1.701117        -0.582811       -2.386730
H       1.218171        0.951510        -1.683068
C       3.005139        0.104692        -0.828906
O       1.564306        -0.969498       1.801898
O       0.476193        0.877030        1.327890
N       3.503446        1.331272        -0.368338
C       3.948238        -0.904594       -0.597765
C       4.741645        1.065333        0.136319
N       5.043710        -0.288676       0.013550
H       3.916862        -1.956643       -0.830451
H       5.416054        1.795114        0.573028
H       5.896936        -0.753457       0.314482
###
31
AspHis5 pm6 E=-0.733824742156 au
N       5.554759        0.274851        -0.244642
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C       4.382660        0.439020        -0.988173
C       3.500259        -0.561836       -0.561649
N       4.112640        -1.340245       0.429730
C       5.356121        -0.811726       0.604824
C       2.106351        -0.797462       -1.013942
C       1.104684        -0.284345       0.035999
C       1.282252        1.241593        0.201537
O       0.746342        2.050569        -0.598408
N       -0.287139       -0.614382       -0.354918
C       -1.339949       -0.282821       0.455512
O       -1.149987       0.343897        1.518047
C       -2.748424       -0.707265       0.006984
C       -3.618848       0.554358        -0.047609
C       -5.050732       0.272980        -0.430293
O       -5.334781       -0.571726       -1.325260
N       -3.183748       -1.737085       0.984366
O       -5.970236       0.918908        0.153852
O       1.988346        1.648386        1.167588
H       -3.977718       -2.262631       0.609710
H       -3.514879       -1.298633       1.847877
H       -2.711690       -1.176630       -1.016989
H       -3.585574       1.099191        0.922048
H       -3.198366       1.280117        -0.785934
H       -0.420146       -1.115693       -1.247947
H       1.318680        -0.772806       1.029686
H       1.936166        -1.884967       -1.201861
H       1.931708        -0.317098       -2.003885
H       4.264936        1.203268        -1.738619
H       6.103885        -1.175539       1.302445
H       6.393694        0.844193        -0.323968
###
34
AspHis pm6 E=-0.247341337805 au
N       3.381002        2.160104        -0.240582
H       2.807105        2.775757        -0.854058
H       4.382313        2.300736        -0.498385
H       3.263104        2.470269        0.744461
C       2.998278        0.698972        -0.414749
H       3.102417        0.442950        -1.520582
C       3.954365        -0.171415       0.396414
C       1.527402        0.485601        0.020091
H       5.011781        0.171021        0.250439
H       3.797081        -0.037204       1.492285
C       3.860469        -1.640249       0.026986
O       1.237242        -0.056834       1.092778
O       3.074591        -2.395250       0.671369
O       4.584001        -2.106541       -0.893045
N       0.576815        0.898316        -0.879452
H       0.854676        1.372282        -1.764256
C       -0.880067       0.746962        -0.694221
H       -1.359469       0.988791        -1.702736
C       -1.296107       -0.672072       -0.274645
C       -1.390723       1.809128        0.293664
H       -0.852502       -1.414248       -0.989815
H       -0.850006       -0.942854       0.715021
C       -2.768317       -0.831305       -0.260350
O       -1.879276       2.883285        -0.008743
O       -1.268628       1.445583        1.592913
N       -3.451585       -1.508707       0.768112
C       -3.730075       -0.417181       -1.183258
H       -3.021143       -1.947103       1.591444
C       -4.798104       -1.503964       0.476302
N       -4.978696       -0.837665       -0.714148
H       -3.605036       0.130299        -2.114261
H       -5.588684       -1.958707       1.087524
H       -5.878052       -0.678985       -1.180669
H       -1.602501       2.153837        2.246484
###
29
CysAsn1 pm6 E=-0.196398694357 au
N       -2.814064       -2.166167       0.096219
H       -2.215382       -3.013652       0.171807
H       -3.688182       -2.434866       -0.407073
H       -3.074319       -1.877352       1.056173
C       -2.092049       -1.065146       -0.661258
H       -1.769972       -1.507371       -1.664913
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C       -3.001908       0.122272        -0.918957
C       -0.849734       -0.625220       0.132521
H       -2.612192       0.725382        -1.777872
H       -4.015267       -0.196224       -1.259868
S       -3.068605       1.194348        0.533944
O       -0.682689       -0.945823       1.312854
H       -4.068705       0.602769        1.236517
N       0.073633        0.123127        -0.560778
H       -0.065678       0.376918        -1.555940
C       1.320215        0.599034        0.076941
H       1.304958        0.366891        1.191975
C       2.545155        -0.055851       -0.572816
C       1.380043        2.127237        -0.039975
H       2.497601        0.016302        -1.688212
H       3.473340        0.519123        -0.319467
C       2.681551        -1.502682       -0.164429
O       2.647707        2.580995        0.112853
O       0.451416        2.900332        -0.199481
O       2.114555        -2.419753       -0.799890
N       3.446655        -1.805948       0.919802
H       3.577353        -2.766790       1.227507
H       3.937269        -1.097428       1.464057
H       2.725743        3.595779        0.072666
###
28
CysAsn2 pm6 E=-0.374220386433 au
N       -2.586848       -0.527229       1.800259
H       -2.169526       -1.342553       2.295874
H       -3.559216       -0.398631       2.160797
H       -2.045589       0.316825        2.057948
C       -2.628906       -0.771395       0.304370
H       -3.301456       -1.688298       0.149654
C       -3.268548       0.388363        -0.440762
C       -1.267180       -1.139696       -0.312134
H       -3.543282       0.068644        -1.478439
H       -4.253477       0.658854        0.012621
S       -2.179433       1.822332        -0.580909
O       -1.218865       -2.090489       -1.109383
H       -2.492879       2.482683        0.563851
N       -0.143619       -0.420950       -0.007266
H       -0.151573       0.402328        0.622863
C       1.134163        -0.672757       -0.715990
H       0.922476        -1.223855       -1.682466
C       1.856011        0.626741        -1.079383
C       2.038249        -1.582432       0.154689
H       2.779616        0.376293        -1.662798
H       1.249175        1.202397        -1.828884
C       2.157628        1.538530        0.077741
O       2.444474        -1.213672       1.285389
O       2.364446        -2.696293       -0.335614
O       1.398612        1.631865        1.073008
N       3.292930        2.290023        0.037775
H       3.511805        2.960795        0.771291
H       3.949773        2.258882        -0.741548
###
27
CysAsn3 pm6 E=-0.534624907583 au
N       -2.877380       -2.102077       0.469431
H       -2.340636       -2.816456       0.996243
H       -3.637177       -2.587817       -0.049300
H       -3.316678       -1.452193       1.151041
C       -1.984076       -1.345514       -0.498223
H       -1.573267       -2.091215       -1.250195
C       -2.791822       -0.260652       -1.202385
C       -0.830646       -0.697094       0.272401
H       -2.193355       0.245932        -1.981674
H       -3.673577       -0.682201       -1.722420
S       -3.325693       0.906553        0.085662
O       -0.760456       -0.695668       1.510691
N       0.168645        -0.138712       -0.492232
H       0.111801        -0.115221       -1.523638
C       1.303210        0.580745        0.133798
H       1.408412        0.261649        1.212866
C       2.611395        0.306485        -0.607807
C       0.935000        2.086411        0.123133
H       2.466320        0.330199        -1.715699
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H       3.335384        1.137759        -0.417556
C       3.210115        -1.021602       -0.211719
O       1.379605        2.864035        -0.751104
O       0.141055        2.489197        1.024530
O       2.948379        -2.069460       -0.844747
N       4.058023        -1.066933       0.852398
H       4.491753        -1.936898       1.153102
H       4.299364        -0.241839       1.399314
###
26
CysAsn4 pm6 E=-0.682735503445 au
N       2.857569        2.521180        0.171052
H       2.025802        3.111542        0.097784
H       3.113595        2.487189        1.158564
C       2.582198        1.162979        -0.360326
H       2.426542        1.268018        -1.470965
C       3.737834        0.204235        -0.087900
C       1.322697        0.551245        0.285638
H       4.615651        0.424575        -0.716451
H       4.077317        0.221814        0.960594
S       3.045792        -1.429844       -0.508218
O       1.220213        0.396101        1.524245
N       0.226316        0.324003        -0.517919
H       0.308792        0.334962        -1.543833
C       -1.100491       -0.030719       0.037687
H       -1.213772       0.447676        1.056005
C       -2.193763       0.500902        -0.897461
C       -1.190791       -1.563261       0.242889
H       -1.864625       1.459113        -1.377228
H       -2.340308       -0.173617       -1.774473
C       -3.507113       0.681700        -0.180508
O       -1.978095       -2.265091       -0.442105
O       -0.467817       -2.094198       1.135959
O       -4.192081       -0.303365       0.194111
N       -3.961439       1.940964        0.051406
H       -4.845600       2.111209        0.526038
H       -3.454373       2.771929        -0.254126
###
42
DLeuTyr3 pm6 E=-0.506406471399 au
C       1.857638        -1.147591       0.061613
C       3.204900        -0.408775       0.083664
C       0.752694        -0.208448       -0.446289
H       3.295951        0.243643        -0.809140
H       3.249001        0.283106        0.950818
C       4.406150        -1.377802       0.134497
O       0.106309        -0.496546       -1.473410
H       4.245617        -2.099378       0.975523
C       4.533265        -2.171360       -1.168737
C       5.690454        -0.591670       0.414347
H       4.718080        -1.523424       -2.032925
H       5.360945        -2.888982       -1.126527
H       3.624283        -2.747499       -1.385903
H       5.642813        -0.057130       1.370590
H       6.564430        -1.252038       0.463579
H       5.900287        0.155050        -0.359969
N       0.516033        0.964726        0.225424
H       0.971252        1.157462        1.130071
C       -0.532826       1.918573        -0.208170
H       -0.795872       1.717296        -1.285371
C       -1.803684       1.816066        0.650240
C       0.084167        3.332957        -0.113632
H       -1.550187       1.906824        1.729444
H       -2.457414       2.693614        0.438857
C       -2.553515       0.543129        0.382961
O       0.201833        3.912935        0.995355
O       0.484062        3.870836        -1.183352
C       -2.538350       -0.497797       1.324270
C       -3.280907       0.393740        -0.811795
H       -1.973408       -0.388870       2.253711
C       -3.251376       -1.674457       1.092220
C       -3.996264       -0.772921       -1.067422
H       -3.292027       1.202367        -1.547611
H       -3.252788       -2.484330       1.822874
C       -3.975463       -1.789886       -0.099976
H       -4.565065       -0.898042       -1.988088
```

```
O       -4.726641       -2.911376       -0.403826
H       -4.699386       -3.590366       0.341002
N       1.405235        -1.697730       1.367499
H       2.010166        -2.483416       1.627700
H       1.525773        -0.999355       2.107875
H       1.922871        -2.004838       -0.671851
###
41
DLeuTyr4 pm6 E=-0.668085049982 au
C       -2.448325       1.316898        0.853249
C       -1.254051       2.281077        0.972814
C       -2.060390       0.101776        0.001601
H       -1.580963       3.185683        1.527506
H       -0.492796       1.819048        1.639118
C       -0.593288       2.696297        -0.359231
O       -2.520658       -0.128652       -1.134055
H       -0.550827       1.808831        -1.039600
C       -1.382098       3.800230        -1.067754
C       0.845299        3.157128        -0.096229
H       -1.470266       4.707308        -0.458784
H       -0.903393       4.097706        -2.009030
H       -2.404380       3.484301        -1.321790
H       1.453824        2.361901        0.350557
H       1.343987        3.468637        -1.021670
H       0.886735        4.014238        0.586653
N       -1.165150       -0.776370       0.569860
H       -0.751062       -0.592783       1.497907
C       -0.619047       -1.936007       -0.177169
H       -0.398475       -1.628132       -1.238041
C       0.672533        -2.455233       0.475225
C       -1.708408       -3.030894       -0.208542
H       0.509348        -2.666190       1.554622
H       0.926352        -3.443765       0.028837
C       1.807469        -1.491158       0.290015
O       -1.999785       -3.696603       0.817877
O       -2.323206       -3.212388       -1.299274
C       2.097455        -0.529619       1.273197
C       2.586912        -1.534222       -0.878299
H       1.499353        -0.493487       2.188094
C       3.136335        0.373953        1.100770
C       3.630780        -0.641427       -1.071979
H       2.366313        -2.279711       -1.645980
H       3.357900        1.112480        1.863237
C       3.924240        0.336393        -0.081962
H       4.230057        -0.680370       -1.974470
O       4.894297        1.182174        -0.261514
N       -3.690939       1.907814        0.292321
H       -4.075002       2.582131        0.961495
H       -3.473777       2.447951        -0.556168
H       -2.697966       0.946723        1.893751
###
41
GluHisOMe2 pm6 E=-0.737786364948E-01 au
N       1.309049        -2.986364       -0.620205
H       1.631127        -2.706455       -1.565757
H       0.361195        -3.405675       -0.711467
H       1.954806        -3.724605       -0.270034
C       1.285295        -1.811823       0.339604
H       0.786129        -2.178170       1.299670
C       2.697792        -1.344742       0.712452
C       0.467854        -0.666420       -0.279520
H       2.604330        -0.578327       1.521467
H       3.241194        -2.194462       1.194878
C       3.517088        -0.794134       -0.453673
O       0.672424        -0.253496       -1.425163
H       3.602627        -1.543383       -1.279639
H       2.998641        0.079301        -0.928677
C       4.885825        -0.379225       -0.023907
O       5.946126        -0.843213       -0.425338
O       5.034768        0.629014        0.893778
N       -0.500382       -0.116079       0.528760
H       -0.692849       -0.482087       1.479413
C       -1.382926       0.961608        0.034528
H       -1.534690       0.853501        -1.084048
C       -2.745707       0.946636        0.747229
C       -0.697676       2.310408        0.317124
```

```
H       -2.614670       0.977131        1.860888
H       -3.299533       1.892965        0.507200
C       -3.551142       -0.236827       0.376466
O       -0.343954       2.775388        1.383192
N       -4.520253       -0.222342       -0.646037
C       -3.553968       -1.520737       0.922911
C       -5.098561       -1.470254       -0.718082
N       -4.514039       -2.271681       0.237444
H       -2.950750       -1.925023       1.732234
H       -5.889867       -1.771298       -1.416562
H       -4.746378       -3.254407       0.417711
O       -0.507446       2.957022        -0.867002
C       0.106047        4.280921        -0.833078
H       -0.505287       4.960322        -0.230221
H       1.128091        4.208975        -0.447451
H       0.100658        4.573032        -1.892617
H       -4.758441       0.582067        -1.237534
H       4.168164        1.041672        1.222737
###
40
GluHisOMe3 pm6 E=-0.248024056025 au
N       -3.354942       -0.448717       -1.696659
H       -3.531790       -1.440032       -1.442716
H       -3.110813       -0.411804       -2.707358
H       -4.250491       0.084336        -1.553584
C       -2.243468       0.147067        -0.850550
H       -2.009160       1.179640        -1.263915
C       -2.661656       0.260154        0.624640
C       -1.012603       -0.767281       -0.972894
H       -2.990533       -0.729684       1.013052
H       -1.756756       0.516480        1.228357
C       -3.723144       1.327777        0.877859
O       -1.133554       -1.973782       -1.215844
H       -3.572430       1.767797        1.889985
H       -3.593968       2.195095        0.190268
C       -5.126956       0.781653        0.759567
O       -5.648541       0.614749        -0.382324
O       -5.785211       0.492062        1.802198
N       0.216884        -0.178741       -0.801574
H       0.302335        0.816588        -0.535012
C       1.464242        -0.961156       -0.923176
H       1.306500        -1.801857       -1.684241
C       2.620749        -0.097417       -1.432168
C       1.764788        -1.681303       0.399836
H       3.488888        -0.773228       -1.669039
H       2.347402        0.316824        -2.442082
C       3.073930        1.003807        -0.550832
O       0.949194        -2.117031       1.195634
N       4.168996        1.812062        -0.921097
C       2.624645        1.476992        0.681610
C       4.374759        2.755488        0.062978
N       3.434527        2.559699        1.045499
H       1.804545        1.135595        1.308530
H       5.156309        3.527715        0.057992
H       3.341176        3.110058        1.906707
O       3.101752        -1.864050       0.563942
C       3.543834        -2.622879       1.730554
H       3.232796        -2.115551       2.649011
H       3.155620        -3.645382       1.679925
H       4.637621        -2.609482       1.620266
H       4.720647        1.713767        -1.782711
###
39
GluHisOMe4 pm6 E=-0.395353097423 au
N       -2.059249       -0.382985       -1.883800
H       -1.087682       -0.745733       -1.815088
H       -2.232627       -0.106129       -2.872427
H       -2.707241       -1.179490       -1.639561
C       -2.299591       0.776398        -0.938844
H       -3.329710       1.201079        -1.196653
C       -2.322805       0.320593        0.529183
C       -1.309252       1.928789        -1.163355
H       -1.539586       -0.443218       0.727342
H       -2.056160       1.188428        1.181206
C       -3.688087       -0.206193       0.960145
O       -1.761888       3.031504        -1.501562
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H       -3.810963       -0.054089       2.059004
H       -4.511163       0.409446        0.522110
C       -3.941568       -1.653928       0.628104
O       -4.895275       -2.257604       1.209299
O       -3.227068       -2.281881       -0.207320
N       0.052420        1.833755        -0.982257
H       0.611706        2.695413        -1.140530
C       0.831944        0.651077        -0.578386
H       0.316434        -0.309748       -0.887854
C       2.229323        0.685372        -1.232743
C       0.991545        0.615789        0.953979
H       2.113709        0.659493        -2.344707
H       2.738099        1.656291        -1.027334
C       3.054715        -0.461994       -0.785134
O       0.735522        -0.339852       1.666109
N       4.011780        -0.352324       0.234184
C       3.036519        -1.772013       -1.277893
C       4.570074        -1.587931       0.355854
N       3.997367        -2.479218       -0.551971
H       2.435991        -2.215870       -2.056248
H       5.354033        -1.862242       1.054196
H       4.230801        -3.461397       -0.673194
O       1.493242        1.779341        1.438643
C       1.732578        1.872317        2.877660
H       0.783648        1.780073        3.416060
H       2.452954        1.108398        3.186033
H       2.152897        2.882989        2.981789
###
21
GlyAla1 pm6 E=-0.114621838226 au
N       -3.700688       -0.259520       0.132550
H       -3.603068       -1.277651       0.299252
C       -2.488198       0.485357        0.618167
H       -3.847648       -0.108813       -0.882302
H       -4.546191       0.073261        0.638342
C       -1.236531       0.073701        -0.125287
H       -2.663556       1.598326        0.530767
H       -2.355920       0.324481        1.729526
O       -1.221027       -0.860268       -0.939738
N       -0.106369       0.811016        0.145451
H       -0.107762       1.568114        0.850756
C       1.168861        0.553047        -0.559492
H       0.957263        0.289397        -1.641972
C       2.076621        1.766955        -0.494813
C       1.847242        -0.676425       0.070878
H       2.262165        2.117399        0.532117
H       3.058118        1.564019        -0.952809
H       1.652410        2.621602        -1.046700
O       1.884568        -1.795938       -0.417403
O       2.430413        -0.420717       1.264564
H       2.883985        -1.231034       1.680904
###
20
GlyAla2 pm6 E=-0.289298126399 au
N       -3.164281       -0.924266       -0.473997
H       -3.427725       -1.046975       0.520860
C       -1.698364       -0.610991       -0.611205
H       -3.389219       -1.803612       -0.981761
H       -3.742397       -0.161462       -0.870789
C       -1.314362       0.587509        0.227234
H       -1.090582       -1.517494       -0.325414
H       -1.451360       -0.438953       -1.700876
O       -2.157431       1.184196        0.920307
N       -0.020464       1.043708        0.228792
H       0.217145        1.853297        0.823865
C       1.105721        0.429555        -0.510939
H       0.736051        0.016751        -1.493990
C       2.183772        1.473974        -0.772028
C       1.738754        -0.735013       0.283612
H       2.573454        1.932143        0.148470
H       3.042273        1.042773        -1.308361
H       1.815530        2.296049        -1.404271
O       2.526060        -1.498311       -0.347058
O       1.495985        -0.920737       1.502833
###
19
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```
GlyAla3 pm6 E=-0.438858015169 au
N       -3.642857       -0.347177       0.258664
H       -3.763354       -0.711451       -0.688169
C       -2.559364       0.657105        0.284723
H       -3.393953       -1.146737       0.843925
C       -1.213677       0.147634        -0.196694
H       -2.858285       1.534515        -0.346700
H       -2.474150       1.070839        1.322197
O       -1.092138       -0.946508       -0.789654
N       -0.119841       0.944924        0.027469
H       -0.199599       1.832830        0.547788
C       1.231495        0.589101        -0.474482
H       1.165930        0.406045        -1.585330
C       2.215372        1.713694        -0.199838
C       1.722581        -0.714883       0.195259
H       2.237542        2.023649        0.854767
H       3.242526        1.431408        -0.476467
H       1.979341        2.616159        -0.785251
O       1.978917        -1.690896       -0.568199
O       1.866277        -0.812271       1.439915
###
24
GlyAsp1 pm6 E=-0.258675276396 au
N       4.525632        -0.560858       -0.398662
H       4.402563        -1.086070       -1.284177
C       3.338533        -0.745311       0.506151
H       4.665065        0.439827        -0.631080
C       2.062025        -0.256492       -0.140997
H       3.248901        -1.832359       0.804405
H       3.517584        -0.215831       1.488043
O       2.039378        0.285801        -1.252282
N       0.905524        -0.437230       0.590018
H       0.909407        -0.893252       1.518674
C       -0.399085       -0.024439       0.037215
H       -0.389075       -0.172942       -1.092700
C       -1.521412       -0.856364       0.666250
C       -0.631771       1.472363        0.308855
H       -1.189546       -1.924949       0.797236
H       -1.725424       -0.547252       1.730336
C       -2.793684       -0.807741       -0.111560
O       -0.028843       2.191053        1.086596
O       -1.605642       2.091586        -0.415416
O       -3.201633       0.096877        -0.836973
O       -3.531766       -1.929437       0.066026
H       5.385568        -0.912416       0.068669
H       -4.414640       -1.923901       -0.445167
H       -2.128078       1.476633        -1.072824
###
23
GlyAsp2 pm6 E=-0.445228497946 au
N       4.478362        -0.384470       -0.069137
H       4.566500        0.047918        -1.006611
C       3.203732        -1.173704       0.045462
H       4.513319        0.369829        0.640842
C       1.987883        -0.320031       -0.242714
H       3.223971        -2.050225       -0.669199
H       3.149061        -1.662453       1.062117
O       2.063878        0.743628        -0.881330
N       0.790169        -0.785811       0.236314
H       0.733579        -1.647962       0.807812
C       -0.485142       -0.115272       -0.111133
H       -0.624224       -0.175952       -1.232744
C       -1.650492       -0.816318       0.593912
C       -0.454072       1.384281        0.286088
H       -1.461567       -1.923526       0.669973
H       -1.726521       -0.516081       1.673991
C       -2.961153       -0.566554       -0.074185
O       -0.951099       2.197520        -0.543269
O       0.033283        1.771627        1.374528
O       -3.393853       0.473998        -0.558277
O       -3.722545       -1.691301       -0.097639
H       5.297489        -1.007697       0.081814
H       -4.633177       -1.560071       -0.534913
###
22
GlyAsp3 pm6 E=-0.616302258614 au
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N       -3.698187       -0.813805       0.699430
H       -4.159496       -0.419840       -0.141488
C       -2.252762       -0.401765       0.763274
H       -4.200669       -0.464636       1.541131
H       -3.791167       -1.846021       0.667172
C       -1.493086       -0.857217       -0.461206
H       -2.191845       0.714203        0.906671
H       -1.775844       -0.823432       1.698006
O       -2.000734       -1.620613       -1.296298
N       -0.193631       -0.444342       -0.659406
H       0.290209        -0.760676       -1.515371
C       0.534816        0.530210        0.185097
H       0.345161        0.299831        1.273067
C       2.034148        0.460546        -0.108293
C       0.064173        1.982407        -0.089645
H       2.249125        0.714264        -1.171943
H       2.574697        1.251826        0.468834
C       2.644426        -0.877612       0.240920
O       0.163337        2.807566        0.856911
O       -0.388824       2.320195        -1.212906
O       2.390708        -1.439462       1.343450
O       3.424547        -1.427424       -0.589549
###
21
GlyAsp4 pm6 E=-0.768927389893 au
N       -3.981423       -1.241594       -0.193478
H       -3.894785       -1.708803       0.711223
C       -2.653342       -1.113477       -0.829298
H       -4.370943       -0.316381       -0.003696
C       -1.650358       -0.330853       -0.004758
H       -2.248670       -2.135097       -1.049671
H       -2.773406       -0.635331       -1.835950
O       -1.946201       0.159667        1.105294
N       -0.387055       -0.156390       -0.521814
H       -0.126616       -0.540535       -1.443645
C       0.669969        0.564426        0.231799
H       0.543086        0.367774        1.334905
C       2.059699        0.117271        -0.203703
C       0.469909        2.082716        -0.006579
H       2.208355        0.277272        -1.296281
H       2.831348        0.770168        0.277294
C       2.377820        -1.314544       0.155358
O       -0.321599       2.692936        0.769701
O       1.059860        2.679082        -0.938504
O       3.165792        -1.965385       -0.591499
O       1.888247        -1.857100       1.187001
###
18
GlyGly1 pm6 E=-0.106115339486 au
N       -3.481457       -0.408106       -0.045590
H       -3.675266       -0.118878       0.931004
C       -2.342726       0.384106        -0.625160
H       -3.266601       -1.421885       -0.045207
C       -1.063880       0.188993        0.160979
H       -2.180680       0.096161        -1.706325
H       -2.627038       1.475877        -0.684394
O       -0.962276       -0.666930       1.053278
N       -0.017871       1.013989        -0.175018
H       -0.091479       1.706066        -0.939006
C       1.290524        0.899676        0.479836
C       2.112671        -0.227166       -0.103063
H       1.839042        1.879626        0.391114
H       1.192272        0.734217        1.590498
O       1.729804        -1.294417       -0.558267
H       -4.342548       -0.257248       -0.608840
O       3.436677        0.069705        -0.052476
H       4.034420        -0.675637       -0.400417
###
17
GlyGly2 pm6 E=-0.279048396968 au
N       2.722104        -1.267179       -0.060983
H       2.899852        -1.163574       0.955284
C       1.344958        -0.779057       -0.421893
H       3.449009        -0.734945       -0.573071
C       1.142369        0.658870        0.001034
H       1.179367        -0.898453       -1.534353
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H       0.572666        -1.454286       0.043704
O       2.057408        1.307299        0.541153
N       -0.060676       1.275811        -0.221242
H       -0.204205       2.235750        0.124794
C       -1.234169       0.626167        -0.818771
C       -2.042014       -0.225609       0.154161
H       -1.903692       1.417783        -1.250798
H       -0.950980       -0.000415       -1.705786
O       -3.104870       -0.748308       -0.289902
O       -1.672149       -0.417870       1.340799
H       2.818005        -2.273486       -0.307785
###
16
GlyGly3 pm6 E=-0.429811431032 au
N       3.512131        0.279117        -0.261001
H       3.711454        0.237098        0.740799
C       2.321190        -0.536881       -0.576333
H       3.331803        1.261163        -0.476431
C       1.058028        -0.119294       0.153982
H       2.127942        -0.495749       -1.680830
H       2.554557        -1.613600       -0.375809
O       0.973283        0.969068        0.765860
N       -0.003740       -0.985910       0.118424
H       0.037948        -1.865885       -0.417585
C       -1.285561       -0.693878       0.781523
C       -2.178487       0.183492        -0.096712
H       -1.800741       -1.656960       1.024695
H       -1.132732       -0.200339       1.772974
O       -1.830398       1.366036        -0.369444
O       -3.252884       -0.299955       -0.541982
###
27
GlyHis2 pm6 E=-0.250892782842 au
N       -5.001466       -0.919640       0.061827
H       -4.726533       -1.914077       -0.039032
C       -3.957188       -0.009352       -0.522174
H       -5.142727       -0.724034       1.069927
C       -2.590893       -0.267226       0.078629
H       -3.923894       -0.133280       -1.644948
H       -4.265052       1.067885        -0.381554
O       -2.399688       -1.153872       0.924243
N       -1.576892       0.558132        -0.346072
H       -1.725804       1.248422        -1.097911
C       -0.182315       0.339883        0.094969
H       -0.176788       -0.299065       1.023181
C       0.646325        -0.355612       -1.004948
C       0.461641        1.704794        0.426054
H       0.149635        -1.309387       -1.300752
H       0.652762        0.253440        -1.936169
C       2.025504        -0.628564       -0.531650
O       0.481770        2.620705        -0.434536
O       1.002042        1.841959        1.557229
N       3.095315        0.247259        -0.766524
C       2.472380        -1.734214       0.201747
C       4.181302        -0.325404       -0.174414
N       3.836785        -1.534842       0.425877
H       1.937937        -2.601883       0.552802
H       5.186423        0.083105        -0.165976
H       4.451712        -2.161672       0.938423
H       -5.907400       -0.781986       -0.428506
###
28
GlyHis3 pm6 E=-0.918413102501E-01 au
N       3.115450        -1.860046       -0.874928
H       3.629130        -2.389853       -0.146685
C       1.632182        -1.898725       -0.630616
H       3.464390        -0.882982       -0.875370
H       3.332834        -2.286017       -1.798570
C       1.277447        -1.389753       0.755087
H       1.092299        -1.338472       -1.450478
H       1.245731        -2.953266       -0.746434
O       1.409464        -2.118341       1.752147
N       0.802682        -0.114192       0.931253
H       0.536015        0.192498        1.880304
C       0.526532        0.850672        -0.154139
H       0.586378        0.333861        -1.160068
```

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C       -0.864576       1.480661        0.020624
C       1.583917        1.983042        -0.134522
H       -0.941217       2.006775        1.006682
H       -0.996764       2.302538        -0.732758
C       -1.963822       0.501218        -0.130081
O       1.978809        2.432762        -1.241975
O       2.015439        2.442035        0.954761
N       -3.216889       0.688464        0.485815
C       -2.039659       -0.693390       -0.847678
H       -3.478785       1.476150        1.089939
C       -4.035294       -0.368728       0.147028
N       -3.324384       -1.218044       -0.667127
H       -1.286766       -1.183288       -1.459951
H       -5.073657       -0.504590       0.474948
H       -3.677650       -2.088260       -1.080323
###
26
GlyHis4 pm6 E=-0.395108366311 au
N       -5.228454       -0.618982       -0.054507
H       -5.106729       -1.627809       -0.163645
C       -4.054438       0.094207        -0.599737
H       -5.307018       -0.448914       0.949966
C       -2.735416       -0.268313       0.057418
H       -3.992291       -0.092593       -1.702994
H       -4.224165       1.198465        -0.510269
O       -2.659250       -1.063052       1.014108
N       -1.607106       0.341503        -0.441222
H       -1.656685       0.965531        -1.260053
C       -0.257818       0.072735        0.096431
H       -0.335624       -0.581931       1.008074
C       0.630174        -0.625266       -0.955322
C       0.396071        1.414035        0.501200
H       0.256757        -1.660152       -1.128611
H       0.532452        -0.126023       -1.946957
C       2.051742        -0.641368       -0.530078
O       0.903412        1.498428        1.654154
O       0.455126        2.366642        -0.316265
N       2.555278        -1.538140       0.420812
C       3.074109        0.215259        -0.959775
C       3.873228        -1.224003       0.569366
N       4.223122        -0.159099       -0.258410
H       3.062963        1.005891        -1.691525
H       4.571019        -1.722305       1.234475
H       5.139216        0.273022        -0.348172
###
33
GlyLys1 pm6 E=-0.638243761387E-03 au
N       4.518345        -1.922867       0.108423
C       3.054205        -1.817599       0.431503
H       4.920447        -2.773310       0.553216
H       5.035365        -1.096971       0.459441
C       2.428860        -0.595849       -0.207149
H       2.520858        -2.758978       0.106166
H       2.904464        -1.803568       1.551753
O       3.086006        0.210552        -0.880226
N       1.078149        -0.430944       -0.003356
H       0.539790        -1.072270       0.602583
C       0.341498        0.695817        -0.612785
H       0.742888        0.878308        -1.662104
C       -1.160472       0.388102        -0.710447
C       0.577807        1.980457        0.185607
H       -1.647366       1.173094        -1.333851
H       -1.304138       -0.547892       -1.297746
C       -1.869415       0.274471        0.642286
O       1.200534        2.107353        1.228635
O       0.076192        3.145793        -0.319168
H       -1.424530       -0.540816       1.251578
H       -1.717942       1.199144        1.237716
C       -3.374761       0.041257        0.477629
H       -3.883284       0.232299        1.448461
H       -3.804588       0.785347        -0.227664
C       -3.673627       -1.381354       0.002907
H       -3.120621       -1.619411       -0.939708
H       -3.337122       -2.135221       0.755495
N       -5.158791       -1.559913       -0.244132
H       -5.489338       -0.925619       -0.992149
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H       -5.364784       -2.532877       -0.534165
H       -5.707322       -1.355880       0.609392
H       -0.441420       3.060774        -1.191155
H       4.668301        -1.991479       -0.915037
###
32
GlyLys2 pm6 E=-0.183628336139 au
N       -5.135390       -0.598676       -0.351633
C       -3.767797       -1.189849       -0.554981
H       -5.857611       -1.230138       -0.752772
H       -5.213301       0.322756        -0.819027
C       -2.692279       -0.363804       0.117670
H       -3.738326       -2.247295       -0.157076
H       -3.569899       -1.319579       -1.659570
O       -2.973477       0.485291        0.983945
N       -1.400635       -0.606661       -0.266393
H       -1.180508       -1.296540       -1.006437
C       -0.249906       0.056269        0.399586
H       -0.446485       0.112768        1.508958
C       1.031132        -0.750785       0.154047
C       -0.142822       1.502408        -0.140030
H       0.861838        -1.814526       0.432166
H       1.275571        -0.781798       -0.928672
C       2.210646        -0.187053       0.954481
O       -0.696496       2.415660        0.540350
O       0.451381        1.765366        -1.213935
H       2.447362        0.846159        0.629312
H       1.932309        -0.093678       2.026230
C       3.451620        -1.078196       0.844729
H       4.166433        -0.819430       1.657710
H       3.176496        -2.138121       1.046881
C       4.147576        -1.013070       -0.512424
H       4.786683        -1.918078       -0.666904
H       3.412537        -1.020821       -1.353632
N       5.021578        0.221800        -0.626745
H       5.758087        0.222036        0.101283
H       5.484649        0.259174        -1.552786
H       4.465109        1.085245        -0.509641
H       -5.340106       -0.469446       0.656035
###
31
GlyLys3 pm6 E=-0.323743516332 au
N       4.582283        -1.649539       -0.396638
C       4.033365        -0.477957       0.339233
H       5.383544        -2.019917       0.122955
H       4.955223        -1.342092       -1.297773
C       2.649165        -0.190999       -0.208893
H       4.016685        -0.698647       1.435466
H       4.643308        0.455264        0.251299
O       2.448328        0.016375        -1.424873
N       1.611685        -0.136592       0.688391
H       1.765817        -0.311305       1.694234
C       0.213933        0.143881        0.270492
H       -0.012957       -0.426954       -0.674183
C       -0.761960       -0.286633       1.372736
C       0.100651        1.655768        -0.034631
H       -0.559505       -1.342622       1.660636
H       -0.576418       0.295388        2.300149
C       -2.228240       -0.141889       0.954275
O       -0.047462       2.496831        0.888642
O       0.193079        2.026486        -1.240800
H       -2.860982       -0.185678       1.867802
H       -2.421742       0.861261        0.524269
C       -2.660410       -1.238078       -0.026149
H       -2.183024       -1.087247       -1.017845
H       -2.283405       -2.227110       0.320772
C       -4.176566       -1.339692       -0.172673
H       -4.452900       -2.288018       -0.698353
H       -4.679296       -1.392262       0.824067
N       -4.744442       -0.169962       -0.953057
H       -4.311644       -0.108610       -1.891130
H       -5.767095       -0.276504       -1.080145
H       -4.573488       0.723758        -0.463185
###
30
GlyLys4 pm6 E=-0.453145263745 au
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N       1.395872        3.320622        -0.852081
C       2.374153        2.548696        -0.037544
H       1.896823        3.826206        -1.587428
H       0.954279        4.035289        -0.269892
C       1.627884        1.353385        0.529854
H       3.245505        2.227781        -0.658682
H       2.826460        3.127261        0.802322
O       1.084923        1.392858        1.651705
N       1.583055        0.208409        -0.228883
H       1.965794        0.188491        -1.183758
C       0.826454        -0.987726       0.210106
H       0.594452        -0.895262       1.309354
C       -0.485146       -1.164163       -0.571134
C       1.736604        -2.217484       0.012596
H       -0.316539       -1.020953       -1.657858
H       -0.836236       -2.213670       -0.469324
C       -1.567677       -0.203532       -0.065785
O       2.071209        -2.871329       1.040386
O       2.134190        -2.553301       -1.132450
H       -1.751968       -0.379057       1.012335
H       -1.214943       0.844201        -0.141093
C       -2.872848       -0.368498       -0.852380
H       -2.694893       -0.152270       -1.926225
H       -3.205757       -1.426049       -0.825851
C       -3.987303       0.551855        -0.340505
H       -3.598113       1.580259        -0.174052
H       -4.762932       0.655956        -1.131415
N       -4.565799       0.072026        0.955711
H       -5.482389       0.505182        1.089534
H       -4.746726       -0.931778       0.900439
###
31
GlyPhe1 pm6 E=-0.716066185036E-01 au
C       4.613952        -0.434858       0.562692
C       3.835084        -1.589940       0.678500
C       2.558311        -1.636741       0.112972
C       2.055261        -0.522931       -0.575020
C       2.838037        0.635685        -0.690708
C       4.113079        0.676958        -0.121573
C       0.682295        -0.571574       -1.185617
C       -0.384258       -0.093535       -0.187423
C       -0.178701       1.406803        0.080821
O       0.295983        1.593717        1.339993
N       -1.742089       -0.288796       -0.735664
C       -2.840002       -0.357610       0.095444
O       -2.734665       -0.209971       1.319360
C       -4.168966       -0.609675       -0.582797
N       -5.310872       -0.539810       0.392620
O       -0.376710       2.351074        -0.661447
H       -5.219403       -1.268795       1.123743
H       -6.212046       -0.687555       -0.103461
H       -5.345026       0.386296        0.858127
H       -4.163558       -1.616150       -1.098203
H       -4.339763       0.120215        -1.427673
H       -1.827098       -0.425819       -1.757111
H       -0.279926       -0.659703       0.788274
H       0.442648        -1.611150       -1.517235
H       0.641597        0.022138        -2.127836
H       1.956283        -2.542058       0.204926
H       2.456351        1.505320        -1.227787
H       4.224549        -2.459738       1.210483
H       4.719218        1.580072        -0.211836
H       5.610759        -0.401103       1.003960
H       0.484744        2.564229        1.575953
###
30
GlyPhe2 pm6 E=-0.247473915835 au
N       -3.351971       -2.439507       0.957505
C       -2.491602       -1.213476       0.809897
H       -4.079767       -2.472240       0.220568
H       -3.824236       -2.431879       1.884765
C       -1.767954       -1.205738       -0.517802
H       -3.129552       -0.291015       0.928139
H       -1.758196       -1.161951       1.668213
O       -1.949959       -2.102684       -1.357819
N       -0.896122       -0.188200       -0.821233
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H       -0.388802       -0.228706       -1.721555
C       -0.535524       0.932762        0.076703
H       -0.453987       0.560801        1.139110
C       0.808444        1.547885        -0.350781
C       -1.612286       2.043943        0.028811
H       0.775709        1.861227        -1.419161
H       0.970618        2.499888        0.208339
C       1.956289        0.608789        -0.107053
O       -2.075841       2.457017        -1.067661
C       2.498231        -0.133525       -1.166553
C       2.491942        0.471375        1.182818
H       2.086359        -0.034777       -2.172517
C       3.568319        -1.002165       -0.936329
C       3.561267        -0.398564       1.406505
H       2.074535        1.043890        2.012067
H       3.988141        -1.576429       -1.763827
C       4.101933        -1.136132       0.348435
H       3.975585        -0.502314       2.410798
H       4.937689        -1.813385       0.525351
O       -1.990275       2.539845        1.123865
H       -2.783187       -3.303508       0.890821
###
29
GlyPhe3 pm6 E=-0.393645785337 au
N       -3.943151       -1.623474       -0.986194
C       -3.537498       -1.282010       0.404995
H       -4.817939       -1.146423       -1.214116
H       -4.144338       -2.625419       -1.039086
C       -2.675419       -0.036869       0.329521
H       -4.392327       -1.082449       1.097181
H       -2.994559       -2.141077       0.870589
O       -3.082041       1.026199        -0.188716
N       -1.414823       -0.103917       0.865177
H       -1.048859       -0.973925       1.285122
C       -0.489244       1.054159        0.819292
H       -0.998769       1.934539        1.309890
C       0.806166        0.758387        1.590696
C       -0.171637       1.449170        -0.642159
H       1.227700        1.724228        1.956030
H       0.570169        0.209397        2.534128
C       1.832017        -0.000561       0.797056
O       0.019826        2.670888        -0.887268
C       2.944187        0.674791        0.270527
C       1.680705        -1.375285       0.560024
H       3.077760        1.741033        0.458403
C       3.892233        -0.017846       -0.486479
C       2.629529        -2.061509       -0.202415
H       0.828575        -1.915726       0.976591
H       4.758222        0.511031        -0.889034
C       3.734821        -1.385605       -0.728284
H       2.508441        -3.131066       -0.385342
H       4.473976        -1.923708       -1.322753
O       -0.114958       0.584208        -1.557408
###
32
GlyTyr1 pm6 E=-0.150471667158 au
N       -1.729831       3.796721        -0.090286
H       -2.615739       3.736859        0.444699
C       -1.563880       2.603867        -0.990624
H       -1.749412       4.669378        -0.655306
H       -0.946626       3.863765        0.584792
C       -1.566289       1.307950        -0.203897
H       -2.381742       2.593026        -1.771107
H       -0.617445       2.709196        -1.597611
O       -1.782177       1.290852        1.014777
N       -1.355587       0.167328        -0.945110
H       -1.169806       0.232475        -1.963589
C       -1.190317       -1.182804       -0.369185
H       -0.772982       -1.843697       -1.195041
C       -0.255485       -1.261216       0.850978
C       -2.569070       -1.723299       0.039968
H       -0.664052       -0.669687       1.699869
H       -0.242251       -2.313549       1.227206
C       1.140543        -0.823148       0.517207
O       -2.873312       -2.825343       -0.686291
O       -3.341760       -1.287379       0.878991
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C       1.626982        0.404317        0.994024
C       1.967802        -1.646214       -0.266840
H       0.987364        1.051127        1.599951
C       2.929280        0.811293        0.703919
C       3.269619        -1.257915       -0.574417
H       1.589825        -2.602330       -0.639694
H       3.317614        1.760426        1.075474
C       3.730169        -0.029444       -0.077493
H       3.917632        -1.886585       -1.183269
O       5.030727        0.300305        -0.419621
H       5.320257        1.163043        0.012587
H       -3.758676       -3.259595       -0.435879
###
31
GlyTyr2 pm6 E=-0.326435931067 au
N       -3.008533       3.032581        -0.800421
H       -3.656858       3.206314        -0.010342
C       -2.447745       1.637350        -0.744196
H       -3.533365       3.167336        -1.688807
H       -2.251406       3.738874        -0.759006
C       -1.807253       1.351202        0.594683
H       -3.267683       0.892752        -0.962268
H       -1.708017       1.496578        -1.586814
O       -1.823977       2.188986        1.512293
N       -1.197867       0.140953        0.819518
H       -0.728322       -0.014150       1.726494
C       -1.067302       -0.950473       -0.171443
H       -0.960135       -0.518983       -1.207818
C       0.163939        -1.822037       0.141924
C       -2.317977       -1.861623       -0.140134
H       0.067121        -2.289683       1.147707
H       0.184626        -2.685652       -0.564231
C       1.442646        -1.042352       0.040969
O       -2.797180       -2.241028       -1.242080
O       -2.817815       -2.240541       0.953286
C       1.971389        -0.709586       -1.216455
C       2.106861        -0.631782       1.209413
H       1.460179        -1.032590       -2.127334
C       3.145490        0.036631        -1.316201
C       3.283443        0.110905        1.134188
H       1.697541        -0.891778       2.190180
H       3.560776        0.303960        -2.288387
C       3.780615        0.438938        -0.135266
H       3.805179        0.433379        2.034094
O       4.942152        1.192792        -0.141581
H       5.225090        1.434191        -1.077380
###
30
GlyTyr3 pm6 E=-0.473638617593 au
N       -3.513186       -2.775653       0.300481
H       -2.558335       -3.010121       0.584217
C       -3.501192       -1.705258       -0.718868
H       -3.994582       -2.452463       1.142390
C       -2.961287       -0.360107       -0.257658
H       -2.918667       -2.046040       -1.613662
H       -4.543802       -1.560511       -1.098286
O       -3.667765       0.670447        -0.303936
N       -1.670756       -0.299312       0.205427
H       -1.061531       -1.134160       0.219747
C       -1.094018       0.965753        0.721544
H       -1.875335       1.474248        1.363720
C       0.129522        0.735220        1.618984
C       -0.806267       1.903674        -0.474605
H       0.358150        1.701143        2.132032
H       -0.160548       0.056031        2.456750
C       1.359671        0.202529        0.945292
O       -1.452232       2.992069        -0.506373
O       -0.019851       1.593365        -1.403359
C       1.431829        -1.142467       0.548111
C       2.459134        1.051288        0.722726
H       0.592833        -1.819007       0.744782
C       2.566500        -1.635800       -0.095103
C       3.605660        0.580761        0.087226
H       2.417371        2.094604        1.048092
H       2.624386        -2.678206       -0.411906
C       3.636186        -0.761388       -0.321113
```

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H       4.460959        1.231271        -0.091157
O       4.797294        -1.159527       -0.959077
H       4.732703        -2.108087       -1.295330
###
29
GlyTyr4 pm6 E=-0.632883856819 au
N       -0.395036       4.143915        -0.328567
H       0.584885        3.930986        -0.524343
C       -1.009809       3.038998        0.437061
H       -0.852453       4.237154        -1.238188
C       -0.918199       1.677578        -0.228270
H       -0.525705       2.976995        1.446889
H       -2.077549       3.298100        0.654480
O       -0.187837       1.473506        -1.219581
N       -1.712319       0.676467        0.283004
H       -2.240450       0.825760        1.156228
C       -1.577567       -0.729470       -0.163613
H       -1.184737       -0.749868       -1.218098
C       -0.630647       -1.540309       0.745263
C       -2.980680       -1.372300       -0.146081
H       -0.888126       -1.377650       1.813249
H       -0.802493       -2.626938       0.575054
C       0.804944        -1.197199       0.483041
O       -3.619186       -1.484305       0.933060
O       -3.453000       -1.795739       -1.236774
C       1.468309        -0.236491       1.263899
C       1.496966        -1.824923       -0.568156
H       0.941120        0.249014        2.088262
C       2.788361        0.105278        1.003509
C       2.816070        -1.502235       -0.846274
H       0.987315        -2.576621       -1.175583
H       3.295748        0.846359        1.610119
C       3.489465        -0.524997       -0.060841
H       3.346184        -1.990130       -1.656131
O       4.720582        -0.212140       -0.317983
###
27
GlyVal1 pm6 E=-0.129743881060 au
N       -4.110473       -0.168420       0.100551
H       -4.183785       0.541439        -0.650574
C       -2.804585       -0.042955       0.835017
H       -4.903530       -0.028821       0.758039
H       -4.204221       -1.105709       -0.331060
C       -1.624911       -0.163357       -0.106428
H       -2.772366       0.935976        1.397728
H       -2.747224       -0.823572       1.650222
O       -1.768641       -0.383418       -1.316257
N       -0.377493       -0.047830       0.465496
H       -0.260108       0.219175        1.456109
C       0.840017        -0.067167       -0.366682
H       0.556198        -0.202668       -1.456939
C       1.685329        1.240719        -0.250043
C       1.687754        -1.265169       0.058450
H       2.625622        1.061182        -0.839070
C       0.921982        2.393757        -0.896506
C       2.068958        1.559737        1.190896
O       1.886885        -1.716416       1.172146
H       -0.040180       2.592934        -0.408202
H       1.498613        3.327675        -0.849790
H       0.714658        2.209618        -1.958617
H       2.589401        0.727792        1.681245
H       2.751789        2.420427        1.234706
H       1.206474        1.822826        1.816968
O       2.264722        -1.837326       -1.035249
H       2.873428        -2.620631       -0.816440
###
26
GlyVal2 pm6 E=-0.304003215149 au
N       3.811836        0.525588        -0.629704
H       4.190565        0.542911        0.334762
C       2.306757        0.512264        -0.621026
H       4.157005        1.369227        -1.131043
H       4.186028        -0.313529       -1.109997
C       1.769476        -0.672993       0.148835
H       1.923551        1.479098        -0.183586
H       1.926265        0.511548        -1.684979
```

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O       2.530854        -1.472283       0.722034
N       0.417117        -0.896781       0.215364
H       0.077982        -1.686659       0.788613
C       -0.627112       -0.012811       -0.346690
H       -0.255753       0.448895        -1.307129
C       -1.897523       -0.854599       -0.677963
C       -0.961366       1.132065        0.632457
H       -1.556353       -1.733780       -1.288122
C       -2.587188       -1.380199       0.579105
C       -2.859896       -0.031719       -1.532929
O       -1.382993       2.218487        0.147129
H       -2.992804       -0.581288       1.209514
H       -3.434400       -2.032151       0.322963
H       -1.917897       -1.987971       1.202946
H       -2.378496       0.364143        -2.436391
H       -3.707157       -0.642249       -1.874752
H       -3.292312       0.817469        -0.992565
O       -0.821334       0.990124        1.875764
###
25
GlyVal3 pm6 E=-0.454128355135 au
N       4.246462        -0.195507       -0.011177
H       4.354514        0.093219        -0.985912
C       2.974473        -0.930098       0.160388
H       4.232698        0.665539        0.539217
C       1.738655        -0.139202       -0.222173
H       3.013537        -1.874678       -0.441830
H       2.891850        -1.278353       1.221844
O       1.810219        1.023818        -0.675335
N       0.517419        -0.746930       -0.075185
H       0.423206        -1.674604       0.365540
C       -0.730044       -0.057038       -0.476800
H       -0.599973       0.310097        -1.537570
C       -1.941452       -1.031370       -0.461779
C       -0.975431       1.183991        0.404177
H       -1.688130       -1.870364       -1.164583
C       -2.208637       -1.629698       0.916908
C       -3.179584       -0.312353       -0.999051
O       -1.338184       2.241686        -0.190454
H       -2.490552       -0.877807       1.661088
H       -3.034665       -2.354237       0.879773
H       -1.344250       -2.181248       1.310431
H       -3.008075       0.134682        -1.986162
H       -4.019224       -1.011159       -1.120497
H       -3.535819       0.481680        -0.333147
O       -0.798307       1.175609        1.649080
###
29
HisGly1 pm6 E=0.853165737491E-01 au
N       0.255756        3.214326        -0.356507
H       -0.606527       3.450801        -0.885736
H       1.050172        3.737356        -0.785137
H       0.142546        3.548416        0.619758
C       0.527379        1.721779        -0.403698
H       0.628476        1.428755        -1.500629
C       1.834790        1.414276        0.344149
C       -0.653923       0.977406        0.240380
H       2.628422        2.153695        0.042669
H       1.712467        1.596824        1.444236
C       2.337744        0.049446        0.074922
O       -1.375112       1.517676        1.090708
N       2.620442        -0.875656       1.098552
C       2.675510        -0.563814       -1.132867
H       2.487501        -0.716083       2.103883
C       3.123953        -2.022441       0.525226
N       3.158114        -1.842747       -0.839443
H       2.595751        -0.178859       -2.146551
H       3.443386        -2.923980       1.063695
H       3.493533        -2.528638       -1.523325
N       -0.865569       -0.308732       -0.180869
H       -0.297435       -0.745881       -0.925766
C       -1.905460       -1.149307       0.425217
C       -3.273979       -0.871114       -0.145667
H       -1.631464       -2.236211       0.288585
H       -1.949008       -1.024628       1.546325
O       -3.686002       0.181696        -0.615903
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```
O       -4.190027       -1.881576       -0.130833
H       -3.865971       -2.751644       0.288113
###
28
HisGly2 pm6 E=-0.957895235520E-01 au
N       0.540161        2.472988        -0.013591
H       -0.132350       2.935320        -0.658120
H       1.502640        2.702998        -0.344567
H       0.425714        2.883462        0.933985
C       0.344692        0.965903        0.003541
H       0.494314        0.581624        -1.059915
C       1.371096        0.310114        0.937000
C       -1.094110       0.620807        0.447902
H       1.658525        1.002255        1.775709
H       0.896605        -0.548635       1.485818
C       2.593664        -0.152319       0.240011
O       -1.325427       0.135546        1.568366
N       3.289175        -1.307323       0.653886
C       3.297016        0.375395        -0.842817
H       3.025953        -1.918507       1.436374
C       4.388720        -1.473607       -0.159680
N       4.400384        -0.451577       -1.079954
H       3.088069        1.261589        -1.440379
H       5.124840        -2.284992       -0.085965
H       5.099821        -0.319220       -1.818306
N       -2.088116       0.827949        -0.466191
H       -1.896108       1.218141        -1.404729
C       -3.502348       0.586335        -0.135703
C       -3.886804       -0.883109       -0.319280
H       -3.737759       0.902189        0.912814
H       -4.146072       1.241406        -0.776711
O       -4.696297       -1.195706       -1.231783
O       -3.411647       -1.758464       0.458303
###
27
HisGly3 pm6 E=-0.245197053894 au
N       0.277637        2.390178        0.174351
H       -0.439118       2.824962        0.789253
H       0.467391        3.042196        -0.615869
H       1.151776        2.289308        0.721609
C       -0.203265       1.049674        -0.356887
H       -1.186794       1.239447        -0.891594
C       0.804586        0.473570        -1.364350
C       -0.393760       0.093597        0.826774
H       0.302964        -0.330825       -1.959538
H       1.048545        1.248843        -2.134278
C       2.040138        -0.052156       -0.735910
O       0.321256        0.204799        1.841184
N       3.085069        0.772645        -0.299156
C       2.353397        -1.391794       -0.471222
C       4.025076        -0.062281       0.224304
N       3.611712        -1.391014       0.134248
H       1.795478        -2.291535       -0.675250
H       4.972437        0.243586        0.656474
N       -1.319951       -0.911036       0.791865
H       -1.419208       -1.523055       1.617097
C       -2.269446       -1.163285       -0.299089
C       -3.555670       -0.350789       -0.184255
H       -1.802166       -1.005429       -1.303861
H       -2.544018       -2.255166       -0.298889
O       -3.966012       0.080249        0.926752
O       -4.212128       -0.144551       -1.243484
H       4.120182        -2.210935       0.453876
###
26
HisGly4 pm6 E=-0.396318164213 au
N       -0.076554       3.059945        -0.516469
H       -1.018171       3.121159        -0.909582
H       -0.129630       3.394914        0.446867
C       0.419888        1.664316        -0.570482
H       0.504154        1.377475        -1.656580
C       1.806862        1.577322        0.094980
C       -0.540721       0.702096        0.157460
H       2.495835        2.291897        -0.414342
H       1.759311        1.945375        1.145868
C       2.377270        0.208624        0.059984
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O       -0.897498       0.907079        1.337963
N       2.839671        -0.400515       -1.113986
C       2.576371        -0.651783       1.147350
C       3.318003        -1.619882       -0.738572
N       3.174749        -1.805957       0.634823
H       2.350558        -0.519855       2.192342
H       3.755531        -2.358191       -1.402046
N       -1.025879       -0.368691       -0.542123
H       -0.779027       -0.529046       -1.530194
C       -1.945679       -1.345974       0.062853
C       -3.395395       -0.866972       -0.023428
H       -1.828792       -2.334846       -0.446668
H       -1.686495       -1.551078       1.131854
O       -3.768973       0.131830        0.657477
O       -4.203764       -1.491126       -0.758962
H       3.455103        -2.620019       1.174079
###
44
HisLys0 pm6 E=0.189569471543 au
N       -0.201094       -3.189017       -1.035400
H       0.609429        -3.002710       -1.661465
H       0.158362        -3.591289       -0.147869
C       -0.995084       -1.918733       -0.795380
H       -1.329280       -1.531151       -1.813879
C       -2.227843       -2.227136       0.065733
C       -0.084678       -0.901253       -0.079438
H       -2.785329       -3.102286       -0.371766
H       -1.924461       -2.596448       1.080670
C       -3.146713       -1.072247       0.167236
O       0.565637        -1.215150       0.923372
N       -3.820260       -0.746336       1.360253
C       -3.551699       -0.146125       -0.795233
C       -4.616538       0.354076        1.126670
N       -4.457885       0.728813        -0.187698
H       -3.254321       -0.059068       -1.838317
H       -5.266986       0.842333        1.863890
H       -4.925727       1.520320        -0.643374
N       -0.058755       0.369017        -0.599084
H       -0.548707       0.601139        -1.483564
C       0.859959        1.391543        -0.050319
H       1.254189        1.045256        0.956937
C       2.048990        1.663339        -0.986683
C       0.069773        2.681581        0.190968
H       1.687983        1.916868        -2.008958
H       2.588660        2.571627        -0.636152
C       3.011407        0.476763        -1.071882
O       -0.073010       3.211761        1.282765
O       -0.535435       3.332567        -0.840225
H       2.464943        -0.447205       -1.355262
H       3.717051        0.652181        -1.913435
C       3.797356        0.255335        0.224598
H       4.383978        1.165027        0.478007
H       3.106304        0.111095        1.082869
C       4.723865        -0.952476       0.078364
H       4.144385        -1.888879       -0.112467
H       5.404959        -0.833730       -0.800339
N       5.563452        -1.138432       1.326754
H       4.966944        -1.307056       2.155195
H       6.200785        -1.948531       1.221303
H       6.139683        -0.299829       1.517107
H       -0.801245       -3.909420       -1.491555
H       -3.738323       -1.247984       2.252758
H       -0.421794       2.910005        -1.759205
###
43
HisLys1 pm6 E=0.619168543221E-02 au
N       2.356106        2.869155        0.110884
H       1.594013        3.572025        0.200845
H       2.573403        2.507194        1.058139
C       1.952733        1.760082        -0.843934
H       1.551325        2.267684        -1.787122
C       3.150170        0.906027        -1.270791
C       0.851795        0.908225        -0.187738
H       2.830615        0.264640        -2.137982
H       3.931313        1.573248        -1.732859
C       3.778165        0.085258        -0.212537
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O       0.932683        0.564190        1.002765
N       3.797927        -1.323350       -0.262959
C       4.494692        0.458381        0.925745
C       4.509640        -1.791340       0.819974
N       4.938344        -0.709522       1.553540
H       4.718003        1.451962        1.310893
H       4.702457        -2.846992       1.053272
H       5.488415        -0.754192       2.419693
N       -0.197011       0.554336        -0.987735
H       -0.231568       0.842795        -1.982561
C       -1.381448       -0.173086       -0.462100
H       -1.647873       0.241283        0.552636
C       -2.568615       0.011329        -1.416273
C       -1.002663       -1.663001       -0.291152
H       -2.678781       1.088521        -1.675846
H       -2.365787       -0.486251       -2.388287
C       -3.878135       -0.521824       -0.828663
O       -1.037888       -2.467955       -1.255076
O       -0.631881       -2.043535       0.857349
H       -4.593808       -0.705991       -1.659490
H       -3.727495       -1.516483       -0.362484
C       -4.498880       0.448716        0.181617
H       -3.814501       0.605942        1.042132
H       -4.619214       1.453391        -0.279323
C       -5.850004       -0.079445       0.666029
H       -6.529816       -0.305359       -0.192046
H       -5.731875       -1.041424       1.221878
N       -6.524521       0.933866        1.569687
H       -6.744012       1.803851        1.053918
H       -7.409789       0.552589        1.950142
H       -5.917048       1.185590        2.368762
H       3.205910        3.359687        -0.243990
H       3.372173        -1.902634       -0.995613
###
42
HisLys2 pm6 E=-0.146490158381 au
N       -2.669972       1.986965        -0.624132
H       -2.432238       2.914170        -0.218313
H       -2.236334       1.920833        -1.567629
C       -2.219321       0.858014        0.283944
H       -2.792279       0.957408        1.262105
C       -2.522254       -0.509131       -0.350291
C       -0.722990       0.968117        0.635465
H       -2.252740       -0.509764       -1.437512
H       -1.850154       -1.283430       0.095893
C       -3.940283       -0.905644       -0.175391
O       -0.391380       1.150207        1.819231
N       -4.341808       -1.834573       0.795607
C       -5.053628       -0.478091       -0.908511
C       -5.688025       -1.970024       0.649424
N       -6.155789       -1.154811       -0.382239
H       -5.124313       0.225118        -1.725152
H       -6.327224       -2.615838       1.241602
H       -7.115643       -1.065415       -0.702870
N       0.207063        0.822130        -0.354553
H       -0.065917       0.713287        -1.347152
C       1.652937        0.704549        -0.034538
H       1.770145        0.184890        0.961493
C       2.367383        -0.114377       -1.117552
C       2.233510        2.131157        0.102344
H       1.807076        -1.056136       -1.310510
H       2.347307        0.424765        -2.087756
C       3.814380        -0.442457       -0.736875
O       2.196684        2.675175        1.243253
O       2.720063        2.736391        -0.886323
H       4.356470        -0.764760       -1.652304
H       4.343980        0.469445        -0.394050
C       3.903197        -1.535367       0.333235
H       3.357400        -1.218688       1.250162
H       3.375524        -2.453699       -0.005453
C       5.343196        -1.860264       0.723034
H       5.944677        -0.932231       0.881787
H       5.367985        -2.408228       1.697916
N       6.024066        -2.714101       -0.329893
H       6.069683        -2.223181       -1.239441
H       6.992512        -2.945507       -0.043737
```

```
H       5.511141        -3.601172       -0.476232
H       -3.703525       1.955804        -0.751393
###
41
HisLys3 pm6 E=-0.296311265839 au
N       2.294505        3.480512        -0.072707
H       1.395726        3.967975        -0.120253
H       2.626161        3.560336        0.890217
C       2.127002        2.061331        -0.462793
H       1.819488        2.038605        -1.547637
C       3.456693        1.299520        -0.294281
C       1.064980        1.357805        0.405734
H       4.217598        1.737491        -0.984291
H       3.878401        1.477499        0.721184
C       3.318671        -0.152956       -0.568171
O       1.217867        1.223085        1.639104
N       3.848590        -1.125542       0.291904
C       2.716305        -0.776435       -1.668344
C       3.573760        -2.327684       -0.288730
N       2.894580        -2.151362       -1.492607
H       2.211461        -0.353160       -2.522154
H       3.851765        -3.298443       0.108667
H       2.566615        -2.876597       -2.125515
N       -0.048245       0.865792        -0.218206
H       -0.168915       0.949290        -1.241897
C       -1.075062       0.081812        0.515412
H       -1.610893       0.771243        1.227878
C       -2.080120       -0.536935       -0.467383
C       -0.392009       -1.038385       1.331069
H       -2.295503       0.178003        -1.295218
H       -1.636917       -1.416742       -0.978574
C       -3.388920       -0.940518       0.218469
O       -0.702839       -1.173728       2.543724
O       0.461365        -1.795872       0.789730
H       -3.901897       -1.702185       -0.407439
H       -3.183440       -1.463948       1.174737
C       -4.324673       0.243285        0.483080
H       -5.102014       -0.053485       1.221309
H       -3.768036       1.067639        0.982367
C       -4.976969       0.803091        -0.778874
H       -5.360265       1.837371        -0.594554
H       -4.237653       0.898393        -1.612891
N       -6.130922       -0.064485       -1.244182
H       -6.871123       -0.117196       -0.523188
H       -6.551080       0.322110        -2.109061
H       -5.818134       -1.030057       -1.444700
###
40
HisLys4 pm6 E=-0.420415777068 au
N       -3.434998       -1.612576       0.919103
H       -3.009509       -2.436061       1.354774
H       -3.191099       -0.811565       1.505097
C       -2.926721       -1.438278       -0.458471
H       -3.303908       -2.320469       -1.059497
C       -3.476036       -0.156424       -1.116324
C       -1.390937       -1.462438       -0.610021
H       -3.166808       -0.137694       -2.188734
H       -4.588514       -0.231545       -1.159274
C       -3.069572       1.109212        -0.457404
O       -0.876942       -2.066861       -1.576151
N       -3.891924       1.790702        0.449602
C       -1.879870       1.827090        -0.642378
C       -3.201055       2.905931        0.817913
N       -1.968312       2.959276        0.171452
H       -1.032446       1.621825        -1.275172
H       -3.545545       3.659908        1.517703
H       -1.260642       3.682535        0.261265
N       -0.593866       -0.846113       0.319158
H       -0.990237       -0.309897       1.104687
C       0.874934        -0.746702       0.120637
H       1.081783        -0.520603       -0.965364
C       1.463730        0.373798        0.986944
C       1.502847        -2.119669       0.448850
H       1.041006        1.348569        0.657857
H       1.138545        0.266344        2.043938
C       2.994548        0.425394        0.933283
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```
O       1.965905        -2.789410       -0.520581
O       1.536887        -2.571009       1.621679
H       3.335972        1.247841        1.596796
H       3.425958        -0.494677       1.375728
C       3.548530        0.632550        -0.481005
H       3.390085        -0.282032       -1.086512
H       2.974963        1.424438        -1.004876
C       5.045806        0.974172        -0.475599
H       5.543417        0.569769        0.432685
H       5.541807        0.467803        -1.332866
N       5.258301        2.456599        -0.496704
H       6.260157        2.646021        -0.566728
H       4.846577        2.844716        -1.347919
###
44
LeuTyr1 pm6 E=-0.183786918523 au
N       1.804349        -3.014459       -1.309528
H       2.089476        -2.785045       -2.280492
H       0.803840        -3.297519       -1.322009
H       2.367195        -3.833901       -1.000002
C       2.026230        -1.842082       -0.369992
H       1.684991        -2.165655       0.664598
C       3.517888        -1.480184       -0.329303
C       1.220723        -0.631388       -0.865242
H       4.104541        -2.385775       -0.052035
H       3.875468        -1.213426       -1.347948
C       3.841031        -0.333749       0.654714
O       1.267422        -0.250763       -2.040548
H       3.230013        0.562826        0.375819
C       3.509465        -0.719282       2.096935
C       5.319664        0.040419        0.519050
H       4.027604        -1.632776       2.412405
H       3.799165        0.070061        2.801139
H       2.435935        -0.896499       2.245124
H       5.573520        0.352723        -0.501248
H       5.585433        0.873527        1.181428
H       5.985503        -0.792512       0.774080
N       0.466840        0.029441        0.077489
H       0.418643        -0.291472       1.061402
C       -0.232749       1.289608        -0.253580
H       -0.660449       1.226628        -1.300000
C       -1.349377       1.596420        0.756883
C       0.799482        2.429134        -0.203163
H       -0.972247       1.497127        1.801975
H       -1.640395       2.672090        0.672753
C       -2.552240       0.726320        0.536903
O       0.794951        3.117632        -1.373845
O       1.554346        2.731248        0.703247
C       -2.805231       -0.354697       1.395677
C       -3.434466       1.002008        -0.522718
H       -2.117486       -0.573661       2.217540
C       -3.933876       -1.153913       1.212738
C       -4.565812       0.215498        -0.726413
H       -3.235376       1.842269        -1.193753
H       -4.144124       -1.991965       1.878375
C       -4.797683       -0.852542       0.153475
H       -5.256641       0.419187        -1.543307
O       -5.944380       -1.587863       -0.093724
H       -6.065914       -2.323532       0.584641
H       1.455962        3.890975        -1.403035
###
43
LeuTyr2 pm6 E=-0.359812603860 au
N       2.192453        -1.764236       -1.254764
H       2.452582        -1.537251       -2.233639
H       1.213712        -2.117120       -1.250355
H       2.810508        -2.538600       -0.937289
C       2.346977        -0.560104       -0.342529
H       2.056800        -0.889268       0.708815
C       3.794659        -0.054550       -0.330809
C       1.416597        0.563981        -0.838817
H       4.218284        -0.063746       -1.358734
H       3.808854        1.016927        -0.030298
C       4.706690        -0.858827       0.623259
O       1.628151        1.158064        -1.905474
H       4.612316        -1.948252       0.379896
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C       6.163266        -0.440488       0.406073
C       4.294195        -0.649351       2.081929
H       6.326606        0.625263        0.604664
H       6.840843        -0.994990       1.066830
H       6.495645        -0.630542       -0.621534
H       3.252254        -0.950274       2.258181
H       4.915577        -1.242357       2.763746
H       4.384037        0.396844        2.396027
N       0.388156        0.915409        -0.003037
H       0.160703        0.342909        0.825546
C       -0.642433       1.896899        -0.418461
H       -0.133463       2.765795        -0.926079
C       -1.668608       1.293025        -1.399680
C       -1.374817       2.419510        0.833854
H       -2.342955       2.103580        -1.757895
H       -1.140094       0.957530        -2.320764
C       -2.457549       0.160478        -0.809782
O       -1.884882       3.570225        0.780635
O       -1.474767       1.699562        1.861902
C       -3.703155       0.404153        -0.210617
C       -1.940404       -1.147543       -0.838755
H       -4.118852       1.414540        -0.203671
C       -4.421855       -0.634575       0.382534
C       -2.642190       -2.201012       -0.258978
H       -0.974078       -1.343580       -1.315433
H       -5.387313       -0.453378       0.855729
C       -3.873044       -1.921646       0.354724
H       -2.249392       -3.217024       -0.273733
O       -4.508374       -3.008268       0.930265
H       -5.337834       -2.731574       1.432303
###
42
LeuTyr3 pm6 E=-0.504428185784 au
N       -2.709378       -1.052817       1.957037
H       -1.892325       -0.605851       2.379302
H       -2.673939       -2.042485       2.211276
C       -2.702992       -0.894650       0.484541
H       -3.668433       -1.334711       0.095704
C       -2.608338       0.581871        0.066024
C       -1.561399       -1.671390       -0.210675
H       -1.822693       1.097500        0.657649
H       -2.269166       0.655392        -0.988605
C       -3.950698       1.329687        0.222969
O       -1.821328       -2.520725       -1.085451
H       -4.340504       1.147486        1.255241
C       -3.724441       2.835192        0.053528
C       -4.988296       0.823468        -0.782932
H       -3.296409       3.084218        -0.924206
H       -4.663054       3.395163        0.142621
H       -3.043296       3.235320        0.813764
H       -5.160559       -0.256105       -0.684167
H       -5.959171       1.313000        -0.641155
H       -4.688556       1.008691        -1.820333
N       -0.268203       -1.426908       0.175328
H       -0.050348       -0.666922       0.836835
C       0.892104        -2.039355       -0.507842
H       0.556138        -2.977467       -1.037309
C       1.516557        -1.090831       -1.551890
C       1.955450        -2.437258       0.535767
H       2.341357        -1.624942       -2.075688
H       0.769890        -0.896483       -2.355217
C       2.005516        0.203745        -0.970150
O       2.090936        -1.793164       1.608067
O       2.692167        -3.424812       0.262513
C       3.336845        0.330442        -0.544231
C       1.126033        1.293873        -0.839778
H       4.032159        -0.503314       -0.666669
C       3.786166        1.514892        0.040677
C       1.553150        2.488425        -0.265806
H       0.092844        1.207246        -1.190225
H       4.816625        1.618940        0.382480
C       2.882338        2.574766        0.175783
H       0.878201        3.336479        -0.156910
O       3.238695        3.782744        0.749366
H       4.172587        3.757318        1.127174
###
```

41
LeuTyr4 pm6 E=-0.663965382932 au
N -2.844403 -0.928979 2.011329
H -2.019624 -0.489829 2.427130
H -2.815647 -1.919319 2.264005
C -2.847353 -0.768857 0.538674
H -3.815120 -1.208254 0.154950
C -2.753190 0.709510 0.125637
C -1.712728 -1.549405 -0.162415
H -2.046872 1.247417 0.793102
H -2.309036 0.798474 -0.887584
C -4.126201 1.417437 0.140906
O -1.983015 -2.411088 -1.022625
H -4.623124 1.213459 1.121881
C -3.928208 2.930689 0.009966
C -5.030520 0.892862 -0.977904
H -3.418118 3.205807 -0.920254
H -4.886815 3.463352 0.016174
H -3.333246 3.338192 0.835784
H -5.190971 -0.190135 -0.900594
H -6.021184 1.361804 -0.949559
H -4.615976 1.086434 -1.973577
N -0.414458 -1.293158 0.196317
H -0.187835 -0.526826 0.846536
C 0.733036 -1.910014 -0.505878
H 0.382604 -2.843192 -1.033075
C 1.340955 -0.953027 -1.554306
C 1.814149 -2.315554 0.513634
H 2.010146 -1.538602 -2.222906
H 0.531765 -0.591888 -2.226734
C 2.077939 0.204249 -0.948934
O 2.548875 -3.299709 0.220838
O 1.975079 -1.679024 1.588457
C 1.390320 1.356412 -0.530250
C 3.471196 0.138162 -0.777544
H 0.308014 1.421762 -0.672594
C 2.064395 2.415014 0.061404
C 4.166873 1.181028 -0.184562
H 4.014650 -0.747694 -1.113568
H 1.528833 3.299755 0.386018
C 3.472528 2.345487 0.245731
H 5.241137 1.123897 -0.050974
O 4.118971 3.325620 0.799251
###
36
LysAla1 pm6 E=-0.103715166280E-01 au
N 0.930149 3.079734 0.705971
H 1.325442 2.576755 1.521641
H 0.200615 3.734686 1.049745
H 1.694870 3.644046 0.279850
C 0.354914 2.121123 -0.320296
H -0.160120 2.754621 -1.115249
C 1.459666 1.305755 -1.006619
C -0.664245 1.195340 0.361165
H 0.999478 0.712787 -1.829725
H 2.148462 2.008031 -1.533475
C 2.260537 0.393921 -0.073134
O -0.484208 0.744205 1.498747
H 2.786265 0.990533 0.701771
H 1.582702 -0.280180 0.489125
C 3.282578 -0.423668 -0.871023
H 2.768432 -1.083268 -1.603542
H 3.905536 0.254018 -1.498399
C 4.217222 -1.238162 0.019577
H 5.109762 -1.578141 -0.563811
H 4.624622 -0.622747 0.858773
N 3.520982 -2.457276 0.594243
H 3.115516 -3.041589 -0.157280
H 4.188904 -3.040098 1.130302
H 2.755083 -2.181513 1.232258
N -1.782947 0.884261 -0.372785
H -1.930035 1.265706 -1.322650
C -2.835082 -0.010507 0.158316
H -2.918251 0.128509 1.282147
C -4.169444 0.287257 -0.507492
C -2.463138 -1.472666 -0.110047

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H       -4.146142       0.153898        -1.600608
H       -4.972989       -0.359008       -0.117977
H       -4.495387       1.324066        -0.325870
O       -1.579778       -1.902331       -0.835324
O       -3.184794       -2.437523       0.535185
H       -3.927852       -2.093313       1.139414
###
35
LysAla2 pm6 E=-0.186379338684 au
N       0.435119        2.872326        1.147108
H       0.630507        3.696936        0.547922
H       1.218647        2.769410        1.820781
H       -0.430424       3.070859        1.689990
C       0.256940        1.614057        0.311217
H       -0.034593       0.777682        1.021105
C       -0.845067       1.821962        -0.738355
C       1.585560        1.299682        -0.384065
H       -0.702358       2.797420        -1.259708
H       -0.741620       1.064874        -1.549614
C       -2.259537       1.761309        -0.157388
O       2.395779        2.212389        -0.627393
H       -2.397299       2.557049        0.606292
H       -2.979623       2.018841        -0.965445
C       -2.639225       0.413518        0.462140
H       -1.951912       0.164883        1.299627
H       -3.642098       0.511047        0.937494
C       -2.645627       -0.711943       -0.571832
H       -3.127156       -0.387239       -1.527253
H       -1.597364       -1.010911       -0.846538
N       -3.382602       -1.925960       -0.041407
H       -4.362684       -1.688788       0.200738
H       -3.401211       -2.682425       -0.748209
H       -2.929505       -2.295759       0.811665
N       1.911191        0.025004        -0.762831
H       2.806225        -0.117284       -1.260918
C       1.096095        -1.194549       -0.555686
H       -0.008826       -0.951168       -0.650685
C       1.462615        -2.246263       -1.594400
C       1.348734        -1.796117       0.846131
H       2.529552        -2.511604       -1.587692
H       0.897151        -3.178436       -1.441253
H       1.228305        -1.913286       -2.617023
O       0.365739        -2.312109       1.443694
O       2.499408        -1.807983       1.360206
###
34
LysAla3 pm6 E=-0.336804867158 au
N       0.869281        3.306453        -0.843744
H       0.221565        3.450536        -1.623314
H       0.507897        3.863586        -0.067077
C       0.913524        1.867690        -0.478082
H       1.441393        1.326439        -1.317828
C       1.701859        1.672415        0.828993
C       -0.510242       1.298336        -0.317960
H       2.627086        2.288379        0.787893
H       1.132641        2.077894        1.690894
C       2.073223        0.212243        1.099909
O       -1.429920       1.997741        0.163804
H       2.539191        0.142074        2.106611
H       1.161454        -0.412331       1.168091
C       3.035635        -0.349949       0.048482
H       2.659345        -0.136797       -0.978715
H       4.009840        0.183959        0.107161
C       3.291874        -1.844580       0.220068
H       4.246125        -2.137039       -0.285152
H       3.424736        -2.119383       1.294969
N       2.160715        -2.668099       -0.367981
H       1.993472        -2.412519       -1.358676
H       2.382854        -3.678380       -0.326508
H       1.277042        -2.510976       0.145408
N       -0.750142       0.022836        -0.748545
H       0.023050        -0.587749       -1.070749
C       -2.112267       -0.571928       -0.785933
H       -2.783292       0.104427        -1.388848
C       -2.064060       -1.946244       -1.431467
C       -2.692561       -0.673362       0.644254
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H       -1.382841       -2.642403       -0.920780
H       -3.058767       -2.416771       -1.452930
H       -1.727717       -1.895938       -2.479384
O       -3.613044       0.137700        0.961893
O       -2.266532       -1.523323       1.464458
###
33
LysAla4 pm6 E=-0.465458651739 au
N       0.941500        2.547707        -1.221604
H       0.130399        2.624178        -1.840871
H       0.919526        3.362487        -0.605767
C       0.877644        1.289520        -0.435517
H       1.067532        0.436958        -1.149950
C       1.958755        1.276319        0.657528
C       -0.511418       1.127402        0.214530
H       2.921963        1.624440        0.224286
H       1.722738        2.018381        1.447134
C       2.144453        -0.108947       1.285382
O       -0.877558       1.835881        1.172686
H       2.772315        -0.007988       2.195807
H       1.172210        -0.496195       1.651222
C       2.774525        -1.131615       0.334354
H       2.666289        -2.148376       0.762708
H       2.212390        -1.160778       -0.622195
C       4.257110        -0.832980       0.066089
H       4.372345        0.203959        -0.321105
H       4.833604        -0.865447       1.015300
N       4.895376        -1.762443       -0.909337
H       4.327117        -1.808345       -1.758713
H       4.886476        -2.712823       -0.533248
N       -1.348339       0.173540        -0.308539
H       -1.086841       -0.367246       -1.144220
C       -2.747628       0.030202        0.164135
H       -2.796686       0.322666        1.250612
C       -3.706727       0.899124        -0.640236
C       -3.177485       -1.443870       0.024763
H       -3.717686       0.651497        -1.710191
H       -4.740319       0.808824        -0.275743
H       -3.447066       1.965627        -0.571529
O       -3.777964       -1.982547       0.995637
O       -2.950908       -2.077632       -1.038740
###
34
LysDAla3 pm6 E=-0.334977409107 au
N       0.191004        -2.600397       -1.285170
H       -0.727383       -2.964462       -1.552100
H       0.391458        -1.804670       -1.894014
C       0.215006        -2.202752       0.138525
H       -0.065442       -3.116894       0.747767
C       1.636061        -1.768343       0.546373
C       -0.792401       -1.121214       0.581493
H       1.668369        -1.615507       1.645451
H       2.329971        -2.617803       0.367698
C       2.144329        -0.518147       -0.179128
O       -0.657660       -0.553829       1.688584
H       2.220662        -0.709284       -1.269536
H       1.415994        0.311704        -0.087057
C       3.508567        -0.091239       0.375801
H       3.406237        0.267930        1.422657
H       4.183560        -0.973295       0.452207
C       4.203143        0.960377        -0.485316
H       5.288504        1.023762        -0.221305
H       4.172460        0.688542        -1.568995
N       3.580913        2.331653        -0.305256
H       3.592438        2.616132        0.690271
H       4.099746        3.044556        -0.848859
H       2.598125        2.338774        -0.625601
N       -1.865376       -0.800871       -0.212996
H       -2.027051       -1.249039       -1.126153
C       -2.902643       0.172322        0.223071
C       -2.317668       1.594312        0.053429
O       -2.272139       2.152901        -1.070683
O       -1.859476       2.169569        1.084621
C       -4.172932       0.008644        -0.591449
H       -4.013789       0.127123        -1.672608
H       -4.628160       -0.984391       -0.453986
```

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H       -3.131287       0.006613        1.313517
H       -4.934763       0.744625        -0.292364
###
33
LysDAla4 pm6 E=-0.470048574202 au
N       -0.114531       3.121686        -0.484052
H       0.655597        3.653052        -0.069486
H       0.175998        2.882347        -1.435988
C       -0.389642       1.902717        0.310608
H       -0.823789       2.241291        1.296105
C       -1.410619       1.003335        -0.409800
C       0.861969        1.070592        0.657072
H       -2.319769       1.602673        -0.634249
H       -1.030617       0.691799        -1.403478
C       -1.785745       -0.219874       0.434116
O       1.064237        0.700192        1.832909
H       -0.906585       -0.886127       0.548183
H       -2.049794       0.095317        1.465201
C       -2.942426       -1.023181       -0.169096
H       -2.743180       -1.248573       -1.235302
H       -2.993313       -2.012068       0.331824
C       -4.290141       -0.299713       -0.027577
H       -4.425349       0.060000        1.015696
H       -4.303502       0.610513        -0.666437
N       -5.469380       -1.136451       -0.388462
H       -5.505308       -1.960427       0.215360
H       -5.354764       -1.503248       -1.335406
N       1.744267        0.720445        -0.332726
H       1.601177        0.999803        -1.314302
C       2.933583        -0.120922       -0.040854
C       2.443837        -1.585293       0.067333
O       2.315776        -2.083763       1.222440
O       2.152428        -2.251333       -0.959735
C       3.984957        0.025851        -1.124202
H       3.609130        -0.210334       -2.129639
H       4.382598        1.051298        -1.176269
H       3.368827        0.185351        0.952195
H       4.845991        -0.634257       -0.937855
###
42
LysGlu1 pm6 E=-0.166585840646 au
N       -1.159610       -2.859207       -1.818367
H       -0.885921       -3.525353       -1.071397
H       -0.384051       -2.803312       -2.508974
H       -1.992110       -3.255428       -2.304823
C       -1.488271       -1.488807       -1.253835
H       -1.771435       -0.816055       -2.127343
C       -2.682093       -1.583465       -0.291776
C       -0.254432       -0.939916       -0.517169
H       -3.511869       -2.141763       -0.785350
H       -2.419868       -2.193109       0.599811
C       -3.170902       -0.193533       0.127068
O       0.073549        -1.342458       0.606978
H       -2.345313       0.390472        0.583798
H       -3.476677       0.387436        -0.768791
C       -4.336718       -0.310113       1.114627
H       -5.164984       -0.904716       0.670866
H       -4.020742       -0.894571       2.008273
C       -4.846152       1.048079        1.589252
H       -5.438563       0.932508        2.531164
H       -4.003592       1.736266        1.844765
N       -5.722637       1.710954        0.543465
H       -6.521314       1.104216        0.288569
H       -6.102960       2.606236        0.900009
H       -5.188804       1.909184        -0.319749
N       0.443987        0.059657        -1.151200
H       0.267550        0.299247        -2.143262
C       1.641865        0.648954        -0.509829
H       1.520539        0.596065        0.617842
C       2.921380        -0.101694       -0.922268
C       1.716335        2.123686        -0.914416
H       2.708344        -1.191654       -1.019038
H       3.240197        0.196346        -1.946477
C       4.061233        0.126663        0.062906
O       2.306143        2.592850        -1.871810
O       1.064924        3.035740        -0.135320
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H       5.034956        -0.168633       -0.412542
H       4.207271        1.218083        0.277956
C       3.887139        -0.614169       1.341950
O       2.902924        -1.231444       1.740175
O       4.939321        -0.641923       2.223786
H       5.755056        -0.112679       1.929983
H       0.570911        2.655155        0.667896
###
41
LysGlu2 pm6 E=-0.351513286958 au
N       2.190243        2.802543        -0.620949
H       2.030073        3.362143        0.237261
H       1.536304        3.133587        -1.357256
H       3.162299        2.993157        -0.946246
C       2.011460        1.316861        -0.363418
H       2.176913        0.776818        -1.351630
C       3.060507        0.827119        0.645760
C       0.589249        1.059505        0.175119
H       4.075366        1.141963        0.303874
H       2.921275        1.332020        1.626529
C       3.027785        -0.690622       0.838954
O       0.306048        1.282176        1.361677
H       3.692782        -0.950473       1.692188
H       2.017367        -1.017594       1.163981
C       3.431869        -1.487816       -0.404373
H       3.277870        -2.572942       -0.210507
H       2.746742        -1.252095       -1.250405
C       4.863926        -1.235257       -0.868780
H       5.031021        -1.688691       -1.877268
H       5.065889        -0.141564       -0.991327
N       5.872140        -1.817802       0.102420
H       5.695557        -2.825526       0.260139
H       6.835898        -1.713687       -0.260199
H       5.822323        -1.341527       1.019847
N       -0.310473       0.575642        -0.736093
H       -0.020955       0.432492        -1.722922
C       -1.701825       0.164090        -0.443278
H       -2.096214       -0.295757       -1.402081
C       -1.791480       -0.897967       0.665245
C       -2.580232       1.400968        -0.134901
H       -1.313825       -1.839699       0.308305
H       -1.192267       -0.599492       1.553022
C       -3.226331       -1.178349       1.111208
O       -3.389473       1.766360        -1.033463
O       -2.521521       2.000047        0.967728
H       -3.221550       -2.001335       1.875527
H       -3.657213       -0.312951       1.667871
C       -4.119426       -1.546624       -0.026219
O       -4.931313       -0.805284       -0.579514
O       -4.070079       -2.807056       -0.545115
H       -3.391324       -3.422929       -0.098755
###
40
LysGlu3 pm6 E=-0.535623097264 au
N       1.183918        3.061070        -0.426744
H       1.015675        3.326100        0.563351
H       0.322153        3.260006        -0.974620
H       1.936412        3.681361        -0.794218
C       1.605680        1.605266        -0.550576
H       1.647695        1.346909        -1.659538
C       3.004255        1.434724        0.063681
C       0.580829        0.673741        0.119904
H       3.635326        2.322419        -0.178143
H       2.942140        1.432924        1.173192
C       3.700421        0.168899        -0.445310
O       0.893521        -0.096973       1.043575
H       3.058478        -0.721218       -0.288168
H       3.846505        0.226769        -1.544697
C       5.047323        -0.016976       0.261404
H       5.695363        0.870348        0.089800
H       4.906010        -0.058809       1.363161
C       5.741831        -1.285657       -0.232884
H       5.130835        -2.195342       -0.015603
H       5.874710        -1.268743       -1.342886
N       7.100748        -1.435314       0.422073
H       7.009501        -1.520244       1.449849
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H       7.584320        -2.281105       0.070568
H       7.700421        -0.615295       0.223482
N       -0.699185       0.676713        -0.372439
H       -0.980134       1.272647        -1.172035
C       -1.781134       -0.087359       0.298798
H       -1.524015       -0.223472       1.391726
C       -3.099860       0.688048        0.192324
C       -1.839870       -1.497806       -0.332632
H       -2.942708       1.741375        0.516951
H       -3.405593       0.779589        -0.872493
C       -4.199138       0.047148        1.044761
O       -2.767529       -1.844771       -1.113452
O       -0.919221       -2.306264       -0.026016
H       -3.889816       -0.933497       1.466173
H       -4.395039       0.660840        1.951210
C       -5.458673       -0.112743       0.231518
O       -5.621033       -1.151992       -0.484203
O       -6.345313       0.784431        0.244694
###
39
LysGlu4 pm6 E=-0.675090297900 au
N       -0.847194       -3.043009       0.748967
H       0.078541        -3.465920       0.665937
H       -1.061378       -2.998513       1.747072
C       -0.859868       -1.687434       0.148537
H       -0.824633       -1.818021       -0.972530
C       -2.132610       -0.912055       0.537597
C       0.375314        -0.869351       0.576530
H       -2.289525       -0.952090       1.635930
H       -2.008631       0.165974        0.301562
C       -3.369452       -1.449033       -0.191764
O       1.097790        -1.225722       1.532167
H       -3.162484       -1.546817       -1.278110
H       -3.594837       -2.477991       0.154677
C       -4.603314       -0.567811       0.030596
H       -5.518257       -1.149166       -0.218202
H       -4.709955       -0.310351       1.106370
C       -4.543114       0.703560        -0.816714
H       -3.673574       1.342222        -0.527030
H       -4.397622       0.462040        -1.898446
N       -5.818367       1.508885        -0.660677
H       -5.989803       1.743523        0.333122
H       -5.760669       2.395114        -1.194118
H       -6.636906       0.979052        -1.007388
N       0.688784        0.255522        -0.142627
H       0.126691        0.542613        -0.958941
C       1.826766        1.134818        0.213172
H       2.371372        0.695769        1.095853
C       2.797787        1.308794        -0.969305
C       1.280972        2.515521        0.642964
H       2.284858        1.105843        -1.934439
H       3.118343        2.372103        -1.052142
C       4.046635        0.439161        -0.834644
O       1.689956        2.988253        1.737968
O       0.473663        3.143217        -0.088501
H       4.718307        0.610366        -1.707678
H       4.653241        0.754918        0.041413
C       3.703403        -1.024880       -0.738045
O       3.821999        -1.625363       0.374412
O       3.288996        -1.661410       -1.749308
###
38
LysGlu5 pm6 E=-0.800653809086 au
N       0.388596        -3.923221       -0.230405
H       1.405839        -4.024138       -0.240402
H       0.055929        -4.409667       0.605248
C       0.010985        -2.488567       -0.184902
H       0.401210        -2.005122       -1.125200
C       -1.521275       -2.345503       -0.146672
C       0.605431        -1.805022       1.059596
H       -1.957633       -2.952969       -0.968569
H       -1.929882       -2.787659       0.784787
C       -1.968265       -0.886277       -0.286003
O       0.445288        -2.290208       2.199217
H       -1.578921       -0.281627       0.558152
H       -1.532331       -0.437227       -1.202080
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C       -3.496711       -0.786869       -0.333573
H       -3.886741       -1.334171       -1.215230
H       -3.940443       -1.296958       0.544967
C       -3.958440       0.677742        -0.377823
H       -3.574388       1.228458        0.507925
H       -3.529301       1.189566        -1.266290
N       -5.440538       0.836157        -0.420177
H       -5.853946       0.387577        0.400776
H       -5.813834       0.318473        -1.219466
N       1.355803        -0.658924       0.966908
H       1.741990        -0.238096       1.824749
C       1.675927        0.043599        -0.294506
H       0.871122        -0.157653       -1.065357
C       1.780512        1.557019        -0.042677
C       2.997694        -0.490946       -0.893168
H       2.474792        1.759597        0.801507
H       2.245053        2.041182        -0.929645
C       0.413340        2.182294        0.228218
O       3.522331        0.145857        -1.847523
O       3.520464        -1.549637       -0.454861
H       -0.309049       1.905534        -0.570924
H       -0.037238       1.769971        1.160511
C       0.503554        3.681516        0.361838
O       -0.299050       4.413353        -0.292678
O       1.356495        4.219750        1.128132
###
48
PheArg1 pm6 E=0.691094022775E-01 au
N       3.224740        2.394991        0.308319
H       -1.987817       3.613818        -0.939074
H       3.901070        1.882923        0.905161
C       2.134098        1.477202        -0.219501
H       1.374614        2.140129        -0.747004
C       2.699703        0.481741        -1.242670
C       1.493766        0.747104        0.966107
H       1.850296        -0.077078       -1.708103
H       3.131786        1.051988        -2.102631
C       3.715142        -0.475734       -0.685787
O       2.163774        0.463870        1.970273
C       3.307101        -1.716724       -0.173458
C       5.077287        -0.140887       -0.688825
H       2.251206        -1.990783       -0.177311
C       4.252830        -2.608353       0.337957
C       6.018857        -1.037132       -0.176923
H       5.405591        0.820616        -1.090291
H       3.931581        -3.572686       0.735341
C       5.609524        -2.270543       0.338009
H       7.077920        -0.772680       -0.180210
H       6.346588        -2.968626       0.736558
N       0.164042        0.394894        0.954504
H       -0.208517       -0.116910       1.775091
C       -0.797862       0.638083        -0.138754
H       -0.273995       0.672236        -1.142215
C       -1.869876       -0.468208       -0.160286
C       -1.488771       1.988884        0.110657
H       -1.372132       -1.456076       -0.292266
H       -2.383357       -0.539950       0.823788
C       -2.883705       -0.233718       -1.281528
O       -1.997829       2.403138        1.139279
O       -1.505280       2.722575        -1.027029
H       -3.495202       0.669058        -1.072104
H       -2.357809       -0.001150       -2.236825
C       -3.789326       -1.442914       -1.529494
H       -4.512704       -1.211323       -2.348953
H       -3.189073       -2.312833       -1.898653
N       -4.525233       -1.927752       -0.331743
H       -3.947817       -2.537262       0.284010
C       -5.459527       -1.123616       0.321208
N       -5.777273       -1.411600       1.636830
N       -6.035836       -0.030267       -0.275047
H       -5.431679       -2.282663       2.052571
H       -6.674390       -1.090711       2.014231
H       -5.860012       0.183917        -1.258634
H       -6.901552       0.361560        0.109002
H       3.754883        2.817125        -0.484224
H       2.816663        3.167734        0.872243
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###
47
PheArg2 pm6 E=-0.105935373123 au
N       1.428668        -2.557211       -2.187223
H       0.656140        -2.498862       -2.881130
H       2.186215        -1.911911       -2.488569
C       0.940060        -2.253597       -0.783933
H       0.147280        -3.040411       -0.542488
C       2.084043        -2.405983       0.232084
C       0.234710        -0.895400       -0.596464
H       1.664727        -2.869843       1.158841
H       2.811424        -3.182707       -0.115239
C       2.823748        -1.141123       0.565153
O       -0.370158       -0.730629       0.477355
C       2.723915        -0.604901       1.859349
C       3.633403        -0.502494       -0.384619
H       2.111377        -1.103198       2.612777
C       3.424830        0.555232        2.196295
C       4.322645        0.665475        -0.046076
H       3.735139        -0.915688       -1.390926
H       3.353624        0.957607        3.208563
C       4.220417        1.197536        1.242462
H       4.948792        1.159855        -0.791511
H       4.765129        2.105094        1.505109
N       0.279952        0.055168        -1.576582
H       0.857809        -0.081276       -2.425094
C       -0.383404       1.383978        -1.538163
H       -0.247043       1.801368        -2.587105
C       -1.897175       1.331045        -1.266503
C       0.332752        2.365070        -0.588238
H       -2.396036       2.076453        -1.925265
H       -2.293694       0.350759        -1.610198
C       -2.303626       1.587632        0.186189
O       1.047136        1.963532        0.369908
O       0.190320        3.595745        -0.818145
H       -1.760348       0.895752        0.863482
H       -1.994934       2.608268        0.502919
C       -3.813888       1.473638        0.413900
H       -4.060311       1.736294        1.472133
H       -4.363394       2.220005        -0.212778
N       -4.393721       0.145059        0.083518
H       -4.591367       0.018953        -0.930405
C       -4.029282       -1.001268       0.782178
N       -3.408957       -0.947535       2.014084
N       -4.226755       -2.235122       0.190049
H       -3.367893       -0.056670       2.517854
H       -3.457395       -1.770534       2.625229
H       -4.777717       -2.289896       -0.674126
H       -4.312196       -3.063072       0.788156
H       1.813101        -3.527071       -2.221789
###
46
PheArg3 pm6 E=-0.258074490912 au
N       -3.596349       -2.247191       0.543332
H       -3.483471       -2.849884       1.362157
H       -4.046234       -1.390490       0.871410
C       -2.275750       -1.950308       -0.062362
H       -1.875696       -2.925240       -0.472376
C       -2.412559       -0.953133       -1.228633
C       -1.284246       -1.411316       0.982538
H       -1.544561       -1.076051       -1.916890
H       -3.286431       -1.247008       -1.855328
C       -2.542295       0.481821        -0.802162
O       -1.691221       -0.858245       2.028271
C       -3.780323       1.000796        -0.395425
C       -1.415113       1.318233        -0.815290
H       -4.668442       0.366914        -0.391976
C       -3.884329       2.337715        -0.001539
C       -1.523924       2.652823        -0.422159
H       -0.442524       0.922501        -1.142909
H       -4.850827       2.736276        0.312242
C       -2.758473       3.165884        -0.012678
H       -0.640132       3.300298        -0.437111
H       -2.841949       4.209105        0.293583
N       0.073837        -1.541797       0.839010
H       0.689448        -1.138161       1.559386
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C       0.765699        -2.080926       -0.350931
H       0.023200        -2.601538       -1.026245
C       1.445743        -0.950123       -1.142152
C       1.799549        -3.144463       0.069736
H       1.684266        -1.313357       -2.164223
H       0.703733        -0.126454       -1.309423
C       2.704197        -0.395182       -0.471420
O       2.368150        -3.796258       -0.851589
O       2.062150        -3.367185       1.279989
H       2.518676        -0.173650       0.600967
H       3.507867        -1.162924       -0.466449
C       3.233967        0.852500        -1.185263
H       4.326170        0.974175        -0.992021
H       3.145074        0.747812        -2.295687
N       2.503909        2.097782        -0.820297
H       1.531944        2.127121        -1.192218
C       2.688019        2.679834        0.437443
N       3.903180        2.636973        1.067683
N       1.651940        3.400472        1.007498
H       4.590608        1.918537        0.831618
H       4.024353        3.079293        1.983063
H       0.832804        3.633143        0.425564
H       1.872893        4.114498        1.710706
###
45
PheArg4 pm6 E=-0.403630237776 au
N       3.117406        3.630891        -0.150346
H       2.262728        4.165511        -0.327621
H       3.351697        3.761642        0.835645
C       2.901006        2.198626        -0.460863
H       2.761150        2.111174        -1.576784
C       4.125512        1.363223        -0.035848
C       1.664205        1.638721        0.270696
H       4.986572        1.624448        -0.693201
H       4.464205        1.662808        0.981356
C       3.862690        -0.115397       -0.097399
O       1.569514        1.654923        1.514386
C       3.755722        -0.858094       1.088843
C       3.721940        -0.764725       -1.333604
H       3.874473        -0.365910       2.055480
C       3.519551        -2.234058       1.037651
C       3.484191        -2.140164       -1.378830
H       3.803505        -0.196398       -2.262051
H       3.454137        -2.808037       1.963789
C       3.383879        -2.877895       -0.194858
H       3.383817        -2.641891       -2.343348
H       3.211570        -3.954141       -0.233798
N       0.660453        1.103146        -0.496051
H       0.715970        1.097082        -1.526522
C       -0.484064       0.387308        0.121188
H       -0.807796       0.931072        1.052100
C       -1.663018       0.296808        -0.854109
C       0.043753        -1.013801       0.519417
H       -1.874199       1.299921        -1.286386
H       -1.400961       -0.335917       -1.727894
C       -2.913232       -0.242147       -0.153630
O       0.178604        -1.916574       -0.344755
O       0.385882        -1.199247       1.721616
H       -2.687228       -1.179613       0.394863
H       -3.250954       0.472034        0.625746
C       -4.035760       -0.490929       -1.171203
H       -4.180224       0.397988        -1.826883
H       -3.758822       -1.323639       -1.859678
N       -5.325226       -0.867978       -0.528323
H       -5.218524       -1.719182       0.050992
C       -6.062301       0.192506        0.103420
N       -6.133254       1.440026        -0.301485
N       -6.952646       -0.246763       1.121627
H       -5.567674       1.704491        -1.112367
H       -6.590401       -0.971316       1.745321
H       -7.396619       0.499921        1.658076
###
22
SerGly1 pm6 E=-0.175098753721 au
N       2.371362        1.610574        -0.131111
H       1.883272        2.297911        -0.741835
```

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H       3.372950        1.595135        -0.414265
H       2.326899        1.948296        0.851973
C       1.773247        0.225265        -0.267426
H       1.741169        -0.038430       -1.378211
C       2.658780        -0.808388       0.450034
C       0.340069        0.170352        0.290905
H       3.126500        -0.414761       1.375683
H       2.094357        -1.731126       0.699704
O       3.686144        -1.132738       -0.507278
O       0.056802        -0.553168       1.254133
H       4.288155        -1.824127       -0.113692
N       -0.607999       0.927115        -0.346948
H       -0.394424       1.509676        -1.173799
C       -1.992870       0.956082        0.141287
C       -2.781329       -0.266875       -0.252629
H       -2.031138       1.091756        1.260634
H       -2.513675       1.878082        -0.255393
O       -2.432637       -1.188986       -0.975896
O       -4.045959       -0.387802       0.252972
H       -4.339787       0.366695        0.871143
###
21
SerGly2 pm6 E=-0.356788167931 au
N       2.228414        -0.440015       1.370963
H       1.767178        -0.976740       2.132028
H       2.703690        0.384975        1.797408
H       2.955230        -1.045519       0.942766
C       1.216091        0.020199        0.340336
H       0.454819        0.668715        0.882572
C       1.902086        0.867447        -0.754895
C       0.528058        -1.200997       -0.275920
H       2.925066        0.502293        -0.987798
H       1.308842        0.890474        -1.695204
O       1.945754        2.232970        -0.346416
O       1.073763        -2.315715       -0.244217
H       2.636107        2.362326        0.366074
N       -0.688724       -1.074703       -0.888535
H       -1.127033       -1.911941       -1.302314
C       -1.467636       0.166623        -0.984121
C       -2.386839       0.383047        0.215791
H       -0.818815       1.061879        -1.147542
H       -2.105353       0.129726        -1.911247
O       -2.617565       1.568142        0.581093
O       -2.930467       -0.595530       0.796929
###
20
SerGly3 pm6 E=-0.507293128965 au
N       1.647719        2.011259        -0.448059
H       0.798018        2.342659        -0.913581
H       1.605382        2.339514        0.519382
C       1.711487        0.531358        -0.501763
H       1.795093        0.223777        -1.585656
C       2.969234        0.051643        0.241093
C       0.454984        -0.096999       0.129862
H       3.872160        0.607438        -0.080226
H       2.884064        0.117039        1.341177
O       3.125499        -1.334161       -0.143597
O       0.274217        -0.094796       1.365302
H       3.883923        -1.724886       0.370594
N       -0.473715       -0.636418       -0.717105
H       -0.340855       -0.632919       -1.739937
C       -1.751326       -1.184329       -0.228831
C       -2.736140       -0.045561       0.049567
H       -2.171746       -1.893614       -0.984398
H       -1.609559       -1.804003       0.689358
O       -3.534122       0.320465        -0.852297
O       -2.718587       0.516547        1.180576
###
34
SerLeu1 pm6 E=-0.214733643334 au
N       -3.927388       -1.258741       0.795118
H       -3.620920       -1.962518       1.495708
H       -4.795654       -1.613236       0.339892
H       -4.163630       -0.381238       1.296968
C       -2.850395       -1.029095       -0.241628
H       -2.647957       -2.028804       -0.758419
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C       -3.308961       -0.028635       -1.322913
C       -1.567989       -0.531773       0.434870
H       -2.596356       -0.026920       -2.178149
H       -4.323483       -0.280108       -1.699508
O       -3.282768       1.317827        -0.845028
O       -1.577381       -0.011112       1.557263
H       -4.047994       1.487277        -0.224819
N       -0.415742       -0.672064       -0.296458
H       -0.424742       -1.109912       -1.236093
C       0.882966        -0.150863       0.191890
H       1.056156        -0.515578       1.252280
C       2.010299        -0.642909       -0.728097
C       0.840284        1.382010        0.198256
H       1.918342        -1.745177       -0.859077
H       1.878157        -0.229843       -1.752203
C       3.425913        -0.304997       -0.210898
O       0.204534        2.107170        -0.553037
O       1.568265        2.046047        1.140728
H       3.493252        0.801326        -0.046844
C       3.722245        -1.010080       1.113727
C       4.455485        -0.693136       -1.275617
H       3.657552        -2.100978       1.029473
H       4.731964        -0.778967       1.475019
H       3.028377        -0.704499       1.908400
H       4.283171        -0.170571       -2.224453
H       5.475304        -0.442782       -0.958890
H       4.444021        -1.767394       -1.495009
H       2.096067        1.462964        1.788157
###
33
SerLeu2 pm6 E=-0.385450226531 au
N       -2.645712       1.142164        0.636677
H       -1.983276       1.918184        0.393084
H       -3.035919       1.332649        1.584637
H       -3.430998       1.158213        -0.040603
C       -1.936199       -0.193740       0.624588
H       -1.143143       -0.187149       1.447285
C       -2.913764       -1.339890       0.961027
C       -1.287284       -0.433362       -0.743275
H       -2.356360       -2.292800       1.076657
H       -3.475388       -1.125834       1.897022
O       -3.927623       -1.482775       -0.033222
O       -1.942929       -0.954719       -1.665285
H       -3.533594       -1.866836       -0.872793
N       0.021162        -0.110416       -0.961557
H       0.440464        -0.334680       -1.880591
C       0.915880        0.564786        0.007687
H       0.682596        0.208942        1.060808
C       2.379177        0.240736        -0.324051
C       0.674831        2.091386        -0.002904
H       2.589332        0.460292        -1.392760
H       3.041941        0.926630        0.243137
C       2.766813        -1.221333       -0.008272
O       -0.390131       2.564292        -0.484338
O       1.542796        2.847257        0.512118
H       2.068465        -1.902966       -0.555408
C       4.187882        -1.491084       -0.511737
C       2.657715        -1.517696       1.489092
H       4.933442        -0.856955       -0.018650
H       4.487254        -2.530752       -0.331654
H       4.281608        -1.315947       -1.590245
H       1.640058        -1.348762       1.866144
H       2.908622        -2.561766       1.711908
H       3.329540        -0.893947       2.089061
###
32
SerLeu3 pm6 E=-0.545736333045 au
N       -3.797613       -1.700990       0.288005
H       -3.346717       -2.476903       0.778556
H       -4.178588       -1.081792       1.005762
C       -2.813697       -0.988834       -0.557395
H       -2.518421       -1.693306       -1.394979
C       -3.440670       0.263893        -1.198990
C       -1.552138       -0.581492       0.220328
H       -2.750964       0.734311        -1.929461
H       -4.389457       0.014297        -1.713336
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O       -3.675475       1.301827        -0.232593
O       -1.589793       -0.405678       1.457446
H       -4.488475       1.101887        0.304910
N       -0.399190       -0.388819       -0.489233
H       -0.380140       -0.522832       -1.514971
C       0.889904        -0.030242       0.156541
H       0.965856        -0.550476       1.153985
C       2.059262        -0.464036       -0.733932
C       0.880467        1.496445        0.410237
H       1.902282        -1.505389       -1.087909
H       2.078738        0.140561        -1.663704
C       3.415017        -0.363080       0.002297
O       0.316474        1.918713        1.464235
O       1.394958        2.300069        -0.405783
H       3.405730        0.545731        0.656669
C       3.647373        -1.591243       0.885241
C       4.548764        -0.202454       -1.013567
H       3.711401        -2.516766       0.300674
H       4.582105        -1.509900       1.452973
H       2.841677        -1.731600       1.615809
H       4.450224        0.718189        -1.600530
H       5.527583        -0.156065       -0.520597
H       4.589784        -1.034478       -1.726264
###
49
TyrArg1 pm6 E=-0.135595530546E-01 au
N       3.161991        3.844882        -0.282446
H       2.337033        4.420120        -0.545707
H       3.390264        4.034924        0.712359
C       2.893874        2.371437        -0.518322
H       2.672919        2.235023        -1.625847
C       4.133811        1.536723        -0.143597
C       1.703945        1.920957        0.346303
H       4.981611        1.814174        -0.815543
H       4.492505        1.807706        0.877257
C       3.845368        0.066946        -0.242110
O       1.659004        2.122563        1.563583
C       3.672765        -0.694478       0.926360
C       3.731325        -0.546825       -1.500481
H       3.776149        -0.221567       1.907476
C       3.367687        -2.052187       0.851887
C       3.426844        -1.903440       -1.599329
H       3.874798        0.042793        -2.410956
H       3.224465        -2.648283       1.752538
C       3.244620        -2.634269       -0.418361
H       3.331339        -2.388875       -2.571568
O       2.902143        -3.973846       -0.427408
N       0.706811        1.239613        -0.313316
H       0.743153        1.084357        -1.336621
C       -0.427185       0.628481        0.414490
H       -0.635646       1.205977        1.365898
C       -1.682006       0.603427        -0.468377
C       0.000827        -0.803157       0.778275
H       -1.912543       1.643211        -0.799843
H       -1.493439       0.044869        -1.411592
C       -2.883154       0.012537        0.274555
O       0.101840        -1.774009       0.049006
O       0.320281        -0.881624       2.094487
H       -2.725964       -1.068273       0.481637
H       -2.994297       0.484290        1.275137
C       -4.152069       0.221534        -0.559601
H       -4.315418       1.311617        -0.748114
H       -4.052539       -0.259675       -1.563146
N       -5.318984       -0.362843       0.155593
H       -5.121338       -1.005747       0.942350
C       -6.616223       -0.095668       -0.188480
N       -6.945891       0.594099        -1.347312
N       -7.635907       -0.541594       0.650382
H       -6.261189       1.241851        -1.749315
H       -7.909548       0.939100        -1.437295
H       -7.438337       -1.340804       1.263847
H       -8.588607       -0.561555       0.270271
H       2.811363        -4.331211       -1.365237
H       3.969789        4.159369        -0.860520
H       0.638617        -1.799265       2.395613
###
```

48
TyrArg2 pm6 E=-0.186719494569 au
N 0.549427 -2.431592 0.377346
H -0.411159 -2.618233 0.022784
H 1.204602 -2.470757 -0.424440
C 0.608676 -1.091757 1.087649
H -0.218587 -1.096386 1.874484
C 1.943060 -0.900035 1.823989
C 0.366558 0.033767 0.067145
H 1.844212 -0.015630 2.499824
H 2.088973 -1.750976 2.535228
C 3.140799 -0.750582 0.933011
O 0.929592 0.059043 -1.035992
C 3.836266 -1.885964 0.481252
C 3.580921 0.529407 0.559595
H 3.506673 -2.885602 0.783036
C 4.945324 -1.754962 -0.351076
C 4.688901 0.685692 -0.273285
H 3.050747 1.414930 0.920038
H 5.486769 -2.629684 -0.709718
C 5.351271 -0.463605 -0.720471
H 5.036090 1.675955 -0.569597
O 6.450750 -0.406359 -1.557656
N -0.479956 1.033610 0.474308
H -1.066178 0.913887 1.319344
C -0.861854 2.138248 -0.437738
H 0.004021 2.361407 -1.130213
C -2.082088 1.802229 -1.311233
C -1.056899 3.397836 0.437319
H -2.495411 2.752666 -1.715158
H -1.736829 1.257147 -2.217638
C -3.197780 1.007049 -0.627595
O -0.017302 3.929811 0.924294
O -2.191485 3.895338 0.644142
H -3.343144 1.345239 0.418241
H -4.158926 1.245141 -1.135778
C -2.942461 -0.508476 -0.652983
H -2.137996 -0.769031 -1.387292
H -2.560976 -0.866513 0.332220
N -4.140416 -1.282866 -1.077776
H -4.554673 -0.938788 -1.968660
C -5.038372 -1.805039 -0.149902
N -6.325321 -2.105988 -0.557947
N -4.707505 -1.975355 1.175092
H -6.563185 -2.031142 -1.551987
H -6.841355 -2.839490 -0.061127
H -3.738948 -1.829413 1.477702
H -5.229239 -2.656648 1.735753
H 6.685209 0.540317 -1.810142
H 0.809324 -3.198556 1.033581
###
47
TyrArg3 pm6 E=-0.335689763980 au
N 2.534262 2.688912 0.122907
H 2.147390 3.173657 0.937318
H 3.449448 2.334099 0.407071
C 1.639097 1.581749 -0.290833
H 0.745325 2.066397 -0.779959
C 2.306215 0.655973 -1.328165
C 1.170570 0.746947 0.914421
H 1.555759 -0.079542 -1.698282
H 2.555709 1.260187 -2.231078
C 3.530127 -0.053584 -0.825343
O 1.910139 0.566183 1.903524
C 4.799198 0.532554 -0.981289
C 3.415335 -1.303343 -0.196049
H 4.897553 1.496296 -1.488791
C 5.940274 -0.101764 -0.496111
C 4.542824 -1.955529 0.303881
H 2.435495 -1.775552 -0.092258
H 6.927190 0.344658 -0.610843
C 5.789222 -1.337466 0.151133
H 4.460512 -2.922180 0.801821
O 6.960369 -1.904445 0.622883
N -0.085071 0.187879 0.957868
H -0.353349 -0.378243 1.776836

```
C       -1.117863       0.345700        -0.091880
H       -0.636727       0.326929        -1.111576
C       -2.149378       -0.791130       -0.007604
C       -1.818540       1.711415        0.106222
H       -1.630338       -1.773853       -0.051817
H       -2.659651       -0.789659       0.977934
C       -3.167632       -0.687644       -1.146269
O       -1.763403       2.552391        -0.829709
O       -2.432376       1.965901        1.178095
H       -3.701917       0.284118        -1.110658
H       -2.642709       -0.684330       -2.128831
C       -4.166966       -1.847163       -1.147503
H       -4.749836       -1.849064       -2.099851
H       -3.633669       -2.831105       -1.124002
N       -5.096124       -1.850704       0.014397
H       -4.678549       -2.256526       0.876184
C       -6.023619       -0.830009       0.206140
N       -6.570319       -0.148059       -0.849062
N       -6.467735       -0.562275       1.494347
H       -6.094680       -0.104576       -1.751606
H       -7.257029       0.593684        -0.680703
H       -6.290646       -1.260979       2.225283
H       -7.364525       -0.076013       1.609161
H       6.783140        -2.749159       1.142610
###
46
TyrArg4 pm6 E=-0.495782411429 au
N       2.707420        2.965376        -0.238075
H       2.503808        3.533818        0.588410
H       3.643025        2.579094        -0.096458
C       1.704922        1.881689        -0.377900
H       0.765523        2.372603        -0.763198
C       2.159522        0.814800        -1.396383
C       1.395276        1.202301        0.966449
H       1.269477        0.222318        -1.715018
H       2.496314        1.326314        -2.325550
C       3.235526        -0.092233       -0.877254
O       2.218162        1.222531        1.906005
C       4.589184        0.274699        -0.968605
C       2.899667        -1.324366       -0.290218
H       4.862483        1.220082        -1.444849
C       5.586432        -0.545921       -0.462497
C       3.877908        -2.161020       0.225914
H       1.852179        -1.631422       -0.243046
H       6.628273        -0.254773       -0.532743
C       5.247469        -1.782927       0.151793
H       3.611262        -3.106831       0.682951
O       6.169910        -2.555915       0.637047
N       0.194419        0.571078        1.190893
H       0.025250        0.123234        2.104359
C       -0.847303       0.365905        0.156948
H       -0.351985       0.110886        -0.828500
C       -1.788195       -0.780923       0.558599
C       -1.658603       1.671044        -0.020479
H       -1.194931       -1.659565       0.896719
H       -2.396724       -0.499043       1.443287
C       -2.685465       -1.188771       -0.613460
O       -1.673739       2.209221        -1.158915
O       -2.288665       2.174049        0.949299
H       -3.164633       -0.300253       -1.074548
H       -2.067003       -1.628234       -1.428399
C       -3.746596       -2.214217       -0.205402
H       -4.138027       -2.746581       -1.105552
H       -3.303706       -3.016603       0.435890
N       -4.874939       -1.627148       0.569050
H       -4.619839       -1.396329       1.550955
C       -5.764750       -0.742203       -0.046990
N       -6.071361       -0.849745       -1.375852
N       -6.408724       0.212869        0.725289
H       -5.457912       -1.348733       -2.022373
H       -6.746641       -0.209867       -1.802937
H       -6.404876       0.103783        1.745522
H       -7.274337       0.632865        0.365347
###
45
TyrArg5 pm6 E=-0.636565699300 au
```

```
N       2.823089        2.571770        2.189590
H       2.871893        3.481410        1.726141
H       1.940228        2.544956        2.705895
C       2.896171        1.476010        1.196505
H       3.920040        1.513379        0.724818
C       2.709115        0.109474        1.885059
C       1.879307        1.617540        0.043290
H       3.490118        -0.010033       2.667924
H       1.750401        0.084716        2.448186
C       2.784392        -1.015978       0.895808
O       2.288957        1.725223        -1.134374
C       1.615238        -1.658231       0.457609
C       4.026526        -1.435675       0.388816
H       0.637769        -1.336482       0.847924
C       1.668597        -2.687859       -0.470631
C       4.105984        -2.459505       -0.543546
H       4.941338        -0.946862       0.732562
H       0.761917        -3.179704       -0.804202
C       2.922303        -3.106614       -0.993561
H       5.065378        -2.778238       -0.935520
O       2.984025        -4.058433       -1.873099
N       0.543392        1.646705        0.333711
H       0.212119        1.530168        1.306982
C       -0.504804       1.661480        -0.717826
H       -0.150953       1.079064        -1.616447
C       -1.809241       1.044654        -0.198932
C       -0.702116       3.132927        -1.150833
H       -2.087897       1.485575        0.782106
H       -2.635571       1.321991        -0.891666
C       -1.716805       -0.479721       -0.085627
O       -1.582732       3.856026        -0.622596
O       0.071543        3.591702        -2.042531
H       -1.543834       -0.929953       -1.084657
H       -0.820288       -0.768541       0.520733
C       -2.951497       -1.095791       0.577141
H       -2.747703       -2.167848       0.810903
H       -3.154678       -0.601433       1.554414
N       -4.136663       -1.031982       -0.339553
H       -4.124991       -0.165714       -0.907290
C       -5.416502       -1.257836       0.269463
N       -5.541979       -2.435441       1.053880
N       -6.419070       -0.487005       -0.091424
H       -4.692641       -2.824512       1.463757
H       -6.298014       -2.422450       1.742381
H       -7.350372       -0.743194       0.246018
###
32
TyrGly1 pm6 E=-0.146930552813 au
N       -0.100137       1.675408        1.071687
H       0.487838        1.748916        1.926001
H       -1.097315       1.653761        1.370270
H       0.038566        2.532979        0.503785
C       0.241260        0.425394        0.280592
H       0.101140        -0.467472       0.971541
C       -0.686396       0.291644        -0.938210
C       1.699724        0.517527        -0.198487
H       -0.613509       1.199701        -1.582328
H       -0.320647       -0.538595       -1.590776
C       -2.108693       0.024546        -0.538188
O       2.215108        1.604924        -0.495097
C       -2.462535       -1.222985       0.001903
C       -3.089675       1.014933        -0.712456
H       -1.700138       -1.996668       0.133082
C       -3.779278       -1.484568       0.376472
C       -4.414709       0.772657        -0.353830
H       -2.815441       1.988164        -1.130613
H       -4.062616       -2.447271       0.802931
C       -4.735447       -0.477721       0.193659
H       -5.182645       1.532790        -0.488471
O       -6.065576       -0.656094       0.533615
H       -6.214794       -1.530161       1.012078
N       2.383348        -0.665420       -0.292768
H       1.966852        -1.563562       0.004860
C       3.750237        -0.730129       -0.825203
C       4.780951        -0.414643       0.232401
H       3.925283        -1.751456       -1.271680
```

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H       3.899685        -0.026506       -1.693741
O       4.698607        0.428762        1.115253
O       5.952177        -1.114066       0.219541
H       6.030111        -1.812673       -0.517808
###
31
TyrGly2 pm6 E=-0.323961547490 au
N       -1.064026       -2.333612       1.278555
H       -1.744463       -2.188158       2.050100
H       -0.114906       -2.420993       1.698548
H       -1.289209       -3.234154       0.813152
C       -1.098354       -1.176836       0.292140
H       -0.803025       -0.242891       0.867357
C       -0.109612       -1.425704       -0.859454
C       -2.526122       -1.017527       -0.244234
H       -0.001288       -2.518885       -1.064404
H       -0.518222       -1.035244       -1.821848
C       1.223698        -0.799662       -0.569508
O       -3.325282       -1.967878       -0.217491
C       2.213444        -1.523321       0.115004
C       1.475671        0.522203        -0.973982
H       2.020835        -2.556283       0.422653
C       3.439597        -0.931551       0.414396
C       2.694356        1.133225        -0.689058
H       0.703563        1.080609        -1.517845
H       4.211686        -1.481134       0.954825
C       3.658528        0.391848        0.011111
H       2.901857        2.156314        -0.999870
O       4.841921        1.057777        0.275383
H       5.459894        0.504705        0.849447
N       -2.940642       0.185574        -0.750402
H       -3.899231       0.267882        -1.122927
C       -2.091722       1.377786        -0.892020
C       -1.906697       2.116973        0.435890
H       -1.093342       1.133137        -1.343324
H       -2.554801       2.075731        -1.638774
O       -2.889747       2.698910        0.971496
O       -0.762317       2.147569        0.959878
###
30
TyrGly3 pm6 E=-0.472666481146 au
N       -0.280774       -0.668493       1.645227
H       -0.949726       -0.357468       2.354516
H       -0.579116       -1.602854       1.351474
C       -0.270809       0.268007        0.497325
H       0.175404        1.240069        0.856526
C       0.565205        -0.274356       -0.677072
C       -1.694408       0.603733        -0.004858
H       0.276016        -1.325844       -0.904939
H       0.315106        0.289748        -1.605819
C       2.041544        -0.174886       -0.421321
O       -2.143461       1.765266        0.106970
C       2.673410        1.079963        -0.413023
C       2.800017        -1.337540       -0.206086
H       2.089058        1.987179        -0.586757
C       4.044729        1.181964        -0.185222
C       4.173305        -1.261040       0.021369
H       2.312820        -2.316308       -0.216857
H       4.543637        2.151509        -0.176324
C       4.773603        0.005603        0.029686
H       4.767771        -2.157843       0.188425
O       6.137442        0.019394        0.267813
H       6.503939        0.956499        0.277462
N       -2.456458       -0.392508       -0.550400
H       -2.116062       -1.364686       -0.600402
C       -3.798030       -0.148062       -1.105136
C       -4.868022       -0.174791       -0.012663
H       -3.845269       0.828497        -1.648490
H       -4.019777       -0.915311       -1.889066
O       -5.704151       -1.115315       0.008725
O       -4.909384       0.755937        0.841299
###
29
TyrGly4 pm6 E=-0.630797718222 au
N       -0.246278       -0.880960       1.562918
H       -0.925336       -0.638815       2.289281
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H       -0.540040       -1.782716       1.177134
C       -0.220697       0.159411        0.508399
H       0.224211        1.090538        0.963005
C       0.629322        -0.272864       -0.703198
C       -1.632465       0.551884        0.016225
H       0.362457        -1.308971       -1.009006
H       0.366725        0.355280        -1.584501
C       2.101139        -0.160094       -0.432466
O       -2.045297       1.723736        0.160497
C       2.714009        1.103268        -0.366458
C       2.885826        -1.310491       -0.252192
H       2.111046        2.002497        -0.511471
C       4.073775        1.224239        -0.121132
C       4.249857        -1.215074       -0.008188
H       2.417676        -2.296196       -0.306029
H       4.541650        2.200631        -0.070470
C       4.869692        0.060401        0.064752
H       4.849503        -2.107460       0.127951
O       6.143103        0.167853        0.298404
N       -2.422177       -0.402489       -0.564000
H       -2.106105       -1.379757       -0.655696
C       -3.757829       -0.102854       -1.106374
C       -4.823074       -0.115042       -0.008376
H       -3.775543       0.882290        -1.634560
H       -4.009052       -0.849149       -1.901735
O       -4.859012       0.822352        0.838765
O       -5.660712       -1.054034       0.024548
###
46
TyrHisOMe3 pm6 E=0.463155803463E-01 au
N       2.028186        3.355312        0.359672
H       2.788851        2.826712        0.824533
H       1.578817        3.967469        1.070131
H       2.462498        3.964881        -0.365732
C       1.010240        2.428575        -0.278546
H       0.181434        3.082393        -0.709812
C       1.634271        1.622531        -1.430171
C       0.436552        1.483195        0.786535
H       0.808588        1.160864        -2.024202
H       2.109609        2.328233        -2.155379
C       2.616593        0.580680        -0.980864
O       1.087019        1.138187        1.780019
C       2.177733        -0.716559       -0.670349
C       3.980729        0.901031        -0.866976
H       1.121222        -0.979345       -0.784338
C       3.076003        -1.679554       -0.212012
C       4.898228        -0.046477       -0.420246
H       4.327925        1.907058        -1.125626
H       2.741054        -2.685789       0.041857
C       4.424604        -1.324530       -0.086288
H       5.956619        0.193102        -0.325747
O       5.382254        -2.209696       0.374202
H       4.969400        -3.071287       0.696275
N       -0.847781       1.041862        0.566650
H       -1.371882       1.319749        -0.280161
C       -1.460953       0.018148        1.432651
H       -0.957853       0.039728        2.453736
C       -2.963025       0.260643        1.648412
C       -1.227458       -1.390865       0.860678
H       -3.335057       -0.462262       2.423845
H       -3.102505       1.260332        2.139933
C       -3.801969       0.151174        0.435533
O       -1.020379       -2.393628       1.522983
O       -1.262095       -1.401390       -0.493953
N       -4.243961       1.265175        -0.302915
C       -4.346498       -0.981606       -0.172540
H       -4.000578       2.244772        -0.110616
C       -5.038787       0.819387        -1.336027
N       -5.109002       -0.553767       -1.263242
H       -4.244164       -2.027612       0.104477
H       -5.532521       1.451070        -2.086243
H       -5.635074       -1.159681       -1.902493
C       -1.084531       -2.680813       -1.175874
H       -0.169107       -3.175973       -0.836115
H       -1.971070       -3.302455       -1.009338
H       -1.003081       -2.379593       -2.229629
```

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###
45
TyrHisOMe4 pm6 E=-0.110355898903 au
N       -2.861140       -3.772222       -0.000845
H       -2.940837       -3.930656       1.021979
H       -2.134109       -4.413578       -0.376227
H       -3.772363       -4.030398       -0.435933
C       -2.524670       -2.328480       -0.318359
H       -2.496594       -2.222606       -1.450562
C       -3.610851       -1.386274       0.236679
C       -1.166214       -1.957188       0.303331
H       -4.570392       -1.571754       -0.302891
H       -3.840794       -1.636879       1.299038
C       -3.198016       0.051423        0.102268
O       -0.988202       -1.900782       1.523362
C       -2.709233       0.745016        1.221816
C       -3.280610       0.700808        -1.141184
H       -2.664633       0.249003        2.195562
C       -2.272489       2.063469        1.104789
C       -2.853756       2.020134        -1.281288
H       -3.674916       0.166027        -2.010545
H       -1.884123       2.607288        1.967057
C       -2.344659       2.678137        -0.151591
H       -2.912096       2.532169        -2.241142
O       -1.906970       3.973639        -0.360358
H       -1.453260       4.350619        0.458896
N       -0.161848       -1.640031       -0.585630
H       -0.278561       -1.757298       -1.607386
C       1.096191        -1.026832       -0.118518
H       1.304798        -1.344057       0.947191
C       2.280766        -1.416020       -1.022128
C       0.921068        0.502714        -0.166318
H       2.370102        -2.528316       -1.057513
H       2.087505        -1.125163       -2.082763
C       3.538953        -0.798799       -0.536085
O       0.424118        1.179101        -1.047647
O       1.425528        1.043071        0.976634
N       4.353859        -1.395663       0.434911
C       4.088112        0.430962        -0.923233
C       5.386934        -0.531432       0.635964
N       5.256138        0.594141        -0.176547
H       3.746304        1.151071        -1.649543
H       6.210155        -0.679980       1.327496
H       5.889563        1.387414        -0.228264
C       1.455416        2.497229        1.103680
H       2.145941        2.913869        0.362679
H       0.446206        2.911327        0.999203
H       1.835600        2.638874        2.125581
###
44
TyrHisOMe5 pm6 E=-0.253267131276 au
N       -0.416358       -1.511653       3.079483
H       0.163282        -2.348451       2.976122
H       0.220662        -0.726384       3.236317
C       -1.242069       -1.298185       1.868712
H       -1.999888       -2.135582       1.831396
C       -1.976492       0.051067        1.954104
C       -0.445923       -1.386591       0.547426
H       -2.504170       0.115283        2.934776
H       -1.248439       0.892850        1.986918
C       -2.968704       0.231195        0.841896
O       -0.738162       -2.233221       -0.312356
C       -2.789350       1.250183        -0.106092
C       -4.098171       -0.603769       0.763827
H       -1.914103       1.903288        -0.050411
C       -3.726651       1.449193        -1.120646
C       -5.044149       -0.428100       -0.242558
H       -4.241480       -1.398243       1.501599
H       -3.599740       2.245605        -1.854667
C       -4.842896       0.606794        -1.168745
H       -5.921874       -1.069165       -0.311875
O       -5.831017       0.742838        -2.128969
H       -5.644060       1.517197        -2.745880
N       0.614736        -0.526108       0.355031
H       0.823866        0.219643        1.037178
C       1.446240        -0.574463       -0.861635
```

```
H       0.901206        -1.155698       -1.670797
C       1.770403        0.820703        -1.422908
C       2.747202        -1.318198       -0.524742
H       2.334673        0.693563        -2.380052
H       0.813906        1.307439        -1.738783
C       2.503066        1.721580        -0.501589
O       3.484466        -1.177104       0.434814
O       2.995652        -2.226777       -1.508618
N       3.869949        1.996853        -0.645199
C       1.985034        2.460384        0.570697
C       4.175314        2.895030        0.333014
N       3.048101        3.198617        1.093959
H       0.982092        2.509151        0.967387
H       5.154947        3.327628        0.509287
H       2.994516        3.840588        1.880791
C       4.203083        -3.039630       -1.414440
H       5.089501        -2.398051       -1.432182
H       4.168736        -3.658775       -0.512589
H       4.148228        -3.654895       -2.324364
###
43
TyrHisOMe6 pm6 E=-0.413262193467 au
N       -1.394715       -2.491949       2.233607
H       -0.454069       -2.734178       2.555381
H       -1.514155       -1.489006       2.397619
C       -1.557240       -2.825642       0.801515
H       -1.602662       -3.954268       0.736738
C       -2.873774       -2.262340       0.224574
C       -0.379617       -2.404735       -0.102250
H       -3.142654       -2.850324       -0.681226
H       -3.696911       -2.477537       0.942306
C       -2.827652       -0.797747       -0.094767
O       0.067904        -3.184581       -0.959601
C       -3.005342       0.167877        0.911353
C       -2.587063       -0.371956       -1.412094
H       -3.229090       -0.150541       1.933053
C       -2.897648       1.522382        0.629827
C       -2.472552       0.977034        -1.718513
H       -2.478904       -1.114199       -2.206696
H       -3.031831       2.260662        1.412169
C       -2.592819       1.951401        -0.691264
H       -2.284004       1.297550        -2.736940
O       -2.406754       3.209551        -0.952306
N       0.199011        -1.162000       0.073228
H       -0.210667       -0.474747       0.723118
C       1.267468        -0.673081       -0.820690
H       1.320900        -1.334018       -1.742663
C       1.040648        0.773802        -1.289074
C       2.598386        -0.782305       -0.063725
H       1.726584        0.969327        -2.151511
H       0.019046        0.851715        -1.740657
C       1.211675        1.813361        -0.246059
O       2.896016        -0.330687       1.028323
O       3.473334        -1.509647       -0.811930
N       2.225287        2.777754        -0.330497
C       0.454732        2.030149        0.913163
C       2.083409        3.571038        0.768479
N       1.014750        3.140960        1.550740
H       -0.395626       1.497486        1.311271
H       2.707339        4.424509        1.016505
H       0.690412        3.551901        2.423607
C       4.813712        -1.727016       -0.273697
H       5.325027        -0.766036       -0.157059
H       4.751329        -2.272976       0.672938
H       5.287666        -2.339095       -1.054057
###
27
ValGly1 pm6 E=-0.128588043258 au
N       2.787528        -1.427771       -0.270011
H       2.581342        -1.447507       -1.287065
H       2.724433        -2.400253       0.089674
H       3.769562        -1.102337       -0.150187
C       1.831137        -0.513424       0.472457
H       2.020751        -0.656245       1.584854
C       2.114898        0.978229        0.112010
C       0.396009        -0.917769       0.125504
```

```
H       3.233006        1.112548        0.141713
C       1.622453        1.333178        -1.287017
C       1.503714        1.894553        1.167851
O       0.138595        -1.523129       -0.926369
H       0.530566        1.304695        -1.381626
H       1.923088        2.356213        -1.559490
H       2.045102        0.679275        -2.061362
H       1.745193        1.575025        2.191421
H       1.884625        2.920649        1.064572
H       0.411249        1.965241        1.104349
N       -0.577830       -0.605805       1.040606
H       -0.375450       -0.044534       1.884458
C       -1.997340       -0.840271       0.747965
C       -2.578354       0.206545        -0.171105
H       -2.164843       -1.858467       0.292820
H       -2.574369       -0.877223       1.717317
O       -1.968151       0.962126        -0.915472
O       -3.937150       0.330484        -0.213549
H       -4.443606       -0.294150       0.411514
###
26
ValGly2 pm6 E=-0.305296095822 au
N       -2.678152       -1.357460       -0.977454
H       -2.936716       -1.812236       -0.081369
H       -2.274690       -2.082155       -1.601381
H       -3.550262       -0.999269       -1.420318
C       -1.694214       -0.221880       -0.761917
H       -1.412764       0.182403        -1.787049
C       -2.365552       0.925411        0.053216
C       -0.450385       -0.784473       -0.069039
H       -3.398496       1.067799        -0.374016
C       -2.498801       0.575259        1.531526
C       -1.594697       2.227182        -0.144604
O       -0.507238       -1.841951       0.584146
H       -1.532506       0.465901        2.037933
H       -3.038403       1.366676        2.072807
H       -3.067827       -0.349251       1.695203
H       -1.378002       2.430127        -1.202475
H       -2.174021       3.085092        0.225938
H       -0.639678       2.252773        0.392950
N       0.718644        -0.094480       -0.211851
H       0.780855        0.787578        -0.741859
C       1.941316        -0.551730       0.476364
C       3.190176        0.145273        -0.043251
H       1.856870        -0.374891       1.580587
H       2.063087        -1.660260       0.367290
O       3.121917        1.021822        -0.943462
O       4.291827        -0.190742       0.472706
###
25
ValGly3 pm6 E=-0.453572850049 au
N       1.465876        1.674464        -0.729377
H       1.595922        2.034290        0.222458
H       2.304429        1.957565        -1.247179
C       1.390932        0.192304        -0.714225
H       1.441602        -0.150953       -1.791133
C       2.526340        -0.536085       0.070668
C       0.040979        -0.298479       -0.185330
H       2.321402        -1.637420       0.006357
C       3.872147        -0.266224       -0.599535
C       2.546090        -0.136232       1.543958
O       -0.318985       -1.466962       -0.465822
H       4.170038        0.788237        -0.545223
H       4.675765        -0.845162       -0.125918
H       3.868304        -0.544100       -1.661197
H       1.633403        -0.441734       2.068862
H       3.382507        -0.610598       2.074768
H       2.658887        0.946114        1.689435
N       -0.772236       0.501442        0.569729
H       -0.517443       1.465779        0.820598
C       -2.058349       0.008378        1.094632
C       -3.119041       0.009916        -0.007988
H       -1.952237       -1.016445       1.526072
H       -2.386794       0.645652        1.953716
O       -3.730024       1.073986        -0.290414
O       -3.356722       -1.065029       -0.629658
```

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###
28
AlaGlyGly1 tri_tetrapeptidos E=-0.200722815272 au
N       -4.621757       -0.343855       -0.783178
H       -4.384362       -1.208035       -1.304463
H       -4.665318       0.443920        -1.459961
H       -5.571775       -0.470617       -0.377825
C       -3.618179       -0.060367       0.323857
H       -3.963226       0.880647        0.861003
C       -3.570934       -1.218869       1.303076
C       -2.222545       0.136318        -0.294629
H       -3.278973       -2.171935       0.836364
H       -2.860869       -1.025878       2.123557
H       -4.551298       -1.391957       1.780391
O       -1.726901       -0.708619       -1.059128
N       -1.564572       1.286557        0.042915
H       -1.946504       1.950398        0.736400
C       -0.222959       1.590818        -0.476290
C       0.870595        0.807698        0.232717
H       -0.160999       1.388310        -1.581800
H       -0.047292       2.700308        -0.389016
O       0.641228        -0.205991       0.919012
N       2.154880        1.263124        0.059852
H       2.369591        2.077575        -0.539073
C       3.308001        0.580362        0.660821
C       3.692473        -0.665099       -0.106495
H       4.175135        1.296123        0.722579
H       3.112355        0.290460        1.732398
O       2.953487        -1.537263       -0.545000
O       5.035524        -0.751900       -0.253112
H       5.348252        -1.595079       -0.730193
###
27
AlaGlyGly2 tri_tetrapeptidos E=-0.379029211882 au
N       -4.262953       -0.976301       -0.619712
H       -3.767041       -1.849222       -0.878892
H       -4.511567       -0.472643       -1.493156
H       -5.146283       -1.242787       -0.137514
C       -3.412447       -0.104942       0.291632
H       -3.990307       0.854588        0.483914
C       -3.148071       -0.821566       1.603091
C       -2.076197       0.194387        -0.405520
H       -2.571690       -1.751681       1.483649
H       -2.589213       -0.181817       2.305977
H       -4.085286       -1.094879       2.118306
O       -1.564868       -0.608003       -1.199883
N       -1.478210       1.389275        -0.096587
H       -1.868970       2.028122        0.613119
C       -0.186779       1.766538        -0.689880
C       0.994886        1.173309        0.071697
H       -0.133934       1.474910        -1.773967
H       -0.097747       2.886140        -0.699474
O       1.778120        1.909627        0.707527
N       1.179313        -0.180018       0.000711
H       0.535642        -0.776294       -0.548196
C       2.247470        -0.879506       0.733990
C       3.585121        -0.812495       -0.006947
H       2.375053        -0.468461       1.767163
H       1.946845        -1.945417       0.894582
O       4.197092        0.290545        -0.097808
O       4.066350        -1.865369       -0.499184
###
26
AlaGlyGly3 tri_tetrapeptidos E=-0.525297822088 au
N       -3.859522       -0.875965       -0.605038
H       -3.451181       -1.399751       -1.379572
H       -4.256167       -0.018554       -0.997284
C       -2.841853       -0.558631       0.422658
H       -3.372019       -0.035113       1.269941
C       -2.171964       -1.825983       0.944239
C       -1.723027       0.350555        -0.130013
H       -1.662575       -2.399152       0.159612
H       -1.440726       -1.606143       1.734534
H       -2.909542       -2.508979       1.393433
O       -1.161772       0.102699        -1.222708
N       -1.338803       1.420576        0.627608
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H       -1.753383       1.604554        1.556344
C       -0.263530       2.337261        0.209452
C       1.040094        1.602176        -0.070259
H       -0.564881       2.912375        -0.704721
H       -0.107721       3.122529        0.999599
O       1.574536        1.678925        -1.195946
N       1.601807        0.858997        0.930656
H       1.163179        0.776952        1.858975
C       2.771045        0.002394        0.685275
C       2.461224        -1.268906       -0.098181
H       3.575572        0.564624        0.143561
H       3.233575        -0.272581       1.670377
O       3.364691        -2.145211       -0.155757
O       1.358738        -1.436314       -0.695141
###
46
AlaLysAla1 tri_tetrapeptidos E=-0.100029872679 au
N       -5.428847       0.490188        -0.352158
H       -5.549611       -0.433958       -0.806944
H       -5.377319       1.215261        -1.093915
C       -4.187648       0.519557        0.526661
H       -4.074645       1.577389        0.924922
C       -4.342180       -0.455674       1.679405
C       -2.968052       0.117132        -0.319621
H       -4.480342       -1.497419       1.350713
H       -3.464773       -0.440538       2.346137
H       -5.209927       -0.207805       2.314654
O       -3.048949       -0.752270       -1.198326
N       -1.789475       0.765455        -0.050226
H       -1.719863       1.481299        0.691911
C       -0.546216       0.429529        -0.780118
H       -0.826936       0.026000        -1.803805
C       0.344748        1.662943        -0.998199
C       0.212576        -0.654817       0.009379
H       1.222073        1.359158        -1.613592
H       -0.205160       2.383928        -1.644343
C       0.818145        2.362827        0.279087
O       0.447228        -0.569298       1.229369
H       -0.031340       2.516672        0.978970
C       1.448647        3.727462        -0.018578
H       0.785446        4.316481        -0.691264
H       1.493038        4.327605        0.917796
C       2.831341        3.645971        -0.659856
H       2.869121        2.859466        -1.452727
H       3.080389        4.608281        -1.173211
N       3.903360        3.359371        0.374748
H       3.740165        2.450607        0.839425
H       4.840561        3.332759        -0.064064
H       3.913064        4.089780        1.108596
N       0.647545        -1.748007       -0.700727
H       0.497528        -1.830631       -1.720455
C       1.279126        -2.910932       -0.030110
H       0.708881        -3.158766       0.920263
C       1.282912        -4.117222       -0.950578
C       2.712510        -2.542081       0.382584
H       1.805061        -3.937793       -1.902460
H       1.767796        -4.984632       -0.474581
H       0.261107        -4.440049       -1.208042
O       2.859720        -1.639878       1.398050
O       3.753922        -2.977589       -0.078286
H       1.961882        -1.269704       1.777113
H       -6.277771       0.674608        0.221300
H       1.532660        1.717053        0.829350
###
45
AlaLysAla2 tri_tetrapeptidos E=-0.285906494777 au
N       5.085639        0.215765        1.213889
H       4.940355        -0.679279       1.716696
H       4.856522        0.994025        1.862215
C       4.239100        0.287863        -0.047922
H       4.433535        1.297665        -0.532891
C       4.626809        -0.832456       -0.994382
C       2.755064        0.176708        0.336845
H       4.432447        -1.834782       -0.581898
H       4.088114        -0.762459       -1.953379
H       5.701187        -0.804718       -1.247649
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O       2.404803        -0.244172       1.449993
N       1.850740        0.575284        -0.610648
H       2.155856        0.869284        -1.555771
C       0.390920        0.577332        -0.346758
H       0.209654        1.179559        0.596022
C       -0.361277       1.207723        -1.533289
C       -0.119759       -0.864237       -0.135859
H       0.330371        1.839342        -2.139883
H       -0.692490       0.424137        -2.248193
C       -1.561016       2.050340        -1.093916
O       0.451495        -1.858126       -0.626290
H       -2.235142       2.192931        -1.966507
C       -1.136076       3.416654        -0.544724
H       -0.431333       3.293499        0.306668
H       -0.553552       3.969216        -1.315865
C       -2.324842       4.280534        -0.132427
H       -2.015319       5.351819        -0.041959
H       -3.130827       4.266717        -0.906605
N       -2.906755       3.830473        1.193608
H       -2.183034       3.825841        1.933081
H       -3.669766       4.463779        1.492183
H       -3.294855       2.873641        1.126369
N       -1.254003       -1.002790       0.619521
H       -1.741683       -0.180436       1.016016
C       -1.865368       -2.328606       0.899486
H       -1.065867       -3.025350       1.281152
C       -2.964485       -2.203190       1.938526
C       -2.430281       -2.911699       -0.417941
H       -3.747955       -1.484115       1.661314
H       -3.461167       -3.171046       2.112748
H       -2.575619       -1.878938       2.916180
O       -1.787150       -3.861746       -0.953004
O       -3.468294       -2.446441       -0.950041
H       6.095750        0.283347        0.970744
H       -2.174089       1.507271        -0.346484
###
44
AlaLysAla3 tri_tetrapeptidos E=-0.430759466599 au
N       -5.541892       0.182958        -0.168335
H       -5.651787       -0.832019       -0.184911
H       -5.587556       0.499195        -1.139489
C       -4.246504       0.565584        0.443306
H       -4.249525       1.688095        0.558498
C       -4.075042       -0.092400       1.807741
C       -3.047851       0.168576        -0.443721
H       -4.015042       -1.187585       1.753087
H       -3.174914       0.267291        2.326801
H       -4.924019       0.134204        2.470546
O       -3.164705       -0.661030       -1.368874
N       -1.841856       0.768747        -0.187683
H       -1.723097       1.406635        0.619589
C       -0.620628       0.480158        -0.973373
H       -0.912738       0.317948        -2.061232
C       0.331525        1.684085        -0.917219
C       -0.000773       -0.857068       -0.520757
H       1.194924        1.505502        -1.598378
H       -0.187447       2.560134        -1.370965
C       0.831794        2.046449        0.484518
O       -0.691856       -1.719439       0.064389
H       0.002077        1.990697        1.224230
C       1.421044        3.460273        0.535137
H       0.682585        4.193632        0.139959
H       1.567717        3.760882        1.597056
C       2.722669        3.624132        -0.245087
H       2.674086        3.115549        -1.238906
H       2.908396        4.704811        -0.467988
N       3.905643        3.079575        0.532269
H       3.783118        2.073851        0.739334
H       4.782903        3.191861        -0.005987
H       4.015563        3.576063        1.433933
N       1.297761        -1.118794       -0.859927
H       1.890616        -0.403006       -1.314770
C       1.916692        -2.455550       -0.656135
H       1.194364        -3.247786       -1.006905
C       3.208245        -2.565337       -1.446381
C       2.171884        -2.676851       0.854328
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H       3.940294        -1.784571       -1.197258
H       3.700596        -3.536155       -1.278769
H       3.034361        -2.494964       -2.531831
O       1.353078        -3.418821       1.475225
O       3.136094        -2.136321       1.448540
H       1.577735        1.304919        0.831696
###
43
AlaLysAla4 tri_tetrapeptidos E=-0.562410518968 au
N       2.715110        2.494501        0.014695
H       2.920976        3.492987        -0.069951
H       2.788271        2.102999        -0.926727
C       1.354329        2.276775        0.574884
H       1.330491        1.224608        0.967192
C       1.062939        3.229575        1.727810
C       0.275313        2.490767        -0.504592
H       1.116785        4.287974        1.439524
H       0.064754        3.057259        2.157042
H       1.781365        3.096932        2.550571
O       0.204945        3.570178        -1.128947
N       -0.634988       1.516426        -0.835469
H       -1.324539       1.709550        -1.580564
C       -0.706521       0.165373        -0.230360
H       -0.789256       0.277579        0.895451
C       -1.933520       -0.596649       -0.758786
C       0.575218        -0.631281       -0.573573
H       -2.015236       -0.496557       -1.862526
H       -1.800339       -1.686816       -0.582400
C       -3.224958       -0.124174       -0.082394
O       1.252996        -0.377641       -1.586844
H       -3.119016       -0.190816       1.021211
C       -4.428410       -0.951703       -0.546877
H       -4.571822       -0.831839       -1.639744
H       -4.231484       -2.033248       -0.402659
C       -5.719362       -0.551334       0.182448
H       -5.870718       0.548233        0.120846
H       -6.592649       -1.004513       -0.336087
N       -5.770224       -0.948063       1.619028
H       -4.934855       -0.601214       2.097370
H       -5.715065       -1.966094       1.692419
N       0.923022        -1.597938       0.331221
H       0.313724        -1.773221       1.152099
C       2.122823        -2.466887       0.258117
H       1.979947        -3.273923       1.038393
C       2.333246        -3.128577       -1.092621
C       3.371532        -1.642224       0.653772
H       2.474874        -2.416201       -1.913903
H       3.214904        -3.788413       -1.081143
H       1.481893        -3.768016       -1.371022
O       3.932698        -1.892960       1.751817
O       3.830894        -0.748155       -0.113880
H       -3.401485       0.948917        -0.295864
###
29
CysGlyGly1 tri_tetrapeptidos E=-0.185818034020 au
N       -3.973770       -1.427928       0.297813
H       -3.873777       -2.345752       -0.182243
H       -4.953827       -1.108100       0.164111
H       -3.827864       -1.576254       1.316852
C       -2.989082       -0.414716       -0.261216
H       -3.178885       -0.325390       -1.379100
C       -3.154301       0.935036        0.420545
C       -1.557171       -0.932869       -0.002798
H       -3.108208       0.844852        1.534332
H       -2.309794       1.613194        0.158710
S       -4.746309       1.675593        -0.008031
O       -1.219281       -1.362686       1.107448
H       -4.421048       2.275286        -1.178337
N       -0.701898       -0.908367       -1.071424
H       -0.961055       -0.480196       -1.973293
C       0.682518        -1.386157       -0.938230
C       1.593234        -0.330722       -0.326870
H       0.711444        -2.352145       -0.365495
H       1.084904        -1.657474       -1.955873
O       1.486483        0.879106        -0.577599
N       2.575385        -0.789666       0.523547
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H       2.692284        -1.791503       0.738216
C       3.542918        0.132024        1.131953
C       4.656341        0.467598        0.163473
H       3.042945        1.065192        1.506442
H       3.996206        -0.332559       2.054453
O       5.381256        -0.291538       -0.457824
O       4.795092        1.815484        0.039543
H       5.554458        2.098995        -0.573511
###
28
CysGlyGly2 tri_tetrapeptidos E=-0.358572603738 au
N       -1.358131       0.115049        2.182905
H       -0.439702       0.601339        2.206228
H       -1.305600       -0.701922       2.829071
H       -2.082716       0.762622        2.550419
C       -1.690326       -0.354986       0.776973
H       -0.849033       -1.046611       0.436793
C       -3.000764       -1.133251       0.779158
C       -1.804175       0.856474        -0.164975
H       -2.854623       -2.153393       1.210260
H       -3.780429       -0.658662       1.414579
S       -3.557332       -1.310914       -0.934181
O       -2.848761       1.516530        -0.241555
H       -4.314908       -0.192831       -1.054729
N       -0.763754       1.181373        -1.002970
H       -0.860280       2.005814        -1.617578
C       0.583987        0.598602        -0.943566
C       1.537746        1.458058        -0.129741
H       0.563595        -0.446989       -0.525463
H       0.967827        0.482303        -1.997786
O       1.165919        2.452700        0.517648
N       2.882476        1.162233        -0.133494
H       3.517676        1.702826        0.469226
C       3.466863        -0.003903       -0.807151
C       3.389632        -1.289750       0.013332
H       3.013763        -0.159365       -1.818962
H       4.550106        0.201074        -1.029219
O       3.518296        -1.273346       1.265856
O       3.235762        -2.373336       -0.616350
###
27
CysGlyGly3 tri_tetrapeptidos E=-0.517371148028 au
N       3.947434        -0.915342       -0.499831
H       4.096209        -1.924895       -0.309660
H       4.851745        -0.411566       -0.354433
H       3.684009        -0.807923       -1.495209
C       2.879587        -0.342383       0.414640
H       3.225435        -0.495735       1.484468
C       2.659682        1.147850        0.146442
C       1.565564        -1.100903       0.173951
H       1.979678        1.318119        -0.708745
H       2.191553        1.623683        1.030292
S       4.261410        1.923655        -0.210268
O       1.367640        -1.730291       -0.879068
N       0.632253        -1.048898       1.174044
H       0.763709        -0.460622       2.015237
C       -0.687750       -1.677338       1.014503
C       -1.595121       -0.856892       0.102160
H       -0.594878       -2.717201       0.604791
H       -1.159788       -1.815307       2.026117
O       -1.920642       -1.288648       -1.024037
N       -2.044961       0.344216        0.569234
H       -1.797029       0.678844        1.514860
C       -2.874433       1.246803        -0.245864
C       -4.346097       0.830531        -0.206021
H       -2.756007       2.296080        0.126047
H       -2.521486       1.289086        -1.306388
O       -5.153613       1.497867        0.490368
O       -4.730560       -0.166039       -0.883021
###
26
CysGlyGly4 tri_tetrapeptidos E=-0.654663883996 au
N       3.515551        1.765412        -0.854214
H       2.745625        2.224205        -1.346282
H       3.760974        2.359394        -0.060635
C       3.107284        0.413971        -0.396957
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H       2.965193        -0.214240       -1.321529
C       4.162245        -0.210351       0.522060
C       1.768614        0.471339        0.374592
H       4.839700        0.553242        0.944676
H       3.708153        -0.723654       1.388315
S       5.140870        -1.430146       -0.413964
O       1.497651        1.402066        1.159796
N       0.882048        -0.558551       0.177431
H       1.048610        -1.288574       -0.529448
C       -0.414709       -0.628119       0.867798
C       -1.484231       0.186713        0.153987
H       -0.712115       -1.707609       0.970085
H       -0.336820       -0.261107       1.927040
O       -1.223064       1.221125        -0.493497
N       -2.772800       -0.260586       0.265928
H       -3.010742       -1.097380       0.817132
C       -3.884792       0.498471        -0.342673
C       -5.191370       -0.285450       -0.230094
H       -4.006746       1.496114        0.150317
H       -3.661653       0.730983        -1.412908
O       -5.742507       -0.413766       0.894412
O       -5.700322       -0.770976       -1.275666
###
31
GlyAlaAla1 tri_tetrapeptidos E=-0.205459894160 au
N       -4.869967       -1.496030       0.233848
H       -5.098057       -1.469192       -0.777455
C       -4.128520       -0.256151       0.648973
H       -5.760598       -1.573066       0.765537
H       -4.306184       -2.345012       0.417395
C       -2.809988       -0.126080       -0.085435
H       -4.777625       0.652253        0.480637
H       -3.960030       -0.260273       1.766142
O       -2.396127       -1.006934       -0.852817
N       -2.097203       1.027103        0.143828
H       -2.429388       1.743725        0.809374
C       -0.819265       1.297613        -0.557760
H       -0.897300       0.915921        -1.619073
C       -0.525732       2.789231        -0.571095
C       0.327391        0.580729        0.192461
H       -0.468199       3.230260        0.434930
H       0.427153        3.007923        -1.078621
H       -1.299982       3.351669        -1.117134
O       0.515801        0.715302        1.409916
N       1.157825        -0.216424       -0.562756
H       1.028313        -0.328292       -1.580519
C       2.276917        -0.964384       0.051584
H       1.990121        -1.273135       1.105372
C       2.619497        -2.194819       -0.772497
C       3.517894        -0.069109       0.147179
H       2.900283        -1.959680       -1.810574
H       3.456649        -2.759271       -0.328232
H       1.772403        -2.896949       -0.828681
O       3.738279        0.975965        -0.444158
O       4.516054        -0.464620       0.993242
H       4.346618        -1.339311       1.486537
###
30
GlyAlaAla2 tri_tetrapeptidos E=-0.388887860451 au
N       -4.867681       -1.329438       0.341586
H       -5.027187       -1.529829       -0.663307
C       -4.120275       -0.037341       0.518121
H       -5.792893       -1.272810       0.813226
H       -4.343319       -2.122129       0.752552
C       -2.735199       -0.100065       -0.091207
H       -4.719452       0.811630        0.076432
H       -4.054272       0.223888        1.615986
O       -2.266653       -1.147561       -0.561080
N       -2.025049       1.076070        -0.099377
H       -2.392218       1.929989        0.352497
C       -0.695670       1.177262        -0.750079
H       -0.770539       0.734048        -1.788084
C       -0.265449       2.633814        -0.836897
C       0.358726        0.416131        0.083869
H       -0.196038       3.125869        0.144249
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H       -0.967917       3.232858        -1.439220
O       0.417662        0.509394        1.323890
N       1.258721        -0.353308       -0.607081
H       1.227246        -0.432803       -1.636086
C       2.357608        -1.079800       0.083658
H       1.962656        -1.527803       1.038741
C       2.912158        -2.183333       -0.797332
C       3.449092        -0.042552       0.445303
H       3.291655        -1.822596       -1.763461
H       3.740369        -2.712464       -0.300719
H       2.154329        -2.947971       -1.028221
O       4.259644        0.377100        -0.420116
O       3.469914        0.400077        1.628977
###
29
GlyAlaAla3 tri_tetrapeptidos E=-0.533191198147 au
N       -5.153218       -1.109821       0.401497
H       -5.418717       -1.031735       -0.582908
C       -4.151153       -0.077371       0.739368
H       -4.748194       -2.040711       0.514627
C       -2.864464       -0.158881       -0.060886
H       -4.620029       0.933591        0.628557
H       -3.897824       -0.150322       1.829781
O       -2.540094       -1.169154       -0.712717
N       -2.047232       0.949941        -0.044623
H       -2.283239       1.781252        0.517917
C       -0.759841       0.985980        -0.775327
H       -0.875711       0.418912        -1.746068
C       -0.350527       2.423655        -1.059022
C       0.343987        0.335789        0.088379
H       -0.264300       3.037344        -0.150389
H       0.616217        2.475953        -1.583282
H       -1.076810       2.931943        -1.713198
O       0.417587        0.509311        1.319166
N       1.269246        -0.432227       -0.570308
H       1.217818        -0.585222       -1.590108
C       2.418044        -1.055084       0.140125
H       2.060766        -1.483576       1.118654
C       3.041498        -2.157574       -0.695135
C       3.445620        0.062271        0.441904
H       3.370650        -1.821192       -1.688084
H       3.920250        -2.589225       -0.190426
H       2.344725        -2.992852       -0.864848
O       4.220615        0.490749        -0.451679
O       3.456121        0.557578        1.604904
###
40
GlyGlyAspAla1 tri_tetrapeptidos E=-0.623824920224 au
N       -5.243706       -1.668167       -1.083369
H       -5.114341       -2.532523       -0.523123
C       -5.118733       -0.437157       -0.230560
H       -4.544280       -1.666076       -1.848285
H       -6.190579       -1.701454       -1.514357
C       -3.729411       -0.188968       0.329663
H       -5.445391       0.466694        -0.821820
H       -5.869441       -0.471984       0.615191
O       -3.145613       0.884518        0.095558
N       -3.161589       -1.146930       1.126362
H       -3.609921       -2.062388       1.297491
C       -1.874983       -0.913104       1.806464
C       -0.763651       -0.555994       0.834009
H       -1.998422       -0.136038       2.610298
H       -1.578189       -1.841864       2.374397
O       -0.655733       -1.090149       -0.286556
N       0.147366        0.385749        1.250361
H       0.059740        0.857425        2.169310
C       1.223704        0.880853        0.359403
H       1.210423        0.298274        -0.606101
C       1.027057        2.366358        0.033574
C       2.560298        0.713334        1.111097
H       0.877135        2.976362        0.964741
H       1.971671        2.800003        -0.401662
C       -0.093927       2.594861        -0.920897
O       2.717676        1.226495        2.230949
O       -0.358047       3.916314        -1.069855
O       -0.752105       1.761123        -1.538470
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N       3.588001        -0.012962       0.570649
H       4.461978        -0.107362       1.118264
C       3.565763        -0.722026       -0.733910
H       3.328666        0.020031        -1.550577
C       4.919344        -1.360138       -1.002289
C       2.490839        -1.832981       -0.748640
H       5.235139        -2.058786       -0.213663
H       4.921157        -1.925398       -1.947801
H       5.719996        -0.609700       -1.096131
O       1.827502        -1.980669       -1.814612
O       2.255145        -2.542329       0.263149
H       -1.094245       4.118311        -1.742970
###
39
GlyGlyAspAla2 tri_tetrapeptidos E=-0.809531320577 au
N       3.693280        -0.426136       2.306290
H       2.714142        -0.192506       2.565886
C       3.733077        -1.528629       1.284967
H       4.144652        0.433687        1.945472
H       4.199154        -0.721184       3.165836
C       2.984709        -1.151367       0.023279
H       4.804647        -1.780723       1.021975
H       3.345199        -2.483467       1.745057
O       2.898099        0.031427        -0.350889
N       2.437812        -2.187115       -0.686495
H       2.468326        -3.162421       -0.340577
C       1.685056        -1.964288       -1.929376
C       0.387220        -1.206354       -1.689740
H       2.301837        -1.407183       -2.683442
H       1.464876        -2.955479       -2.418722
O       0.156591        -0.139365       -2.295196
N       -0.509585       -1.707839       -0.784673
H       -0.329372       -2.590334       -0.271847
C       -1.772302       -0.992135       -0.475148
H       -2.421425       -1.008268       -1.403599
C       -2.508150       -1.662914       0.680269
C       -1.509076       0.497005        -0.147899
H       -2.541720       -2.775323       0.528284
H       -1.945023       -1.560448       1.638408
C       -3.927670       -1.176684       0.853090
O       -2.277188       1.351013        -0.646054
O       -4.527722       -0.568795       -0.084110
O       -4.520079       -1.396115       1.944358
N       -0.466965       0.855245        0.653651
H       0.155897        0.152807        1.089760
C       -0.091904       2.284211        0.848075
H       -0.986840       2.843489        1.243842
C       1.062068        2.402946        1.823618
C       0.288978        2.875822        -0.532661
H       1.993641        1.940663        1.470486
H       1.293817        3.457637        2.044508
H       0.837974        1.931650        2.795013
O       -0.447454       3.781334        -1.006910
O       1.271051        2.424580        -1.184770
###
43
GlyGlyGluAla1 tri_tetrapeptidos E=-0.631604142924 au
N       -5.751722       -1.200645       1.287310
H       -5.960297       -0.210023       1.522358
C       -5.375114       -1.347775       -0.160293
H       -4.992206       -1.533614       1.907426
H       -6.603628       -1.764097       1.487193
C       -4.088511       -0.637534       -0.547600
H       -5.288690       -2.442571       -0.418886
H       -6.222635       -0.991328       -0.817567
O       -3.128975       -1.284655       -1.008626
N       -4.048321       0.723562        -0.426696
H       -4.816014       1.256171        0.017355
C       -2.879509       1.507245        -0.860955
C       -1.597450       1.086798        -0.152962
H       -2.775392       1.453413        -1.979285
H       -3.064529       2.599877        -0.655780
O       -1.599154       0.630180        1.003053
N       -0.452316       1.193426        -0.904511
H       -0.492143       1.601245        -1.858187
C       0.910664        0.875458        -0.431141
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H       1.618343        1.333481        -1.194580
C       1.252558        1.439240        0.961333
C       1.119402        -0.655263       -0.405469
H       0.556137        1.034898        1.729228
H       2.259587        1.075705        1.268750
C       1.213877        2.962685        1.007149
O       0.215476        -1.455436       -0.079823
H       0.231693        3.358240        0.643971
H       1.242527        3.308954        2.076205
C       2.336247        3.600657        0.265476
O       3.338999        3.069800        -0.197445
O       2.282592        4.957825        0.055340
N       2.366775        -1.100525       -0.740337
H       3.118615        -0.444043       -1.011232
C       2.725370        -2.542891       -0.730996
H       1.894180        -3.132101       -1.213341
C       4.018198        -2.776966       -1.489480
C       2.857375        -3.003332       0.741614
H       4.870626        -2.214564       -1.083956
H       4.301263        -3.841646       -1.476852
H       3.932206        -2.495444       -2.550540
O       1.877356        -3.628143       1.245611
O       3.885258        -2.755374       1.417518
H       1.458391        5.413227        0.432270
###
42
GlyGlyGluAla2 tri_tetrapeptidos E=-0.813864664767 au
C       4.592167        -0.906683       -1.456322
C       4.035376        -1.209136       -0.074096
C       4.959004        -0.583712       0.995798
O       5.665153        -1.373751       1.679788
N       2.626391        -0.780731       0.110912
C       2.096618        0.402078        -0.313758
O       2.795894        1.346615        -0.735482
C       0.569924        0.627184        -0.253915
C       0.200335        1.191274        1.132017
C       -1.230759       1.717817        1.204635
C       -1.576033       2.669167        0.089687
O       -0.783247       3.585658        -0.267085
N       -0.191415       -0.602099       -0.565291
C       -1.181044       -0.610401       -1.512940
O       -1.395638       0.375305        -2.246580
C       -2.011705       -1.879246       -1.663986
N       -2.777954       -2.198686       -0.448626
C       -3.701590       -1.334680       0.073457
O       -3.907121       -0.209153       -0.419792
C       -4.475197       -1.829745       1.277055
N       -5.138762       -0.706282       2.023880
O       -2.677520       2.520352        -0.529734
O       5.029829        0.663630        1.166679
H       -5.785562       -0.181504       1.408972
H       -4.436937       -0.045816       2.404266
H       -5.688011       -1.089184       2.821516
H       -3.820178       -2.419712       1.984066
H       -5.248727       -2.584824       0.943397
H       -2.583099       -3.117922       -0.014967
H       -1.348764       -2.752046       -1.924967
H       -2.691263       -1.772784       -2.550727
H       -0.077922       -1.398567       0.087249
H       0.349044        1.398150        -1.053222
H       0.340969        0.411105        1.915430
H       0.916995        1.997633        1.401874
H       -1.957252       0.877105        1.246698
H       -1.386218       2.238797        2.181805
H       2.023748        -1.493135       0.560499
H       4.039624        -2.330847       0.081171
H       4.638851        0.165135        -1.684867
H       5.613309        -1.302602       -1.572870
H       3.992196        -1.377151       -2.249592
###
25
GlyGlyGly1 tri_tetrapeptidos E=-0.191181499568 au
N       4.846535        -1.020423       0.052311
H       4.443855        -1.969249       0.147792
C       3.908961        0.023546        0.590208
H       5.051070        -0.853690       -0.950879
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C       2.577034        0.014349        -0.132878
H       3.737545        -0.136216       1.696417
H       4.406359        1.036444        0.548253
O       2.156417        -0.994663       -0.722790
N       1.865817        1.186886        -0.101430
H       2.176068        1.995981        0.459976
C       0.559978        1.314738        -0.763517
C       -0.565172       0.717947        0.067678
H       0.375089        2.403244        -0.986337
H       0.564807        0.821663        -1.774557
O       -0.375318       -0.183274       0.906697
N       -1.827188       1.203601        -0.167925
H       -2.009661       1.928639        -0.882399
C       -2.997923       0.709464        0.568532
C       -3.480832       -0.621149       0.034903
H       -2.783821       0.592731        1.668982
H       -3.818227       1.479883        0.527103
O       -2.816438       -1.616290       -0.222465
O       -4.826055       -0.623193       -0.118691
H       5.745632        -0.994179       0.575450
H       -5.205991       -1.509701       -0.442064
###
24
GlyGlyGly2 tri_tetrapeptidos E=-0.368241482281 au
N       4.097464        -1.336679       0.112745
H       4.640195        -0.678388       0.702641
C       3.145211        -0.592549       -0.780816
H       3.591890        -1.991473       0.736029
C       2.095379        0.153524        0.017962
H       3.724461        0.093544        -1.465823
H       2.638091        -1.305638       -1.495463
O       1.777693        -0.182697       1.168346
N       1.493131        1.211634        -0.616677
H       1.733639        1.477549        -1.584516
C       0.462965        2.021015        0.052355
C       -0.894790       1.325607        0.029188
H       0.762569        2.280469        1.102863
H       0.376993        3.015221        -0.463256
O       -1.737080       1.571952        -0.855410
N       -1.157849       0.438003        1.037978
H       -0.434633       0.175850        1.724914
C       -2.441433       -0.278830       1.121314
C       -2.714176       -1.113151       -0.127184
H       -2.444339       -0.946979       2.022116
H       -3.279698       0.437742        1.303717
O       -3.841674       -1.006299       -0.684559
O       -1.827134       -1.877310       -0.595552
H       4.768230        -1.887459       -0.461058
###
23
GlyGlyGly3 tri_tetrapeptidos E=-0.517579064660 au
N       -4.287269       1.538215        0.134147
H       -4.860480       0.829615        0.595661
C       -3.329046       0.893947        -0.788741
H       -3.786159       2.030603        0.875884
C       -2.431236       -0.138111       -0.132194
H       -3.894860       0.416779        -1.630307
H       -2.704260       1.683530        -1.280253
O       -2.526901       -0.419203       1.079783
N       -1.496037       -0.757783       -0.926299
H       -1.387059       -0.515594       -1.923295
C       -0.577251       -1.782868       -0.406117
C       0.617769        -1.122557       0.272468
H       -1.082886       -2.459308       0.331196
H       -0.267118       -2.463804       -1.245035
O       0.491659        -0.558365       1.384699
N       1.814779        -1.144923       -0.378685
H       1.917627        -1.582805       -1.308868
C       3.035359        -0.566191       0.207366
C       3.116850        0.942805        -0.025963
H       3.107321        -0.779734       1.303783
H       3.931294        -1.076870       -0.229600
O       2.298890        1.712161        0.557988
O       4.012802        1.403765        -0.779248
###
45
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GlyGlyHisAla1 tri_tetrapeptidos E=-0.274884976257 au
N 6.896067 -0.025698 -1.037703
H 7.220530 -1.009868 -0.988759
C 5.855441 0.248844 0.011213
H 7.717722 0.595834 -0.893438
H 6.524096 0.145442 -1.988613
C 4.631229 -0.624364 -0.170609
H 6.311717 0.132113 1.037544
H 5.553333 1.337686 -0.013691
O 4.344351 -1.133512 -1.266267
N 3.851097 -0.817719 0.941451
H 4.048418 -0.340793 1.835880
C 2.653395 -1.667821 0.905473
C 1.441774 -0.942862 0.339365
H 2.825121 -2.596248 0.292507
H 2.459308 -2.057474 1.944832
O 1.530986 -0.083419 -0.557273
N 0.220164 -1.299591 0.858288
H 0.143725 -2.013368 1.606143
C -1.056703 -0.798726 0.300058
H -0.860404 -0.240116 -0.660353
C -1.987780 -1.992549 -0.001624
C -1.708933 0.110111 1.362598
H -1.516941 -2.637617 -0.788206
H -2.064881 -2.670932 0.886291
C -3.338205 -1.561374 -0.422509
O -2.008638 -0.335275 2.484470
N -3.676920 -1.260207 -1.755348
C -4.493663 -1.385282 0.341431
H -3.041388 -1.304658 -2.559652
C -5.005832 -0.900522 -1.798475
N -5.513725 -0.972540 -0.520710
H -4.647167 -1.535476 1.405987
H -5.562415 -0.604901 -2.697919
N -2.005532 1.422889 1.097390
H -2.465079 1.978477 1.838895
C -1.642618 2.164992 -0.133655
H -1.878892 1.531305 -1.036843
C -2.427380 3.466307 -0.208834
C -0.134638 2.498866 -0.149822
H -2.228320 4.142210 0.635235
H -2.197773 4.024863 -1.129459
H -3.514757 3.290538 -0.223444
O 0.422394 2.636551 -1.274735
O 0.528321 2.611521 0.915681
H -6.479828 -0.757593 -0.249187
###
44
GlyGlyHisAla2 tri_tetrapeptidos E=-0.431287573688 au
N -7.580714 -0.126286 -0.620826
H -7.659570 -0.616724 0.288526
C -6.263137 -0.425722 -1.280363
H -8.362492 -0.440872 -1.229966
H -7.690582 0.889871 -0.449790
C -5.099911 0.128644 -0.486901
H -6.159711 -1.538774 -1.444646
H -6.252105 -0.005847 -2.329581
O -5.268866 0.898511 0.474622
N -3.847454 -0.248867 -0.895363
H -3.701972 -0.933411 -1.654963
C -2.637804 0.290729 -0.258595
C -2.270440 -0.439768 1.022069
H -1.798468 0.260301 -1.014212
H -2.752288 1.385955 -0.019820
O -3.127675 -0.893489 1.802724
N -0.944118 -0.611598 1.357878
H -0.709219 -1.026815 2.272083
C 0.177059 -0.050733 0.575755
H -0.117767 -0.021264 -0.522562
C 0.527644 1.383164 1.031074
C 1.425901 -0.927847 0.773203
H -0.362391 2.041831 0.874888
H 0.703322 1.417074 2.129430
C 1.689196 1.914913 0.278320
O 1.918790 -1.140258 1.897518
N 2.906413 2.235477 0.894729

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C       1.764119        2.199793        -1.091117
C       3.712526        2.709885        -0.096686
N       3.043249        2.711985        -1.319059
H       1.027033        2.078784        -1.869547
H       4.729120        3.067097        0.031520
N       2.014761        -1.415857       -0.361169
H       1.610172        -1.245924       -1.297606
C       3.330083        -2.106732       -0.315144
H       3.404961        -2.710585       0.632743
C       3.501161        -3.020764       -1.512623
C       4.404845        -0.991106       -0.272468
H       3.402788        -2.500709       -2.475416
H       4.486968        -3.510927       -1.503404
H       2.757534        -3.832995       -1.520148
O       4.768431        -0.571809       0.865047
O       4.875368        -0.492304       -1.324578
H       3.403897        3.037999        -2.212673
###
48
GlyGlyLysAla1 tri_tetrapeptidos E=-0.502089391493 au
N       -4.508964       1.783205        1.793616
H       -3.545146       1.564386        2.062897
C       -5.224207       0.536241        1.441611
H       -4.444520       2.394785        0.977235
C       -4.622622       -0.170387       0.236306
H       -5.266994       -0.129196       2.338940
H       -6.296228       0.766898        1.215961
O       -4.643824       0.344728        -0.898343
N       -4.033826       -1.394784       0.441046
H       -3.980316       -1.820128       1.378755
C       -3.374714       -2.126252       -0.646917
C       -1.963347       -1.677790       -0.999241
H       -3.337253       -3.221902       -0.386240
H       -3.993213       -2.087998       -1.585658
O       -1.370478       -2.252375       -1.933527
N       -1.355140       -0.648931       -0.323037
H       -1.784868       -0.198148       0.499145
C       -0.014676       -0.144951       -0.716073
H       0.040071        -0.124916       -1.849179
C       0.186385        1.270340        -0.147426
C       1.075984        -1.121232       -0.230901
H       -0.794236       1.706288        0.157894
H       0.758463        1.244341        0.803802
C       0.863189        2.204307        -1.156791
O       0.791344        -2.172089       0.380890
H       1.938462        1.947748        -1.268156
H       0.430032        2.053047        -2.169367
C       0.703743        3.678545        -0.772637
H       0.917201        4.315371        -1.660626
H       -0.360679       3.895258        -0.529469
C       1.568508        4.110294        0.408743
H       1.141397        5.022714        0.894680
H       1.594277        3.329805        1.207843
N       2.987543        4.415468        -0.031547
H       2.998795        5.157202        -0.754346
H       3.557826        4.739661        0.768807
H       3.440533        3.576867        -0.434008
N       2.374408        -0.819265       -0.536694
H       2.625500        0.062012        -1.018548
C       3.490351        -1.763484       -0.259631
H       3.166805        -2.805905       -0.543228
C       4.715205        -1.382280       -1.070507
C       3.795210        -1.751139       1.257711
H       5.069034        -0.360729       -0.871369
H       5.555523        -2.064524       -0.870316
H       4.524735        -1.437293       -2.154096
O       3.278718        -2.663382       1.968177
O       4.519566        -0.862977       1.772736
###
47
GlyGlyLysAla2 tri_tetrapeptidos E=-0.643434590506 au
N       6.184866        -1.957366       0.737725
H       5.766847        -2.526556       1.475539
C       5.219363        -0.944678       0.262543
H       6.421918        -2.598696       -0.022351
C       3.872222        -1.503049       -0.160787
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H       5.040523        -0.194161       1.077536
H       5.691831        -0.353533       -0.562807
O       3.414409        -2.563597       0.315180
N       3.157754        -0.783228       -1.086840
H       3.508110        0.114797        -1.458449
C       1.808756        -1.173612       -1.526189
C       0.782811        -0.728076       -0.488212
H       1.607876        -0.733898       -2.540567
H       1.722769        -2.279335       -1.682540
O       0.616937        -1.391547       0.559705
N       0.070089        0.407409        -0.746283
H       0.187369        0.911183        -1.646496
C       -0.853438       1.039334        0.234127
H       -0.252863       1.380648        1.131826
C       -1.564770       2.249772        -0.385583
C       -1.857295       -0.011476       0.746753
H       -2.063719       1.968177        -1.340416
H       -2.393456       2.563090        0.288526
C       -0.628326       3.434122        -0.644753
O       -1.754337       -0.437864       1.918499
H       0.239154        3.117458        -1.258771
H       -1.164941       4.172758        -1.278852
C       -0.145299       4.107072        0.643271
H       -1.009949       4.394582        1.273806
H       0.429256        3.383559        1.257858
C       0.737484        5.331671        0.361832
H       1.270914        5.621338        1.294273
H       1.533067        5.070382        -0.369956
N       0.012119        6.530113        -0.147589
H       -0.721615       6.794198        0.512553
H       -0.479283       6.290678        -1.011703
N       -2.805491       -0.514127       -0.095372
H       -2.932245       -0.153568       -1.054850
C       -3.695933       -1.628464       0.325907
H       -3.884536       -1.561937       1.435916
C       -5.016834       -1.570189       -0.415050
C       -2.918513       -2.940191       0.049529
H       -4.902636       -1.590308       -1.508281
H       -5.665957       -2.415615       -0.139974
H       -5.581754       -0.655243       -0.178660
O       -2.006708       -3.268854       0.869621
O       -3.163227       -3.647267       -0.956128
###
47
GlyGlyTyrAla1 tri_tetrapeptidos E=-0.657448853819 au
N       -5.183405       2.618462        -0.882104
H       -4.373580       2.901496        -0.326677
C       -5.675092       1.301816        -0.424498
H       -4.855113       2.553366        -1.847696
C       -4.619994       0.211337        -0.432808
H       -6.113538       1.414524        0.600404
H       -6.539870       0.982079        -1.062163
O       -3.514924       0.370214        -0.999041
N       -4.912290       -0.962974       0.211861
H       -5.792825       -1.090164       0.733505
C       -3.960252       -2.089145       0.258016
C       -2.596109       -1.635826       0.748911
H       -4.352689       -2.886337       0.949289
H       -3.902691       -2.589580       -0.745139
O       -2.455029       -0.800057       1.660800
N       -1.495233       -2.164290       0.117180
H       -1.579215       -2.868183       -0.634533
C       -0.134912       -1.669505       0.436727
H       0.019594        -1.719685       1.556758
C       0.933152        -2.526790       -0.266652
C       -0.027241       -0.205059       -0.048571
H       1.007872        -3.515044       0.245396
H       0.612939        -2.789375       -1.302336
C       2.267241        -1.837607       -0.275767
O       -0.486861       0.166598        -1.146379
C       2.976521        -1.647851       0.922887
C       2.797755        -1.357952       -1.484560
H       2.577770        -2.042790       1.862505
C       4.181023        -0.946006       0.927947
C       4.003262        -0.657167       -1.504712
H       2.263714        -1.532339       -2.423606
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H       4.736866        -0.789829       1.854004
C       4.668353        -0.451415       -0.288636
H       4.424870        -0.286954       -2.438366
O       5.813308        0.322971        -0.360630
H       6.301701        0.354987        0.521532
N       0.581282        0.680919        0.797068
H       0.982852        0.375293        1.699876
C       0.787465        2.107066        0.434971
H       0.127598        2.377588        -0.436469
C       0.463099        3.014197        1.608539
C       2.266309        2.244502        -0.005114
H       1.020969        2.760172        2.520526
H       0.686490        4.066857        1.376586
H       -0.604765       2.978526        1.871180
O       2.508971        2.278819        -1.242916
O       3.188922        2.288080        0.847829
###
46
GlyGlyTyrAla2 tri_tetrapeptidos E=-0.814204473405 au
N       -5.435920       -1.789227       -2.013922
H       -4.666318       -1.883189       -2.679272
C       -4.958371       -1.128022       -0.782087
H       -5.750983       -2.737770       -1.802251
C       -3.768551       -1.811494       -0.131854
H       -4.698082       -0.062899       -1.014870
H       -5.802476       -1.057091       -0.048254
O       -3.232336       -2.825443       -0.627207
N       -3.299004       -1.265345       1.037684
H       -3.707051       -0.401734       1.429672
C       -2.163554       -1.832138       1.780554
C       -0.842601       -1.468329       1.111522
H       -2.201683       -1.470244       2.844861
H       -2.238973       -2.947029       1.868949
O       -0.405835       -2.131359       0.144360
N       -0.151883       -0.394959       1.598973
H       -0.510273       0.163278        2.394557
C       1.133066        0.042031        1.000371
H       1.041628        -0.005930       -0.122924
C       1.462609        1.486777        1.424626
C       2.260357        -0.890409       1.477700
H       1.354808        1.603393        2.526909
H       2.540041        1.694830        1.228916
C       0.606159        2.473637        0.689528
O       2.237494        -1.430043       2.599174
C       0.975387        2.905098        -0.596271
C       -0.575698       2.965615        1.268385
H       1.897264        2.528224        -1.047195
C       0.186137        3.801505        -1.300397
C       -1.380848       3.864588        0.583582
H       -0.864798       2.634746        2.269872
H       0.475118        4.134031        -2.290731
C       -1.016368       4.294956        -0.722297
H       -2.291591       4.242997        1.033591
O       -1.772193       5.120436        -1.379972
N       3.330807        -1.159172       0.663359
H       4.093281        -1.754827       1.028179
C       3.534429        -0.632267       -0.709264
H       2.910069        0.291532        -0.882922
C       4.998376        -0.281655       -0.918901
C       3.055306        -1.722250       -1.699269
H       5.676817        -1.124754       -0.730147
H       5.182820        0.065745        -1.946551
H       5.321442        0.538656        -0.259824
O       1.810450        -1.924797       -1.808858
O       3.874411        -2.383407       -2.384847
###
35
GlyHisGly2 tri_tetrapeptidos E=-0.182841211269 au
N       -3.702656       -2.644197       -0.975495
H       -4.180086       -2.723481       -0.059297
C       -2.211113       -2.728655       -0.816571
H       -4.035687       -3.420103       -1.584482
H       -3.979414       -1.747727       -1.413431
C       -1.672657       -1.686288       0.138569
H       -1.923574       -3.768064       -0.473856
H       -1.709553       -2.635128       -1.826343
```

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O       -2.390877       -0.803583       0.642136
N       -0.329817       -1.760572       0.409241
H       0.265627        -2.487277       -0.031456
C       0.325146        -0.871427       1.398357
H       -0.102932       -1.116169       2.425362
C       1.837572        -1.119868       1.472574
C       -0.002031       0.616492        1.153403
H       2.225780        -0.629568       2.406046
H       2.021297        -2.213650       1.663295
C       2.626030        -0.696159       0.295163
O       -0.367786       1.302876        2.131767
N       3.591154        0.330337        0.362104
C       2.656139        -1.193969       -1.008003
H       3.816512        0.891082        1.192239
C       4.185523        0.456679        -0.873468
N       3.618880        -0.470207       -1.719131
H       2.076380        -1.997167       -1.457628
H       4.976884        1.170753        -1.135602
N       0.070365        1.144081        -0.101440
H       0.343961        0.577202        -0.918038
C       -0.289843       2.543840        -0.378799
C       -1.798049       2.763005        -0.490648
H       0.113488        3.233716        0.407872
H       0.217371        2.868766        -1.324476
O       -2.595435       2.193145        0.310710
O       -2.229357       3.546216        -1.376577
H       3.865812        -0.610422       -2.704910
###
34
GlyHisGly3 tri_tetrapeptidos E=-0.331441365896 au
N       0.316475        3.816029        0.861643
H       0.019413        3.497436        1.803826
C       -0.450970       3.114674        -0.222774
H       0.147521        4.841220        0.803147
H       1.335521        3.653242        0.765940
C       -0.162833       1.625296        -0.343487
H       -1.560863       3.277907        -0.081522
H       -0.242329       3.608717        -1.215274
O       0.314173        1.165096        -1.389421
N       -0.463221       0.831408        0.738916
H       -0.888814       1.243599        1.589528
C       -0.437537       -0.647278       0.702739
H       -0.880074       -1.002347       1.685824
C       -1.259267       -1.251283       -0.452323
C       1.020348        -1.157474       0.667581
H       -0.905965       -0.868253       -1.439427
H       -1.073196       -2.351143       -0.495596
C       -2.707302       -0.971183       -0.299735
O       1.523571        -1.653803       1.695717
N       -3.594773       -1.875724       0.298439
C       -3.403979       0.171471        -0.713279
C       -4.820218       -1.283534       0.248529
N       -4.740296       -0.032485       -0.362213
H       -3.051281       1.064267        -1.205295
H       -5.743451       -1.708464       0.626500
N       1.724249        -1.083634       -0.499578
H       1.345033        -0.579279       -1.323021
C       3.086543        -1.624994       -0.629697
C       4.141343        -0.591124       -0.235755
H       3.222621        -2.547432       -0.010863
H       3.244350        -1.967557       -1.683504
O       4.158652        -0.122260       0.935876
O       4.978894        -0.223194       -1.102143
H       -5.504618       0.614793        -0.531747
###
50
GlyHisLys3 tri_tetrapeptidos E=-0.788368065828E-01 au
N       -4.884673       2.435450        -0.547604
H       -4.889430       1.916677        -1.446161
C       -3.506451       2.936257        -0.217519
H       -5.535366       3.241677        -0.638765
H       -5.249979       1.811017        0.196888
C       -2.438227       1.859803        -0.133873
H       -3.195463       3.707237        -0.980493
H       -3.530995       3.524428        0.748661
O       -1.435149       1.920995        -0.868127
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N       -2.564063       0.894607        0.829888
H       -3.408685       0.847367        1.434776
C       -1.607330       -0.230159       0.984439
H       -1.822165       -0.717354       1.992995
C       -1.787639       -1.284118       -0.118495
C       -0.187028       0.356851        1.098764
H       -1.525819       -0.863931       -1.123205
H       -1.053433       -2.121137       0.034339
C       -3.152363       -1.862491       -0.150111
O       0.013512        1.294509        1.901138
N       -3.635565       -2.554299       -1.279179
C       -4.166437       -1.894763       0.807841
C       -4.914735       -2.994138       -1.010347
N       -5.248505       -2.593393       0.261240
H       -4.187653       -1.476054       1.811616
H       -5.551427       -3.567519       -1.696226
H       -6.137890       -2.779822       0.735121
N       0.843204        -0.122595       0.341239
H       0.729913        -0.899098       -0.329756
C       2.209606        0.456218        0.451173
H       2.353436        0.879227        1.489733
C       3.244701        -0.650241       0.198689
C       2.329878        1.647913        -0.529464
H       2.856684        -1.626472       0.566780
H       3.390062        -0.807916       -0.889969
C       4.580631        -0.344924       0.885868
O       3.273436        1.727978        -1.351671
O       1.454638        2.567345        -0.470330
H       5.027478        0.584240        0.480222
H       4.412446        -0.134482       1.963992
C       5.565743        -1.511192       0.758407
H       6.353769        -1.417877       1.539183
H       5.054378        -2.469933       1.000582
C       6.199864        -1.637288       -0.624555
H       6.542388        -2.686924       -0.803846
H       5.466050        -1.421991       -1.438457
N       7.390228        -0.708238       -0.771985
H       8.123829        -0.931745       -0.075310
H       7.807552        -0.791813       -1.716111
H       7.115351        0.278667        -0.630410
H       -3.122179       -2.710171       -2.154357
###
49
GlyHisLys4 tri_tetrapeptidos E=-0.229998309948 au
N       -4.532507       -3.422155       -0.131955
H       -3.744382       -4.058063       0.089685
C       -4.201064       -2.529405       -1.293560
H       -5.362757       -4.005486       -0.364679
H       -4.759973       -2.869662       0.716627
C       -2.899078       -1.755785       -1.163566
H       -4.168861       -3.142421       -2.240617
H       -5.050892       -1.807781       -1.481477
O       -2.023396       -1.851570       -2.035229
N       -2.750060       -0.905998       -0.093536
H       -3.443066       -0.863625       0.670600
C       -1.579181       -0.002853       0.014480
H       -1.397724       0.474472        -0.996706
C       -1.836788       1.092517        1.065930
C       -0.335657       -0.811365       0.444548
H       -2.220542       0.644467        2.013182
H       -0.867934       1.570335        1.352855
C       -2.758802       2.137691        0.558846
O       -0.388662       -1.695410       1.320310
N       -4.022075       2.371066        1.116621
C       -2.533903       3.033461        -0.494906
C       -4.558766       3.401688        0.404129
N       -3.678459       3.828039        -0.588311
H       -1.681653       3.146224        -1.145051
H       -5.536061       3.842732        0.570720
H       -3.825765       4.580242        -1.255917
N       0.839685        -0.517421       -0.189060
H       0.908839        0.248199        -0.879826
C       2.102757        -1.216055       0.156123
H       1.947253        -2.322786       -0.017659
C       3.252912        -0.745537       -0.745368
C       2.473335        -1.034860       1.642777
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H       4.115948        -1.435089       -0.610612
H       2.960786        -0.878803       -1.811172
C       3.696920        0.700820        -0.501778
O       2.159020        -0.000434       2.288599
O       3.099260        -1.980250       2.200306
H       2.824322        1.385810        -0.557543
H       4.096587        0.814853        0.525773
C       4.737775        1.159030        -1.528612
H       4.383573        0.925508        -2.558243
H       4.816692        2.269100        -1.506806
C       6.115032        0.527948        -1.342705
H       6.040411        -0.567772       -1.134990
H       6.711654        0.613037        -2.285184
N       6.886823        1.194890        -0.219854
H       6.384187        1.113828        0.679756
H       7.818490        0.758403        -0.105895
H       7.024284        2.202858        -0.414071
###
48
GlyHisLys5 tri_tetrapeptidos E=-0.375682515625 au
N       -6.320458       -2.584193       -0.365196
H       -6.781516       -1.916683       -0.986746
C       -5.363330       -1.881387       0.514204
H       -5.824388       -3.243646       -0.967725
C       -4.282043       -1.114922       -0.224218
H       -5.928303       -1.189019       1.190613
H       -4.883851       -2.622028       1.205826
O       -4.110704       -1.216306       -1.454144
N       -3.463795       -0.298917       0.527204
H       -3.583652       -0.212889       1.550386
C       -2.441454       0.564671        -0.102321
H       -2.795670       0.881767        -1.131368
C       -2.209015       1.822719        0.748840
C       -1.162645       -0.273331       -0.330813
H       -3.138466       2.444161        0.748227
H       -2.071371       1.555982        1.826120
C       -1.067352       2.629196        0.250954
O       -1.060515       -0.954308       -1.368998
N       -0.059259       3.092957        1.107722
C       -0.809698       3.058469        -1.057132
C       0.802812        3.796842        0.320329
N       0.373870        3.799283        -1.004272
H       -1.364114       2.897067        -1.967523
H       1.702330        4.300001        0.660769
H       0.826891        4.254215        -1.792836
N       -0.183965       -0.292811       0.627813
H       -0.256193       0.311919        1.460485
C       1.158201        -0.862794       0.335898
H       1.026303        -1.882296       -0.121648
C       1.952011        0.039369        -0.628789
C       1.903621        -1.000043       1.678253
H       1.267941        0.429313        -1.415316
H       2.316769        0.949020        -0.109050
C       3.110444        -0.690836       -1.313374
O       2.295911        -2.141233       2.034421
O       2.109525        0.023227        2.384252
H       2.791301        -1.699498       -1.648354
H       3.363300        -0.150461       -2.252514
C       4.361801        -0.797332       -0.434994
H       4.658171        0.207905        -0.065356
H       4.153107        -1.399663       0.472607
C       5.509195        -1.426402       -1.228118
H       5.230169        -2.441056       -1.605901
H       5.750378        -0.820555       -2.136232
N       6.755107        -1.545248       -0.372697
H       6.582496        -2.142271       0.455027
H       7.531243        -1.968183       -0.913701
H       7.067594        -0.616953       -0.036367
###
47
GlyHisLys6 tri_tetrapeptidos E=-0.511338759245 au
N       -2.219741       4.360549        -0.560737
H       -3.011428       4.280632        0.080519
C       -2.049402       3.101584        -1.316405
H       -1.399398       4.531270        0.024716
C       -1.842518       1.872226        -0.450323
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H       -2.947613       2.938981        -1.968443
H       -1.198154       3.221397        -2.034164
O       -1.975893       1.896766        0.787259
N       -1.466060       0.710643        -1.092237
H       -1.463455       0.653735        -2.123337
C       -1.347207       -0.573939       -0.366145
H       -1.254886       -0.376647       0.743809
C       -2.574168       -1.474431       -0.616531
C       -0.064475       -1.276601       -0.856245
H       -2.833575       -1.487980       -1.701118
H       -2.315962       -2.531570       -0.376095
C       -3.741962       -1.028679       0.181278
O       -0.095480       -2.200481       -1.691296
N       -4.150416       -1.687145       1.348891
C       -4.593388       0.054574        -0.072040
C       -5.244151       -1.008333       1.797202
N       -5.542436       0.059400        0.954076
H       -4.591093       0.772982        -0.875590
H       -5.817232       -1.251460       2.686232
H       -6.304024       0.724770        1.055582
N       1.121218        -0.855249       -0.320523
H       1.160397        -0.115158       0.397442
C       2.420076        -1.432419       -0.746218
H       2.359330        -1.695719       -1.847127
C       3.541057        -0.399514       -0.562250
C       2.714044        -2.754982       -0.012936
H       4.458148        -0.778170       -1.061412
H       3.283554        0.524853        -1.126557
C       3.840951        -0.050981       0.899508
O       1.782909        -3.389683       0.560083
O       3.881373        -3.231493       -0.042903
H       2.921169        0.296913        1.414216
H       4.154054        -0.959058       1.452531
C       4.933724        1.016839        1.016820
H       5.285480        1.066251        2.067761
H       5.825054        0.719917        0.428768
C       4.441813        2.400849        0.567196
H       4.061331        2.349448        -0.477365
H       3.578396        2.720666        1.189732
N       5.482128        3.466137        0.630580
H       6.286765        3.193874        0.062282
H       5.840662        3.541704        1.584643
###
29
GlySerGly1 tri_tetrapeptidos E=-0.268371885085 au
N       -2.746251       -3.244766       -0.031693
H       -2.477110       -3.443268       -1.012855
C       -3.047433       -1.784706       0.159932
H       -3.587927       -3.812574       0.196295
H       -1.972060       -3.549025       0.585822
C       -1.860427       -0.912301       -0.185159
H       -3.942185       -1.488794       -0.464988
H       -3.398576       -1.603443       1.219210
O       -0.844067       -1.364791       -0.739714
N       -1.970834       0.415659        0.143610
H       -2.788463       0.772581        0.671028
C       -0.907392       1.395569        -0.180137
H       -0.838510       1.485479        -1.309445
C       -1.248270       2.786503        0.400811
C       0.439602        0.920252        0.395084
H       -2.104655       2.755697        1.107837
H       -0.381288       3.253083        0.917366
O       -1.533885       3.700301        -0.659389
O       0.531897        0.382687        1.511369
H       -2.380968       3.445240        -1.120516
N       1.542843        1.105679        -0.398424
H       1.487983        1.545048        -1.331837
C       2.878242        0.676891        0.037749
C       3.048512        -0.819322       -0.080637
H       3.663210        1.213798        -0.566426
H       3.089943        0.981338        1.102899
O       4.356510        -1.150889       -0.164559
O       2.177184        -1.681736       -0.081206
H       4.532196        -2.153056       -0.206710
###
28
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GlySerGly2 tri_tetrapeptidos E=-0.448136526111 au
C 3.607539 -1.038033 -0.672756
C 2.382539 -0.518984 0.059900
N 1.735124 0.551539 -0.505917
C 0.509928 1.122595 0.094174
C -0.629931 0.085044 0.071296
N -1.581243 0.194072 1.045670
C -2.681726 -0.779431 1.167816
C -3.436206 -0.971671 -0.146254
O -3.430529 -2.111860 -0.687486
N 4.845991 -0.951084 0.175052
O 1.976221 -1.046986 1.106235
C 0.085768 2.401972 -0.664138
O -0.229983 3.436111 0.269336
O -0.683478 -0.817872 -0.786566
O -4.048656 -0.004003 -0.673893
H 5.070500 0.037415 0.400392
H 5.653377 -1.360271 -0.336881
H 4.733424 -1.471364 1.063814
H 3.789573 -0.516486 -1.657478
H 3.418558 -2.107708 -0.983974
H 2.060029 0.964532 -1.399842
H 0.734104 1.402811 1.172020
H 0.917724 2.840346 -1.260431
H -0.776858 2.232271 -1.337993
H -1.025340 3.190705 0.820688
H -1.576897 0.972620 1.727136
H -2.297207 -1.759221 1.545070
H -3.396154 -0.439413 1.962612
###
27
GlySerGly3 tri_tetrapeptidos E=-0.593329524749 au
N 4.826738 -1.540955 -0.147115
H 4.547377 -2.231864 0.551927
C 3.636894 -1.033177 -0.861557
H 5.278376 -0.781712 0.366552
C 2.600202 -0.390385 0.041052
H 3.964672 -0.308889 -1.650629
H 3.159916 -1.872609 -1.431424
O 2.662761 -0.450128 1.282731
N 1.561711 0.276825 -0.572323
H 1.465484 0.308126 -1.601698
C 0.512754 0.955290 0.210655
H 0.937717 1.266054 1.214643
C -0.001469 2.222939 -0.502461
C -0.652631 -0.012085 0.499380
H 0.038316 2.142399 -1.607781
H -1.040232 2.469105 -0.194175
O 0.761275 3.349664 -0.058059
O -0.958955 -0.260364 1.682912
H 1.604887 3.421617 -0.583199
N -1.324675 -0.572033 -0.547482
H -1.094623 -0.337848 -1.527105
C -2.469435 -1.475861 -0.341209
C -3.755629 -0.672460 -0.131291
H -2.569175 -2.155931 -1.224230
H -2.304835 -2.159940 0.527404
O -3.931860 -0.057450 0.958305
O -4.615522 -0.640589 -1.048298
###
58
PHEAlaArg1 tri_tetrapeptidos E=-0.232334727168E-01 au
N -4.524008 -1.773102 0.823508
H -4.537978 -0.870079 1.336268
H -4.197411 -2.515596 1.474335
H -5.509159 -1.992576 0.557784
C -3.658513 -1.714905 -0.419231
H -3.745673 -2.734393 -0.926885
C -4.169710 -0.655730 -1.406582
C -2.162665 -1.505736 -0.126502
H -3.697572 -0.844798 -2.402088
H -5.257820 -0.830684 -1.601286
C -3.935656 0.764892 -0.978341
O -1.336555 -2.178943 -0.761121
C -2.766944 1.434078 -1.375591
C -4.883262 1.432707 -0.189704

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H       -2.027411       0.923497        -1.994778
C       -2.545936       2.753965        -0.977098
C       -4.658489       2.754791        0.203534
H       -5.799081       0.923034        0.118938
H       -1.633464       3.268479        -1.282778
C       -3.491215       3.416403        -0.187511
H       -5.398306       3.270039        0.818472
H       -3.317442       4.447609        0.122202
N       -1.762195       -0.581295       0.803594
H       -2.434334       0.006724        1.325391
C       -0.327427       -0.226172       0.957235
H       0.143041        -0.145823       -0.075005
C       -0.178584       1.100700        1.682044
C       0.373047        -1.324743       1.781865
H       -0.693411       1.129290        2.653477
H       0.883060        1.343378        1.872387
H       -0.572772       1.940025        1.085607
O       -0.079635       -1.742128       2.857820
N       1.547288        -1.891432       1.325942
H       2.041810        -2.566417       1.934348
C       2.257743        -1.490030       0.093802
H       1.615096        -0.775158       -0.515069
C       3.603431        -0.826550       0.424883
C       2.480289        -2.766031       -0.729391
H       3.441014        -0.042236       1.199174
H       4.287785        -1.556762       0.910995
C       4.294170        -0.220046       -0.795645
O       1.507142        -2.890822       -1.671539
O       3.355245        -3.603312       -0.617898
H       5.282754        0.181891        -0.478456
H       4.544299        -1.012448       -1.536221
C       3.498624        0.871139        -1.519586
H       4.129803        1.329465        -2.318340
H       2.624237        0.429516        -2.060934
N       2.943644        1.930907        -0.633299
H       2.107198        1.603045        -0.104216
C       3.802604        2.771014        0.089507
N       4.997038        3.183822        -0.436014
N       3.382319        3.269366        1.308525
H       5.457229        2.656047        -1.179121
H       5.599880        3.820929        0.092467
H       2.403367        3.137262        1.590244
H       3.810109        4.126828        1.673830
H       1.603909        -3.714781       -2.260774
###
57
PHEAlaArg2 tri_tetrapeptidos E=-0.204562908735 au
N       -4.585818       -2.483127       -1.442354
H       -4.695098       -3.034051       -0.566863
H       -3.837470       -2.921063       -2.015191
H       -5.479972       -2.558178       -1.974246
C       -4.276680       -1.025274       -1.162516
H       -4.276033       -0.485973       -2.166812
C       -5.365759       -0.416504       -0.265574
C       -2.885972       -0.801027       -0.542202
H       -6.367473       -0.568767       -0.740032
H       -5.436795       -0.975560       0.697796
C       -5.135915       1.050334        -0.031383
O       -2.149212       0.068625        -1.036481
C       -4.837482       1.518329        1.256248
C       -5.223495       1.958095        -1.098265
H       -4.773899       0.820992        2.093433
C       -4.625026       2.882439        1.472711
C       -5.007315       3.319567        -0.876101
H       -5.463613       1.602532        -2.101915
H       -4.395665       3.242563        2.477231
C       -4.706287       3.784215        0.408211
H       -5.075293       4.022790        -1.708027
H       -4.538483       4.848319        0.578688
N       -2.497018       -1.516352       0.557159
H       -3.088921       -2.256021       0.972357
C       -1.215755       -1.215336       1.251493
H       -1.183596       -0.107163       1.479691
C       -1.120453       -2.008079       2.543800
C       -0.033125       -1.603615       0.337561
H       -1.156713       -3.097070       2.393662
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H -0.190789 -1.782798 3.089439
H -1.944601 -1.764958 3.235060
O 0.012411 -2.690108 -0.267497
N 0.977520 -0.687438 0.212572
H 0.988554 0.189458 0.760088
C 2.150320 -0.949307 -0.653123
H 1.769068 -1.323283 -1.651956
C 2.959315 0.330301 -0.917928
C 3.048771 -2.066044 -0.082356
H 3.808437 0.075043 -1.590596
H 2.330400 1.017741 -1.530628
C 3.458119 1.098693 0.305818
O 3.088578 -2.334786 1.145074
O 3.728994 -2.729051 -0.917722
H 3.629403 2.159369 0.011192
H 2.664396 1.169086 1.083230
C 4.723414 0.539863 0.959953
H 4.937440 1.097420 1.904298
H 4.579884 -0.520618 1.279526
N 5.925762 0.550175 0.083352
H 5.875768 -0.158003 -0.675729
C 6.530337 1.761665 -0.280724
N 7.250196 1.819526 -1.462463
N 6.501421 2.848885 0.546002
H 7.460797 0.944789 -1.956052
H 7.983877 2.530579 -1.558923
H 5.801232 2.937949 1.284115
H 7.002481 3.705854 0.296561
###
56
PHEAlaArg3 tri_tetrapeptidos E=-0.348875264180 au
N 2.434793 2.675187 -0.076945
H 1.448432 2.917961 0.038961
H 2.741231 2.231182 0.792034
C 2.622697 1.775263 -1.235870
H 2.334728 2.365538 -2.158552
C 4.091806 1.350699 -1.408395
C 1.688042 0.545165 -1.222132
H 4.205334 0.863868 -2.405012
H 4.715998 2.271525 -1.490626
C 4.637690 0.461437 -0.327807
O 0.907398 0.349507 -2.181136
C 4.710593 -0.925773 -0.534650
C 5.087283 1.001588 0.886442
H 4.377782 -1.354389 -1.481038
C 5.209265 -1.760385 0.467628
C 5.584363 0.162125 1.886716
H 5.053692 2.078876 1.054981
H 5.259651 -2.837911 0.302546
C 5.644062 -1.218877 1.681189
H 5.926945 0.587707 2.831378
H 6.030423 -1.871962 2.463970
N 1.673470 -0.290570 -0.139269
H 2.315878 -0.146741 0.658238
C 0.795328 -1.490537 -0.062887
H 1.074332 -2.188938 -0.907419
C 0.977005 -2.197099 1.269231
C -0.679495 -1.046991 -0.207548
H 0.705940 -1.577542 2.135684
H 0.365287 -3.112508 1.323873
H 2.020652 -2.517298 1.426803
O -1.092655 -0.000886 0.328981
N -1.474393 -1.840456 -0.985462
H -1.112983 -2.734570 -1.362575
C -2.878016 -1.538726 -1.357365
H -3.084651 -2.152966 -2.298224
C -3.899149 -2.010246 -0.308222
C -3.067171 -0.085113 -1.820814
H -4.919329 -1.809609 -0.703047
H -3.842470 -3.122667 -0.266514
C -3.764138 -1.463809 1.114465
O -2.096271 0.556757 -2.331705
O -4.208924 0.438679 -1.785181
H -3.771198 -2.322952 1.825281
H -2.773239 -1.000581 1.281957
C -4.880187 -0.505303 1.540088

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H       -5.875933       -0.860543       1.176020
H       -4.969707       -0.493294       2.653443
N       -4.719540       0.886982        1.035802
H       -4.929471       0.969719        0.015285
C       -3.659733       1.678929        1.486557
N       -3.190628       2.699827        0.659769
N       -3.076463       1.484810        2.701280
H       -3.807469       3.026622        -0.092658
H       -2.670356       3.471640        1.099560
H       -3.331799       0.698868        3.302908
H       -2.416212       2.163953        3.089082
###
55
PHEAlaArg4 tri_tetrapeptidos E=-0.499334211883 au
N       -2.860727       -1.973091       -2.499517
H       -1.875703       -1.960791       -2.774811
H       -3.024876       -2.859492       -2.014995
C       -3.175548       -0.818187       -1.631263
H       -3.017116       0.115646        -2.246190
C       -4.641137       -0.879666       -1.164824
C       -2.263400       -0.675309       -0.391205
H       -5.297946       -1.066931       -2.046246
H       -4.808054       -1.765759       -0.512671
C       -5.062016       0.391730        -0.482966
O       -1.705303       0.421666        -0.158241
C       -5.206573       1.574046        -1.226143
C       -5.316229       0.405133        0.895993
H       -5.016769       1.571658        -2.300363
C       -5.600806       2.754756        -0.593830
C       -5.712775       1.589512        1.523246
H       -5.213181       -0.508835       1.482291
H       -5.712628       3.671633        -1.175122
C       -5.854051       2.765364        0.781489
H       -5.911697       1.594866        2.596423
H       -6.162062       3.688878        1.272615
N       -2.055537       -1.750814       0.424666
H       -2.526951       -2.656178       0.247496
C       -1.231197       -1.696778       1.662645
H       -1.800203       -1.110821       2.445987
C       -0.952778       -3.101073       2.169053
C       0.093459        -0.947593       1.416400
H       -0.433044       -3.737218       1.436651
H       -0.331695       -3.089045       3.079175
H       -1.880872       -3.630793       2.441550
O       0.368452        0.047978        2.119157
N       0.940521        -1.377172       0.434040
H       0.727749        -2.212323       -0.135933
C       2.186964        -0.637217       0.110090
H       2.865789        -0.668407       1.011488
C       2.903099        -1.272366       -1.088972
C       1.835908        0.837859        -0.192911
H       3.061963        -2.358681       -0.900955
H       2.261299        -1.239301       -1.994541
C       4.240900        -0.588082       -1.377277
O       1.045001        1.140976        -1.125419
O       2.345999        1.725081        0.546111
H       4.600367        -0.903025       -2.381513
H       4.115838        0.508967        -1.466243
C       5.297665        -0.931311       -0.317946
H       4.878646        -0.853885       0.709328
H       5.618327        -1.994972       -0.428197
N       6.529665        -0.106735       -0.428700
H       6.930703        -0.133978       -1.383309
C       6.540320        1.191619        0.160548
N       7.714832        1.941141        -0.139503
N       5.643413        1.551642        1.057075
H       8.184471        1.750708        -1.025582
H       7.653651        2.945860        0.033593
H       5.804807        2.447198        1.528012
###
# Conformations of ALANINE optimized with pm6
# opt freq pm6 scf=(xqc,tight) scrf(smd,solvent=water)
###
14
ala100 pm6_conformaciones E=-0.293533286616E-01 au
N       1.299707        -1.188197       0.058708
```

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H       1.225793        -1.386851       -0.958043
H       0.862991        -1.976986       0.574846
H       2.310824        -1.160531       0.307821
C       0.640530        0.133838        0.414077
H       0.742907        0.288122        1.541112
C       1.316323        1.270171        -0.330841
C       -0.850374       0.123863        0.094427
H       1.227303        1.182561        -1.425954
H       0.897059        2.249203        -0.048299
H       2.395571        1.325806        -0.105054
O       -1.605866       1.077861        0.156551
O       -1.284354       -1.106271       -0.265549
H       -2.277518       -1.143903       -0.491371
###
14
ala101 pm6_conformaciones E=-0.293535141525E-01 au
N       1.299394        -1.188329       0.058613
H       1.225465        -1.386574       -0.958197
H       0.862428        -1.977120       0.574489
H       2.310539        -1.160989       0.307758
C       0.640541        0.133823        0.414158
H       0.742776        0.287834        1.541188
C       1.316601        1.270007        -0.330720
C       -0.850319       0.124029        0.094329
H       1.228509        1.181827        -1.425899
H       0.896867        2.249106        -0.048991
H       2.395650        1.326045        -0.104026
O       -1.605807       1.078017        0.156393
O       -1.284372       -1.106187       -0.265363
H       -2.277492       -1.143626       -0.491461
###
14
ala102 pm6_conformaciones E=-0.289970834244E-01 au
N       -1.546390       -0.960841       -0.284354
H       -1.579513       -1.334509       0.684103
H       -1.257691       -1.729540       -0.922026
H       -2.513288       -0.672342       -0.545631
C       -0.603271       0.225909        -0.391521
H       -0.594367       0.571969        -1.476319
C       -1.066610       1.350127        0.516237
C       0.809473        -0.199377       0.002441
H       -1.073572       1.072458        1.582840
H       -0.422236       2.239729        0.421928
H       -2.090075       1.682403        0.269578
O       1.144876        -1.171640       0.653823
O       1.710862        0.691714        -0.475496
H       2.672020        0.475172        -0.213560
###
14
ala103 pm6_conformaciones E=-0.293533408085E-01 au
N       1.299216        -1.188503       0.058308
H       1.225059        -1.386564       -0.958508
H       0.862290        -1.977321       0.574152
H       2.310424        -1.161315       0.307248
C       0.640555        0.133669        0.414174
H       0.742752        0.287377        1.541236
C       1.316827        1.269913        -0.330423
C       -0.850301       0.124115        0.094311
H       1.228505        1.182154        -1.425618
H       0.897446        2.249055        -0.048316
H       2.395927        1.325589        -0.103891
O       -1.605563       1.078313        0.156017
O       -1.284636       -1.106101       -0.264988
H       -2.277798       -1.143350       -0.491066
###
14
ala104 pm6_conformaciones E=-0.293533760118E-01 au
N       1.299073        -1.188629       0.058105
H       0.861920        -1.977470       0.573681
H       2.310230        -1.161632       0.307219
H       1.225050        -1.386471       -0.958802
C       0.640563        0.133568        0.414168
H       0.742768        0.287061        1.541255
C       1.316983        1.269862        -0.330203
C       -0.850282       0.124216        0.094256
H       1.229172        1.181999        -1.425436
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```
H       0.897308        2.248952        -0.048350
H       2.395983        1.325715        -0.103209
O       -1.605417       1.078519        0.155747
O       -1.284782       -1.106062       -0.264710
H       -2.277931       -1.143282       -0.490720
###
14
ala105 pm6_conformaciones E=-0.289970025200E-01 au
N       -1.546282       -0.960867       -0.284633
H       -1.578813       -1.335221       0.683569
H       -1.257937       -1.729106       -0.923035
H       -2.513313       -0.672176       -0.545136
C       -0.603229       0.225973        -0.391503
H       -0.594292       0.572303        -1.476185
C       -1.066799       1.349925        0.516407
C       0.809488        -0.199304       0.002493
H       -1.074462       1.071818        1.582867
H       -0.422191       2.239407        0.422769
H       -2.090069       1.682491        0.269295
O       1.144831        -1.171305       0.654263
O       1.710937        0.691567        -0.475788
H       2.672140        0.474899        -0.213901
###
14
ala106 pm6_conformaciones E=-0.293535823775E-01 au
N       1.299418        -1.188323       0.058658
H       0.862501        -1.977056       0.574583
H       2.310594        -1.160929       0.307783
H       1.225505        -1.386628       -0.958152
C       0.640542        0.133837        0.414151
H       0.742785        0.287894        1.541171
C       1.316591        1.270000        -0.330780
C       -0.850313       0.124007        0.094341
H       1.228734        1.181595        -1.425953
H       0.896658        2.249091        -0.049318
H       2.395574        1.326269        -0.103813
O       -1.605810       1.077998        0.156462
O       -1.284405       -1.106185       -0.265396
H       -2.277470       -1.143531       -0.491697
###
14
ala107 pm6_conformaciones E=-0.293533587265E-01 au
N       1.299248        -1.188504       0.058246
H       0.862206        -1.977371       0.573923
H       2.310392        -1.161351       0.307339
H       1.225258        -1.386525       -0.958611
C       0.640559        0.133630        0.414154
H       0.742758        0.287307        1.541220
C       1.316831        1.269927        -0.330348
C       -0.850303       0.124111        0.094292
H       1.228735        1.182078        -1.425568
H       0.897220        2.249018        -0.048363
H       2.395873        1.325737        -0.103613
O       -1.605525       1.078352        0.155932
O       -1.284694       -1.106105       -0.264913
H       -2.277946       -1.143351       -0.490790
###
14
ala108 pm6_conformaciones E=-0.289970888215E-01 au
N       -1.546218       -0.960924       -0.284455
H       -1.257466       -1.729425       -0.922340
H       -2.513211       -0.672525       -0.545562
H       -1.579196       -1.334884       0.683900
C       -0.603260       0.225919        -0.391482
H       -0.594314       0.572015        -1.476268
C       -1.066841       1.349996        0.516268
C       0.809518        -0.199265       0.002440
H       -1.074177       1.072114        1.582793
H       -0.422336       2.239543        0.422487
H       -2.090128       1.682525        0.269134
O       1.144890        -1.171480       0.653978
O       1.710839        0.691730        -0.475531
H       2.672022        0.475215        -0.213891
###
13
ala200 pm6_conformaciones E=-0.208885289779 au
```

```
N       -1.425243       -1.027930       -0.228508
H       -1.102922       -1.797871       -0.842279
H       -1.398214       -1.362341       0.751630
C       -0.565114       0.209786        -0.408773
H       -0.610177       0.506550        -1.500000
C       -1.091730       1.335846        0.462116
C       0.903537        -0.086871       -0.044882
H       -1.074595       1.093753        1.536191
H       -0.505399       2.258092        0.333979
H       -2.134781       1.594894        0.215491
O       1.195289        -1.130376       0.590353
O       1.772012        0.751402        -0.400505
H       -2.415779       -0.818345       -0.465006
###
13
ala201 pm6_conformaciones E=-0.208900459185 au
N       -1.414538       -1.051271       -0.146549
H       -1.078639       -1.857768       -0.702592
H       -1.386369       -1.315936       0.855249
C       -0.570639       0.183050        -0.409623
H       -0.624669       0.412166        -1.517706
C       -1.108773       1.353069        0.393651
C       0.904187        -0.079478       -0.049441
H       -1.064081       1.184582        1.480782
H       -0.548508       2.277462        0.188202
H       -2.162379       1.570633        0.152184
O       1.239448        -1.180703       0.453635
O       1.738612        0.833346        -0.283309
H       -2.406716       -0.873234       -0.400416
###
13
ala202 pm6_conformaciones E=-0.208885493908 au
N       -1.425230       -1.028139       -0.228007
H       -1.101786       -1.798843       -0.840178
H       -1.399599       -1.361168       0.752696
C       -0.565102       0.209553        -0.408675
H       -0.610199       0.506005        -1.500031
C       -1.092008       1.335867        0.461753
C       0.903539        -0.086838       -0.044867
H       -1.074966       1.094091        1.535886
H       -0.505798       2.258129        0.333286
H       -2.135044       1.594678        0.214811
O       1.771660        0.752216        -0.399762
O       1.195945        -1.130753       0.589341
H       -2.415409       -0.819116       -0.466317
###
13
ala203 pm6_conformaciones E=-0.208885338732 au
N       -1.425132       -1.028101       -0.228297
H       -1.102623       -1.798089       -0.841869
H       -1.398099       -1.362255       0.751991
C       -0.565109       0.209735        -0.408733
H       -0.610330       0.506357        -1.500057
C       -1.092043       1.335775        0.461931
C       0.903540        -0.086747       -0.044931
H       -1.075661       1.093471        1.535985
H       -0.505300       2.257850        0.334416
H       -2.134808       1.595128        0.214521
O       1.771927        0.751792        -0.400103
O       1.195579        -1.130499       0.589903
H       -2.415629       -0.818668       -0.464910
###
13
ala204 pm6_conformaciones E=-0.207146208010 au
N       1.197548        -1.222604       -0.343695
H       0.680985        -2.102465       -0.168084
H       1.194797        -1.044801       -1.366521
C       0.585481        -0.055391       0.415126
H       0.642233        -0.283544       1.524106
C       1.373530        1.205492        0.122761
C       -0.911989       0.059824        0.049579
H       1.368520        1.480303        -0.942140
H       0.978058        2.063857        0.686574
H       2.431442        1.106536        0.418586
O       -1.636941       -0.949745       0.254559
O       -1.381314       1.130285        -0.407012
```

```
H       2.185037        -1.365530       -0.051832
###
13
ala205 pm6_conformaciones E=-0.208885211343 au
N       -1.425319       -1.027920       -0.228627
H       -1.103832       -1.797368       -0.843452
H       -1.397340       -1.363295       0.751175
C       -0.565101       0.209770        -0.408721
H       -0.610187       0.506748        -1.499890
C       -1.091701       1.335805        0.462273
C       0.903514        -0.086928       -0.044868
H       -1.074705       1.093541        1.536275
H       -0.505408       2.258032        0.334053
H       -2.134743       1.594961        0.215561
O       1.771955        0.751359        -0.400739
O       1.195453        -1.130246       0.590544
H       -2.416089       -0.817964       -0.463877
###
13
ala206 pm6_conformaciones E=-0.208900489290 au
N       -1.414503       -1.051311       -0.146625
H       -1.077634       -1.858159       -0.701531
H       -1.387485       -1.315154       0.855382
C       -0.570632       0.183029        -0.409625
H       -0.624801       0.412284        -1.517666
C       -1.108877       1.353025        0.393720
C       0.904190        -0.079419       -0.049449
H       -1.065162       1.184043        1.480828
H       -0.547960       2.277182        0.189142
H       -2.162175       1.571124        0.151466
O       1.738627        0.833337        -0.283411
O       1.239502        -1.180615       0.453757
H       -2.406378       -0.873731       -0.401883
###
13
ala207 pm6_conformaciones E=-0.208885369263 au
N       -1.425215       -1.028028       -0.228296
H       -1.102538       -1.798234       -0.841532
H       -1.398591       -1.361987       0.752041
C       -0.565102       0.209699        -0.408737
H       -0.610256       0.506354        -1.500013
C       -1.091872       1.335861        0.461961
C       0.903522        -0.086840       -0.044908
H       -1.075079       1.093739        1.536024
H       -0.505423       2.258027        0.333908
H       -2.134814       1.595003        0.214959
O       1.771908        0.751734        -0.400159
O       1.195537        -1.130531       0.589927
H       -2.415650       -0.818646       -0.465345
###
12
ala300 pm6_conformaciones E=-0.350675629512 au
N       -1.434998       -1.111163       -0.339891
H       -0.901707       -1.898333       -0.714043
H       -1.638489       -1.339291       0.634839
C       -0.628562       0.134538        -0.423992
H       -0.657609       0.469736        -1.498451
C       -1.213504       1.222399        0.471046
C       0.849036        -0.051485       -0.039689
H       -1.180851       0.960015        1.537446
H       -0.687739       2.179058        0.356280
H       -2.268914       1.417987        0.233317
O       1.226572        -1.044330       0.646219
O       1.690737        0.813863        -0.423011
###
12
ala301 pm6_conformaciones E=-0.350675542706 au
N       -1.434754       -1.111175       -0.340271
H       -0.901406       -1.898092       -0.714926
H       -1.637826       -1.339780       0.634443
C       -0.628556       0.134668        -0.424036
H       -0.657561       0.470072        -1.498422
C       -1.213667       1.222306        0.471221
C       0.849035        -0.051345       -0.039643
H       -1.180279       0.960097        1.537629
H       -0.688468       2.179229        0.355975
```

```
H       -2.269309       1.417245        0.234064
O       1.226123        -1.043945       0.646942
O       1.691035        0.813405        -0.423457
###
12
ala302 pm6_conformaciones E=-0.350675555240 au
N       -1.435091       -1.111016       -0.339883
H       -0.902121       -1.898228       -0.714418
H       -1.638274       -1.339271       0.634913
C       -0.628577       0.134634        -0.424095
H       -0.657584       0.469910        -1.498498
C       -1.213284       1.222564        0.471068
C       0.849052        -0.051492       -0.039729
H       -1.180519       0.960082        1.537466
H       -0.687359       2.179111        0.356240
H       -2.268734       1.418197        0.233516
O       1.226185        -1.044452       0.646322
O       1.690950        0.813587        -0.423010
###
12
ala303 pm6_conformaciones E=-0.350675392467 au
N       -1.435036       -1.111055       -0.339804
H       -0.902278       -1.897955       -0.715297
H       -1.637215       -1.339895       0.634971
C       -0.628600       0.134584        -0.424027
H       -0.657736       0.469866        -1.498471
C       -1.213451       1.222431        0.471092
C       0.849001        -0.051461       -0.039734
H       -1.179587       0.960560        1.537551
H       -0.688429       2.179421        0.355388
H       -2.269192       1.417166        0.234261
O       1.690904        0.813659        -0.423094
O       1.226345        -1.044298       0.646373
###
12
ala304 pm6_conformaciones E=-0.350675704289 au
N       -1.435201       -1.110977       -0.340371
H       -0.901305       -1.898524       -0.712847
H       -1.640605       -1.338284       0.634151
C       -0.628491       0.134635        -0.423956
H       -0.657422       0.470139        -1.498293
C       -1.213408       1.222286        0.471233
C       0.849129        -0.051578       -0.039697
H       -1.181217       0.959557        1.537565
H       -0.687460       2.178895        0.356893
H       -2.268724       1.418207        0.233270
O       1.690921        0.813566        -0.423317
O       1.226550        -1.044217       0.646615
###
12
ala305 pm6_conformaciones E=-0.350675579936 au
N       -1.434955       -1.111108       -0.340155
H       -0.901607       -1.898214       -0.714368
H       -1.638498       -1.339390       0.634532
C       -0.628549       0.134607        -0.424017
H       -0.657593       0.470001        -1.498412
C       -1.213518       1.222340        0.471202
C       0.849031        -0.051473       -0.039670
H       -1.180619       0.959895        1.537579
H       -0.687924       2.179083        0.356369
H       -2.269003       1.417737        0.233682
O       1.690869        0.813574        -0.423346
O       1.226400        -1.044099       0.646672
###
12
ala306 pm6_conformaciones E=-0.350675473730 au
N       -1.435094       -1.111058       -0.339900
H       -0.902151       -1.898122       -0.714803
H       -1.637877       -1.339629       0.634878
C       -0.628571       0.134552        -0.424013
H       -0.657619       0.469800        -1.498447
C       -1.213416       1.222436        0.471128
C       0.849027        -0.051511       -0.039699
H       -1.179980       0.960353        1.537572
H       -0.688127       2.179272        0.355723
H       -2.269064       1.417483        0.234034
```

```
O       1.690800        0.813673        -0.423191
O       1.226479        -1.044250       0.646422
###
12
ala307 pm6_conformaciones E=-0.350675337638 au
N       -1.435031       -1.111098       -0.339855
H       -0.902332       -1.897938       -0.715567
H       -1.637075       -1.340155       0.634962
C       -0.628588       0.134558        -0.423983
H       -0.657632       0.469829        -1.498428
C       -1.213469       1.222426        0.471135
C       0.848996        -0.051461       -0.039677
H       -1.179175       0.960788        1.537656
H       -0.688805       2.179524        0.354981
H       -2.269377       1.416817        0.234656
O       1.690801        0.813652        -0.423252
O       1.226447        -1.044191       0.646485
###
# Conformations of ARGININE optimized with pm6
# opt freq pm6 scf=(xqc,tight) scrf(smd,solvent=water)
###
28
arg101 pm6_conformaciones E=0.118039470556 au
N       3.277107        -0.205888       -0.852554
H       2.982130        -0.466948       -1.813764
H       3.832518        -0.990653       -0.455220
H       3.903809        0.624406        -0.930601
C       2.088331        0.124976        0.030059
H       2.487055        0.419797        1.055642
C       1.281186        1.288548        -0.570381
C       1.195301        -1.107958       0.168822
H       1.981501        1.999826        -1.075615
H       0.621819        0.930614        -1.391093
C       0.486064        2.073908        0.470904
O       0.688534        -1.767153       -0.720655
H       1.143775        2.366593        1.321965
H       0.176481        3.045072        0.017642
C       -0.739787       1.358340        1.041072
H       -0.447005       0.420255        1.566314
H       -1.210271       1.999444        1.831420
N       -1.768074       1.127424        -0.009475
H       -1.748816       1.805222        -0.796489
C       -2.369553       -0.091828       -0.231221
N       -2.479298       -1.041409       0.766490
N       -2.970144       -0.329142       -1.464757
H       -1.757802       -1.093705       1.492353
H       -2.902574       -1.947458       0.537840
H       -3.161807       0.476135        -2.072434
H       -3.712774       -1.036939       -1.508289
O       0.987269        -1.375151       1.475693
H       0.339142        -2.146048       1.646562
###
28
arg102 pm6_conformaciones E=0.117218506640 au
N       3.128541        -1.258996       0.137970
H       2.822447        -1.298723       1.129339
H       4.112994        -0.925492       0.118454
H       3.107283        -2.227636       -0.244720
C       2.232980        -0.352689       -0.686241
H       2.673781        -0.296140       -1.741852
C       0.811915        -0.922031       -0.788020
C       2.218863        1.071870        -0.148778
H       0.278232        -0.393390       -1.611533
H       0.868148        -1.980282       -1.140451
C       0.010377        -0.837871       0.511656
O       1.490437        1.976776        -0.514595
H       0.588124        -1.270640       1.359835
H       -0.162659       0.220040        0.800618
C       -1.318779       -1.591684       0.413263
H       -1.166773       -2.608553       -0.031089
H       -1.729800       -1.779966       1.434436
N       -2.333381       -0.912876       -0.436112
H       -2.097145       -0.933684       -1.449391
C       -3.002536       0.226901        0.010754
N       -3.065647       0.568589        1.338704
N       -3.581083       1.070463        -0.922665
```

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H       -2.679156       -0.052448       2.052104
H       -3.793777       1.211058        1.663772
H       -3.636118       0.764126        -1.899292
H       -4.366122       1.662662        -0.632255
O       3.165421        1.257616        0.801452
H       3.177735        2.196699        1.196080
###
28
arg103 pm6_conformaciones E=0.122573726610 au
N       0.947511        -1.313895       0.206079
H       1.188669        -1.505525       1.200165
H       1.229926        -2.135737       -0.363306
H       -0.087617       -1.221412       0.144449
C       1.621784        -0.047562       -0.287000
H       1.290757        0.129492        -1.367219
C       1.236555        1.160370        0.581420
C       3.138400        -0.199490       -0.320972
H       1.210442        0.878390        1.660216
H       2.046899        1.925785        0.526919
C       -0.079251       1.811869        0.154879
O       3.933810        0.656768        -0.665931
H       -0.058364       2.885291        0.452765
H       -0.150989       1.849024        -0.955712
C       -1.315488       1.151691        0.777658
H       -1.032166       0.282202        1.416862
H       -1.823851       1.864379        1.473281
N       -2.268644       0.748877        -0.294062
H       -2.469005       1.472196        -1.009426
C       -3.123725       -0.320402       -0.177400
N       -3.060245       -1.211176       0.886951
N       -4.188522       -0.423977       -1.059284
H       -2.175355       -1.279498       1.408379
H       -3.516808       -2.122911       0.767131
H       -4.204439       0.168294        -1.895209
H       -4.632546       -1.338122       -1.188012
O       3.536024        -1.433809       0.061042
H       4.545424        -1.573191       0.018529
###
28
arg104 pm6_conformaciones E=0.116999073562 au
N       2.805342        0.505480        1.292074
H       3.606000        0.706553        0.662877
H       3.048565        -0.318137       1.877889
H       2.681901        1.325405        1.924204
C       1.528400        0.256373        0.510240
H       0.701051        0.056324        1.266012
C       1.187789        1.490123        -0.344570
C       1.649818        -0.979188       -0.374118
H       1.214404        2.400838        0.301022
H       1.992664        1.658771        -1.097558
C       -0.161551       1.400455        -1.055863
O       0.724864        -1.655991       -0.785640
H       -0.135012       2.089193        -1.935582
H       -0.314307       0.398493        -1.507186
C       -1.359613       1.800669        -0.191349
H       -1.124333       2.713860        0.411960
H       -2.218544       2.094977        -0.842946
N       -1.792227       0.758124        0.776035
H       -1.155932       0.652783        1.592413
C       -2.433340       -0.402308       0.346992
N       -3.026083       -0.495154       -0.893590
N       -2.421885       -1.515390       1.162290
H       -3.139232       0.347710        -1.464240
H       -3.756083       -1.201566       -1.040924
H       -2.014393       -1.453655       2.100093
H       -3.159344       -2.219060       1.061252
O       2.937524        -1.260768       -0.682554
H       3.048459        -2.086570       -1.269388
###
28
arg105 pm6_conformaciones E=0.119353815050 au
N       2.431240        0.333410        1.742959
H       3.377695        0.563149        1.382277
H       2.499726        -0.537158       2.307923
H       2.137378        1.105666        2.379329
C       1.425593        0.178515        0.617597
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H       0.415956        -0.057115       1.084151
C       1.339883        1.480434        -0.196703
C       1.844015        -0.969004       -0.298071
H       1.177351        2.338843        0.498904
H       2.321886        1.695361        -0.678191
C       0.243160        1.457658        -1.259833
O       2.952602        -1.215542       -0.734650
H       0.454722        2.273259        -1.991444
H       0.301682        0.533784        -1.875728
C       -1.169450       1.665060        -0.700331
H       -1.134970       2.046557        0.346380
H       -1.695117       2.464093        -1.283768
N       -2.011172       0.444909        -0.824795
H       -1.937861       -0.034630       -1.743250
C       -2.431027       -0.307144       0.253902
N       -2.855940       -1.614731       0.038776
N       -2.539333       0.236968        1.518180
H       -3.079516       -1.899683       -0.922325
H       -3.495493       -2.030231       0.726856
H       -1.903949       0.993399        1.792577
H       -2.816475       -0.374210       2.293220
O       0.762594        -1.715379       -0.623504
H       0.968807        -2.470736       -1.276892
###
28
arg106 pm6_conformaciones E=0.118125941860 au
N       3.473757        0.150355        -0.374956
H       3.355621        -0.070010       -1.383458
H       4.077165        -0.581677       0.050904
H       3.974939        1.062495        -0.306971
C       2.138721        0.238933        0.338694
H       2.342348        0.460395        1.437343
C       1.276956        1.358427        -0.268764
C       1.395436        -1.089442       0.221131
H       1.891601        2.283420        -0.374374
H       0.995693        1.100355        -1.314730
C       0.047590        1.659321        0.593409
O       1.340145        -1.841868       -0.732720
H       -0.155052       0.838723        1.314982
H       0.253328        2.540926        1.242648
C       -1.203317       1.951551        -0.238151
H       -1.993115       2.412403        0.402305
H       -0.982873       2.713267        -1.028313
N       -1.746890       0.760235        -0.945668
H       -1.147649       0.452594        -1.739209
C       -2.374632       -0.268072       -0.237623
N       -2.880278       -0.086391       1.024993
N       -2.449368       -1.524391       -0.813306
H       -2.885065       0.842393        1.453525
H       -3.597307       -0.727110       1.379654
H       -2.168870       -1.639336       -1.792580
H       -3.198925       -2.158866       -0.518519
O       0.733195        -1.348847       1.375168
H       0.186373        -2.207225       1.347590
###
28
arg107 pm6_conformaciones E=0.117873703517 au
N       -3.551269       -0.869653       -0.482478
H       -3.495759       -0.628759       -1.491533
H       -4.394722       -0.412648       -0.080812
H       -3.679578       -1.902266       -0.409031
C       -2.298207       -0.449650       0.261703
H       -2.431123       -0.735478       1.356764
C       -1.059996       -1.155969       -0.315061
C       -2.111172       1.061570        0.156935
H       -1.311662       -2.216347       -0.558366
H       -0.769848       -0.704601       -1.290010
C       0.105313        -1.124755       0.676896
O       -2.339722       1.781647        -0.797502
H       0.280287        -0.092642       1.048764
H       -0.156902       -1.713603       1.585321
C       1.386097        -1.704000       0.070545
H       2.051148        -2.096619       0.876625
H       1.157725        -2.592739       -0.571090
N       2.119973        -0.740132       -0.794344
H       1.581765        -0.461994       -1.640193
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C       2.915842        0.258995        -0.227123
N       3.398614        0.165906        1.057812
N       3.188651        1.396003        -0.958381
H       3.287998        -0.705581       1.582067
H       4.212637        0.726825        1.328537
H       2.891591        1.452175        -1.936722
H       4.018904        1.952783        -0.732895
O       -1.605215       1.544206        1.315385
H       -1.402011       2.542670        1.287875
###
28
arg108 pm6_conformaciones E=0.118308297147 au
N       -2.405954       1.989108        -0.288206
H       -1.990736       2.377331        0.581627
H       -3.440268       2.080573        -0.224037
H       -2.081273       2.576438        -1.086102
C       -1.994422       0.546460        -0.510671
H       -2.425401       0.211026        -1.511016
C       -0.462141       0.432178        -0.547297
C       -2.559734       -0.333829       0.602206
H       -0.067367       1.156607        -1.301738
H       -0.021796       0.747480        0.423979
C       -0.016840       -0.986664       -0.903299
O       -2.356616       -0.266519       1.798440
H       -0.192400       -1.678737       -0.051908
H       -0.642428       -1.388227       -1.734439
C       1.445582        -1.051140       -1.348706
H       1.617332        -2.010395       -1.904372
H       1.680684        -0.245548       -2.083819
N       2.420205        -1.052494       -0.226251
H       2.293336        -1.842949       0.435956
C       2.922946        0.127867        0.317262
N       2.743432        1.358051        -0.284849
N       3.707177        0.037637        1.442864
H       2.374154        1.400870        -1.240284
H       3.390547        2.118864        -0.052388
H       3.631851        -0.769559       2.064903
H       4.119363        0.878147        1.855516
O       -3.361885       -1.287226       0.065155
H       -3.763968       -1.917306       0.757484
###
28
arg109 pm6_conformaciones E=0.118395299441 au
N       -2.688788       1.902376        -0.373567
H       -3.118108       1.989353        0.568412
H       -3.449012       1.936099        -1.082080
H       -2.073956       2.730247        -0.523252
C       -1.883924       0.622490        -0.498711
H       -1.420550       0.597868        -1.539591
C       -0.775018       0.592546        0.565349
C       -2.784067       -0.602441       -0.363721
H       -0.185956       1.539144        0.501910
H       -1.215535       0.602561        1.587829
C       0.148433        -0.615230       0.394363
O       -2.671502       -1.647151       -0.977035
H       -0.404528       -1.557717       0.606863
H       0.478727        -0.709412       -0.662029
C       1.356871        -0.546699       1.333104
H       1.051608        -0.198930       2.353146
H       1.781556        -1.567955       1.490619
N       2.416853        0.389562        0.875300
H       2.143238        1.390529        0.943860
C       3.268354        0.056345        -0.177298
N       3.373608        -1.235197       -0.653976
N       4.100537        1.031585        -0.678440
H       2.988917        -2.005429       -0.099586
H       4.197825        -1.491016       -1.208619
H       3.859745        2.018854        -0.563544
H       4.717433        0.820143        -1.467335
O       -3.750586       -0.419854       0.566540
H       -4.374063       -1.218644       0.673640
###
28
arg110 pm6_conformaciones E=0.118419336323 au
N       2.576727        1.223688        -1.302283
H       2.251544        0.641136        -2.097875
```

```
H       3.595282        1.400996        -1.416778
H       2.088531        2.143224        -1.358700
C       2.277756        0.560763        0.029607
H       2.524341        1.304179        0.856722
C       0.800991        0.144844        0.121186
C       3.153930        -0.677299       0.199052
H       0.531651        -0.513775       -0.736708
H       0.663787        -0.489741       1.028443
C       -0.133477       1.355452        0.183451
O       3.581995        -1.417174       -0.666832
H       0.275280        2.125083        0.880222
H       -0.178770       1.866410        -0.803649
C       -1.539590       0.994314        0.662634
H       -1.500765       0.446819        1.636298
H       -2.122120       1.930509        0.852666
N       -2.248014       0.175075        -0.361592
H       -1.692475       -0.138800       -1.176374
C       -3.480245       -0.382764       -0.136974
N       -3.921091       -1.404065       -0.971775
N       -4.317744       0.080660        0.866562
H       -3.481633       -1.501476       -1.893598
H       -4.923459       -1.623260       -0.979877
H       -3.908233       0.543046        1.683336
H       -5.142995       -0.483263       1.099571
O       3.411029        -0.886611       1.512602
H       3.970509        -1.720167       1.690009
###
28
arg111 pm6_conformaciones E=0.116944758758 au
N       2.753590        -1.602711       -0.285179
H       3.056614        -1.710918       0.702951
H       3.599405        -1.627218       -0.889267
H       2.158905        -2.422234       -0.528417
C       1.978137        -0.313245       -0.481191
H       1.686905        -0.241365       -1.583360
C       0.715137        -0.297207       0.394507
C       2.832146        0.908340        -0.166854
H       0.956165        -0.632680       1.430031
H       0.361356        0.752554        0.518903
C       -0.401790       -1.153541       -0.205457
O       2.528265        2.066856        -0.386235
H       -0.744331       -0.724195       -1.170905
H       -0.022115       -2.166952       -0.470764
C       -1.576368       -1.330080       0.759322
H       -2.233469       -2.163148       0.412575
H       -1.213213       -1.645194       1.771261
N       -2.377591       -0.096296       0.971979
H       -1.900192       0.613209        1.563357
C       -3.225158       0.396526        -0.016536
N       -3.604329       1.729635        0.032956
N       -3.768050       -0.426230       -0.971944
H       -3.428798       2.259119        0.893536
H       -4.460853       2.013589        -0.454613
H       -3.295393       -1.290953       -1.242100
H       -4.400563       -0.039105       -1.678214
O       4.012305        0.576861        0.405763
H       4.597047        1.380221        0.631372
###
28
arg112 pm6_conformaciones E=0.116809005885 au
N       -1.965727       1.789491        -0.591822
H       -1.979203       2.224867        0.351224
H       -2.744029       2.192918        -1.151226
H       -1.071050       2.057276        -1.053872
C       -2.077337       0.278867        -0.508927
H       -1.974771       -0.138992       -1.564226
C       -0.985501       -0.309645       0.397456
C       -3.445154       -0.106883       0.046810
H       -0.961591       0.221752        1.376969
H       -1.255953       -1.361619       0.655378
C       0.395058        -0.276333       -0.259952
O       -4.147261       0.517463        0.819203
H       0.350725        -0.707178       -1.283675
H       0.741052        0.770506        -0.400338
C       1.399780        -1.053607       0.600541
H       1.443874        -0.643219       1.636672
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H       1.077250        -2.118746       0.720755
N       2.754754        -1.091083       -0.011906
H       2.789788        -1.645733       -0.891975
C       3.574095        0.041043        0.020256
N       4.502148        0.229823        -0.987406
N       3.557590        0.896764        1.092776
H       4.694243        -0.538998       -1.638275
H       5.314988        0.829087        -0.807107
H       2.734929        0.952477        1.697449
H       4.145928        1.735667        1.084009
O       -3.817260       -1.316282       -0.440366
H       -4.697014       -1.655126       -0.051046
###
28
arg113 pm6_conformaciones E=0.118488666458 au
N       -3.459683       1.568199        -0.343964
H       -3.639165       1.774401        0.658504
H       -4.362847       1.319863        -0.792826
H       -3.104356       2.439408        -0.792456
C       -2.444768       0.451052        -0.503619
H       -2.313693       0.250189        -1.621919
C       -1.102455       0.870845        0.116074
C       -2.940210       -0.845023       0.124017
H       -0.923972       1.958401        -0.065854
H       -1.140159       0.780580        1.225247
C       0.060801        0.060660        -0.462267
O       -2.291564       -1.856718       0.317759
H       -0.114998       -1.029461       -0.338005
H       0.126786        0.216611        -1.562268
C       1.366304        0.474729        0.223896
H       1.528856        1.578055        0.140268
H       1.323086        0.248979        1.317481
N       2.506010        -0.250973       -0.401818
H       2.304069        -0.826526       -1.237785
C       3.801345        -0.099543       0.015265
N       4.116398        0.503321        1.223624
N       4.828036        -0.586891       -0.791875
H       3.477106        1.202197        1.613846
H       5.102607        0.724370        1.405629
H       4.598189        -1.325573       -1.467217
H       5.747545        -0.724872       -0.358597
O       -4.255205       -0.777276       0.446837
H       -4.616339       -1.626582       0.877231
###
28
arg114 pm6_conformaciones E=0.118380151771 au
N       -2.787214       1.734105        -0.069399
H       -2.464564       1.811784        0.915324
H       -3.821432       1.631798        -0.063033
H       -2.552519       2.624332        -0.555904
C       -2.128874       0.564658        -0.776629
H       -2.536668       0.530792        -1.845679
C       -0.606513       0.751528        -0.844685
C       -2.493935       -0.766188       -0.134475
H       -0.193030       0.003461        -1.560294
H       -0.393347       1.731617        -1.336674
C       0.113569        0.686851        0.502607
O       -2.039767       -1.856981       -0.426779
H       0.833763        1.532357        0.572222
H       -0.586297       0.876985        1.348334
C       0.825908        -0.641871       0.768047
H       1.124650        -0.707916       1.842848
H       0.136613        -1.507354       0.601529
N       2.010428        -0.874404       -0.098430
H       1.790601        -1.272181       -1.031473
C       3.151416        -0.091595       -0.004774
N       3.495833        0.539895        1.171112
N       4.012148        -0.032840       -1.090660
H       2.766549        0.792023        1.843052
H       4.301400        1.175844        1.174568
H       3.924032        -0.745205       -1.824124
H       4.978929        0.271781        -0.933268
O       -3.444861       -0.622880       0.819517
H       -3.719455       -1.498815       1.261762
###
28
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arg115 pm6_conformaciones E=0.118093237808 au
N 1.578586 0.459314 1.559720
H 1.294793 1.420755 1.281426
H 2.430860 0.527891 2.150336
H 0.810212 0.058299 2.143259
C 1.818128 -0.419271 0.347802
H 2.041139 -1.475762 0.718562
C 0.588142 -0.436528 -0.574805
C 3.035128 0.042391 -0.446661
H 0.158060 0.586749 -0.673857
H 0.914579 -0.687895 -1.613507
C -0.476986 -1.447375 -0.154247
O 3.609335 -0.602350 -1.306053
H -1.116814 -1.672188 -1.037232
H -0.002613 -2.425969 0.092312
C -1.350188 -1.028907 1.031163
H -2.090829 -1.833941 1.258192
H -0.738715 -0.927645 1.965507
N -2.054294 0.269712 0.851953
H -1.443450 1.092096 1.049722
C -2.976115 0.440704 -0.184115
N -3.762456 -0.594364 -0.620635
N -3.177878 1.710580 -0.696382
H -3.482226 -1.564694 -0.471213
H -4.422340 -0.445816 -1.389865
H -2.807515 2.515470 -0.180603
H -4.044814 1.906604 -1.206960
O 3.432670 1.287882 -0.099757
H 4.247264 1.619014 -0.617018
###
28
arg116 pm6_conformaciones E=0.119061620929 au
N -2.988368 1.574509 -0.108806
H -3.115318 1.760394 0.906390
H -3.927308 1.525566 -0.551785
H -2.486597 2.387576 -0.522695
C -2.202692 0.297969 -0.340762
H -2.056500 0.164584 -1.466588
C -0.834214 0.357046 0.351259
C -2.996672 -0.909336 0.154790
H -0.946811 0.685170 1.410108
H -0.422157 -0.676684 0.408979
C 0.151118 1.269195 -0.384101
O -2.608518 -1.811164 0.872862
H 0.142642 1.056907 -1.477469
H -0.172564 2.332594 -0.304792
C 1.565390 1.158554 0.186285
H 2.132088 2.104102 -0.002746
H 1.537451 1.032408 1.296179
N 2.287205 0.013157 -0.438408
H 1.830537 -0.445634 -1.246493
C 3.556541 -0.352950 -0.079667
N 4.161281 0.128488 1.070664
N 4.247710 -1.261937 -0.879536
H 3.868513 1.031503 1.453404
H 5.160115 -0.063564 1.207223
H 3.701856 -1.865809 -1.504577
H 5.049615 -1.747864 -0.461924
O -4.249439 -0.901162 -0.363204
H -4.823517 -1.685029 -0.054691
###
28
arg117 pm6_conformaciones E=0.118426967715 au
N -1.556937 1.802349 0.507237
H -1.146496 1.381278 1.367755
H -2.414085 2.327759 0.773642
H -0.862028 2.485430 0.132401
C -1.861561 0.749426 -0.539594
H -2.311611 1.287204 -1.442258
C -0.593355 0.019861 -1.005570
C -2.895296 -0.237664 -0.012257
H -0.851534 -0.541266 -1.937658
H 0.150249 0.774806 -1.357341
C 0.040492 -0.949148 -0.009512
O -3.178767 -0.486794 1.143854
H -0.729893 -1.596797 0.464908

```
H       0.673925        -1.666514       -0.581443
C       0.878257        -0.306415       1.100057
H       0.250324        0.337869        1.767157
H       1.284070        -1.098580       1.777707
N       1.977489        0.558268        0.597866
H       1.631556        1.449571        0.181031
C       3.090814        -0.007050       -0.031854
N       3.422601        -1.334984       0.132886
N       3.927386        0.822772        -0.743271
H       2.987712        -1.872200       0.888556
H       4.370298        -1.644043       -0.108857
H       3.561780        1.688041        -1.149731
H       4.748350        0.434322        -1.215531
O       -3.507831       -0.857272       -1.052450
H       -4.199722       -1.547234       -0.762214
###
27
arg201 pm6_conformaciones E=-0.624162579969E-01 au
N       1.627981        1.346359        1.047863
H       1.596987        2.086269        0.323703
H       2.406092        1.560842        1.699091
H       0.738229        1.393285        1.586199
C       1.807268        -0.023148       0.422389
H       1.835915        -0.783190       1.260140
C       0.660823        -0.342737       -0.548933
C       3.152162        -0.080959       -0.333395
H       0.142874        0.588837        -0.873122
H       1.073922        -0.750724       -1.500877
C       -0.352248       -1.348663       -0.001684
O       3.666401        0.979148        -0.767842
H       -0.993693       -1.695241       -0.842621
H       0.168830        -2.269059       0.345561
C       -1.225245       -0.832226       1.144852
H       -1.888753       -1.650876       1.514394
H       -0.600462       -0.539858       2.026336
N       -2.043043       0.362378        0.798214
H       -1.484236       1.244204        0.789196
C       -3.033992       0.275023        -0.184466
N       -3.352835       1.404285        -0.918449
N       -3.760261       -0.872428       -0.362583
H       -3.005771       2.314915        -0.599794
H       -4.262003       1.449275        -1.390203
H       -4.480370       -0.919708       -1.088205
O       3.684600        -1.207317       -0.503524
H       -3.411066       -1.771523       -0.026764
###
27
arg202 pm6_conformaciones E=-0.625653058087E-01 au
N       2.259670        1.719276        -0.406865
H       1.893841        1.424265        -1.329984
H       3.235512        2.047671        -0.534417
H       1.686822        2.524502        -0.081757
C       2.198659        0.589766        0.598929
H       2.673219        0.962585        1.558484
C       0.750030        0.182260        0.900005
C       3.007141        -0.631353       0.115549
H       0.768079        -0.594596       1.698027
H       0.224676        1.040383        1.380231
C       -0.041327       -0.335586       -0.304022
O       3.433635        -1.421995       0.998669
H       0.635661        -0.631373       -1.135238
H       -0.556404       -1.280979       -0.026603
C       -1.057864       0.671723        -0.850829
H       -0.607528       1.692541        -0.944059
H       -1.361203       0.390759        -1.888018
N       -2.256416       0.826554        0.013872
H       -2.077571       1.346292        0.895065
C       -3.261566       -0.133730       0.050159
N       -4.257944       0.002073        0.994909
N       -3.344041       -1.148276       -0.883066
H       -4.075034       0.527288        1.854140
H       -4.982224       -0.716892       1.072047
H       -4.231919       -1.652275       -0.986203
O       3.216652        -0.810643       -1.107340
H       -2.807550       -1.074933       -1.753046
###
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27
arg203 pm6_conformaciones E=-0.621686421566E-01 au
N       2.473307        1.838651        -0.196602
H       2.821335        1.864714        -1.172909
H       3.221703        2.200892        0.424219
H       1.661918        2.486274        -0.134007
C       2.061305        0.436430        0.205484
H       1.682667        0.475525        1.269494
C       0.965082        -0.101068       -0.723591
C       3.282690        -0.511270       0.143754
H       1.217528        0.123743        -1.784959
H       0.953978        -1.215464       -0.673686
C       -0.428643       0.442897        -0.409015
O       3.935996        -0.610584       -0.924431
H       -0.389164       1.524170        -0.156487
H       -1.047307       0.391736        -1.331834
C       -1.099780       -0.344298       0.723293
H       -1.076957       -1.441393       0.520439
H       -0.541708       -0.208582       1.682895
N       -2.496248       0.100217        0.980769
H       -2.554015       1.005065        1.490182
C       -3.499012       -0.136872       0.039060
N       -4.592003       0.707510        -0.007675
N       -3.479575       -1.256390       -0.757148
H       -4.737290       1.382756        0.749495
H       -5.457259       0.378083        -0.447649
H       -4.201422       -1.380125       -1.474240
O       3.566299        -1.175811       1.171800
H       -2.600583       -1.741060       -0.949222
###
27
arg204 pm6_conformaciones E=-0.606683274157E-01 au
N       1.494315        1.568734        0.228070
H       1.401650        1.797705        -0.778775
H       2.117781        2.271954        0.663580
H       0.548627        1.654400        0.663038
C       2.036108        0.166523        0.421396
H       2.252003        0.023861        1.526294
C       1.014346        -0.877621       -0.048408
C       3.374971        0.006053        -0.325048
H       0.540315        -0.565192       -1.004732
H       1.553377        -1.816085       -0.314102
C       -0.042437       -1.203453       1.008924
O       3.937689        -1.117909       -0.299937
H       -0.385433       -2.254526       0.867114
H       0.413970        -1.202781       2.025814
C       -1.241132       -0.255336       1.024618
H       -1.774639       -0.330888       2.005727
H       -0.917539       0.812651        0.937899
N       -2.178849       -0.593410       -0.082593
H       -1.947517       -1.422612       -0.657029
C       -3.358039       0.068852        -0.294321
N       -4.280108       -0.470564       -1.191189
N       -3.647012       1.269377        0.333397
H       -3.933314       -1.129988       -1.897183
H       -5.006198       0.154325        -1.559064
H       -4.600816       1.639095        0.255363
O       3.876903        0.996672        -0.912413
H       -3.200339       1.488905        1.228102
###
27
arg205 pm6_conformaciones E=-0.628353775685E-01 au
N       -1.853815       1.950617        0.328031
H       -1.513927       1.676771        1.267076
H       -2.738991       2.478119        0.446788
H       -1.149796       2.590651        -0.091280
C       -2.061522       0.740609        -0.558214
H       -2.533393       1.102755        -1.523875
C       -0.731290       0.057603        -0.897522
C       -3.036241       -0.260383       0.094116
H       -0.926898       -0.730744       -1.659894
H       -0.070749       0.784913        -1.423747
C       -0.001376       -0.541031       0.307036
O       -3.274082       -0.196500       1.322893
H       0.377339        0.260596        0.977232
H       -0.699448       -1.131957       0.938918
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C       1.151151        -1.458195       -0.116025
H       1.507885        -2.053953       0.757836
H       0.806467        -2.215530       -0.864243
N       2.283819        -0.731639       -0.752341
H       2.022445        -0.314664       -1.671182
C       3.144668        0.050874        0.027836
N       3.749663        1.155315        -0.543342
N       3.473065        -0.314253       1.306125
H       3.698611        1.279669        -1.559963
H       4.612561        1.522687        -0.126690
H       4.119797        0.259198        1.854833
O       -3.569133       -1.118836       -0.657476
H       2.872352        -0.942968       1.842179
###
27
arg206 pm6_conformaciones E=-0.629207851590E-01 au
N       3.509111        -1.310191       -0.402798
H       3.872341        -1.313200       0.567963
H       4.262526        -0.971722       -1.029839
H       3.292182        -2.294195       -0.663044
C       2.271682        -0.441894       -0.524163
H       1.946950        -0.449225       -1.607686
C       1.153080        -1.016928       0.355549
C       2.599258        1.011257        -0.117809
H       0.995342        -2.089836       0.093671
H       1.463881        -1.030544       1.423419
C       -0.157309       -0.242965       0.193332
O       1.986367        1.936183        -0.707203
H       -0.046978       0.788359        0.588102
H       -0.410366       -0.128387       -0.882199
C       -1.292414       -0.970908       0.924814
H       -1.511764       -1.953430       0.445351
H       -0.993690       -1.214434       1.976271
N       -2.528686       -0.151068       1.022513
H       -2.471005       0.606594        1.731023
C       -3.316358       0.109782        -0.096551
N       -4.118346       1.238264        -0.104104
N       -3.388479       -0.777555       -1.141953
H       -4.255721       1.754715        0.771908
H       -4.932219       1.263230        -0.728122
H       -3.960412       -0.550629       -1.961247
O       3.453133        1.230946        0.777414
H       -2.629901       -1.440539       -1.313901
###
27
arg207 pm6_conformaciones E=-0.618926338208E-01 au
N       -1.899061       1.764626        -0.079990
H       -1.757536       1.675316        0.942563
H       -2.788415       2.272409        -0.239737
H       -1.120169       2.343130        -0.457276
C       -1.920814       0.408248        -0.751474
H       -2.187569       0.567630        -1.841905
C       -0.545273       -0.269472       -0.683516
C       -3.002378       -0.495650       -0.128565
H       -0.607881       -1.239547       -1.226594
H       0.177734        0.325369        -1.286765
C       -0.014126       -0.502245       0.732519
O       -3.380827       -1.493236       -0.796760
H       -0.845257       -0.514021       1.470159
H       0.406296        -1.530735       0.802157
C       1.031986        0.527912        1.178350
H       0.944734        1.485552        0.614693
H       0.860243        0.808080        2.249089
N       2.427018        0.006445        1.116282
H       2.571633        -0.809470       1.748534
C       3.104394        -0.074471       -0.107646
N       2.977252        0.904545        -1.057397
N       4.014339        -1.094734       -0.305194
H       2.168121        1.529561        -1.060981
H       3.472699        0.822534        -1.949630
H       4.748075        -0.985439       -1.012692
O       -3.479841       -0.218583       0.997765
H       4.283054        -1.687925       0.486426
###
27
arg208 pm6_conformaciones E=0.322612038231E-01 au
```

```
N       -3.125413       -0.649431       0.609853
H       -2.716397       -0.782170       1.550668
H       -3.291855       -1.589674       0.204477
H       -4.039154       -0.172699       0.719549
C       -2.195935       0.153858        -0.286220
H       -2.790160       0.469969        -1.193057
C       -1.726578       1.404760        0.464902
C       -1.046623       -0.769707       -0.812314
H       -2.582798       2.108023        0.566536
H       -1.447713       1.150852        1.511477
C       -0.561064       2.117752        -0.224563
O       -1.336999       -2.053635       -0.743258
H       -0.658541       2.061183        -1.328383
H       -0.612536       3.206323        0.007017
C       0.812263        1.615106        0.228293
H       1.608636        2.290466        -0.173546
H       0.895971        1.654307        1.338378
N       1.082959        0.239223        -0.316244
H       -0.683085       -0.421108       -1.798192
C       2.379889        -0.302851       0.096131
N       3.486848        0.245919        -0.461291
N       2.457993        -1.386096       0.912281
H       3.439465        1.097220        -1.026919
H       4.422143        -0.117639       -0.256827
H       3.338346        -1.887293       1.062103
O       0.113549        -0.660818       0.181185
H       1.616862        -1.812932       1.303738
###
27
arg210 pm6_conformaciones E=-0.636019438370E-01 au
N       1.859687        1.334598        1.272881
H       1.592715        2.050327        0.573422
H       2.732139        1.645286        1.739818
H       1.109850        1.294614        1.992056
C       2.045365        -0.022001       0.623867
H       2.278264        -0.767412       1.442526
C       0.781400        -0.447119       -0.135405
C       3.236469        0.008350        -0.356833
H       0.445109        0.367050        -0.815905
H       1.034912        -1.294054       -0.813764
C       -0.356326       -0.863273       0.800197
O       3.671906        1.107006        -0.779840
H       0.022253        -1.559487       1.582232
H       -0.741623       0.012488        1.363840
C       -1.495232       -1.558624       0.048759
H       -1.099098       -2.377252       -0.603717
H       -2.178138       -2.067984       0.770621
N       -2.266281       -0.649353       -0.842390
H       -1.707282       -0.308013       -1.652065
C       -3.171553       0.269823        -0.304465
N       -3.487458       1.400042        -1.026696
N       -3.719449       0.106196        0.947717
H       -3.134076       1.509773        -1.981238
H       -4.363591       1.895437        -0.835591
H       -4.590253       0.594688        1.179188
O       3.731424        -1.093134       -0.709498
H       -3.574050       -0.769758       1.455978
###
27
arg211 pm6_conformaciones E=-0.621815861250E-01 au
N       -2.785366       1.404156        0.551823
H       -2.739632       1.106510        1.543975
H       -3.783714       1.465679        0.278370
H       -2.375869       2.357208        0.487867
C       -2.036236       0.436200        -0.341803
H       -2.148841       0.790144        -1.411136
C       -0.551565       0.384384        0.044590
C       -2.649889       -0.975382       -0.239565
H       -0.442361       0.393438        1.153915
H       -0.116544       -0.587229       -0.276656
C       0.238584        1.534395        -0.583325
O       -2.385996       -1.792413       -1.158476
H       0.305177        1.400608        -1.684387
H       -0.303908       2.498477        -0.449728
C       1.634552        1.702650        0.020158
H       2.041817        2.706851        -0.269226
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H       1.592997        1.714634        1.135079
N       2.617498        0.703882        -0.470628
H       2.892813        0.803602        -1.464355
C       2.875922        -0.492087       0.163230
N       3.860923        -1.313951       -0.359462
N       2.247808        -0.861954       1.342265
H       4.107868        -1.231092       -1.350649
H       3.977247        -2.256073       0.024568
H       2.689592        -1.589108       1.916886
O       -3.379049       -1.269565       0.738707
H       1.769464        -0.143719       1.895924
###
27
arg212 pm6_conformaciones E=-0.623400302529E-01 au
N       0.957903        1.424429        0.263801
H       0.952677        1.692425        -0.739209
H       1.426710        2.176027        0.799701
H       -0.033001       1.371923        0.575845
C       1.654181        0.093116        0.467529
H       1.606023        -0.160982       1.571555
C       0.957084        -0.997592       -0.355284
C       3.144371        0.194186        0.086621
H       0.734633        -0.618646       -1.379926
H       1.662268        -1.838176       -0.534019
C       -0.308896       -1.530150       0.326506
O       3.875580        -0.804081       0.315802
H       -0.109301       -2.542044       0.744928
H       -0.574890       -0.921500       1.217373
C       -1.507455       -1.628212       -0.620191
H       -1.213976       -2.118874       -1.582178
H       -2.292124       -2.290712       -0.181963
N       -2.093915       -0.309159       -0.985801
H       -1.436641       0.275911        -1.547725
C       -2.849876       0.404468        -0.044121
N       -3.394194       -0.199023       1.068372
N       -3.035831       1.753562        -0.228079
H       -3.357042       -1.217456       1.162266
H       -4.197372       0.238248        1.532014
H       -3.827633       2.227071        0.213033
O       3.590875        1.254785        -0.415033
H       -2.646164       2.217611        -1.052259
###
27
arg214 pm6_conformaciones E=-0.611127903655E-01 au
N       -1.125718       1.424949        0.646944
H       -1.434534       1.401656        1.636097
H       -1.534877       2.267772        0.203121
H       -0.092125       1.527547        0.633830
C       -1.553395       0.168513        -0.084517
H       -1.099021       0.191071        -1.121442
C       -1.104496       -1.092886       0.663559
C       -3.088418       0.155031        -0.245410
H       -1.569815       -1.117999       1.675928
H       -1.518966       -1.981851       0.135561
C       0.408451        -1.255518       0.815779
O       -3.772586       1.030894        0.339911
H       0.833563        -0.425821       1.419565
H       0.591882        -2.157369       1.446961
C       1.169567        -1.424582       -0.503619
H       1.909664        -2.256016       -0.420090
H       0.483144        -1.733169       -1.330964
N       1.861974        -0.191191       -0.969481
H       1.212758        0.511468        -1.382198
C       2.920551        0.342088        -0.228125
N       3.204838        1.689936        -0.337344
N       3.758491        -0.470113       0.500483
H       2.764701        2.232871        -1.087715
H       4.136496        2.025699        -0.072449
H       4.517956        -0.048712       1.045265
O       -3.606017       -0.732001       -0.970410
H       3.417345        -1.359236       0.872296
###
27
arg215 pm6_conformaciones E=0.599873629250E-01 au
N       1.870809        -1.773937       0.695754
H       2.872907        -1.888583       0.481141
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H       1.420042        -2.692398       0.591240
H       1.788034        -1.494983       1.687551
C       1.272537        -0.778953       -0.178072
H       -0.751000       -0.790595       2.343842
C       2.004604        0.499350        -0.385942
C       -0.069484       -0.933265       -0.613929
H       3.062287        0.395004        -0.057416
H       2.062880        0.724373        -1.471721
C       1.388677        1.705348        0.345688
O       -0.577517       -1.981370       -1.119417
H       1.313271        1.476667        1.435298
H       2.097396        2.562812        0.303347
C       0.047400        2.193955        -0.204725
H       -0.442633       2.886590        0.529493
H       0.214112        2.802694        -1.128927
N       -0.964415       1.122501        -0.543022
H       -1.837986       1.553836        -0.941982
C       -1.205182       -0.101483       0.420128
N       -0.779159       0.125731        1.845346
N       -2.550063       -0.595003       0.424382
H       0.189827        0.533588        1.905181
H       -1.427572       0.755721        2.361778
H       -3.255388       0.102479        0.692350
O       -0.442174       0.284382        -1.570628
H       -2.820169       -1.016058       -0.466923
###
27
arg217 pm6_conformaciones E=-0.587173126139E-01 au
N       3.015903        1.658911        -0.441771
H       3.682908        1.344619        -1.171545
H       3.560214        1.997648        0.372508
H       2.484421        2.465987        -0.828877
C       2.066104        0.543036        -0.045189
H       1.350016        0.954739        0.729816
C       1.279631        0.072884        -1.274467
C       2.874733        -0.591258       0.631655
H       1.024454        0.941234        -1.926746
H       1.918522        -0.570535       -1.917401
C       0.001872        -0.679668       -0.898303
O       3.461177        -0.317991       1.711184
H       -0.339353       -1.267383       -1.782080
H       0.204636        -1.436976       -0.112706
C       -1.100053       0.281831        -0.438995
H       -0.877905       0.675927        0.582520
H       -1.158782       1.170320        -1.114959
N       -2.410377       -0.426194       -0.448826
H       -2.473999       -1.298538       -1.002949
C       -3.510399       0.030023        0.224775
N       -4.625501       -0.795553       0.324470
N       -3.549735       1.297474        0.794466
H       -4.750973       -1.530817       -0.379140
H       -5.507439       -0.376967       0.638145
H       -4.286194       1.482360        1.487254
O       2.932564        -1.730412       0.112723
H       -2.663810       1.752058        1.039675
###
26
arg301 pm6_conformaciones E=-0.204414195256 au
N       -3.465598       -0.585024       -0.420454
H       -3.034724       -0.717417       -1.340148
H       -3.878646       -1.492290       -0.181096
C       -2.416692       -0.252236       0.579399
H       -2.926216       -0.201214       1.585513
C       -1.274994       -1.282525       0.691656
C       -1.843867       1.140743        0.305702
H       -0.583783       -0.982953       1.505788
H       -1.712250       -2.241951       1.049932
C       -0.501531       -1.554772       -0.599208
O       -1.974429       1.729067        -0.802166
H       -0.085339       -2.587553       -0.555099
H       -1.191185       -1.583098       -1.473059
C       0.616390        -0.558460       -0.907439
H       0.978185        -0.708932       -1.956577
H       0.251783        0.492548        -0.863422
N       1.751478        -0.743025       0.039737
H       1.658924        -1.490831       0.749159
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C       2.881470        0.029424        0.006545
N       2.977002        1.143569        -0.818213
N       3.950849        -0.306217       0.828124
H       2.449773        1.150487        -1.697178
H       3.897529        1.591882        -0.906421
H       3.765460        -0.874065       1.662484
H       4.687892        0.393458        0.970644
O       -1.217843       1.715154        1.250315
###
26
arg303 pm6_conformaciones E=-0.204112356687 au
N       3.271402        0.584312        -1.098765
H       2.975965        0.205296        -2.002073
H       3.573017        1.544909        -1.286431
C       2.121410        0.603263        -0.148436
H       2.419338        1.216979        0.745431
C       0.826710        1.183597        -0.738338
C       1.965995        -0.858425       0.299061
H       1.085052        2.045610        -1.394848
H       0.340963        0.456908        -1.418373
C       -0.162958       1.674455        0.319630
O       1.265085        -1.677835       -0.356190
H       0.321954        2.443100        0.963064
H       -0.987251       2.220669        -0.187119
C       -0.738045       0.588984        1.232840
H       0.065609        0.123668        1.853234
H       -1.437252       1.047616        1.974840
N       -1.416827       -0.527542       0.519780
H       -0.748572       -1.146105       0.012148
C       -2.639257       -0.312746       -0.130857
N       -3.107614       -1.289488       -0.973657
N       -3.417568       0.796424        0.124503
H       -2.473340       -1.983062       -1.374129
H       -3.999548       -1.172539       -1.462129
H       -3.211062       1.381198        0.940081
H       -4.411117       0.774507        -0.132097
O       2.602085        -1.244598       1.326437
###
26
arg305 pm6_conformaciones E=-0.204660754868 au
N       2.766356        -1.442696       -0.771869
H       2.588125        -1.922098       0.115571
H       2.443166        -2.087505       -1.500005
C       1.965370        -0.190049       -0.843569
H       2.078064        0.214289        -1.889919
C       0.457966        -0.340280       -0.575446
C       2.599654        0.821245        0.120113
H       -0.036804       0.642711        -0.721691
H       0.028551        -0.996696       -1.365397
C       0.117528        -0.898654       0.806790
O       2.805657        0.557531        1.335007
H       0.782216        -1.757851       1.051267
H       0.322015        -0.141362       1.591234
C       -1.329242       -1.388760       0.911458
H       -1.581363       -2.082632       0.076750
H       -1.450286       -1.997337       1.845156
N       -2.325817       -0.289318       1.014465
H       -2.182387       0.319737        1.845321
C       -2.859253       0.331559        -0.111848
N       -2.978150       -0.330418       -1.308000
N       -3.377599       1.612278        0.012103
H       -2.359354       -1.112316       -1.534868
H       -3.396984       0.143436        -2.113570
H       -3.523952       1.993460        0.953424
H       -4.088081       1.920650        -0.661717
O       2.953268        1.942997        -0.355437
###
26
arg306 pm6_conformaciones E=-0.207163991957 au
N       2.827704        0.043540        1.404040
H       3.606203        0.448393        0.878485
H       2.720544        0.638029        2.232367
C       1.578898        0.106167        0.595824
H       0.722617        -0.114342       1.290931
C       1.345270        1.462629        -0.092952
C       1.652628        -1.007017       -0.458368
```

```
H       1.344361        2.263753        0.678068
H       2.210664        1.707951        -0.744264
C       0.059045        1.530410        -0.919224
O       2.609579        -1.073247       -1.280936
H       0.177286        2.323432        -1.695108
H       -0.093773       0.600739        -1.502060
C       -1.192957       1.867713        -0.105633
H       -1.004244       2.747009        0.560647
H       -2.020392       2.185450        -0.784694
N       -1.650009       0.765383        0.782159
H       -1.006460       0.589427        1.581773
C       -2.317268       -0.347926       0.278973
N       -2.925091       -0.344394       -0.951150
N       -2.303556       -1.524021       1.015939
H       -2.984365       0.522003        -1.494219
H       -3.658729       -1.032982       -1.154360
H       -1.941247       -1.500842       1.975507
H       -3.069479       -2.194052       0.880854
O       0.715420        -1.856675       -0.500636
###
26
arg307 pm6_conformaciones E=-0.203925878848 au
N       1.803951        -0.101193       1.735118
H       2.431158        0.673620        1.965760
H       0.930888        0.093976        2.238763
C       1.525021        -0.110598       0.273565
H       0.638478        -0.775971       0.095163
C       1.264549        1.268513        -0.357285
C       2.747163        -0.746006       -0.407980
H       2.134749        1.934804        -0.175223
H       1.210044        1.166557        -1.462611
C       0.001795        1.959228        0.161468
O       2.597763        -1.853815       -1.002374
H       -0.023210       1.947040        1.273106
H       0.062036        3.042428        -0.095296
C       -1.300211       1.410445        -0.425398
H       -2.053823       2.231285        -0.522796
H       -1.135355       1.020261        -1.458054
N       -1.874694       0.356257        0.461821
H       -1.262943       0.023744        1.230576
C       -2.903436       -0.463829       0.045914
N       -3.619433       -0.215386       -1.107409
N       -3.148300       -1.638747       0.741975
H       -3.532698       0.686947        -1.579814
H       -4.529973       -0.669557       -1.229414
H       -2.702264       -1.772493       1.654837
H       -4.075267       -2.069787       0.668232
O       3.873265        -0.176922       -0.393309
###
26
arg308 pm6_conformaciones E=-0.205056770312 au
N       -3.275440       0.909280        0.109915
H       -2.943159       1.146219        1.048484
H       -3.488780       1.804684        -0.339793
C       -2.192898       0.229169        -0.649660
H       -2.585014       0.040273        -1.691883
C       -0.895873       1.050525        -0.771804
C       -1.897936       -1.149122       -0.047767
H       -0.233282       0.565101        -1.518033
H       -1.130009       2.042685        -1.212798
C       -0.169627       1.231581        0.562795
O       -0.940115       -1.826263       -0.531869
H       -0.756619       1.902814        1.229219
H       -0.110049       0.272581        1.115907
C       1.228341        1.832449        0.396289
H       1.170046        2.825977        -0.114416
H       1.680342        2.035753        1.397036
N       2.156387        0.999459        -0.416770
H       2.006312        1.103477        -1.441667
C       2.570170        -0.259281       0.009945
N       3.009139        -1.174263       -0.933240
N       2.500278        -0.650893       1.325726
H       3.152086        -0.858519       -1.899170
H       3.668865        -1.903569       -0.640609
H       2.214930        0.016487        2.046355
H       3.101188        -1.413317       1.655027
```

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O       -2.601442       -1.645943       0.877887
###
26
arg309 pm6_conformaciones E=-0.204378939137 au
N       1.289292        1.470712        -0.264434
H       1.066507        1.336808        -1.254509
H       0.390096        1.657641        0.199013
C       1.873089        0.220859        0.303154
H       1.964993        0.357507        1.417450
C       1.055774        -1.052867       0.028562
C       3.298577        0.134409        -0.263243
H       0.586209        -1.005661       -0.975125
H       1.735948        -1.930624       -0.020304
C       -0.003045       -1.327040       1.099545
O       4.187988        0.880574        0.248787
H       -0.385869       -2.365369       0.972622
H       0.467634        -1.328433       2.108693
C       -1.167020       -0.335659       1.121229
H       -1.720259       -0.418202       2.090142
H       -0.803857       0.721013        1.068928
N       -2.096727       -0.610566       -0.009510
H       -1.898556       -1.444433       -0.588212
C       -3.215721       0.138096        -0.257287
N       -3.445142       1.345959        0.382498
N       -4.135857       -0.322451       -1.197341
H       -3.024195       1.512890        1.301216
H       -4.369233       1.780183        0.278756
H       -3.804783       -0.978304       -1.913491
H       -4.822296       0.348195        -1.560899
O       3.597858        -0.642521       -1.210603
###
26
arg310 pm6_conformaciones E=-0.206428027753 au
N       2.646304        -1.289151       1.270527
H       1.777127        -1.145850       1.791395
H       2.729439        -2.302752       1.147886
C       2.550539        -0.644053       -0.065123
H       3.440573        -0.989995       -0.665106
C       1.282351        -0.981601       -0.872263
C       2.663910        0.876571        0.090897
H       1.344890        -0.511258       -1.875882
H       1.272359        -2.074863       -1.076246
C       -0.018588       -0.570044       -0.179025
O       2.200360        1.495515        1.089207
H       -0.078063       -1.036871       0.828052
H       -0.040950       0.524357        -0.002046
C       -1.231064       -0.982403       -1.023277
H       -1.319112       -0.350057       -1.935801
H       -1.118235       -2.031539       -1.398139
N       -2.497547       -0.963192       -0.241050
H       -2.518379       -1.697737       0.496228
C       -3.106461       0.247380        0.110356
N       -3.044369       1.339157        -0.712172
N       -3.870681       0.302284        1.263008
H       -2.314231       1.425237        -1.420646
H       -3.526160       2.205794        -0.458893
H       -4.092417       -0.571590       1.753418
H       -4.604300       1.014753        1.339753
O       3.245562        1.522432        -0.833652
###
26
arg311 pm6_conformaciones E=-0.207347370412 au
N       -2.093030       1.733698        -0.610994
H       -2.086734       2.150297        0.323607
H       -1.212340       2.027507        -1.046466
C       -2.108211       0.249216        -0.504487
H       -1.927719       -0.166120       -1.534339
C       -1.072740       -0.349146       0.464268
C       -3.519175       -0.163377       -0.061427
H       -1.099414       0.179747        1.438952
H       -1.339477       -1.401494       0.700533
C       0.336095        -0.291998       -0.131809
O       -4.017267       0.240605        1.025566
H       0.356669        -0.821308       -1.108363
H       0.619447        0.756908        -0.361339
C       1.359944        -0.912608       0.826475
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H       1.442438        -0.320031       1.765740
H       1.038878        -1.935407       1.146578
N       2.695213        -1.078284       0.187454
H       2.683136        -1.783583       -0.578155
C       3.507336        0.039183        -0.045250
N       3.560423        1.069596        0.854785
N       4.341092        0.050756        -1.148706
H       2.811113        1.209202        1.535366
H       4.146848        1.887964        0.667547
H       4.468962        -0.816338       -1.682657
H       5.168776        0.656724        -1.141561
O       -4.184728       -0.925861       -0.824294
###
26
arg312 pm6_conformaciones E=-0.206519535856 au
N       1.446553        1.166583        -0.931529
H       1.455301        0.621099        -1.797930
H       0.483416        1.507865        -0.833957
C       1.775383        0.289341        0.225016
H       1.453370        0.814523        1.166281
C       1.137737        -1.109619       0.201680
C       3.307622        0.188046        0.236552
H       1.317403        -1.604014       -0.774878
H       1.650762        -1.754968       0.947231
C       -0.358924       -1.075022       0.522208
O       3.952775        0.913214        1.052511
H       -0.623281       -1.964105       1.135319
H       -0.597995       -0.205936       1.171525
C       -1.229724       -1.050973       -0.740183
H       -0.924259       -0.244622       -1.443978
H       -1.113636       -2.001851       -1.317219
N       -2.679502       -0.934584       -0.410406
H       -3.028540       -1.761398       0.118021
C       -3.184395       0.299240        0.034398
N       -2.737334       1.476020        -0.500513
N       -4.218521       0.314579        0.951359
H       -1.850972       1.526107        -1.008336
H       -3.108639       2.369039        -0.165026
H       -4.717341       -0.558297       1.154580
H       -4.805926       1.152165        1.027863
O       3.927947        -0.575698       -0.554998
###
26
arg313 pm6_conformaciones E=-0.203314495790 au
N       2.877978        -0.362697       1.582141
H       2.269117        -0.001412       2.320233
H       3.216678        -1.269391       1.917664
C       2.100273        -0.559477       0.325190
H       2.728508        -1.172053       -0.378288
C       0.748021        -1.263958       0.517544
C       1.939140        0.846972        -0.267713
H       0.900542        -2.152119       1.170117
H       0.048413        -0.618932       1.083951
C       0.124109        -1.725146       -0.801936
O       1.033415        1.627538        0.126484
H       0.913930        -1.922997       -1.560573
H       -0.356344       -2.718281       -0.654835
C       -0.887266       -0.747950       -1.406065
H       -0.455781       0.271817        -1.507817
H       -1.136378       -1.063229       -2.452163
N       -2.176482       -0.739573       -0.656562
H       -2.475893       -1.687417       -0.345762
C       -2.525576       0.316691        0.179592
N       -2.185663       1.612185        -0.142485
N       -3.320750       0.077895        1.285425
H       -1.378249       1.793806        -0.741510
H       -2.427712       2.370958        0.503020
H       -3.797583       -0.828400       1.365911
H       -3.860221       0.854762        1.685126
O       2.773234        1.225640        -1.147033
###
26
arg314 pm6_conformaciones E=-0.204804760935 au
N       3.071621        -0.903085       1.121778
H       2.244512        -1.277671       1.597082
H       3.645936        -1.719069       0.888176
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C       2.666137        -0.215323       -0.131962
H       3.609075        0.012676        -0.706710
C       1.744637        -1.030482       -1.060069
C       2.008645        1.123163        0.222610
H       1.572267        -0.466688       -2.001084
H       2.297752        -1.939803       -1.384686
C       0.415604        -1.457561       -0.433821
O       1.232211        1.260257        1.210162
H       0.164005        -2.487782       -0.769026
H       0.514661        -1.556792       0.669689
C       -0.725862       -0.504191       -0.803735
H       -0.406004       0.562927        -0.753877
H       -1.049085       -0.674599       -1.859500
N       -1.872511       -0.731704       0.119928
H       -1.758419       -1.456334       0.851288
C       -3.013205       0.029198        0.100632
N       -3.325095       0.855841        -0.966254
N       -3.887469       -0.054661       1.176901
H       -2.574858       1.188874        -1.577404
H       -4.074779       1.546465        -0.838932
H       -3.841541       -0.883802       1.779772
H       -4.839076       0.309814        1.060109
O       2.269538        2.115771        -0.520573
###
26
arg315 pm6_conformaciones E=-0.206381283238 au
N       2.052332        0.616641        1.804012
H       1.789903        1.571109        1.545844
H       1.306471        0.291137        2.428090
C       2.081305        -0.245939       0.592750
H       2.283695        -1.298235       0.936568
C       0.794039        -0.237982       -0.253548
C       3.250819        0.198265        -0.295196
H       0.457525        0.801959        -0.438925
H       1.004626        -0.653897       -1.262201
C       -0.320314       -1.045953       0.417585
O       4.026697        -0.697925       -0.744898
H       0.091679        -1.984499       0.852279
H       -0.731995       -0.490930       1.286053
C       -1.437377       -1.428685       -0.556745
H       -1.014998       -1.898255       -1.480753
H       -2.090629       -2.212706       -0.105922
N       -2.256721       -0.273955       -1.013071
H       -1.751428       0.359635        -1.663723
C       -3.171621       0.335660        -0.155055
N       -3.797500       -0.368838       0.841834
N       -3.528281       1.654366        -0.385576
H       -3.367148       -1.207002       1.238259
H       -4.478524       0.099976        1.446986
H       -3.274617       2.083888        -1.282339
H       -4.414498       2.001472        -0.001545
O       3.438306        1.408757        -0.596080
###
26
arg316 pm6_conformaciones E=-0.206657964907 au
N       -2.665451       -0.926061       1.621331
H       -2.148370       -1.802758       1.516064
H       -2.524850       -0.643555       2.596455
C       -2.091191       0.113001        0.722956
H       -2.550441       1.099857        1.005190
C       -0.558892       0.237687        0.790654
C       -2.531683       -0.239237       -0.704445
H       -0.245950       0.324551        1.855929
H       -0.080222       -0.695558       0.434717
C       -0.053325       1.446472        0.002099
O       -2.132101       -1.295969       -1.270213
H       -0.250063       1.321339        -1.082825
H       -0.629963       2.354556        0.291456
C       1.430825        1.737760        0.241499
H       1.658860        2.791172        -0.069510
H       1.680255        1.694440        1.327078
N       2.344858        0.879302        -0.557010
H       2.253452        1.014589        -1.584022
C       2.754922        -0.376776       -0.132270
N       2.825418        -0.701247       1.200661
N       3.209225        -1.283997       -1.081355
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H       2.230917        -0.223827       1.881012
H       3.136689        -1.637115       1.477627
H       3.440362        -0.931129       -2.017649
H       3.833176        -2.038970       -0.774933
O       -3.306164       0.556342        -1.312905
###
26
arg317 pm6_conformaciones E=-0.204934631692 au
N       1.112848        -1.492040       -1.111303
H       0.340018        -1.527233       -0.440994
H       0.665657        -1.420961       -2.031881
C       1.928091        -0.270436       -0.874436
H       2.722462        -0.242027       -1.675020
C       1.128993        1.044717        -0.943810
C       2.648323        -0.366616       0.473855
H       1.828906        1.900021        -1.033855
H       0.566201        1.061883        -1.903536
C       0.186595        1.266549        0.244781
O       2.367655        -1.254977       1.326706
H       0.105057        0.355518        0.873652
H       0.613796        2.036598        0.923304
C       -1.211050       1.724884        -0.179694
H       -1.731168       2.229355        0.668501
H       -1.148998       2.501276        -0.983046
N       -2.046915       0.619771        -0.727807
H       -1.620157       0.179858        -1.570867
C       -2.690554       -0.270986       0.140244
N       -2.963084       0.052649        1.447206
N       -3.033334       -1.524966       -0.320453
H       -2.775060       0.997604        1.792693
H       -3.701589       -0.451402       1.949012
H       -2.882962       -1.759701       -1.306255
H       -3.810419       -2.026514       0.121416
O       3.557254        0.481121        0.728011
###
25
arg400 pm6_conformaciones E=-0.331490048955 au
N       -1.059522       -0.007736       1.949322
H       -0.094712       0.339082        1.984712
H       -1.598275       0.654598        2.517045
C       -1.561445       0.044303        0.544214
H       -2.615581       -0.352507       0.579227
C       -1.651314       1.476060        -0.016745
C       -0.769092       -0.935804       -0.382175
H       -2.490360       1.519380        -0.743111
H       -1.968453       2.156056        0.803861
C       -0.406323       2.049679        -0.693531
O       -1.472144       -2.230755       -0.082543
H       -0.275281       1.597819        -1.695694
H       -0.587966       3.126850        -0.901370
C       0.887780        1.914133        0.113203
H       1.438434        2.884421        0.095789
H       0.681443        1.719452        1.189917
N       1.793242        0.880080        -0.478349
H       2.771497        1.225922        -0.486598
C       1.667185        -0.468907       -0.008641
N       2.881719        -1.024730       0.494144
N       0.622771        -1.258395       -0.039048
H       3.744448        -0.643955       0.091953
H       2.931336        -2.043708       0.513113
H       -1.150340       -2.942776       -0.664456
O       -0.959656       -0.749489       -1.680559
###
25
arg401 pm6_conformaciones E=-0.340131963027 au
N       1.516784        1.618551        0.121580
H       1.336655        1.712090        -0.881766
H       0.621706        1.807175        0.581822
C       1.942869        0.224125        0.435402
H       1.965376        0.107907        1.555216
C       1.023013        -0.856295       -0.156886
C       3.392044        0.109418        -0.056286
H       0.774847        -0.607276       -1.208273
H       1.559409        -1.824594       -0.215676
C       -0.252039       -1.028308       0.678917
O       4.296903        0.696992        0.611825
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H       -0.080259       -1.799937       1.458303
H       -0.477380       -0.103799       1.248608
C       -1.472013       -1.434945       -0.160227
H       -1.164330       -2.069769       -1.022372
H       -2.144817       -2.078817       0.449348
N       -2.184842       -0.231665       -0.684240
H       -2.268460       -0.241229       -1.712971
C       -3.334536       0.242038        0.000999
N       -4.189436       1.076900        -0.790026
N       -3.582890       -0.080258       1.252402
H       -3.779246       1.487395        -1.631762
H       -4.685109       1.800154        -0.262066
H       -4.372916       0.394972        1.697524
O       3.703244        -0.547638       -1.087508
###
25
arg402 pm6_conformaciones E=-0.341261126920 au
N       3.291991        0.072891        -1.249787
H       2.769510        -0.240981       -2.071320
H       3.795356        0.914710        -1.544709
C       2.354240        0.420083        -0.145406
H       2.938553        0.962051        0.647204
C       1.165440        1.297246        -0.570119
C       1.880970        -0.923818       0.429077
H       1.548422        2.200022        -1.091263
H       0.562172        0.772449        -1.338468
C       0.298759        1.720318        0.622969
O       2.408033        -1.336917       1.505063
H       0.616029        1.206079        1.552889
H       0.468139        2.797483        0.842119
C       -1.202109       1.513003        0.395730
H       -1.774918       1.982571        1.227418
H       -1.526235       2.028384        -0.535615
N       -1.535943       0.052223        0.369008
H       -0.771797       -0.497946       -0.065962
C       -2.833996       -0.296131       -0.118787
N       -2.964757       -1.673170       -0.490099
N       -3.837073       0.546063        -0.021196
H       -2.140338       -2.117447       -0.895955
H       -3.785639       -1.883977       -1.064397
H       -4.757557       0.199208        -0.306001
O       1.016837        -1.624689       -0.166589
###
25
arg403 pm6_conformaciones E=-0.347905403257 au
N       2.142478        -0.679039       1.625839
H       1.149157        -0.540530       1.846810
H       2.337347        -1.658079       1.860435
C       2.363732        -0.477019       0.168733
H       3.452199        -0.700791       -0.026736
C       1.530456        -1.386401       -0.754904
C       2.122999        0.993183        -0.184248
H       2.018368        -1.424231       -1.753057
H       1.595441        -2.431560       -0.380053
C       0.064546        -0.993394       -0.943230
O       2.802497        1.502465        -1.124577
H       -0.027225       0.065766        -1.250768
H       -0.344233       -1.566298       -1.806045
C       -0.791371       -1.270211       0.299698
H       -0.705775       -2.342990       0.596482
H       -0.431090       -0.687618       1.177765
N       -2.239256       -1.011134       0.074008
H       -2.597181       -1.550031       -0.735453
C       -2.711026       0.334238        0.116336
N       -4.056216       0.477127        -0.339948
N       -2.035674       1.285665        0.728222
H       -4.365241       -0.151803       -1.083139
H       -4.349554       1.435524        -0.540328
H       -2.510477       2.189440        0.819029
O       1.275369        1.704096        0.430064
###
25
arg404 pm6_conformaciones E=-0.349252171576 au
N       -3.506045       -0.442401       -0.033379
H       -3.549505       -0.453214       0.988668
H       -4.208622       0.243282        -0.329140
```

```
C       -2.162415       0.013339        -0.483743
H       -2.193868       0.091029        -1.605538
C       -1.723810       1.372987        0.091964
C       -1.150965       -1.068731       -0.098043
H       -2.459663       2.143627        -0.224236
H       -1.790291       1.369929        1.198916
C       -0.323703       1.787400        -0.369876
O       -1.052151       -1.496224       1.084688
H       -0.072938       1.297888        -1.333031
H       -0.321316       2.871243        -0.613541
C       0.753954        1.505010        0.689556
H       0.878986        2.398582        1.346886
H       0.441891        0.689876        1.375619
N       2.094397        1.230444        0.089363
H       2.215155        1.770970        -0.788731
C       2.473594        -0.144107       -0.081012
N       2.328534        -0.992575       1.055826
N       2.916378        -0.540782       -1.249697
H       2.181486        -0.531285       1.955765
H       3.051731        -1.713252       1.142228
H       3.356050        -1.463775       -1.304925
O       -0.393084       -1.540412       -1.001790
###
25
arg405 pm6_conformaciones E=-0.348042624984 au
N       3.662232        -0.751882       0.358418
H       3.559963        -0.693212       1.375219
H       3.933168        -1.721116       0.164218
C       2.358579        -0.465010       -0.306042
H       2.473109        -0.682784       -1.404060
C       1.185713        -1.293680       0.238237
C       2.136386        1.046145        -0.147530
H       1.448253        -2.372519       0.205026
H       1.034220        -1.081245       1.316179
C       -0.102107       -1.048010       -0.551631
O       2.724374        1.826294        -0.955099
H       -0.235544       0.033049        -0.754728
H       -0.032008       -1.511534       -1.556472
C       -1.318886       -1.600354       0.204692
H       -1.404868       -2.701169       0.048190
H       -1.202541       -1.463831       1.302321
N       -2.610351       -1.004598       -0.233031
H       -2.807113       -1.211462       -1.228369
C       -2.895724       0.346251        0.131573
N       -4.070976       0.860698        -0.492931
N       -2.248031       0.956404        1.102863
H       -4.308747       0.497503        -1.417291
H       -4.178831       1.875739        -0.464201
H       -2.608342       1.873530        1.383844
O       1.402550        1.526536        0.763486
###
25
arg407 pm6_conformaciones E=-0.343140899046 au
N       -0.821225       -1.736225       0.344748
H       -0.341606       -1.530198       -0.535295
H       -0.080019       -1.954408       1.016494
C       -1.557275       -0.527058       0.804838
H       -2.012428       -0.775344       1.806283
C       -0.665014       0.716830        0.977570
C       -2.719118       -0.215094       -0.144624
H       -1.212020       1.488135        1.556966
H       0.189607        0.449993        1.635086
C       -0.168313       1.313948        -0.343045
O       -3.545103       0.683075        0.202968
H       -0.296021       0.596445        -1.180268
H       -0.810706       2.174709        -0.624168
C       1.290419        1.788159        -0.278979
H       1.398215        2.741578        -0.851670
H       1.588119        2.042335        0.763006
N       2.269294        0.839669        -0.883494
H       2.013751        0.647192        -1.870493
C       2.604423        -0.363237       -0.180289
N       2.728621        -0.288771       1.234729
N       2.805952        -1.451625       -0.891180
H       2.773204        0.643654        1.648209
H       3.452707        -0.891248       1.634085
```

```
H       3.211488        -2.256460       -0.406651
O       -2.887834       -0.832950       -1.232721
###
25
arg408 pm6_conformaciones E=-0.344623447097 au
N       1.656586        1.648771        -0.643384
H       2.029118        1.569837        -1.592890
H       0.669328        1.898936        -0.758827
C       1.749907        0.338239        0.053467
H       1.237844        0.447985        1.048747
C       1.134489        -0.856129       -0.700054
C       3.233959        0.033310        0.300280
H       1.586021        -0.943336       -1.710514
H       1.404336        -1.801859       -0.182887
C       -0.385319       -0.759437       -0.840061
O       3.606069        -0.269139       1.471285
H       -0.679617       0.227347        -1.251049
H       -0.723161       -1.495148       -1.602178
C       -1.111857       -1.017999       0.487857
H       -0.837682       -2.019612       0.894667
H       -0.801832       -0.281197       1.259542
N       -2.594629       -1.014163       0.332768
H       -2.885027       -1.671118       -0.415622
C       -3.246209       0.257729        0.241664
N       -4.536746       0.199246        -0.371750
N       -2.776757       1.309537        0.873680
H       -4.658891       -0.479132       -1.125413
H       -4.934019       1.102148        -0.638060
H       -3.353158       2.155620        0.846998
O       4.076149        0.058079        -0.642614
###
25
arg409 pm6_conformaciones E=-0.338214307899 au
N       -1.702319       0.196218        1.608069
H       -1.893554       -0.770672       1.885955
H       -0.737888       0.378347        1.913429
C       -1.767566       0.320883        0.125410
H       -1.340056       1.321554        -0.156631
C       -1.029386       -0.779163       -0.657640
C       -3.259515       0.306261        -0.242174
H       -1.239837       -1.775276       -0.216905
H       -1.437769       -0.834409       -1.690198
C       0.482317        -0.548175       -0.741618
O       -3.946160       -0.748516       -0.130877
H       0.886004        -1.133659       -1.593964
H       0.700887        0.509064        -0.994101
C       1.199741        -0.946734       0.553736
H       0.901097        -0.268814       1.385397
H       0.892923        -1.969676       0.872967
N       2.686746        -0.990015       0.356354
H       3.125642        -1.379154       1.215178
C       3.282010        0.314021        0.060204
N       3.848294        0.370740        -1.232638
N       3.214038        1.306112        0.907085
H       4.024063        -0.510484       -1.709621
H       4.614401        1.031997        -1.366055
H       3.669955        2.186531        0.652154
O       -3.796189       1.377357        -0.651273
###
25
arg410 pm6_conformaciones E=-0.340375052552 au
N       2.434686        -0.832481       1.606815
H       2.646152        -0.032460       2.208823
H       1.641735        -1.309023       2.047346
C       2.030117        -0.358596       0.253117
H       1.580150        -1.227529       -0.300898
C       1.030747        0.808910        0.243816
C       3.338922        0.029409        -0.449376
H       1.357321        1.594660        0.955941
H       1.039443        1.303889        -0.750435
C       -0.391646       0.363768        0.595045
O       3.881270        -0.825450       -1.213382
H       -0.376806       -0.379432       1.417305
H       -0.957272       1.225017        1.002332
C       -1.120722       -0.208702       -0.629497
H       -1.225394       0.567777        -1.418852
```

```
H       -0.519234       -1.028303       -1.087993
N       -2.438933       -0.788545       -0.237908
H       -2.631297       -1.672157       -0.738982
C       -3.569565       0.071243        -0.143406
N       -4.798191       -0.632240       0.089731
N       -3.455369       1.379458        -0.083621
H       -4.870466       -1.564672       -0.321482
H       -5.640576       -0.094364       -0.126885
H       -4.316254       1.906872        0.084147
O       3.889983        1.149222        -0.263329
###
25
arg411 pm6_conformaciones E=-0.341955222530 au
N       2.733433        -1.275737       1.209080
H       1.919065        -1.104466       1.804585
H       2.792390        -2.293713       1.110590
C       2.517388        -0.669125       -0.131040
H       3.352857        -1.030059       -0.796741
C       1.185065        -1.035467       -0.812240
C       2.639412        0.854749        -0.023394
H       1.163403        -0.609246       -1.836825
H       1.158783        -2.136092       -0.968766
C       -0.053075       -0.589792       -0.030277
O       3.160029        1.475492        -1.000246
H       -0.010208       -0.978669       1.007941
H       -0.074021       0.516648        0.067123
C       -1.332950       -1.081116       -0.723278
H       -1.471065       -0.571465       -1.702055
H       -1.242933       -2.167139       -0.965936
N       -2.513901       -0.916550       0.177475
H       -3.115390       -1.757692       0.155562
C       -3.265180       0.296641        0.128364
N       -2.561659       1.503362        -0.155094
N       -4.561059       0.225221        0.345289
H       -1.543341       1.477002        -0.048959
H       -2.938480       2.331460        0.314884
H       -5.062513       1.107982        0.470023
O       2.246196        1.500262        0.988061
###
25
arg412 pm6_conformaciones E=-0.345840158125 au
N       -2.194993       1.715288        1.033314
H       -1.440557       1.348867        1.617991
H       -1.887951       2.648107        0.741152
C       -2.366110       0.861978        -0.171285
H       -3.121550       1.375160        -0.833167
C       -1.090530       0.629985        -1.004687
C       -2.954705       -0.497511       0.220401
H       -1.341083       0.014436        -1.894281
H       -0.757243       1.602168        -1.426902
C       0.054594        -0.013326       -0.219355
O       -2.739506       -1.048352       1.335939
H       0.455239        0.700622        0.528973
H       -0.307667       -0.879202       0.370079
C       1.172944        -0.468905       -1.168467
H       0.815735        -1.302674       -1.817870
H       1.461766        0.349020        -1.863057
N       2.371623        -0.978011       -0.445763
H       2.117222        -1.736893       0.211787
C       3.275620        -0.020066       0.109658
N       4.145755        -0.558698       1.106106
N       3.418607        1.172412        -0.426000
H       3.774440        -1.303009       1.697338
H       4.647719        0.131332        1.668109
H       4.158703        1.763247        -0.036322
O       -3.674569       -1.091779       -0.640316
###
25
arg414 pm6_conformaciones E=-0.346343819248 au
N       1.405591        1.367567        -0.868148
H       1.579940        1.092453        -1.838136
H       0.415388        1.627317        -0.828384
C       1.645122        0.213341        0.042604
H       1.208550        0.466357        1.049340
C       1.057801        -1.129675       -0.420672
C       3.170940        0.129136        0.191177
```

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H       1.487242        -1.417153       -1.402824
H       1.374301        -1.929442       0.281695
C       -0.468026       -1.109003       -0.532266
O       3.878936        -0.538698       -0.613752
H       -0.791500       -0.315611       -1.236198
H       -0.808658       -2.058838       -0.997408
C       -1.149278       -0.925023       0.830418
H       -0.906244       -1.779007       1.505872
H       -0.763706       -0.018768       1.351869
N       -2.636012       -0.861159       0.739730
H       -3.013537       -1.757016       0.379281
C       -3.219839       0.267130        0.071082
N       -2.583046       1.528187        0.226389
N       -4.312926       0.064733        -0.632423
H       -1.893708       1.613634        0.974725
H       -3.213194       2.332985        0.221834
H       -4.806925       0.892160        -0.976496
O       3.720625        0.773722        1.133993
###
25
arg415 pm6_conformaciones E=-0.342524677257 au
N       2.699954        -0.916249       1.641457
H       1.987896        -0.325928       2.080061
H       2.467961        -1.875436       1.917799
C       2.605896        -0.801349       0.161616
H       3.329903        -1.546806       -0.274578
C       1.211688        -1.101095       -0.421835
C       3.061056        0.597736        -0.268687
H       1.280892        -1.191183       -1.525464
H       0.896663        -2.111746       -0.081586
C       0.153663        -0.061385       -0.042519
O       3.659644        0.708660        -1.381217
H       0.186174        0.144609        1.049075
H       0.379342        0.906699        -0.533740
C       -1.246574       -0.545213       -0.437878
H       -1.301227       -0.759148       -1.528909
H       -1.479442       -1.504095       0.077069
N       -2.254921       0.515723        -0.125330
H       -1.947255       1.147447        0.633881
C       -3.616767       0.109375        -0.015569
N       -4.484765       1.129029        0.490858
N       -4.029023       -1.028517       -0.528568
H       -4.063063       1.817590        1.117867
H       -5.357778       0.782053        0.895553
H       -5.035924       -1.209808       -0.505173
O       2.855777        1.621019        0.441024
###
25
arg416 pm6_conformaciones E=-0.344985706051 au
N       3.515177        -0.449510       -0.699799
H       3.999327        -0.411217       0.200865
H       3.750895        -1.363694       -1.099367
C       2.042801        -0.375619       -0.490816
H       1.550600        -0.605798       -1.476296
C       1.508481        -1.353557       0.570640
C       1.706359        1.071665        -0.109395
H       1.685780        -2.392980       0.219757
H       2.101694        -1.267669       1.505339
C       0.026770        -1.160410       0.902386
O       2.202941        1.621738        0.911763
H       -0.265564       -1.897698       1.680177
H       -0.134481       -0.172194       1.385997
C       -0.867106       -1.322564       -0.333995
H       -0.550798       -0.632023       -1.146010
H       -0.742781       -2.350584       -0.750854
N       -2.315224       -1.150197       0.004254
H       -2.884863       -1.807255       -0.561864
C       -2.857491       0.178149        -0.032623
N       -2.084908       1.209749        0.578645
N       -4.017168       0.360331        -0.618468
H       -1.371338       0.902394        1.251010
H       -2.638929       1.973679        0.977166
H       -4.469350       1.271418        -0.505673
O       0.912783        1.720140        -0.857995
###
25
```

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arg417 pm6_conformaciones E=-0.346426586653 au
N       -1.360550       1.596215        0.106043
H       -1.465980       1.755573        1.110741
H       -0.367008       1.750144        -0.094248
C       -1.712647       0.190165        -0.224588
H       -1.401416       0.004401        -1.289350
C       -1.083437       -0.887123       0.679568
C       -3.238654       0.053572        -0.132958
H       -1.503729       -0.817672       1.705274
H       -1.381894       -1.892168       0.312961
C       0.440704        -0.801139       0.770039
O       -3.878421       0.464084        0.876787
H       0.747048        0.168197        1.213346
H       0.796032        -1.568243       1.492171
C       1.131544        -1.004933       -0.584918
H       0.820112        -1.974117       -1.040319
H       0.824707        -0.221346       -1.314668
N       2.619416        -1.038623       -0.477952
H       2.920144        -1.843622       0.102452
C       3.286453        0.171674        -0.086627
N       2.759895        1.397631        -0.574024
N       4.339584        0.069935        0.694795
H       2.085992        1.346589        -1.339844
H       3.450708        2.130916        -0.746190
H       4.892111        0.917756        0.846454
O       -3.855206       -0.497310       -1.092276
###
# Conformations of ASPARTIC ACID optimized with pm6
# opt freq pm6 scf=(xqc,tight) scrf(smd,solvent=water)
###
17
asp101 pm6_conformaciones E=-0.172468991456 au
N       1.672244        1.717745        0.212775
H       2.495227        1.544391        0.826557
H       1.239357        2.623686        0.499516
H       2.011098        1.822111        -0.765842
C       0.659165        0.594765        0.332848
H       0.308525        0.552778        1.419995
C       -0.524252       0.851053        -0.598835
C       1.331616        -0.737311       -0.012100
H       -0.756533       1.958019        -0.659849
H       -0.267651       0.607297        -1.665976
C       -1.785851       0.152950        -0.207375
O       2.392954        -0.903198       -0.579497
O       -1.939123       0.052490        1.140227
O       -2.644718       -0.281851       -0.960225
O       0.566315        -1.766290       0.417336
H       0.967874        -2.683529       0.205735
H       -2.791109       -0.426920       1.420478
###
17
asp102 pm6_conformaciones E=-0.173447088520 au
C       -0.601289       0.876355        -0.560771
C       -1.830464       0.138826        -0.141350
O       -2.707971       -0.295539       -0.872882
C       0.628558        0.605277        0.303907
C       1.166697        -0.801379       0.030740
O       2.505666        -0.802000       -0.118714
N       1.681575        1.664911        0.044852
O       0.499027        -1.818115       -0.026074
O       -1.923836       -0.011621       1.207062
H       2.520505        1.506471        0.640855
H       1.303020        2.611818        0.264178
H       1.984356        1.662250        -0.950978
H       0.350743        0.647937        1.414592
H       -0.850696       1.981153        -0.561423
H       -0.387164       0.678172        -1.646853
H       2.903430        -1.728081       -0.290256
H       -2.759315       -0.510361       1.505629
###
17
asp103 pm6_conformaciones E=-0.173446364430 au
C       -0.611273       0.884632        -0.528149
C       -1.842474       0.144032        -0.123683
O       -2.786194       -0.151026       -0.841784
C       0.623740        0.594069        0.323058
```

```
C       1.178389        -0.792988       -0.009413
O       2.517062        -0.771780       -0.163296
N       1.662644        1.677372        0.107646
O       0.524499        -1.815953       -0.104392
O       -1.854174       -0.192967       1.194919
H       2.502826        1.508030        0.698709
H       1.269482        2.609754        0.362580
H       1.966840        1.717493        -0.886835
H       0.346903        0.586938        1.434914
H       -0.858647       1.989913        -0.505135
H       -0.402097       0.709349        -1.619891
H       2.924494        -1.686135       -0.370896
H       -2.688152       -0.701606       1.478583
###
17
asp104 pm6_conformaciones E=-0.170426314691 au
C       0.677677        0.763512        0.613709
C       1.888383        0.092867        0.037480
O       2.886751        0.661815        -0.381435
C       -0.559151       0.652494        -0.274598
C       -1.261551       -0.690881       -0.066378
O       -2.597613       -0.576726       -0.160143
N       -1.502576       1.808215        0.001467
O       -0.708781       -1.762660       0.130140
O       1.933729        -1.267421       -0.018666
H       -2.358654       1.738401        -0.587722
H       -1.035276       2.714783        -0.215423
H       -1.795179       1.827736        1.000562
H       -0.263060       0.700114        -1.381919
H       0.927231        1.844582        0.818003
H       0.478206        0.374123        1.651268
H       -3.096466       -1.462284       -0.035550
H       1.076399        -1.742962       0.320069
###
17
asp105 pm6_conformaciones E=-0.172603566509 au
C       -0.779881       0.059181        1.139579
C       -1.671589       -0.168264       -0.040047
O       -2.498057       -1.056836       -0.176205
C       0.667726        0.437613        0.853892
C       1.364095        -0.633822       0.016038
O       2.026933        -0.098722       -1.032273
N       0.775192        1.815109        0.229150
O       1.363067        -1.827626       0.246459
O       -1.506026       0.776409        -1.003062
H       1.772159        2.075457        0.073855
H       0.348656        2.529707        0.858079
H       0.282534        1.856673        -0.688135
H       1.226914        0.469046        1.859488
H       -1.259325       0.842632        1.801284
H       -0.801612       -0.847997       1.806887
H       2.532821        -0.787142       -1.593215
H       -2.097937       0.641823        -1.818418
###
17
asp106 pm6_conformaciones E=-0.172244883831 au
C       -0.846488       0.471835        0.994580
C       -1.698632       -0.230208       -0.012351
O       -2.908551       -0.133722       -0.137874
C       0.581445        0.827100        0.601982
C       1.406794        -0.412749       0.264929
O       2.015119        -0.298923       -0.936834
N       0.609383        1.855562        -0.513135
O       1.551732        -1.387105       0.978515
O       -0.994307       -1.073932       -0.817191
H       1.587826        2.143633        -0.727153
H       0.076189        2.706942        -0.230495
H       0.184265        1.484973        -1.385343
H       1.088104        1.301152        1.520367
H       -1.381874       1.405444        1.338776
H       -0.834975       -0.147520       1.940138
H       2.618695        -1.089094       -1.170374
H       -1.574571       -1.580867       -1.481736
###
17
asp107 pm6_conformaciones E=-0.171979336457 au
```

```
C       -0.770577       0.477816        1.001290
C       -1.664531       -0.279264       0.072624
O       -2.872600       -0.160670       -0.043799
C       0.608750        0.884541        0.499480
C       1.419528        -0.302227       -0.021413
O       1.813691        -1.084251       1.010486
N       0.518297        1.955445        -0.572921
O       1.719973        -0.543081       -1.174789
O       -0.995905       -1.213866       -0.661605
H       1.468294        2.282809        -0.851941
H       -0.011674       2.779890        -0.213455
H       0.032931        1.608353        -1.422528
H       1.183736        1.332576        1.386713
H       -1.317386       1.393645        1.372221
H       -0.657120       -0.127993       1.949672
H       2.390990        -1.876420       0.716300
H       -1.598143       -1.751227       -1.280757
###
17
asp108 pm6_conformaciones E=-0.169331855800 au
C       -0.654872       0.274762        1.119965
C       -1.641669       -0.267481       0.130954
O       -2.482583       0.372317        -0.481389
C       0.655415        0.800561        0.546491
C       1.415296        -0.290534       -0.213863
O       2.260146        -0.927730       0.625852
N       0.440064        2.005881        -0.349425
O       1.309679        -0.582722       -1.388865
O       -1.644789       -1.609202       -0.130013
H       1.350449        2.374824        -0.704760
H       -0.023997       2.772155        0.187609
H       -0.155000       1.782237        -1.169928
H       1.304899        1.142505        1.429159
H       -1.152532       1.084358        1.729150
H       -0.426840       -0.496854       1.911028
H       2.789483        -1.676787       0.173045
H       -0.951566       -2.148763       0.384703
###
17
asp109 pm6_conformaciones E=-0.172152550209 au
C       0.722367        -0.035989       -1.113436
C       1.674474        -0.248912       0.016988
O       2.744098        -0.836146       -0.032624
C       -0.658257       0.526514        -0.799652
C       -1.440631       -0.381495       0.149381
O       -1.745152       -1.543570       -0.473629
N       -0.579330       1.933159        -0.238144
O       -1.788970       -0.146703       1.289829
O       1.254000        0.309260        1.184533
H       -1.530936       2.310372        -0.043887
H       -0.116788       2.566925        -0.927042
H       -0.030332       1.962982        0.646173
H       -1.246853       0.580874        -1.784280
H       0.603859        -1.004269       -1.681152
H       1.233436        0.619777        -1.881633
H       -2.268823       -2.189389       0.121592
H       1.912222        0.197182        1.952683
###
17
asp110 pm6_conformaciones E=-0.173512804312 au
C       0.724280        0.328855        -0.982967
C       1.578333        -0.239502       0.101413
O       1.267841        -0.576284       1.234358
C       -0.683144       0.755879        -0.587073
C       -1.472800       -0.394335       0.039809
O       -1.907396       -1.230077       -0.929424
N       -0.665432       1.954106        0.342186
O       -1.714963       -0.578332       1.217444
O       2.861653        -0.388371       -0.329015
H       -1.635489       2.261437        0.572272
H       -0.176839       2.756047        -0.116399
H       -0.171714       1.749298        1.231525
H       -1.231040       1.072535        -1.545825
H       0.664762        -0.416638       -1.830742
H       1.257744        1.190614        -1.482123
H       -2.460055       -2.012843       -0.569059
```

```
H       3.473564        -0.800064       0.371063
###
16
asp201 pm6_conformaciones E=-0.355904043573 au
N       1.864042        1.532703        -0.007820
H       2.685487        1.319387        0.589709
H       1.582110        2.519668        0.167107
H       2.159127        1.457671        -1.000544
C       0.721850        0.586418        0.297254
H       0.446013        0.709245        1.391720
C       -0.476436       0.924153        -0.588173
C       1.169324        -0.883081       0.088060
H       -0.690640       2.031926        -0.567697
H       -0.249141       0.731164        -1.669425
C       -1.718139       0.196445        -0.189934
O       2.375099        -1.120977       -0.146687
O       -1.992205       0.313721        1.138373
O       -2.466191       -0.448659       -0.912248
O       0.292070        -1.776566       0.179476
H       -2.831026       -0.181733       1.429328
###
16
asp202 pm6_conformaciones E=-0.355943075598 au
C       0.453653        -0.992976       -0.503781
C       1.704910        -0.239382       -0.198203
O       2.487999        0.252769        -0.998214
C       -0.737296       -0.570807       0.355168
C       -1.136405       0.895435        0.050211
O       -2.279202       1.138905        -0.397172
N       -1.904376       -1.500619       0.095660
O       -0.280452       1.786096        0.277403
O       1.944575        -0.128314       1.138845
H       -2.709855       -1.253762       0.701748
H       -1.639969       -2.488499       0.292454
H       -2.215159       -1.445288       -0.893347
H       -0.470521       -0.640021       1.455903
H       0.664404        -2.095033       -0.376337
H       0.214562        -0.905694       -1.597047
H       2.794639        0.383370        1.359747
###
16
asp203 pm6_conformaciones E=-0.353887422679 au
C       0.592031        0.722698        0.564073
C       1.860014        0.049594        0.147425
O       2.983122        0.528955        0.150909
C       -0.564975       0.523583        -0.414636
C       -1.465224       -0.653019       0.056922
O       -2.314215       -0.454160       0.954052
N       -1.392310       1.788849        -0.527092
O       -1.286178       -1.764995       -0.494920
O       1.678049        -1.241679       -0.249131
H       -2.107087       1.694407        -1.276445
H       -0.789561       2.605657        -0.759590
H       -1.881413       2.000058        0.363123
H       -0.166828       0.282339        -1.447691
H       0.811242        1.816525        0.721660
H       0.324453        0.385798        1.602937
H       2.538062        -1.708833       -0.524331
###
16
asp204 pm6_conformaciones E=-0.354552368219 au
C       0.600351        0.802657        0.538920
C       1.840083        0.097303        0.077361
O       2.954357        0.616568        0.043787
C       -0.616739       0.587652        -0.357904
C       -1.362400       -0.714716       0.013557
O       -2.575293       -0.690365       0.284351
N       -1.558338       1.770385        -0.247141
O       -0.688468       -1.795992       0.011932
O       1.785052        -1.190759       -0.310333
H       -2.406856       1.619677        -0.827173
H       -1.092741       2.642093        -0.575410
H       -1.860800       1.919077        0.735433
H       -0.295423       0.500491        -1.445704
H       0.829439        1.899532        0.644149
H       0.384335        0.507875        1.602492
```

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H       0.777464        -1.634432       -0.273301
###
16
asp205 pm6_conformaciones E=-0.354528230482 au
C       -0.686648       0.133324        1.162882
C       -1.605601       -0.131722       0.013424
O       -2.420891       -1.035812       -0.090231
C       0.762567        0.432077        0.804132
C       1.361003        -0.652139       -0.128202
O       1.843728        -0.298767       -1.228507
N       0.906775        1.808102        0.185422
O       1.349572        -1.837801       0.277303
O       -1.472537       0.788321        -0.980731
H       1.898873        1.999800        -0.057221
H       0.586809        2.543721        0.848645
H       0.343309        1.890580        -0.683971
H       1.374735        0.419849        1.764270
H       -1.118973       0.970928        1.784449
H       -0.721345       -0.733444       1.877131
H       -2.097735       0.635093        -1.767341
###
16
asp206 pm6_conformaciones E=-0.355278693883 au
C       -0.723077       0.492495        1.015861
C       -1.636641       -0.231604       0.080413
O       -2.808354       0.019411        -0.147378
C       0.671519        0.844178        0.513738
C       1.460487        -0.409202       0.062514
O       1.708648        -0.581813       -1.152893
N       0.622085        1.882302        -0.589358
O       1.834650        -1.203156       0.960690
O       -1.049001       -1.305865       -0.526816
H       1.582812        2.170162        -0.864704
H       0.111142        2.731492        -0.269542
H       0.143748        1.519582        -1.432804
H       1.244906        1.303145        1.385082
H       -1.240481       1.427132        1.375588
H       -0.636938       -0.111547       1.964127
H       -1.681055       -1.819897       -1.136212
###
16
asp207 pm6_conformaciones E=-0.355278650828 au
C       -0.722966       0.492112        1.016136
C       -1.636598       -0.231752       0.080562
O       -2.808154       0.019609        -0.147598
C       0.671494        0.844126        0.513803
C       1.460650        -0.409020       0.062399
O       1.834993        -1.203030       0.960375
N       0.621567        1.882349        -0.589239
O       1.708697        -0.581379       -1.153089
O       -1.049134       -1.306214       -0.526628
H       1.582130        2.171622        -0.863603
H       0.109043        2.730739        -0.269805
H       0.144579        1.518971        -1.433194
H       1.244877        1.303272        1.385003
H       -1.240422       1.426537        1.376356
H       -0.636540       -0.112264       1.964130
H       -1.681331       -1.820016       -1.136088
###
16
asp208 pm6_conformaciones E=-0.351954791225 au
C       0.655968        0.616547        -0.917254
C       1.700778        -0.173296       -0.193986
O       2.907000        -0.024987       -0.388706
C       -0.692694       0.885660        -0.267134
C       -1.561836       -0.394287       -0.161766
O       -2.637039       -0.441297       -0.784539
N       -0.550050       1.552633        1.086014
O       -1.146385       -1.364308       0.547641
O       1.390480        -1.132857       0.699943
H       -1.481837       1.826566        1.463005
H       0.025239        2.418426        1.003609
H       -0.093717       0.931325        1.779167
H       -1.249208       1.617396        -0.943347
H       1.111256        1.604022        -1.219335
H       0.485499        0.124678        -1.919877
```

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H       0.327373        -1.290997       0.880805
###
16
asp210 pm6_conformaciones E=-0.357671830296 au
C       -0.716555       0.490657        0.957850
C       -1.503303       -0.322758       -0.016834
O       -1.109939       -1.206456       -0.769596
C       0.709712        0.816613        0.533091
C       1.478753        -0.452875       0.091024
O       1.783021        -1.279740       0.984856
N       0.731876        1.870962        -0.555477
O       1.768329        -0.610665       -1.117389
O       -2.821148       0.003617        0.019480
H       1.709524        2.090282        -0.833616
H       0.287025        2.750677        -0.218545
H       0.221655        1.557249        -1.399949
H       1.255518        1.247091        1.434777
H       -0.703670       -0.055594       1.944247
H       -1.268069       1.435638        1.225812
H       -3.398856       -0.565953       -0.593972
###
15
asp301 pm6_conformaciones E=-0.537575847722 au
N       1.987179        -1.398411       -0.045075
H       2.807571        -1.085499       -0.598188
H       1.831534        -2.409153       -0.239254
H       2.221213        -1.301377       0.961557
C       0.756766        -0.590431       -0.405521
H       0.573069        -0.713608       -1.516348
C       -0.441806       -1.103148       0.388712
C       0.991118        0.913094        -0.124113
H       -0.650857       -2.173537       0.136772
H       -0.216796       -1.133677       1.481211
C       -1.686654       -0.283665       0.131221
O       1.982014        1.271973        0.549919
O       -2.197417       -0.238417       -1.023049
O       -2.209247       0.363921        1.084330
O       0.150585        1.726352        -0.592702
###
15
asp302 pm6_conformaciones E=-0.537576006204 au
C       -0.441764       -1.103220       0.388604
C       -1.686628       -0.283710       0.131245
O       -2.209143       0.363803        1.084451
C       0.756807        -0.590434       -0.405587
C       0.991027        0.913102        -0.124103
O       1.981685        1.271998        0.550273
N       1.987268        -1.398309       -0.045131
O       0.150681        1.726351        -0.593014
O       -2.197448       -0.238348       -1.022983
H       2.807696        -1.085144       -0.598050
H       1.831822        -2.409030       -0.239576
H       2.221150        -1.301481       0.961562
H       0.573150        -0.713602       -1.516406
H       -0.650838       -2.173569       0.136531
H       -0.216724       -1.133875       1.481090
###
15
asp303 pm6_conformaciones E=-0.534189147701 au
C       0.630784        0.635066        0.565565
C       1.881771        -0.072582       0.089534
O       2.996074        0.486944        0.279913
C       -0.542838       0.502108        -0.402392
C       -1.462249       -0.659924       0.051440
O       -2.502237       -0.407225       0.697979
N       -1.327262       1.797812        -0.471655
O       -1.100250       -1.829207       -0.243367
O       1.821380        -1.200972       -0.478333
H       -2.055665       1.747282        -1.210714
H       -0.698135       2.597594        -0.692488
H       -1.796145       2.003116        0.430363
H       -0.169188       0.274064        -1.446190
H       0.873387        1.709962        0.760086
H       0.372035        0.258974        1.586111
###
15
```

```
asp304 pm6_conformaciones E=-0.534189147701 au
C       0.630784        0.635066        0.565565
C       1.881771        -0.072582       0.089534
O       2.996074        0.486944        0.279913
C       -0.542838       0.502108        -0.402392
C       -1.462249       -0.659924       0.051440
O       -2.502237       -0.407225       0.697979
N       -1.327262       1.797812        -0.471655
O       -1.100250       -1.829207       -0.243367
O       1.821380        -1.200972       -0.478333
H       -2.055665       1.747282        -1.210714
H       -0.698135       2.597594        -0.692488
H       -1.796145       2.003116        0.430363
H       -0.169188       0.274064        -1.446190
H       0.873387        1.709962        0.760086
H       0.372035        0.258974        1.586111
###
15
asp305 pm6_conformaciones E=-0.533884541316 au
C       0.633718        0.067844        -1.147417
C       1.613828        -0.201992       -0.029756
O       2.456057        -1.135023       -0.152563
C       -0.735005       0.570219        -0.701168
C       -1.426662       -0.508365       0.168498
O       -1.184592       -0.591593       1.396976
N       -0.622319       1.892394        0.030528
O       -2.197733       -1.301673       -0.426087
O       1.597999        0.508301        1.018230
H       -1.538355       2.186148        0.422564
H       -0.294119       2.636329        -0.618396
H       0.064232        1.823957        0.812452
H       -1.374049       0.741474        -1.622537
H       1.102922        0.799286        -1.856427
H       0.506473        -0.840283       -1.784739
###
15
asp306 pm6_conformaciones E=-0.535780673428 au
C       -0.775112       0.452440        0.999071
C       -1.574503       -0.349209       -0.005088
O       -2.778659       -0.047498       -0.220718
C       0.635273        0.825537        0.559127
C       1.404598        -0.415233       0.055757
O       1.684658        -0.532681       -1.161831
N       0.606711        1.914665        -0.495980
O       1.722651        -1.280879       0.911309
O       -1.044227       -1.328818       -0.609275
H       1.570683        2.166804        -0.792969
H       0.151545        2.772816        -0.120206
H       0.081682        1.616951        -1.335978
H       1.197675        1.238172        1.455843
H       -1.337064       1.370345        1.301543
H       -0.728423       -0.129947       1.954541
###
15
asp307 pm6_conformaciones E=-0.535780183353 au
C       -0.774757       0.451718        0.999324
C       -1.574530       -0.349407       -0.004954
O       -2.778769       -0.047446       -0.220003
C       0.635277        0.825605        0.559030
C       1.405058        -0.414887       0.055685
O       1.723788        -1.280199       0.911273
N       0.605926        1.914578        -0.496189
O       1.684480        -0.532604       -1.162018
O       -1.044789       -1.328886       -0.609725
H       1.569810        2.168780        -0.791766
H       0.148414        2.771802        -0.121265
H       0.082865        1.615679        -1.336960
H       1.197722        1.238736        1.455506
H       -1.336818       1.369242        1.302765
H       -0.727442       -0.131375       1.954313
###
15
asp308 pm6_conformaciones E=-0.535780183353 au
C       -0.774757       0.451718        0.999324
C       -1.574530       -0.349407       -0.004954
O       -2.778769       -0.047446       -0.220003
```

```
C       0.635277        0.825605        0.559030
C       1.405058        -0.414887       0.055685
O       1.723788        -1.280199       0.911273
N       0.605926        1.914578        -0.496189
O       1.684480        -0.532604       -1.162018
O       -1.044789       -1.328886       -0.609725
H       1.569810        2.168780        -0.791766
H       0.148414        2.771802        -0.121265
H       0.082865        1.615679        -1.336960
H       1.197722        1.238736        1.455506
H       -1.336818       1.369242        1.302765
H       -0.727442       -0.131375       1.954313
###
15
asp309 pm6_conformaciones E=-0.535780231831 au
C       -0.774863       0.451769        0.999348
C       -1.574540       -0.349438       -0.004941
O       -2.778748       -0.047543       -0.220191
C       0.635212        0.825583        0.559060
C       1.405020        -0.414855       0.055665
O       1.723832        -1.280195       0.911218
N       0.605896        1.914597        -0.496150
O       1.684459        -0.532513       -1.162051
O       -1.044588       -1.328942       -0.609552
H       1.569785        2.168673        -0.791834
H       0.148530        2.771880        -0.121131
H       0.082666        1.615777        -1.336868
H       1.197627        1.238607        1.455620
H       -0.727563       -0.131248       1.954398
H       -1.336933       1.369320        1.302686
###
15
asp310 pm6_conformaciones E=-0.533883919358 au
C       0.633658        0.067600        -1.147503
C       1.613788        -0.202034       -0.029818
O       1.598549        0.508995        1.017700
C       -0.735047       0.570112        -0.701286
C       -1.426678       -0.508261       0.168637
O       -2.197748       -1.301794       -0.425658
N       -0.622330       1.892357        0.030308
O       -1.184349       -0.591163       1.397099
O       2.455448        -1.135606       -0.152211
H       -1.538036       2.185397        0.423656
H       -0.295524       2.636562        -0.619005
H       0.065269        1.824317        0.811410
H       -1.374119       0.741253        -1.622625
H       0.506291        -0.840768       -1.784440
H       1.102902        0.798782        -1.856773
###
14
asp401 pm6_conformaciones E=-0.683583788931 au
N       1.938983        -1.539674       -0.159541
H       2.798021        -1.099653       -0.499835
H       2.063571        -1.674883       0.846467
C       0.778099        -0.655345       -0.429296
H       0.560599        -0.725653       -1.531523
C       -0.441282       -1.127215       0.373591
C       1.035067        0.830112        -0.101702
H       -0.688439       -2.182376       0.109198
H       -0.207640       -1.181341       1.460136
C       -1.648870       -0.257375       0.131910
O       1.849968        1.165464        0.797776
O       -2.133960       -0.136225       -1.030928
O       -2.165671       0.375608        1.098770
O       0.395028        1.707724        -0.754953
###
14
asp402 pm6_conformaciones E=-0.597854265193 au
C       -0.637000       0.934323        -0.581279
C       -1.617809       -0.089430       -0.156591
O       -1.628843       -1.289336       -0.422048
C       0.696079        0.853089        0.248498
C       1.308124        -0.548598       0.127334
O       1.407011        -1.167895       -0.978929
N       1.731905        1.716905        -0.235947
O       1.807513        -1.087298       1.167874
```

```
O       -2.593706       0.419935        0.649716
H       1.783543        2.542623        0.349344
H       0.397831        1.012624        1.317090
H       -1.044814       1.963365        -0.477607
H       -0.426875       0.833458        -1.666517
H       -3.265186       -0.269954       0.968638
###
14
asp403 pm6_conformaciones E=-0.680979708575 au
C       0.609457        0.604814        0.656417
C       1.842468        -0.095589       0.134593
O       2.897954        0.572835        -0.047472
C       -0.522554       0.588313        -0.382617
C       -1.480223       -0.566430       -0.025441
O       -2.541813       -0.351654       0.614931
N       -1.185446       1.913023        -0.459027
O       -1.160027       -1.738654       -0.383599
O       1.814934        -1.333438       -0.136428
H       -1.995577       1.860033        -1.082644
H       -1.543240       2.193328        0.455940
H       -0.104734       0.376057        -1.407370
H       0.860020        1.650632        0.947016
H       0.298374        0.149433        1.623079
###
14
asp404 pm6_conformaciones E=-0.681215952678 au
C       0.630697        0.716838        0.533710
C       1.821287        -0.112623       0.121160
O       2.968599        0.415598        0.154915
C       -0.550824       0.593867        -0.443041
C       -1.457061       -0.555022       0.029667
O       -2.304306       -0.400145       0.946692
N       -1.378615       1.816480        -0.581787
O       -1.306329       -1.683301       -0.528482
O       1.687722        -1.314573       -0.258072
H       -0.807481       2.573834        -0.970656
H       -1.689163       2.142426        0.336589
H       -0.158137       0.341167        -1.467178
H       0.935845        1.784387        0.630702
H       0.339158        0.443830        1.573659
###
14
asp406 pm6_conformaciones E=-0.681858247956 au
C       -0.643014       0.342036        1.110622
C       -1.553960       -0.398626       0.161067
O       -2.536274       0.193967        -0.370839
C       0.618471        0.901698        0.435968
C       1.471525        -0.261651       -0.099067
O       1.322757        -0.757650       -1.252752
N       0.278296        1.837692        -0.674559
O       2.321929        -0.764908       0.691586
O       -1.321973       -1.612187       -0.122590
H       1.118349        2.351259        -0.957424
H       -0.383089       2.541573        -0.334563
H       1.226112        1.414654        1.236803
H       -1.198724       1.173785        1.602247
H       -0.360364       -0.319628       1.960072
###
14
asp407 pm6_conformaciones E=-0.681858214767 au
C       -0.643001       0.342043        1.110619
C       -1.553937       -0.398674       0.161131
O       -2.536315       0.193974        -0.370735
C       0.618476        0.901738        0.435910
C       1.471523        -0.261633       -0.099023
O       2.322067        -0.764731       0.691574
N       0.278148        1.837639        -0.674677
O       1.322673        -0.757806       -1.252638
O       -1.321960       -1.612184       -0.122627
H       1.118352        2.350521        -0.958295
H       -0.382512       2.542049        -0.334401
H       1.226029        1.414788        1.236730
H       -1.198719       1.173846        1.602195
H       -0.360268       -0.319539       1.960094
###
14
```

```
asp408 pm6_conformaciones E=-0.681858214767 au
C       -0.643001       0.342043        1.110619
C       -1.553937       -0.398674       0.161131
O       -2.536315       0.193974        -0.370735
C       0.618476        0.901738        0.435910
C       1.471523        -0.261633       -0.099023
O       2.322067        -0.764731       0.691574
N       0.278148        1.837639        -0.674677
O       1.322673        -0.757806       -1.252638
O       -1.321960       -1.612184       -0.122627
H       1.118352        2.350521        -0.958295
H       -0.382512       2.542049        -0.334401
H       1.226029        1.414788        1.236730
H       -1.198719       1.173846        1.602195
H       -0.360268       -0.319539       1.960094
###
14
asp409 pm6_conformaciones E=-0.683068798351 au
C       -0.601648       0.277096        1.095172
C       -1.611624       -0.384079       0.186415
O       -2.711997       0.195288        -0.039044
C       0.582587        0.909409        0.347742
C       1.580716        -0.204849       -0.022657
O       2.474218        -0.526232       0.805412
N       0.121738        1.710937        -0.812407
O       1.475828        -0.806267       -1.131640
O       -1.359033       -1.500577       -0.359313
H       0.913813        2.207712        -1.230945
H       -0.259050       1.107780        -1.542208
H       1.105806        1.614260        1.056064
H       -0.239460       -0.450882       1.855228
H       -1.105593       1.061404        1.705367
###
14
asp410 pm6_conformaciones E=-0.683068554931 au
C       -0.601715       0.277263        1.095137
C       -1.611690       -0.384008       0.186426
O       -1.359146       -1.500646       -0.359062
C       0.582620        0.909398        0.347750
C       1.580724        -0.204900       -0.022627
O       2.474364        -0.526215       0.805293
N       0.121937        1.710911        -0.812472
O       1.475650        -0.806458       -1.131555
O       -2.712001       0.195375        -0.039196
H       0.914090        2.207606        -1.230972
H       -0.258822       1.107727        -1.542277
H       1.105894        1.614214        1.056087
H       -0.239594       -0.450597       1.855341
H       -1.105691       1.061703        1.705164
###
# Conformations of CYSTEINE optimized with pm6
# opt freq pm6 scf=(xqc,tight) scrf(smd,solvent=water)
###
15
cys100 pm6_conformaciones E=-0.159212782148E-01 au
N       0.011102        1.717902        -0.286903
H       -0.723331       2.220755        -0.828953
H       0.933090        1.995582        -0.680348
H       -0.029569       2.048536        0.699862
C       -0.180991       0.214275        -0.375993
H       -0.018211       -0.104128       -1.460642
C       0.773040        -0.522666       0.553325
C       -1.623223       -0.134562       0.000655
H       0.676633        -0.183434       1.611212
H       0.514127        -1.611365       0.589878
S       2.471390        -0.384162       -0.050129
O       -2.425881       0.558047        0.595960
H       2.898828        0.662258        0.699002
O       -1.926034       -1.379454       -0.434182
H       -2.869147       -1.677961       -0.181771
###
15
cys101 pm6_conformaciones E=-0.161601608700E-01 au
N       -0.165624       1.691420        -0.103690
H       -0.920604       2.156978        -0.649827
H       0.737728        2.115155        -0.392457
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H       -0.314193       1.908940        0.903584
C       -0.167907       0.192700        -0.349426
H       0.059902        0.013543        -1.456383
C       0.849238        -0.511998       0.536127
C       -1.553910       -0.405700       -0.101094
H       0.764479        -0.199140       1.603664
H       0.651949        -1.613934       0.561324
S       2.523691        -0.283090       -0.104737
O       -1.853453       -1.579519       -0.211594
H       2.892123        0.817511        0.596420
O       -2.454395       0.538732        0.250742
H       -3.392818       0.166733        0.408478
###
15
cys102 pm6_conformaciones E=-0.159085209813E-01 au
N       -0.067619       1.746332        -0.401526
H       -0.842571       2.156983        -0.964376
H       0.827101        2.040607        -0.844644
H       -0.101285       2.163131        0.551878
C       -0.172003       0.232146        -0.352722
H       0.032677        -0.169513       -1.400838
C       0.800035        -0.360438       0.658183
C       -1.598048       -0.168270       0.041767
H       0.782188        0.186532        1.630434
H       0.500320        -1.404217       0.933891
S       2.464502        -0.456632       -0.036768
O       -2.338018       0.367483        0.842502
H       2.920362        0.781722        0.272975
O       -1.959407       -1.274749       -0.651056
H       -2.878000       -1.635959       -0.395284
###
15
cys103 pm6_conformaciones E=-0.197092573187E-01 au
N       0.074593        1.700619        -0.837732
H       0.945094        2.109195        -1.240207
H       -0.566952       2.489199        -0.602679
H       -0.379079       1.123540        -1.571679
C       0.381820        0.891002        0.407975
H       0.927192        1.577855        1.142553
C       -0.887697       0.377091        1.065525
C       1.318025        -0.273961       0.081956
H       -0.647423       -0.172575       2.005996
H       -1.528378       1.227962        1.412540
S       -1.863879       -0.620100       -0.079644
O       2.391748        -0.502785       0.602237
H       -1.089387       -1.731779       -0.167838
O       0.780297        -1.085483       -0.858710
H       1.389600        -1.864781       -1.121230
###
15
cys104 pm6_conformaciones E=-0.197093439404E-01 au
N       0.075887        1.700400        -0.837934
H       0.946815        2.108486        -1.240152
H       -0.565345       2.489462        -0.603504
H       -0.377795       1.123498        -1.572015
C       0.381891        0.890815        0.407973
H       0.927188        1.577270        1.143184
C       -0.888283       0.377901        1.064906
C       1.317993        -0.274298       0.082348
H       -0.648854       -0.170894       2.006185
H       -1.528684       1.229396        1.410878
S       -1.864435       -0.619844       -0.079716
O       2.391740        -0.503091       0.602554
H       -1.090073       -1.731596       -0.167006
O       0.780446        -1.085938       -0.858476
H       1.389407        -1.865192       -1.120568
###
15
cys105 pm6_conformaciones E=-0.192076173553E-01 au
N       0.465073        1.850242        -0.480076
H       1.444811        2.142659        -0.678500
H       -0.054502       2.688494        -0.137882
H       0.031508        1.548837        -1.372935
C       0.425047        0.753963        0.569925
H       0.959198        1.145116        1.507925
C       -1.005797       0.412949        0.943607
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C       1.238221        -0.447161       0.087818
H       -1.024749       -0.228010       1.855749
H       -1.569999       1.330224        1.248788
S       -1.875343       -0.355595       -0.439813
O       2.396778        -0.421973       -0.287206
H       -1.479425       -1.647121       -0.301680
O       0.529857        -1.595769       0.135210
H       1.085230        -2.418940       -0.116052
###
15
cys106 pm6_conformaciones E=-0.197092606269E-01 au
N       0.076155        1.700444        -0.838009
H       0.947192        2.107942        -1.240523
H       -0.564455       2.489955        -0.603542
H       -0.378105       1.123766        -1.571877
C       0.381980        0.890826        0.407971
H       0.927296        1.577222        1.143165
C       -0.888315       0.378109        1.064823
C       1.317948        -0.274418       0.082370
H       -0.648993       -0.170528       2.006204
H       -1.528710       1.229717        1.410577
S       -1.864495       -0.619729       -0.079728
O       2.391892        -0.503065       0.602254
H       -1.090114       -1.731474       -0.167103
O       0.780091        -1.086377       -0.857998
H       1.389188        -1.865605       -1.120225
###
15
cys107 pm6_conformaciones E=-0.226137359418E-01 au
N       2.018609        -1.053475       0.029486
H       2.811988        -0.524688       -0.386248
H       2.147612        -2.062856       -0.200131
H       2.065013        -0.953708       1.063079
C       0.691417        -0.564677       -0.516604
H       0.730778        -0.654359       -1.652604
C       -0.470138       -1.381752       0.034950
C       0.454948        0.912896        -0.169030
H       -0.689176       -2.271012       -0.595551
H       -0.264096       -1.801399       1.050179
S       -1.853622       -0.223058       0.163847
O       0.193720        1.798180        -0.966717
H       -2.414889       -0.367124       -1.062302
O       0.633224        1.158230        1.147555
H       0.467552        2.128320        1.413021
###
15
cys108 pm6_conformaciones E=-0.226133569377E-01 au
N       2.018650        -1.053222       0.029478
H       2.812046        -0.524698       -0.386505
H       2.147550        -2.062717       -0.199724
H       2.065102        -0.952966       1.063050
C       0.691439        -0.564570       -0.516755
H       0.730953        -0.654179       -1.652746
C       -0.469958       -1.381898       0.034642
C       0.454713        0.912967        -0.169144
H       -0.689060       -2.270913       -0.596123
H       -0.263822       -1.801885       1.049723
S       -1.853472       -0.223243       0.164155
O       0.192950        1.798242        -0.966646
H       -2.414803       -0.366783       -1.062022
O       0.633443        1.158181        1.147399
H       0.468739        2.128205        1.413033
###
15
cys109 pm6_conformaciones E=-0.226138269600E-01 au
N       2.018466        -1.053598       0.029096
H       2.811862        -0.525464       -0.387439
H       2.147021        -2.063200       -0.199843
H       2.065439        -0.953050       1.062603
C       0.691157        -0.564729       -0.516691
H       0.730209        -0.654407       -1.652694
C       -0.470236       -1.381751       0.035230
C       0.454910        0.912863        -0.169148
H       -0.689421       -2.271114       -0.595038
H       -0.264090       -1.801205       1.050477
S       -1.853639       -0.222894       0.163942
```

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O       0.193374        1.798314        -0.966469
H       -2.414753       -0.366974       -1.062282
O       0.633885        1.157989        1.147484
H       0.469640        2.128176        1.413010
###
15
cys110 pm6_conformaciones E=-0.226135974283E-01 au
N       2.018641        -1.053420       0.029135
H       2.811961        -0.525061       -0.387275
H       2.147356        -2.062950       -0.199967
H       2.065600        -0.953071       1.062655
C       0.691291        -0.564663       -0.516592
H       0.730309        -0.654349       -1.652613
C       -0.470032       -1.381782       0.035352
C       0.454828        0.912914        -0.169066
H       -0.688976       -2.271324       -0.594703
H       -0.263904       -1.801002       1.050697
S       -1.853623       -0.223082       0.163723
O       0.193532        1.798344        -0.966506
H       -2.414579       -0.367393       -1.062543
O       0.633308        1.158085        1.147622
H       0.468471        2.128160        1.413146
###
15
cys111 pm6_conformaciones E=-0.226588846029E-01 au
N       2.152563        -0.853969       0.003628
H       2.870729        -0.146171       -0.251870
H       2.427619        -1.762582       -0.430432
H       2.166200        -0.980511       1.035301
C       0.780702        -0.443844       -0.493414
H       0.831359        -0.389248       -1.632414
C       -0.288474       -1.440865       -0.063738
C       0.392228        0.937216        0.050501
H       -0.432407       -2.244812       -0.818763
H       -0.028095       -1.986376       0.877762
S       -1.786491       -0.480487       0.255642
O       0.616621        1.411788        1.148348
H       -2.105445       -0.097703       -1.006746
O       -0.236219       1.638589        -0.926172
H       -0.563995       2.554920        -0.626003
###
14
cys200 pm6_conformaciones E=-0.203458001756 au
N       1.847730        -1.327917       0.002941
H       1.941112        -1.327868       1.035871
H       2.705740        -0.906947       -0.402470
H       1.798176        -2.320264       -0.309630
C       0.610088        -0.573775       -0.444860
H       0.585249        -0.603762       -1.577368
C       -0.642505       -1.229188       0.114381
C       0.686308        0.907280        0.009425
H       -0.891278       -2.163895       -0.440252
H       -0.528150       -1.550510       1.172714
S       -1.994835       -0.040031       -0.092372
O       0.700385        1.785998        -0.890077
H       -2.150247       0.376188        1.188822
O       0.749527        1.189888        1.229577
###
14
cys201 pm6_conformaciones E=-0.203310535715 au
N       0.586049        1.892015        -0.261065
H       0.258643        1.688429        -1.221152
H       1.583944        2.175672        -0.321826
H       0.042217        2.702884        0.100320
C       0.428689        0.692532        0.651605
H       0.951216        0.938374        1.631172
C       -1.032188       0.396122        0.932371
C       1.117907        -0.550703       0.043682
H       -1.138514       -0.222379       1.850782
H       -1.612480       1.321229        1.154519
S       -1.704509       -0.447970       -0.529555
O       1.255536        -1.557065       0.787617
H       -2.526026       -1.350804       0.063661
O       1.560007        -0.512648       -1.128002
###
14
```

```
cys202 pm6_conformaciones E=-0.203457540616 au
N       1.848254        -1.327305       0.003082
H       1.943854        -1.323282       1.035772
H       2.705739        -0.908587       -0.405814
H       1.797031        -2.320793       -0.305522
C       0.610383        -0.573673       -0.444964
H       0.585752        -0.603650       -1.577471
C       -0.642146       -1.229425       0.114058
C       0.685784        0.907402        0.009508
H       -0.890705       -2.164133       -0.440606
H       -0.527731       -1.551008       1.172292
S       -1.994559       -0.040319       -0.092444
O       0.699871        1.786208        -0.889930
H       -2.152024       0.373383        1.189332
O       0.748769        1.189854        1.229672
###
14
cys203 pm6_conformaciones E=-0.203457358273 au
N       1.848281        -1.327063       0.003305
H       1.943415        -1.323797       1.036071
H       2.705804        -0.907730       -0.404928
H       1.797806        -2.320393       -0.306115
C       0.610199        -0.573770       -0.444878
H       0.585805        -0.603959       -1.577448
C       -0.642200       -1.229708       0.113779
C       0.685673        0.907366        0.009414
H       -0.890887       -2.164144       -0.441366
H       -0.528002       -1.551950       1.171828
S       -1.994314       -0.040150       -0.092499
O       0.748166        1.189713        1.229748
H       -2.151987       0.372810        1.189466
O       0.700216        1.786245        -0.889816
###
14
cys204 pm6_conformaciones E=-0.203310747416 au
N       0.586350        1.892003        -0.261111
H       0.259241        1.688430        -1.221303
H       1.584204        2.175788        -0.321600
H       0.042322        2.702788        0.100184
C       0.428819        0.692464        0.651523
H       0.951292        0.938296        1.631156
C       -1.032116       0.396224        0.932293
C       1.117920        -0.550747       0.043656
H       -1.138476       -0.222153       1.850753
H       -1.612246       1.321477        1.154435
S       -1.704801       -0.447867       -0.529425
O       1.559817        -0.512919       -1.128145
H       -2.525994       -1.350839       0.064004
O       1.255719        -1.557029       0.787660
###
14
cys205 pm6_conformaciones E=-0.203457638923 au
N       1.848555        -1.327028       0.003342
H       1.943815        -1.323179       1.036088
H       2.706069        -0.907984       -0.405131
H       1.797771        -2.320454       -0.305503
C       0.610634        -0.573622       -0.444973
H       0.586250        -0.603605       -1.577489
C       -0.641896       -1.229495       0.113840
C       0.685640        0.907509        0.009459
H       -0.890425       -2.164089       -0.441100
H       -0.527424       -1.551372       1.172020
S       -1.994584       -0.040744       -0.092360
O       0.748096        1.190081        1.229607
H       -2.150270       0.374686        1.189064
O       0.699580        1.786263        -0.890048
###
14
cys206 pm6_conformaciones E=-0.203457676821 au
N       1.848053        -1.327464       0.003128
H       1.942099        -1.326015       1.035983
H       2.705848        -0.907139       -0.403396
H       1.798148        -2.320196       -0.308093
C       0.610261        -0.573725       -0.444924
H       0.585675        -0.603721       -1.577417
C       -0.642304       -1.229405       0.114054
```

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C       0.685904        0.907354        0.009465
H       -0.891021       -2.163963       -0.440859
H       -0.527937       -1.551266       1.172199
S       -1.994603       -0.040205       -0.092356
O       0.700050        1.786091        -0.890037
H       -2.150969       0.374678        1.189177
O       0.748984        1.189884        1.229617
###
14
cys207 pm6_conformaciones E=-0.203457536320 au
N       1.847903        -1.327535       0.002767
H       1.942268        -1.325744       1.035596
H       2.705620        -0.907430       -0.404182
H       1.797752        -2.320386       -0.308090
C       0.610069        -0.573747       -0.445076
H       0.585211        -0.603782       -1.577597
C       -0.642394       -1.229330       0.114240
C       0.686056        0.907266        0.009312
H       -0.891268       -2.164041       -0.440360
H       -0.527837       -1.550871       1.172470
S       -1.994759       -0.040164       -0.092058
O       0.750211        1.189662        1.229478
H       -2.149753       0.375887        1.189250
O       0.699344        1.786163        -0.890026
###
14
cys208 pm6_conformaciones E=-0.203458067053 au
N       1.847760        -1.327842       0.003050
H       1.941999        -1.326166       1.035870
H       2.705611        -0.907950       -0.403797
H       1.797441        -2.320652       -0.307901
C       0.610124        -0.573750       -0.444912
H       0.585409        -0.603749       -1.577421
C       -0.642462       -1.229181       0.114224
C       0.686203        0.907288        0.009487
H       -0.891164       -2.163904       -0.440334
H       -0.528268       -1.550639       1.172521
S       -1.994732       -0.039935       -0.092559
O       0.700844        1.786105        -0.889878
H       -2.151393       0.374834        1.188960
O       0.748976        1.189637        1.229741
###
14
cys209 pm6_conformaciones E=-0.203457760940 au
N       1.847899        -1.327566       0.002995
H       1.942471        -1.325320       1.035803
H       2.705624        -0.907843       -0.404338
H       1.797461        -2.320554       -0.307385
C       0.610141        -0.573741       -0.444962
H       0.585474        -0.603748       -1.577454
C       -0.642359       -1.229367       0.114202
C       0.685991        0.907308        0.009466
H       -0.891080       -2.164051       -0.440476
H       -0.527904       -1.550900       1.172453
S       -1.994578       -0.040077       -0.092424
O       0.700186        1.786131        -0.889927
H       -2.151344       0.374534        1.189142
O       0.749142        1.189728        1.229655
###
14
cys210 pm6_conformaciones E=-0.203458044934 au
N       1.847761        -1.327821       0.002919
H       1.942212        -1.325900       1.035739
H       2.705563        -0.908028       -0.404166
H       1.797318        -2.320708       -0.307763
C       0.610096        -0.573775       -0.444957
H       0.585313        -0.603748       -1.577461
C       -0.642468       -1.229176       0.114315
C       0.686212        0.907276        0.009424
H       -0.891263       -2.163937       -0.440221
H       -0.528060       -1.550562       1.172625
S       -1.994792       -0.040043       -0.092354
O       0.749541        1.189732        1.229592
H       -2.150359       0.375839        1.188936
O       0.700282        1.786084        -0.889986
###
```

```
14
cys211 pm6_conformaciones E=-0.203459035567 au
N       1.847082        -1.329187       0.002876
H       1.941126        -1.329041       1.035814
H       2.705272        -0.909075       -0.403132
H       1.796464        -2.321639       -0.309358
C       0.609932        -0.573935       -0.444499
H       0.584959        -0.603564       -1.577086
C       -0.643028       -1.228485       0.114775
C       0.687185        0.907179        0.009537
H       -0.891613       -2.163620       -0.439514
H       -0.529071       -1.549270       1.173490
S       -1.995321       -0.039588       -0.092637
O       0.749978        1.190241        1.229560
H       -2.150949       0.377460        1.188226
O       0.701878        1.785749        -0.890216
###
13
cys302 pm6_conformaciones E=-0.346154100133 au
N       0.102772        1.587089        -0.289377
H       -0.225880       1.958620        0.619627
H       -0.376911       2.111553        -1.043901
H       1.130648        1.767766        -0.359576
C       -0.176133       0.101302        -0.401248
H       -0.006433       -0.205022       -1.475281
C       0.760323        -0.678052       0.518272
C       -1.639671       -0.208479       -0.036776
H       0.612829        -0.422109       1.583090
H       0.592086        -1.766319       0.426411
S       2.457150        -0.271209       0.007891
O       -2.148031       -1.262922       -0.499334
O       -2.280376       0.574998        0.707776
###
13
cys304 pm6_conformaciones E=-0.356630623675 au
N       0.754585        1.855661        -0.323459
H       0.363197        1.673593        -1.261862
H       1.780161        1.969442        -0.418561
H       0.359563        2.753486        0.022645
C       0.417135        0.729430        0.631454
H       0.931409        0.943531        1.613660
C       -1.089725       0.617548        0.815082
C       0.915137        -0.628186       0.090180
H       -1.340131       0.183647        1.799181
H       -1.609865       1.590249        0.764564
S       -1.641108       -0.493640       -0.517931
O       0.941314        -1.598437       0.904011
O       1.438187        -0.716324       -1.052613
###
13
cys305 pm6_conformaciones E=-0.346154022842 au
N       0.102814        1.587112        -0.289256
H       -0.225491       1.958581        0.619869
H       -0.377101       2.111614        -1.043556
H       1.130681        1.767690        -0.359788
C       -0.176115       0.101341        -0.401094
H       -0.006356       -0.205009       -1.475118
C       0.760351        -0.677887       0.518447
C       -1.639704       -0.208490       -0.036800
H       0.612917        -0.421714       1.583220
H       0.592103        -1.766177       0.426654
S       2.457117        -0.271229       0.007803
O       -2.280691       0.575108        0.707299
O       -2.147748       -1.263221       -0.499131
###
13
cys310 pm6_conformaciones E=-0.356429717930 au
N       1.975283        -0.982793       0.130582
H       1.888382        -1.004130       1.162444
H       2.777379        -0.375020       -0.114395
H       2.194591        -1.950680       -0.183353
C       0.690995        -0.497027       -0.518210
H       0.858492        -0.479503       -1.633868
C       -0.475103       -1.413841       -0.174733
C       0.357285        0.942415        -0.052150
H       -0.732322       -2.087509       -1.009494
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H       -0.285427       -2.056358       0.704156
S       -1.837983       -0.263079       0.193468
O       0.612436        1.306973        1.131509
O       0.067637        1.799618        -0.939572
###
12
cys400 pm6_conformaciones E=-0.501270170223 au
N       -1.765225       1.417720        -0.064175
H       -1.794744       1.549211        0.949803
H       -1.723277       2.361851        -0.459000
C       -0.534226       0.669056        -0.450110
H       -0.471733       0.683830        -1.571851
C       0.767114        1.207466        0.133677
C       -0.728462       -0.780959       0.005059
H       1.123768        2.092520        -0.417149
H       0.668407        1.505497        1.190283
S       1.975642        -0.155187       -0.004358
O       -0.852037       -1.684750       -0.883921
O       -0.908298       -1.091167       1.220809
###
12
cys401 pm6_conformaciones E=-0.498428140451 au
N       0.815848        1.917067        -0.391894
H       0.471682        1.702254        -1.328905
H       0.338247        2.783833        -0.124077
C       0.410638        0.835857        0.548293
H       0.890641        1.079419        1.537444
C       -1.097811       0.680426        0.734502
C       0.948164        -0.526368       0.092291
H       -1.351446       0.357096        1.757103
H       -1.645850       1.620192        0.560401
S       -1.629051       -0.595097       -0.458945
O       1.041780        -1.442840       0.975997
O       1.468803        -0.729686       -1.046760
###
12
cys402 pm6_conformaciones E=-0.490586801545 au
N       -0.002326       1.632034        -0.402847
H       -0.049846       1.983495        0.556804
H       0.952292        1.845163        -0.716253
C       -0.170226       0.151510        -0.399255
H       -0.000160       -0.206699       -1.450492
C       0.770280        -0.595373       0.547024
C       -1.623353       -0.165444       -0.021450
H       0.664071        -0.260273       1.591787
H       0.579553        -1.681927       0.537119
S       2.473006        -0.278230       -0.020229
O       -2.299220       -0.894403       -0.809459
O       -2.145521       0.269842        1.042798
###
12
cys403 pm6_conformaciones E=-0.501268555786 au
N       -1.765788       1.417033        -0.063988
H       -1.793429       1.551766        0.949630
H       -1.726039       2.359898        -0.462053
C       -0.534539       0.668902        -0.450053
H       -0.471961       0.683651        -1.571771
C       0.766590        1.207557        0.134050
C       -0.728176       -0.781129       0.005227
H       1.122928        2.093020        -0.416307
H       0.667614        1.504979        1.190830
S       1.975701        -0.154555       -0.004639
O       -0.907686       -1.091486       1.220905
O       -0.851446       -1.684971       -0.883847
###
12
cys404 pm6_conformaciones E=-0.498427539739 au
N       0.814262        1.917718        -0.391733
H       0.469141        1.703396        -1.328486
H       0.336750        2.784238        -0.122846
C       0.410304        0.835919        0.548292
H       0.890340        1.079822        1.537449
C       -1.097948       0.679316        0.734847
C       0.948794        -0.525940       0.092382
H       -1.350963       0.355051        1.757302
H       -1.646609       1.618896        0.561613
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S       -1.628960       -0.595630       -0.459296
O       1.470355        -0.728619       -1.046504
O       1.041892        -1.442770       0.975593
###
12
cys405 pm6_conformaciones E=-0.490504042130 au
N       -0.015963       1.616083        0.327619
H       -0.059987       1.515028        1.344684
H       0.935352        1.953218        0.137156
C       -0.175664       0.281074        -0.317474
H       -0.032918       0.419371        -1.422746
C       0.789689        -0.793767       0.179370
C       -1.626971       -0.151752       -0.070014
H       0.674337        -0.993068       1.257403
H       0.630341        -1.750757       -0.345878
S       2.483692        -0.202618       -0.142492
O       -2.010509       -0.554669       1.064312
O       -2.451588       -0.098809       -1.031233
###
12
cys406 pm6_conformaciones E=-0.501269399799 au
N       -1.765635       1.417171        -0.064177
H       -1.793099       1.552548        0.949358
H       -1.726057       2.359769        -0.462867
C       -0.534384       0.668908        -0.450006
H       -0.471551       0.683617        -1.571695
C       0.766661        1.207406        0.134414
C       -0.728314       -0.781087       0.005229
H       1.122985        2.093079        -0.415579
H       0.667612        1.504295        1.191311
S       1.975806        -0.154697       -0.004848
O       -0.907763       -1.091293       1.221025
O       -0.851876       -1.684923       -0.883718
###
12
cys407 pm6_conformaciones E=-0.501268920315 au
N       -1.765651       1.417132        -0.063946
H       -1.793164       1.551904        0.949651
H       -1.725879       2.359978        -0.461999
C       -0.534453       0.668961        -0.450067
H       -0.471950       0.683682        -1.571780
C       0.766739        1.207508        0.133968
C       -0.728289       -0.781094       0.005137
H       1.123201        2.092894        -0.416461
H       0.667894        1.505099        1.190732
S       1.975706        -0.154728       -0.004611
O       -0.907819       -1.091341       1.220921
O       -0.851660       -1.684919       -0.883793
###
12
cys408 pm6_conformaciones E=-0.501267845432 au
N       -1.765956       1.416972        -0.064087
H       -1.794421       1.550021        0.949721
H       -1.725184       2.360493        -0.460470
C       -0.534717       0.668818        -0.450196
H       -0.472366       0.683595        -1.571891
C       0.766409        1.207746        0.133844
C       -0.728040       -0.781220       0.005130
H       1.122721        2.093029        -0.416760
H       0.667521        1.505287        1.190509
S       1.975626        -0.154383       -0.004510
O       -0.851062       -1.685236       -0.883765
O       -0.907502       -1.091409       1.220890
###
12
cys409 pm6_conformaciones E=-0.501268544127 au
N       -1.765893       1.416738        -0.064154
H       -1.793392       1.552139        0.949379
H       -1.726779       2.359329        -0.462895
C       -0.534456       0.668942        -0.450055
H       -0.471450       0.683767        -1.571635
C       0.766559        1.207536        0.134516
C       -0.728065       -0.781045       0.005398
H       1.122737        2.093275        -0.415323
H       0.667271        1.504281        1.191461
S       1.975694        -0.154509       -0.004910
```

```
O       -0.851619       -1.684852       -0.883803
O       -0.907440       -1.091450       1.220990
###
12
cys410 pm6_conformaciones E=-0.501268419202 au
N       -1.765783       1.417012        -0.063914
H       -1.793154       1.552064        0.949672
H       -1.726251       2.359752        -0.462308
C       -0.534573       0.668884        -0.450068
H       -0.472017       0.683578        -1.571771
C       0.766571        1.207580        0.134020
C       -0.728175       -0.781144       0.005218
H       1.122829        2.093042        -0.416347
H       0.667580        1.504946        1.190804
S       1.975693        -0.154534       -0.004655
O       -0.907602       -1.091490       1.220931
O       -0.851465       -1.684990       -0.883830
###
12
cys411 pm6_conformaciones E=-0.501577306356 au
N       1.904805        -1.233190       0.009246
H       1.887464        -1.348210       1.025463
H       1.990153        -2.181732       -0.369449
C       0.622985        -0.634469       -0.459992
H       0.639148        -0.654110       -1.583466
C       -0.645786       -1.318104       0.037214
C       0.588762        0.832640        -0.008959
H       -0.958901       -2.143492       -0.620919
H       -0.540955       -1.734868       1.051698
S       -1.903870       0.006026        0.044374
O       0.589199        1.733939        -0.911303
O       0.750252        1.180802        1.200352
###
# Conformations of GLUTAMIC ACID optimized with pm6
# opt freq pm6 scf=(xqc,tight) scrf(smd,solvent=water)
###
20
glu100 pm6_conformaciones E=-0.183764447762 au
N       -0.628598       1.517551        -0.429242
H       -1.116723       1.950156        -1.240936
H       0.391159        1.724274        -0.515123
H       -0.972905       1.974549        0.438007
C       -0.859654       0.018511        -0.397405
H       -0.616688       -0.394138       -1.434661
C       0.024237        -0.664737       0.659772
C       -2.325095       -0.307734       -0.120030
H       0.130609        -0.022446       1.565599
H       -0.493788       -1.578632       1.045928
C       1.388201        -1.084910       0.125860
O       -2.871787       -1.372166       -0.342824
H       1.788751        -1.927590       0.753851
H       1.301500        -1.556299       -0.889465
C       2.391413        0.013558        0.084059
O       3.671401        -0.304128       -0.303369
O       2.234148        1.197411        0.353582
O       -2.980812       0.740070        0.426726
H       -3.960923       0.548814        0.637789
H       3.810974        -1.279173       -0.542751
###
20
glu102 pm6_conformaciones E=-0.183339360667 au
N       -0.581247       1.686903        -0.141273
H       -1.313706       2.357531        -0.450145
H       0.303820        1.932831        -0.631373
H       -0.427514       1.814892        0.879347
C       -0.973215       0.258140        -0.464998
H       -1.028142       0.152725        -1.600330
C       0.044474        -0.742032       0.107690
C       -2.356064       -0.036087       0.110977
H       0.239091        -0.523578       1.185478
H       -0.420293       -1.759430       0.123095
C       1.337146        -0.809211       -0.700012
O       -2.939769       0.557837        0.996627
H       1.619575        -1.883876       -0.868980
H       1.186564        -0.421146       -1.739854
C       2.494573        -0.110559       -0.066884
```

```
O       2.932266        -0.518917       1.169499
O       3.159362        0.795537        -0.552483
O       -2.899322       -1.105040       -0.520769
H       -3.805602       -1.382038       -0.141797
H       2.413160        -1.293067       1.569839
###
20
glu103 pm6_conformaciones E=-0.184306845110 au
N       -0.602208       1.415630        -0.700087
H       -1.329087       1.912899        -1.253766
H       0.307367        1.528405        -1.193808
H       -0.525316       1.878152        0.228175
C       -0.940115       -0.055354       -0.556730
H       -0.931827       -0.521784       -1.600914
C       0.072216        -0.776521       0.348029
C       -2.344801       -0.252872       0.007560
H       0.192442        -0.221165       1.314201
H       -0.360789       -1.759956       0.661488
C       1.416646        -1.027396       -0.321202
O       -2.906881       -1.322050       0.159472
H       1.752955        -2.078686       -0.097942
H       1.315077        -1.037445       -1.439388
C       2.533697        -0.113358       0.053289
O       2.438727        0.718384        1.136682
O       3.612424        -0.040531       -0.528628
O       -2.931281       0.922039        0.327858
H       -3.865883       0.818095        0.724888
H       1.530747        0.702346        1.608937
###
20
glu104 pm6_conformaciones E=-0.185630289992 au
N       -1.373554       1.796075        -0.732467
H       -1.983733       1.717533        -1.572101
H       -0.571978       2.417222        -0.975092
H       -1.916105       2.255448        0.026130
C       -0.864263       0.433482        -0.304478
H       -0.287338       -0.013113       -1.180319
C       0.048457        0.544322        0.929605
C       -2.038230       -0.485604       0.019132
H       -0.340826       1.317322        1.637227
H       0.010586        -0.402408       1.519831
C       1.490990        0.872209        0.568189
O       -3.156369       -0.181948       0.385263
H       1.552046        1.753692        -0.125538
H       2.032125        1.241798        1.481195
C       2.226974        -0.277423       -0.026246
O       3.580841        -0.139429       -0.223405
O       1.785672        -1.361774       -0.387723
O       -1.663394       -1.777893       -0.145918
H       -2.399930       -2.443271       0.092587
H       3.962477        0.749685        0.080402
###
20
glu105 pm6_conformaciones E=-0.185544260785 au
N       1.487455        1.756634        0.233823
H       2.108886        1.837617        1.064232
H       0.762014        2.500569        0.297504
H       2.056207        1.936812        -0.617210
C       0.833958        0.388947        0.179587
H       0.269661        0.235635        1.163212
C       -0.134206       0.290978        -1.011317
C       1.870523        -0.725940       0.100540
H       0.293832        0.813694        -1.902581
H       -0.223042       -0.770817       -1.344513
C       -1.514137       0.865715        -0.704717
O       1.632452        -1.920173       0.093651
H       -1.442338       1.828195        -0.136953
H       -2.014640       1.170990        -1.660545
C       -2.381100       -0.118922       0.010957
O       -2.509367       -0.025716       1.370708
O       -3.025155       -1.032429       -0.493358
O       3.132728        -0.246549       0.056956
H       3.844909        -0.977586       0.032809
H       -1.963164       0.722726        1.793333
###
20
```

glu106 pm6_conformaciones E=-0.185665808939 au
N -0.983252 1.734971 -0.181275
H -1.592131 2.005716 -0.980626
H -0.086738 2.258704 -0.272978
H -1.446819 2.038408 0.697437
C -0.721627 0.242535 -0.181546
H -0.141156 -0.009874 -1.131963
C 0.074454 -0.190634 1.061265
C -2.023865 -0.551182 -0.229039
H -0.452729 0.141775 1.990354
H 0.075577 -1.306001 1.124798
C 1.504260 0.335081 1.096105
O -2.133638 -1.722913 -0.538326
H 1.528338 1.455118 1.110030
H 1.971344 0.058311 2.078715
C 2.347148 -0.200049 -0.013744
O 2.532636 0.579723 -1.125457
O 2.928782 -1.277448 -0.054558
O -3.087873 0.202562 0.127255
H -3.972505 -0.307160 0.106434
H 1.998105 1.450310 -1.122828
###
20
glu107 pm6_conformaciones E=-0.185487665179 au
N -0.935899 1.829174 -0.008650
H -1.518776 2.194561 -0.788920
H -0.011818 2.310553 -0.049304
H -1.393315 2.086301 0.888396
C -0.748187 0.329307 -0.122980
H -0.202224 0.114258 -1.103130
C 0.054563 -0.226488 1.065020
C -2.111215 -0.350967 -0.201897
H -0.444445 0.047856 2.027674
H 0.015654 -1.342616 1.037702
C 1.502660 0.245486 1.111340
O -3.207692 0.175266 -0.186352
H 1.570487 1.357482 1.226805
H 1.980350 -0.134935 2.053386
C 2.303444 -0.216762 -0.060720
O 2.493616 0.638197 -1.114439
O 2.853767 -1.303370 -0.199393
O -1.963663 -1.692008 -0.318933
H -2.852315 -2.190013 -0.379812
H 1.991880 1.524195 -1.043884
###
20
glu108 pm6_conformaciones E=-0.184847448172 au
N 2.056165 1.849726 -0.041949
H 3.030536 1.807421 0.320168
H 1.615997 2.722507 0.323377
H 2.096414 1.924995 -1.077826
C 1.252968 0.642362 0.400818
H 1.205041 0.652822 1.541007
C -0.165882 0.707953 -0.187403
C 1.948389 -0.638192 -0.052434
H -0.531683 1.765421 -0.175276
H -0.156209 0.424777 -1.266004
C -1.124454 -0.180643 0.604424
O 2.732262 -0.775038 -0.973308
H -0.713287 -1.215761 0.716618
H -1.223042 0.185811 1.660060
C -2.468550 -0.235732 -0.041684
O -3.255261 0.888389 -0.038691
O -2.987905 -1.201417 -0.588638
O 1.569979 -1.676448 0.728865
H 1.997682 -2.562624 0.452623
H -2.842037 1.688182 0.430748
###
20
glu109 pm6_conformaciones E=-0.184031849945 au
N 0.961331 1.842934 -0.159970
H 1.773198 2.078712 -0.765925
H 0.781297 2.653368 0.470235
H 0.123959 1.716985 -0.769049
C 1.236284 0.597247 0.660183
H 2.127353 0.831506 1.342845

```
C       0.041421        0.228459        1.553323
C       1.667128        -0.572240       -0.213679
H       0.441326        -0.282816       2.466273
H       -0.423421       1.158906        1.962005
C       -1.022121       -0.670402       0.936327
O       2.096114        -1.639782       0.184598
H       -0.583435       -1.621549       0.537396
H       -1.687211       -1.054115       1.762005
C       -1.869014       -0.032190       -0.106626
O       -2.922278       -0.759665       -0.610197
O       -1.761088       1.079794        -0.608915
O       1.535774        -0.299952       -1.531871
H       1.854747        -1.054714       -2.139917
H       -3.047504       -1.675227       -0.192166
###
20
glu110 pm6_conformaciones E=-0.185771376517 au
N       1.409207        1.732153        0.440786
H       2.301688        1.971019        0.916904
H       0.645212        2.276951        0.894359
H       1.473818        2.038259        -0.550383
C       1.122260        0.245874        0.539984
H       1.057954        -0.025259       1.649152
C       -0.194166       -0.107652       -0.169140
C       2.255470        -0.585387       -0.051891
H       -0.285790       0.462232        -1.126519
H       -0.179890       -1.180482       -0.480284
C       -1.404232       0.148030        0.728683
O       2.380665        -1.791400       0.051707
H       -1.328903       -0.446277       1.673022
H       -1.431454       1.212639        1.082450
C       -2.679167       -0.175955       0.022934
O       -3.120372       0.658418        -0.973705
O       -3.424815       -1.122557       0.243571
O       3.147660        0.173480        -0.728857
H       3.915726        -0.364425       -1.132193
H       -2.498908       1.437288        -1.177151
###
20
glu111 pm6_conformaciones E=-0.185598018876 au
N       1.631503        1.797312        -0.624976
H       2.654404        1.937635        -0.758226
H       1.216473        2.710068        -0.338389
H       1.219581        1.535268        -1.540864
C       1.362154        0.749566        0.437162
H       1.895466        1.085467        1.393126
C       -0.134477       0.624606        0.749517
C       1.960948        -0.588734       0.017939
H       -0.246280       0.020599        1.683272
H       -0.534336       1.633849        1.015073
C       -0.962770       0.004472        -0.372804
O       2.357756        -0.918319       -1.083403
H       -0.861781       0.582410        -1.330812
H       -0.583330       -1.015501       -0.642437
C       -2.407382       -0.070994       -0.020875
O       -3.213287       -0.879810       -0.788542
O       -3.009573       0.509466        0.873818
O       2.017843        -1.421148       1.085420
H       2.419897        -2.332705       0.863922
H       -2.733362       -1.373284       -1.533817
###
20
glu112 pm6_conformaciones E=-0.185381642109 au
N       -1.425415       1.798354        0.213167
H       -2.297879       2.201773        -0.185432
H       -0.649227       2.465385        0.018040
H       -1.540477       1.730352        1.243658
C       -1.124642       0.444223        -0.399025
H       -0.983609       0.591588        -1.525093
C       0.142260        -0.177380       0.209009
C       -2.289657       -0.523946       -0.219978
H       0.108920        -0.124654       1.322807
H       0.163838        -1.269417       -0.026285
C       1.410399        0.486185        -0.321433
O       -2.407999       -1.603410       -0.769668
H       1.387474        0.555826        -1.441923
```

```
H       1.469109        1.561977        -0.002805
C       2.645070        -0.217524       0.117028
O       3.846028        0.232585        -0.383201
O       2.759738        -1.162081       0.887571
O       -3.216196       -0.053217       0.645812
H       -4.004811       -0.686457       0.784313
H       3.771420        1.004785        -1.037169
###
20
glu113 pm6_conformaciones E=-0.186207092630 au
N       2.170606        -1.551459       -0.440647
H       2.760793        -1.303813       -1.261205
H       1.823694        -2.525174       -0.577405
H       2.771684        -1.548477       0.407805
C       1.003347        -0.592908       -0.302499
H       0.405686        -0.628064       -1.271009
C       0.112630        -1.012023       0.880555
C       1.530830        0.825207        -0.090749
H       -0.226023       -2.065982       0.733890
H       0.709852        -1.044223       1.824491
C       -1.084864       -0.093740       1.079447
O       2.462098        1.178508        0.607110
H       -1.591242       -0.352813       2.052635
H       -0.769109       0.966517        1.256423
C       -2.095085       -0.172565       -0.011038
O       -3.005237       0.851803        -0.125452
O       -2.245447       -1.057875       -0.843938
O       0.785327        1.701054        -0.802485
H       1.069927        2.674177        -0.678721
H       -2.924588       1.576321        0.581450
###
20
glu114 pm6_conformaciones E=-0.183805968638 au
N       -2.204481       1.520299        -0.404576
H       -2.887390       1.239141        -1.137799
H       -1.845982       2.470374        -0.642769
H       -2.707735       1.590860        0.502894
C       -1.052908       0.536351        -0.325760
H       -0.584323       0.475551        -1.364313
C       -0.007834       0.993470        0.708114
C       -1.585886       -0.846037       0.040258
H       -0.359579       1.905884        1.253547
H       0.104979        0.244242        1.527951
C       1.344477        1.297328        0.071306
O       -2.595027       -1.117497       0.661896
H       1.224919        1.874516        -0.878913
H       1.920139        1.999643        0.731858
C       2.146375        0.060723        -0.165698
O       2.710868        -0.576296       0.912077
O       2.385786        -0.480829       -1.238244
O       -0.747781       -1.801443       -0.428221
H       -1.049017       -2.749788       -0.197439
H       2.519252        -0.135010       1.807626
###
20
glu115 pm6_conformaciones E=-0.185794845775 au
N       -1.640584       1.803919        -0.217362
H       -2.667133       1.972604        -0.206409
H       -1.198424       2.542945        -0.804596
H       -1.287421       1.911572        0.753611
C       -1.324008       0.431778        -0.778206
H       -1.821006       0.358526        -1.810138
C       0.185149        0.230526        -0.969146
C       -1.924799       -0.684910       0.064652
H       0.340339        -0.701916       -1.563580
H       0.579479        1.050731        -1.619309
C       0.979862        0.169792        0.332909
O       -1.784203       -1.878957       -0.125778
H       0.877076        1.122379        0.914488
H       0.570373        -0.604374       1.035404
C       2.416857        -0.137356       0.089867
O       3.336990        0.333637        0.996224
O       2.915856        -0.785654       -0.822123
O       -2.685643       -0.206346       1.075704
H       -3.116948       -0.935761       1.643380
H       2.945389        0.895440        1.746010
```

```
###
20
glu116 pm6_conformaciones E=-0.184738932964 au
N       -1.060201       1.713670        0.927427
H       -1.924195       1.731403        1.509611
H       -0.874914       2.687535        0.601331
H       -0.264613       1.425898        1.532665
C       -1.235326       0.795614        -0.263921
H       -2.203952       1.104546        -0.792322
C       -0.095643       0.927249        -1.288843
C       -1.399620       -0.649404       0.198829
H       -0.181248       0.099458        -2.032660
H       -0.278111       1.854716        -1.891926
C       1.320877        0.999653        -0.734021
O       -0.904993       -1.188124       1.172006
H       2.022229        1.270476        -1.572144
H       1.448392        1.866994        -0.038050
C       1.793457        -0.276493       -0.124024
O       2.139420        -0.282228       1.201049
O       1.935757        -1.356335       -0.685299
O       -2.200903       -1.314335       -0.663866
H       -2.356944       -2.291076       -0.409373
H       1.978057        0.602805        1.681642
###
20
glu117 pm6_conformaciones E=-0.184286541704 au
N       2.691411        -0.957761       -0.033016
H       3.429271        -0.403617       -0.513738
H       2.819107        -1.960153       -0.296278
H       2.838003        -0.879565       0.993281
C       1.307217        -0.486415       -0.435792
H       1.227809        -0.562490       -1.571395
C       0.234441        -1.375151       0.217920
C       1.128085        0.970707        -0.016374
H       0.579160        -2.441740       0.193286
H       0.139652        -1.151500       1.307992
C       -1.112258       -1.291571       -0.486879
O       1.546993        1.520390        0.983297
H       -0.983533       -1.230886       -1.597736
H       -1.661844       -2.266647       -0.354650
C       -2.010485       -0.199919       -0.012467
O       -2.093506       0.082581        1.326277
O       -2.738637       0.493632        -0.714248
O       0.385183        1.627967        -0.939625
H       0.192295        2.599245        -0.691126
H       -1.502060       -0.500789       1.917433
###
19
glu200 pm6_conformaciones E=-0.364857166437 au
N       0.541942        1.639576        -0.810919
H       0.094813        1.021094        -1.510655
H       1.293360        2.173227        -1.290567
H       -0.173218       2.319388        -0.476500
C       1.108507        0.845999        0.347599
H       1.780957        1.546347        0.938640
C       0.013802        0.337724        1.292981
C       1.980255        -0.319405       -0.165832
H       0.505381        0.022537        2.247178
H       -0.635269       1.192744        1.611542
C       -0.834799       -0.817223       0.775702
O       1.872986        -0.695134       -1.357429
H       -0.219625       -1.569438       0.224291
H       -1.214105       -1.410602       1.657251
C       -2.023915       -0.450425       -0.046208
O       -2.634959       0.763383        0.109552
O       -2.574289       -1.180627       -0.865984
O       2.771039        -0.856540       0.650333
H       -2.167199       1.398995        0.758021
###
19
glu201 pm6_conformaciones E=-0.365354783571 au
N       0.842307        1.764786        0.657713
H       0.117070        1.875445        -0.077934
H       1.676577        2.313480        0.373466
H       0.469321        2.173899        1.539728
C       1.198863        0.305090        0.858514
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H       2.022907        0.268263        1.640147
C       0.009897        -0.500758       1.395944
C       1.756136        -0.297213       -0.448626
H       0.416166        -1.343114       2.010076
H       -0.555823       0.108070        2.142187
C       -0.950889       -1.091258       0.366346
O       1.361176        0.152432        -1.553292
H       -0.415248       -1.675048       -0.422863
H       -1.567235       -1.882989       0.871711
C       -1.831362       -0.078506       -0.284727
O       -3.187289       -0.219092       -0.191408
O       -1.473821       0.897206        -0.940558
O       2.592687        -1.228759       -0.357974
H       -3.497783       -1.029926       0.340630
###
19
glu202 pm6_conformaciones E=-0.368497198393 au
N       -2.383854       -0.924091       -0.494605
H       -1.990709       -0.840864       -1.448555
H       -3.260389       -0.369137       -0.457602
H       -2.628302       -1.924093       -0.338233
C       -1.401764       -0.448027       0.555908
H       -1.932408       -0.486316       1.560257
C       -0.181550       -1.374093       0.632040
C       -0.991439       1.014328        0.300453
H       0.344371        -1.199218       1.600793
H       -0.532012       -2.433822       0.714110
C       0.797932        -1.270714       -0.535646
O       -1.205554       1.537383        -0.820530
H       1.386918        -2.225672       -0.607917
H       0.271734        -1.229266       -1.519071
C       1.737945        -0.121821       -0.394246
O       2.689069        -0.151159       0.589539
O       1.759648        0.902956        -1.071449
O       -0.423446       1.634351        1.235860
H       2.703295        -1.009260       1.140049
###
19
glu203 pm6_conformaciones E=-0.364699235695 au
N       2.358897        -0.935683       0.569528
H       1.919149        -0.949382       1.509444
H       3.193430        -0.322350       0.614028
H       2.680277        -1.902354       0.356506
C       1.383187        -0.457328       -0.489549
H       1.926547        -0.456363       -1.489933
C       0.201161        -1.422836       -0.607003
C       0.993195        1.008936        -0.206738
H       -0.262863       -1.298324       -1.615821
H       0.577153        -2.475475       -0.620725
C       -0.852460       -1.283555       0.486214
O       -0.218542       1.356991        -0.221800
H       -1.481656       -2.213140       0.522695
H       -0.384281       -1.248673       1.499882
C       -1.754964       -0.111712       0.294903
O       -2.310387       0.122959        -0.947286
O       -2.202873       0.628486        1.173095
O       1.916858        1.831578        0.001329
H       -1.981189       -0.505302       -1.672422
###
19
glu204 pm6_conformaciones E=-0.365990914885 au
N       2.085749        1.766099        -0.368608
H       2.147902        1.613171        -1.392546
H       3.051547        1.799246        0.012131
H       1.646514        2.696252        -0.213876
C       1.274036        0.678212        0.307212
H       1.269448        0.888101        1.419595
C       -0.165111       0.695597        -0.221348
C       1.937900        -0.700798       0.066437
H       -0.580583       1.730258        -0.137555
H       -0.186004       0.465272        -1.310310
C       -1.049610       -0.282599       0.553308
O       2.413244        -1.298490       1.064062
H       -0.643915       -1.321791       0.513863
H       -1.052970       -0.035794       1.646412
C       -2.442743       -0.266495       0.017062
```

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O       -3.252459       0.803961        0.300062
O       -2.979875       -1.126843       -0.670653
O       1.974301        -1.185976       -1.090185
H       -2.820700       1.517870        0.880226
###
19
glu205 pm6_conformaciones E=-0.368382737940 au
N       -1.998218       1.542742        -0.791727
H       -2.572988       1.780375        0.037669
H       -2.625920       1.164624        -1.526811
H       -1.579878       2.425392        -1.153777
C       -0.911327       0.546674        -0.444753
H       -0.317678       0.345225        -1.386563
C       0.009249        1.137727        0.633761
C       -1.533557       -0.784307       0.041465
H       0.487116        2.070273        0.248714
H       -0.588540       1.476904        1.513757
C       1.081522        0.163175        1.114455
O       -2.475636       -0.768311       0.865856
H       1.657483        0.636526        1.954692
H       0.637335        -0.741215       1.594015
C       2.003809        -0.234559       0.010185
O       3.088413        0.549474        -0.268712
O       1.895892        -1.219182       -0.715807
O       -1.033464       -1.847814       -0.408022
H       3.190790        1.357105        0.343180
###
19
glu206 pm6_conformaciones E=-0.367627061140 au
N       2.249913        -1.424478       -0.425900
H       2.845365        -1.340458       0.418976
H       2.819794        -1.157969       -1.251528
H       1.985152        -2.425710       -0.527699
C       1.014728        -0.553222       -0.317858
H       0.426203        -0.664372       -1.276816
C       0.161163        -1.010655       0.874485
C       1.419944        0.931160        -0.162660
H       -0.142143       -2.074260       0.729978
H       0.771487        -1.024100       1.808550
C       -1.068917       -0.139570       1.100166
O       0.764839        1.781420        -0.815621
H       -1.588464       -0.469467       2.044214
H       -0.790384       0.915263        1.346105
C       -2.049576       -0.189747       -0.017732
O       -2.963764       0.832067        -0.126332
O       -2.165182       -1.045636       -0.886197
O       2.362686        1.240128        0.604623
H       -2.929083       1.520795        0.619338
###
19
glu207 pm6_conformaciones E=-0.367531936279 au
N       2.602528        -1.002115       0.316281
H       2.431350        -1.015374       1.339302
H       3.445926        -0.425480       0.134393
H       2.806640        -1.978675       0.017352
C       1.402872        -0.458663       -0.433366
H       1.658378        -0.442228       -1.535844
C       0.194735        -1.381603       -0.204053
C       1.093874        0.984933        0.021179
H       0.451927        -2.408039       -0.565907
H       0.003243        -1.519860       0.885668
C       -1.064270       -0.909419       -0.926821
O       0.738174        1.804244        -0.867497
H       -0.818078       -0.397924       -1.888236
H       -1.660100       -1.801474       -1.260949
C       -1.921033       -0.038218       -0.070031
O       -2.583347       -0.589727       0.991705
O       -2.119229       1.166267        -0.204498
O       1.169552        1.295149        1.231828
H       -2.415249       -1.585778       1.126511
###
19
glu208 pm6_conformaciones E=-0.367395099546 au
N       -2.540594       -1.165393       -0.417402
H       -2.350898       -1.120819       -1.436153
H       -3.424415       -0.656242       -0.228234
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H       -2.683215       -2.165886       -0.165846
C       -1.394615       -0.578691       0.382296
H       -1.646122       -0.686110       1.481102
C       -0.103258       -1.356960       0.080658
C       -1.225511       0.921390        0.060785
H       -0.263151       -2.432669       0.340828
H       0.100416        -1.371785       -1.014624
C       1.104843        -0.838812       0.860543
O       -1.316434       1.333233        -1.119878
H       0.802618        -0.329492       1.807644
H       1.711176        -1.707621       1.229080
C       1.950859        0.070333        0.031503
O       3.015265        -0.453741       -0.650386
O       1.808090        1.278355        -0.136010
O       -0.958558       1.689326        1.022322
H       3.156936        -1.452574       -0.515089
###
19
glu209 pm6_conformaciones E=-0.365178010484 au
N       -2.137457       1.772765        0.096746
H       -2.239871       1.747090        1.128183
H       -3.086487       1.743460        -0.323806
H       -1.705038       2.685269        -0.156227
C       -1.283940       0.626802        -0.407613
H       -1.230667       0.702168        -1.535734
C       0.127577        0.729729        0.183176
C       -1.939122       -0.725177       -0.029604
H       0.512254        1.770968        0.056243
H       0.103323        0.564114        1.283428
C       1.081114        -0.255647       -0.494092
O       -2.126983       -1.011159       1.176517
H       0.716212        -1.310407       -0.404757
H       1.113075        -0.077711       -1.598454
C       2.441129        -0.168414       0.112794
O       3.505638        0.129269        -0.699395
O       2.746595        -0.341383       1.286456
O       -2.255728       -1.497166       -0.968687
H       3.262672        0.285453        -1.673190
###
19
glu210 pm6_conformaciones E=-0.365005371646 au
N       2.251119        -1.617847       -0.411020
H       2.379414        -1.867908       0.586951
H       3.183333        -1.406821       -0.814005
H       1.868578        -2.450999       -0.902780
C       1.317435        -0.433446       -0.564277
H       1.226995        -0.201219       -1.668764
C       -0.061685       -0.780937       0.013884
C       1.907375        0.802612        0.151383
H       -0.349599       -1.813864       -0.295447
H       -0.021448       -0.811684       1.125906
C       -1.124365       0.209890        -0.458055
O       2.746137        0.639175        1.071929
H       -0.833916       1.262667        -0.207507
H       -1.191845       0.217092        -1.578414
C       -2.463495       -0.083568       0.119223
O       -3.510858       0.731656        -0.244249
O       -2.784773       -0.975125       0.894667
O       1.524773        1.935281        -0.226790
H       -3.273163       1.462456        -0.906202
###
19
glu211 pm6_conformaciones E=-0.364959030409 au
N       -1.634292       1.769995        -0.458664
H       -2.174748       2.013076        0.392423
H       -2.292829       1.731567        -1.260674
H       -0.957771       2.541023        -0.635025
C       -0.901789       0.453916        -0.291518
H       -0.316153       0.264741        -1.241533
C       0.050807        0.510791        0.909400
C       -1.911320       -0.708736       -0.117930
H       -0.362087       1.172808        1.709267
H       0.113433        -0.489167       1.402366
C       1.444390        0.999186        0.526663
O       -1.828835       -1.656715       -0.938354
H       1.384954        1.884382        -0.155464
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H       1.967539        1.405333        1.434267
C       2.299169        -0.060774       -0.081630
O       2.414395        -1.276288       0.550846
O       2.959237        0.023244        -1.109447
O       -2.755071       -0.679902       0.808150
H       1.872352        -1.362738       1.405551
###
19
glu212 pm6_conformaciones E=-0.368555945231 au
N       2.745198        0.817027        -0.014184
H       2.885959        0.602810        -1.018691
H       3.429797        0.262573        0.535138
H       2.961326        1.825864        0.127384
C       1.326896        0.513727        0.423557
H       1.243231        0.758820        1.525629
C       0.337283        1.383957        -0.368613
C       1.017378        -0.986718       0.223986
H       0.687934        2.446463        -0.350004
H       0.344393        1.109395        -1.446321
C       -1.077318       1.337369        0.196503
O       1.273421        -1.539641       -0.873920
H       -1.071388       1.432193        1.313685
H       -1.634504       2.264818        -0.117893
C       -1.866916       0.152046        -0.229384
O       -3.036325       -0.127257       0.431375
O       -1.612195       -0.652041       -1.122888
O       0.475156        -1.601348       1.177246
H       -3.287543       0.537880        1.159563
###
19
glu214 pm6_conformaciones E=-0.365585361454 au
N       -2.148854       1.749282        0.177267
H       -2.284117       1.644141        1.199873
H       -3.084223       1.755860        -0.273380
H       -1.704526       2.674112        0.008610
C       -1.288700       0.633487        -0.381666
H       -1.236469       0.762063        -1.504639
C       0.121748        0.716568        0.217436
C       -1.932954       -0.736571       -0.065817
H       0.517333        1.752271        0.084612
H       0.090507        0.561065        1.319993
C       1.064466        -0.297284       -0.432100
O       -1.911764       -1.610723       -0.966446
H       0.780529        -1.341019       -0.152414
H       0.968597        -0.278571       -1.549419
C       2.482257        -0.005231       -0.069970
O       3.190811        -0.941688       0.639872
O       3.128891        0.998542        -0.344640
O       -2.451097       -0.930732       1.060350
H       2.658730        -1.763908       0.905508
###
19
glu215 pm6_conformaciones E=-0.365336224908 au
N       0.668840        1.519844        0.890927
H       0.271786        1.796088        -0.027339
H       1.466148        2.147941        1.101773
H       -0.064183       1.673065        1.613233
C       1.114754        0.072120        0.883955
H       1.641625        -0.132374       1.871005
C       -0.079428       -0.881827       0.780039
C       2.149183        -0.166045       -0.234822
H       0.296996        -1.926777       0.884590
H       -0.729737       -0.748104       1.677549
C       -0.892250       -0.760906       -0.510251
O       2.494974        0.798955        -0.959439
H       -0.348244       -0.183643       -1.296750
H       -1.016728       -1.770550       -0.982257
C       -2.248183       -0.186176       -0.260170
O       -2.545265       1.058888        -0.742788
O       -3.176003       -0.728784       0.331524
O       2.638671        -1.316677       -0.360876
H       -1.763020       1.543398        -1.178169
###
19
glu216 pm6_conformaciones E=-0.365553709465 au
N       -1.533740       1.808630        -0.147884
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H       -1.690909       1.943666        0.867749
H       -2.395952       2.091848        -0.652170
H       -0.768838       2.449910        -0.439526
C       -1.174965       0.371320        -0.462066
H       -1.074014       0.274497        -1.585947
C       0.136716        -0.038520       0.216708
C       -2.305553       -0.576899       0.006537
H       0.138732        0.278556        1.286383
H       0.197318        -1.152967       0.249083
C       1.358675        0.521969        -0.510388
O       -2.595909       -1.539223       -0.747497
H       1.241742        0.416162        -1.618563
H       1.440697        1.631940        -0.361245
C       2.634509        -0.116934       -0.077372
O       2.902775        -0.268448       1.258830
O       3.524853        -0.531016       -0.812302
O       -2.885974       -0.368467       1.097374
H       2.185157        0.097598        1.877661
###
19
glu217 pm6_conformaciones E=-0.366346115114 au
N       1.507840        1.806621        -0.337305
H       1.688285        1.678353        -1.349683
H       2.348429        2.244479        0.088632
H       0.716358        2.474186        -0.237717
C       1.186712        0.489574        0.338102
H       1.052019        0.691416        1.444193
C       -0.087059       -0.141853       -0.236397
C       2.360548        -0.502106       0.156396
H       -0.102514       -0.058348       -1.347077
H       -0.078018       -1.238988       -0.030695
C       -1.350725       0.475667        0.360248
O       2.937856        -0.581354       -0.954179
H       -1.304020       0.474729        1.481035
H       -1.424407       1.568112        0.111709
C       -2.585935       -0.212704       -0.100762
O       -3.767537       0.093435        0.535818
O       -2.714268       -1.040087       -0.995017
O       2.680933        -1.212393       1.141777
H       -3.688140       0.791439        1.268024
###
18
glu300 pm6_conformaciones E=-0.545091223427 au
N       -2.122157       1.747424        0.172622
H       -2.225349       1.657486        1.200163
H       -3.070608       1.733526        -0.249997
H       -1.697506       2.676301        -0.024009
C       -1.260534       0.638307        -0.396226
H       -1.250137       0.749316        -1.521667
C       0.170580        0.750720        0.149451
C       -1.854513       -0.742633       -0.035365
H       0.548030        1.786373        -0.016170
H       0.176740        0.616938        1.253903
C       1.099840        -0.260433       -0.519565
O       -2.236877       -0.970489       1.137286
H       0.739669        -1.299935       -0.366570
H       1.101376        -0.127996       -1.626114
C       2.510134        -0.117418       0.000846
O       3.036231        -1.062540       0.660953
O       3.173852        0.933966        -0.232394
O       -1.905726       -1.605340       -0.947437
###
18
glu301 pm6_conformaciones E=-0.544598008016 au
N       1.689565        1.726149        -0.524737
H       1.422616        1.415267        -1.476471
H       2.709886        1.920002        -0.523907
H       1.191331        2.617750        -0.330537
C       1.339559        0.682811        0.515038
H       1.836544        0.988956        1.487969
C       -0.174569       0.606282        0.749881
C       1.889142        -0.703693       0.119209
H       -0.360181       -0.093393       1.596981
H       -0.538921       1.595477        1.111140
C       -0.967993       0.171354        -0.479932
O       2.205535        -0.937118       -1.071349
```

```
H       -0.960741       0.970201        -1.260346
H       -0.495836       -0.702440       -0.977284
C       -2.403689       -0.144933       -0.139712
O       -2.933787       -1.202381       -0.594927
O       -3.094486       0.646287        0.567542
O       1.981943        -1.565012       1.031074
###
18
glu303 pm6_conformaciones E=-0.543243596411 au
N       -1.368271       1.789298        -0.338534
H       -1.424420       2.057611        0.661222
H       -2.250685       2.078189        -0.803059
H       -0.589920       2.327346        -0.769714
C       -1.136926       0.300071        -0.495850
H       -1.100058       0.071645        -1.603735
C       0.173850        -0.132488       0.174429
C       -2.310975       -0.490402       0.126923
H       0.290919        0.373943        1.159564
H       0.122257        -1.217939       0.422607
C       1.386101        0.131513        -0.717926
O       -2.644962       -1.564032       -0.434416
H       1.340293        -0.489920       -1.639006
H       1.388471        1.179106        -1.094045
C       2.666236        -0.141804       0.034916
O       3.232956        0.795867        0.672762
O       3.186311        -1.295148       0.022622
O       -2.882889       -0.049988       1.151652
###
18
glu304 pm6_conformaciones E=-0.552317130297 au
N       2.322488        -0.740158       0.613905
H       1.779078        -0.940588       1.471779
H       3.038352        -0.024562       0.844497
H       2.816771        -1.614744       0.339518
C       1.428590        -0.267083       -0.512699
H       2.083306        -0.127369       -1.430319
C       0.351852        -1.313109       -0.842494
C       0.789768        1.092434        -0.185151
H       -0.087594       -1.070290       -1.835176
H       0.844694        -2.303380       -1.002734
C       -0.746128       -1.468206       0.205456
O       0.777830        1.523016        0.993901
H       -1.315932       -2.409876       0.004262
H       -0.316869       -1.643607       1.216369
C       -1.718254       -0.318633       0.226755
O       -2.262927       0.100262        -0.839421
O       -1.979266       0.271467        1.319700
O       0.247589        1.725643        -1.131271
###
18
glu305 pm6_conformaciones E=-0.543748254633 au
N       0.579798        1.704907        0.784953
H       -0.134479       1.783044        0.028917
H       1.352968        2.363350        0.572771
H       0.133790        2.001375        1.677970
C       1.089783        0.282966        0.899032
H       1.870976        0.271596        1.722290
C       -0.036711       -0.682685       1.295736
C       1.763468        -0.174459       -0.411167
H       0.428772        -1.564410       1.798187
H       -0.657946       -0.221482       2.098710
C       -0.929577       -1.182847       0.162527
O       1.348302        0.259549        -1.517305
H       -0.336509       -1.555953       -0.700074
H       -1.471209       -2.095481       0.505240
C       -1.921533       -0.145997       -0.308775
O       -1.524882       0.853109        -0.985439
O       -3.147918       -0.288017       -0.048123
O       2.694807        -1.011924       -0.326982
###
18
glu306 pm6_conformaciones E=-0.543888722076 au
N       1.665823        1.799522        0.193898
H       1.328387        1.914077        -0.778944
H       2.693119        1.945431        0.192864
H       1.234139        2.546721        0.774682
```

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C       1.316902        0.430433        0.741225
H       1.799254        0.337223        1.765408
C       -0.198199       0.265560        0.904272
C       1.917001        -0.676098       -0.148026
H       -0.383264       -0.611018       1.565684
H       -0.606972       1.136529        1.468300
C       -0.944847       0.095805        -0.417141
O       1.694968        -1.871980       0.166317
H       -0.763482       0.964039        -1.088532
H       -0.567167       -0.781155       -0.990151
C       -2.427088       -0.081013       -0.192955
O       -2.868741       -0.990216       0.569903
O       -3.239066       0.682393        -0.796004
O       2.615667        -0.352275       -1.139073
###
18
glu307 pm6_conformaciones E=-0.543930011532 au
N       1.701265        1.792258        0.155616
H       1.351324        1.901654        -0.813372
H       2.731937        1.909422        0.137238
H       1.298680        2.559360        0.731204
C       1.322923        0.442757        0.729962
H       1.804288        0.358348        1.755485
C       -0.195061       0.314517        0.896978
C       1.894303        -0.697414       -0.136135
H       -0.399018       -0.572122       1.539033
H       -0.578359       1.182229        1.483345
C       -0.952824       0.199031        -0.424516
O       2.605204        -0.413854       -1.130327
H       -0.828867       1.122976        -1.031354
H       -0.537241       -0.609668       -1.066703
C       -2.417991       -0.079834       -0.190669
O       -2.786731       -1.087496       0.482419
O       -3.285565       0.696987        -0.688160
O       1.634629        -1.879681       0.201329
###
18
glu309 pm6_conformaciones E=-0.548618006287 au
N       2.370843        1.218230        0.368355
H       2.837829        1.173996        -0.556698
H       3.001964        0.790593        1.071531
H       2.247350        2.222720        0.613915
C       1.030951        0.509101        0.341307
H       0.594903        0.574435        1.383697
C       0.087756        1.182332        -0.671726
C       1.228496        -0.982226       -0.003928
H       0.487425        2.181050        -0.975134
H       0.059524        0.609497        -1.623656
C       -1.323047       1.385925        -0.121329
O       0.293421        -1.784771       0.266584
H       -1.299336       1.957448        0.831913
H       -1.902755       2.040748        -0.813347
C       -2.040111       0.074226        0.055057
O       -2.205122       -0.419522       1.211892
O       -2.451881       -0.572608       -0.955620
O       2.297698        -1.359879       -0.536230
###
18
glu310 pm6_conformaciones E=-0.551282269303 au
N       -2.719209       0.579537        -0.094284
H       -2.884180       0.467562        0.923287
H       -3.308697       -0.111947       -0.596909
H       -3.040452       1.533127        -0.364347
C       -1.256170       0.401253        -0.441674
H       -1.144648       0.554728        -1.557120
C       -0.404029       1.439990        0.308800
C       -0.790639       -1.026489       -0.083686
H       -0.865945       2.450739        0.188643
H       -0.430311       1.250157        1.402909
C       1.032856        1.503506        -0.198147
O       -0.211856       -1.694979       -0.982095
H       1.051937        1.743764        -1.284849
H       1.553304        2.373427        0.273609
C       1.833515        0.258776        0.078944
O       2.455830        -0.305397       -0.874492
O       1.887717        -0.255724       1.235172
```

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O       -0.930410       -1.466468       1.082583
###
18
glu311 pm6_conformaciones E=-0.543621332385 au
N       2.162508        1.676706        0.020583
H       2.197985        1.784295        -1.010500
H       3.129602        1.517763        0.358082
H       1.819779        2.572554        0.423881
C       1.251981        0.532783        0.422577
H       1.200505        0.516502        1.555334
C       -0.151303       0.739147        -0.167756
C       1.851904        -0.813897       -0.033984
H       -0.351699       1.824682        -0.321194
H       -0.203761       0.299438        -1.188337
C       -1.230908       0.146055        0.739099
O       2.964102        -0.823285       -0.615924
H       -0.904485       -0.814922       1.188386
H       -1.406723       0.805486        1.620011
C       -2.525201       -0.045086       -0.012532
O       -3.128737       0.946980        -0.517539
O       -3.018494       -1.206199       -0.129484
O       1.208428        -1.867091       0.206177
###
18
glu312 pm6_conformaciones E=-0.549765443598 au
N       1.948337        -1.556725       -0.702676
H       2.552898        -1.728041       0.122522
H       2.547582        -1.218658       -1.479800
H       1.534732        -2.468346       -0.989351
C       0.854198        -0.556318       -0.386051
H       0.223385        -0.433396       -1.315604
C       -0.010984       -1.085851       0.769642
C       1.465672        0.815789        -0.026084
H       -0.417343       -2.087424       0.499177
H       0.621381        -1.276959       1.667953
C       -1.148431       -0.143110       1.149713
O       2.551111        0.876389        0.593518
H       -1.715336       -0.573044       2.009791
H       -0.760881       0.815975        1.553592
C       -2.089088       0.098984        -0.005032
O       -2.099589       1.232166        -0.577938
O       -2.857861       -0.817449       -0.411966
O       0.824717        1.845144        -0.373948
###
18
glu313 pm6_conformaciones E=-0.546708398792 au
N       0.740310        1.602419        -1.146591
H       0.035173        1.054263        -1.664043
H       1.576991        1.702171        -1.756307
H       0.351208        2.554266        -0.982191
C       1.112472        0.944898        0.167152
H       1.982523        1.539110        0.595098
C       -0.044693       1.000680        1.175952
C       1.602269        -0.496674       -0.059123
H       0.394591        1.159180        2.191305
H       -0.648813       1.922447        1.008613
C       -0.951910       -0.224145       1.236509
O       1.318092        -1.092553       -1.131726
H       -0.371403       -1.148636       1.440691
H       -1.611801       -0.143593       2.135700
C       -1.821743       -0.396243       0.016016
O       -2.735626       0.431638        -0.248586
O       -1.628897       -1.396079       -0.745439
O       2.262805        -1.046410       0.855531
###
18
glu314 pm6_conformaciones E=-0.543748142721 au
N       0.579773        1.704721        0.785278
H       -0.134750       1.782817        0.029469
H       1.352838        2.363241        0.572876
H       0.134108        2.001234        1.678481
C       1.089856        0.282793        0.899150
H       1.871081        0.271321        1.722405
C       -0.036708       -0.682890       1.295683
C       1.763409        -0.174344       -0.411156
H       0.428676        -1.564704       1.798109
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H       -0.658005       -0.221765       2.098678
C       -0.929485       -1.182886       0.162321
O       1.348439        0.260236        -1.517145
H       -0.336366       -1.555787       -0.700336
H       -1.471090       -2.095609       0.504852
C       -1.921450       -0.145927       -0.308796
O       -3.147863       -0.288145       -0.048404
O       -1.524795       0.853421        -0.985134
O       2.694389        -1.012296       -0.327404
###
18
glu315 pm6_conformaciones E=-0.550871633021 au
N       -2.733511       0.505724        0.144275
H       -2.701111       0.571119        1.178738
H       -3.345769       -0.291963       -0.112269
H       -3.177499       1.377555        -0.214635
C       -1.348586       0.346876        -0.447637
H       -1.445436       0.419147        -1.573434
C       -0.430954       1.474566        0.058247
C       -0.754735       -1.031963       -0.094542
H       -0.873901       2.457674        -0.234358
H       -0.412000       1.496618        1.169174
C       0.982875        1.386838        -0.506318
O       -0.736844       -1.439676       1.092098
H       0.958009        1.289699        -1.614210
H       1.507502        2.361068        -0.342675
C       1.818298        0.291821        0.105121
O       2.465073        -0.491418       -0.660444
O       1.883002        0.121003        1.356049
O       -0.233307       -1.693635       -1.032137
###
18
glu316 pm6_conformaciones E=-0.541457999431 au
N       -0.593834       1.597259        -0.386896
H       -0.824464       2.018608        0.532314
H       -1.158134       2.078431        -1.114710
H       0.406202        1.787472        -0.582077
C       -0.870702       0.107389        -0.389955
H       -0.693788       -0.275869       -1.440496
C       0.032119        -0.640289       0.602759
C       -2.351769       -0.149960       -0.031054
H       0.233819        -0.016075       1.501371
H       -0.522826       -1.518452       1.011758
C       1.331878        -1.143876       -0.019038
O       -2.975279       0.686995        0.665137
H       1.669582        -2.063814       0.517132
H       1.162257        -1.491898       -1.061732
C       2.456875        -0.140711       0.022176
O       3.045683        0.183187        -1.052625
O       2.844752        0.352093        1.122530
O       -2.878433       -1.209091       -0.455619
###
17
glu400 pm6_conformaciones E=-0.695433964967 au
N       2.018458        -1.453326       -0.877785
H       2.520068        -1.797817       -0.054627
H       1.669359        -2.287889       -1.359510
C       0.869497        -0.607620       -0.460819
H       0.222988        -0.443057       -1.365631
C       0.011921        -1.212607       0.666450
C       1.437745        0.748041        -0.018477
H       -0.430872       -2.167864       0.312035
H       0.651846        -1.508681       1.525430
C       -1.086732       -0.270906       1.158328
O       2.309424        0.834497        0.884979
H       -1.675456       -0.767834       1.964230
H       -0.659578       0.621488        1.660511
C       -2.006608       0.130054        0.034624
O       -2.796121       -0.713721       -0.479311
O       -1.971086       1.314570        -0.422715
O       0.984970        1.790050        -0.585277
###
17
glu401 pm6_conformaciones E=-0.695355553532 au
N       -1.906282       1.525489        -0.940983
H       -2.404481       1.934886        -0.146608
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H       -1.468971       2.313155        -1.430796
C       -0.849122       0.598068        -0.463820
H       -0.190910       0.361027        -1.344023
C       0.021677        1.155610        0.679267
C       -1.517782       -0.701863       0.006048
H       0.492844        2.106030        0.349516
H       -0.613138       1.447249        1.543171
C       1.091240        0.168094        1.147404
O       -1.074581       -1.795318       -0.463914
H       1.655791        0.600932        2.004300
H       0.636157        -0.749703       1.573985
C       2.035787        -0.171198       0.021650
O       1.857605        -1.235231       -0.651074
O       2.984247        0.607670        -0.276067
O       -2.449036       -0.700155       0.852811
###
17
glu402 pm6_conformaciones E=-0.697604952154 au
N       -2.073899       0.929242        0.836924
H       -1.354958       1.231814        1.498104
H       -2.606327       1.774128        0.603708
C       -1.439437       0.397389        -0.396230
H       -2.244622       0.324708        -1.186286
C       -0.304478       1.277572        -0.961449
C       -0.934169       -1.029349       -0.170230
H       0.040808        0.861336        -1.929606
H       -0.729781       2.271655        -1.228751
C       0.880162        1.490414        -0.018915
O       -0.491662       -1.668981       -1.175371
H       1.566779        2.255279        -0.454297
H       0.549552        1.950894        0.937439
C       1.650446        0.223584        0.235202
O       1.717580        -0.265568       1.403555
O       2.209885        -0.398429       -0.721439
O       -0.913215       -1.583542       0.964624
###
17
glu405 pm6_conformaciones E=-0.690969638706 au
N       2.170789        1.706031        -0.443331
H       2.058678        1.599197        -1.454919
H       1.882677        2.667142        -0.234974
C       1.277651        0.757305        0.276590
H       1.315029        1.010538        1.371394
C       -0.186503       0.791056        -0.191920
C       1.887347        -0.637211       0.073451
H       -0.574474       1.827827        -0.093164
H       -0.250952       0.568639        -1.277319
C       -1.058140       -0.178890       0.606305
O       2.502395        -1.178785       1.037651
H       -0.647399       -1.209631       0.581402
H       -1.057670       0.087094        1.686439
C       -2.467809       -0.165877       0.070204
O       -3.260572       0.768258        0.389781
O       -2.860592       -1.090603       -0.702932
O       1.789183        -1.235285       -1.034915
###
17
glu406 pm6_conformaciones E=-0.698305338290 au
N       -2.748424       0.515183        -0.012046
H       -2.818651       0.581281        1.006655
H       -3.142701       1.390511        -0.373134
C       -1.322690       0.413803        -0.423487
H       -1.284250       0.493971        -1.544777
C       -0.407110       1.493411        0.183829
C       -0.843586       -0.984159       -0.016641
H       -0.851432       2.494604        -0.021060
H       -0.392307       1.419357        1.289404
C       1.012958        1.466620        -0.379695
O       -0.497956       -1.789722       -0.932988
H       0.994783        1.575899        -1.485863
H       1.567736        2.370855        -0.032332
C       1.784634        0.237253        0.019397
O       1.986339        -0.052602       1.235796
O       2.231091        -0.544170       -0.879294
O       -0.741905       -1.325297       1.194612
###
```

```
17
glu407 pm6_conformaciones E=-0.698306790083 au
N       -2.748192       0.515505        -0.012617
H       -2.818714       0.581943        1.006066
H       -3.142341       1.390768        -0.374057
C       -1.322284       0.414055        -0.423527
H       -1.283431       0.494349        -1.544794
C       -0.406900       1.493423        0.184309
C       -0.843720       -0.984133       -0.016722
H       -0.851165       2.494721        -0.020335
H       -0.392254       1.419096        1.289905
C       1.013273        1.466841        -0.378986
O       -0.497787       -1.789499       -0.933102
H       0.995301        1.576942        -1.485082
H       1.568140        2.370744        -0.030883
C       1.784615        0.237085        0.019429
O       2.231135        -0.543941       -0.879539
O       1.986152        -0.053489       1.235722
O       -0.743013       -1.325661       1.194479
###
17
glu409 pm6_conformaciones E=-0.698487691643 au
N       -2.734991       0.537951        -0.142566
H       -2.886684       0.552111        0.869411
H       -3.088311       1.437615        -0.486047
C       -1.281767       0.436508        -0.441713
H       -1.152267       0.571215        -1.550764
C       -0.412350       1.473670        0.295123
C       -0.847029       -0.983483       -0.063922
H       -0.861428       2.483577        0.152636
H       -0.447579       1.306528        1.390134
C       1.032922        1.512677        -0.196763
O       -0.354494       -1.724298       -0.969326
H       1.068208        1.775355        -1.276828
H       1.574323        2.353371        0.299917
C       1.781230        0.233217        0.059364
O       2.325767        -0.381238       -0.911394
O       1.865892        -0.267382       1.221098
O       -0.924585       -1.412201       1.120492
###
17
glu410 pm6_conformaciones E=-0.698428731277 au
N       -2.730484       0.550405        -0.119811
H       -2.870691       0.590248        0.892994
H       -3.086861       1.441052        -0.482855
C       -1.280919       0.438211        -0.433870
H       -1.163289       0.556471        -1.546072
C       -0.396651       1.480870        0.276368
C       -0.855455       -0.981611       -0.042885
H       -0.842586       2.490772        0.123975
H       -0.419165       1.330327        1.374188
C       1.042740        1.505148        -0.234892
O       -0.429257       -1.752972       -0.955870
H       1.064798        1.741168        -1.321456
H       1.591124        2.356503        0.234327
C       1.788456        0.228282        0.041786
O       2.284862        -0.432213       -0.924659
O       1.908154        -0.230901       1.217527
O       -0.882381       -1.382013       1.153570
###
17
glu411 pm6_conformaciones E=-0.689488729020 au
N       -0.500462       -1.491499       -0.513744
H       -0.655801       -1.369948       -1.518036
H       0.480222        -1.758422       -0.411915
C       -0.751549       -0.212803       0.206620
H       -0.475814       -0.366452       1.286108
C       0.010813        1.010271        -0.333793
C       -2.269625       0.014404        0.135660
H       0.134896        0.939002        -1.433591
H       -0.592759       1.932193        -0.179168
C       1.364087        1.206063        0.346026
O       -2.971969       -0.305822       1.137983
H       1.829488        2.155931        -0.008491
H       1.230886        1.363367        1.438492
C       2.321962        0.072263        0.089950
```

```
O       2.869167        -0.518299       1.071223
O       2.601074        -0.292177       -1.090484
O       -2.811022       0.491752        -0.899218
###
17
glu412 pm6_conformaciones E=-0.689753967704 au
N       0.404876        -1.412350       -0.615516
H       0.252945        -1.862148       0.290150
H       -0.493723       -1.445732       -1.101889
C       0.816403        0.003271        -0.425588
H       0.727473        0.525001        -1.418114
C       0.018394        0.789321        0.631479
C       2.297926        0.002491        -0.018840
H       -0.088376       0.192345        1.560613
H       0.592253        1.690832        0.942755
C       -1.349254       1.238088        0.121865
O       2.719530        -0.695915       0.943556
H       -1.767019       2.017791        0.801436
H       -1.255230       1.754973        -0.856949
C       -2.331287       0.098670        0.032457
O       -2.858324       -0.199230       -1.080018
O       -2.645078       -0.560400       1.069967
O       3.094428        0.733337        -0.678208
###
17
glu414 pm6_conformaciones E=-0.692830006127 au
N       0.375742        -0.670320       1.788371
H       -0.227468       0.151474        1.761394
H       -0.231507       -1.456402       2.039866
C       0.979540        -0.917597       0.452115
H       1.731497        -1.747677       0.592073
C       -0.005328       -1.365160       -0.646962
C       1.734887        0.329894        -0.015490
H       0.565448        -1.869862       -1.457938
H       -0.660218       -2.166589       -0.241885
C       -0.852339       -0.252900       -1.264014
O       2.717903        0.186604        -0.794646
H       -0.217071       0.528490        -1.728599
H       -1.431526       -0.660946       -2.125913
C       -1.806244       0.348576        -0.264811
O       -2.773858       -0.328329       0.186342
O       -1.622078       1.537629        0.144172
O       1.370228        1.486207        0.348804
###
17
glu416 pm6_conformaciones E=-0.691027405514 au
N       2.224664        1.636980        -0.515750
H       2.050999        1.524126        -1.518276
H       2.014653        2.619078        -0.310680
C       1.306791        0.763923        0.266740
H       1.426482        1.022338        1.354776
C       -0.175052       0.906572        -0.114578
C       1.805489        -0.673109       0.052316
H       -0.477109       1.971344        -0.014691
H       -0.314592       0.676063        -1.191301
C       -1.072946       0.023221        0.753983
O       2.564007        -1.185881       0.925908
H       -0.611615       -0.966294       0.954639
H       -1.199911       0.465525        1.766161
C       -2.411534       -0.157536       0.083909
O       -2.647400       -1.214905       -0.575508
O       -3.293883       0.746081        0.160489
O       1.480021        -1.338977       -0.971465
###
# Conformations of HISTIDINE optimized with pm6
# opt freq pm6 scf=(xqc,tight) scrf(smd,solvent=water)
###
22
his1010 pm6_conformaciones E=0.168829104579 au
N       -3.047159       -0.151737       -0.725688
C       -1.843461       -0.860011       -0.780666
C       -1.081618       -0.486644       0.327783
N       -1.842894       0.449545        1.054150
C       -3.038655       0.644041        0.399033
C       0.256097        -0.949017       0.756696
C       1.334445        -0.644147       -0.296559
```

```
C       1.640266        0.852243        -0.316119
O       2.812767        1.134147        0.292586
N       2.577147        -1.466797       -0.019800
O       0.938767        1.714863        -0.811446
H       3.319188        -1.263959       -0.720424
H       2.352226        -2.484271       -0.071322
H       2.959858        -1.270936       0.926412
H       0.953403        -0.924818       -1.337583
H       0.540518        -0.520687       1.753754
H       0.214425        -2.058526       0.948325
H       -1.555219       0.908398        1.927205
H       -1.605654       -1.563491       -1.574900
H       -3.845999       1.315670        0.719055
H       3.052568        2.125524        0.288660
H       -3.809687       -0.210861       -1.409936
###
22
his1011 pm6_conformaciones E=0.168695183802 au
N       -2.738866       -0.831597       -0.217742
C       -1.635872       -0.958043       0.630170
C       -0.939831       0.252409        0.604638
N       -1.638381       1.110149        -0.265541
C       -2.727979       0.433583        -0.764034
C       0.267395        0.647559        1.361821
C       1.591370        0.526722        0.595732
C       1.689477        -0.812731       -0.126657
O       1.780641        -0.656442       -1.466131
N       1.805806        1.694874        -0.347337
O       1.697850        -1.909496       0.399892
H       2.756462        1.658921        -0.769165
H       1.715471        2.596148        0.170336
H       1.113915        1.702747        -1.120459
H       2.441958        0.546516        1.365822
H       0.338294        0.026702        2.297251
H       0.157922        1.693193        1.764096
H       -1.367698       2.074480        -0.502981
H       -1.420233       -1.865284       1.189133
H       -3.463127       0.834331        -1.475305
H       1.871742        -1.534620       -1.977050
H       -3.439902       -1.556609       -0.407448
###
22
his1012 pm6_conformaciones E=0.168421091225 au
N       -2.742556       -0.918039       -0.092373
C       -1.586523       -1.012748       0.686682
C       -0.924988       0.215112        0.616047
N       -1.698278       1.051142        -0.212698
C       -2.799677       0.345641        -0.639602
C       0.313377        0.640934        1.303545
C       1.591256        0.615049        0.455558
C       1.674893        -0.669852       -0.366068
O       2.406500        -1.591252       0.300333
N       1.693175        1.825942        -0.451383
O       1.172581        -0.896385       -1.450529
H       2.626506        1.863428        -0.912908
H       1.571692        2.701144        0.104626
H       0.967023        1.822252        -1.193160
H       2.482228        0.648993        1.173096
H       0.475843        -0.009642       2.207338
H       0.183683        1.664769        1.752949
H       -1.467692       2.021341        -0.468745
H       -1.308535       -1.913533       1.229060
H       -3.590223       0.725719        -1.300788
H       2.486217        -2.480218       -0.197132
H       -3.435800       -1.661286       -0.234559
###
22
his1013 pm6_conformaciones E=0.170663960080 au
N       -2.467985       -0.804097       -0.939895
C       -1.126519       -0.410078       -0.878249
C       -0.979634       0.435843        0.220944
N       -2.251814       0.547085        0.819485
C       -3.147370       -0.212503       0.097660
C       0.179383        1.158280        0.793958
C       1.560173        0.814843        0.235825
C       1.829903        -0.686588       0.197250
```

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O       1.635585        -1.224007       1.424601
N       1.789196        1.438266        -1.129011
O       2.194037        -1.351889       -0.752625
H       2.786942        1.344371        -1.413708
H       1.559220        2.456453        -1.095645
H       1.201627        1.003680        -1.864883
H       2.340472        1.270166        0.946974
H       0.206611        1.001141        1.910376
H       0.008113        2.270234        0.708056
H       -2.474723       1.108200        1.651002
H       -0.396041       -0.740024       -1.612160
H       -4.218165       -0.321167       0.315469
H       1.839704        -2.223187       1.465034
H       -2.872125       -1.430257       -1.644709
###
22
his1014 pm6_conformaciones E=0.169822954661 au
N       -3.207657       0.465454        0.712954
C       -1.821966       0.653797        0.754318
C       -1.247304       -0.215404       -0.173266
N       -2.304040       -0.927447       -0.776382
C       -3.491456       -0.500020       -0.224392
C       0.159848        -0.482980       -0.548661
C       1.177531        0.408964        0.168716
C       2.547335        -0.272346       0.127339
O       2.678765        -1.085896       1.201388
N       1.262317        1.775476        -0.482264
O       3.420099        -0.151397       -0.709330
H       1.949347        2.382238        0.012303
H       0.334096        2.248705        -0.451189
H       1.546292        1.705746        -1.480579
H       0.883928        0.554868        1.263316
H       0.392125        -1.566498       -0.343307
H       0.283344        -0.408937       -1.665182
H       -2.205522       -1.645870       -1.503758
H       -1.349227       1.378686        1.413908
H       -4.490191       -0.869904       -0.489615
H       3.562518        -1.595205       1.219722
H       -3.895890       0.968076        1.283433
###
22
his101 pm6_conformaciones E=0.169197798217 au
N       -2.993685       -0.168914       -0.703016
C       -1.794221       -0.881813       -0.785201
C       -1.021343       -0.538436       0.325414
N       -1.771288       0.383918        1.080169
C       -2.971304       0.600231        0.440017
C       0.318926        -1.016851       0.727530
C       1.396058        -0.621809       -0.296500
C       1.714594        0.867946        -0.166031
O       0.923128        1.577285        -1.003312
N       2.653985        -1.439890       -0.078128
O       2.534472        1.396120        0.559944
H       3.399612        -1.162595       -0.749618
H       2.449309        -2.453118       -0.222983
H       3.022047        -1.326896       0.887149
H       1.022808        -0.830286       -1.355306
H       0.288022        -2.137506       0.838428
H       0.594092        -0.661076       1.755001
H       -1.473677       0.821932        1.960625
H       -1.565990       -1.566506       -1.598274
H       -3.771776       1.268629        0.783171
H       1.057764        2.586995        -0.934240
H       -3.762341       -0.208231       -1.381560
###
22
his102 pm6_conformaciones E=0.168818324913 au
N       -3.046344       -0.153193       -0.745347
C       -1.842770       -0.862605       -0.787715
C       -1.090019       -0.486345       0.325962
N       -1.856902       0.452389        1.043006
C       -3.047001       0.645746        0.377017
C       0.245219        -0.945897       0.765796
C       1.330158        -0.639453       -0.280109
C       1.645703        0.854310        -0.292618
O       2.889462        1.108626        0.169165
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N       2.567257        -1.470596       -0.003178
O       0.900908        1.738245        -0.674461
H       3.302214        -1.287914       -0.716701
H       2.332273        -2.486520       -0.033321
H       2.964056        -1.259954       0.933974
H       0.952246        -0.911218       -1.325202
H       0.203881        -2.055208       0.958096
H       0.521614        -0.516086       1.764364
H       -1.577012       0.912637        1.917833
H       -1.598580       -1.568496       -1.577866
H       -3.856361       1.319303        0.687631
H       3.139479        2.097199        0.158647
H       -3.802586       -0.213451       -1.436459
###
22
his103 pm6_conformaciones E=0.168371618842 au
N       -2.668507       -1.053235       -0.151324
C       -1.464829       -1.112185       0.557159
C       -0.941107       0.180809        0.612344
N       -1.846352       1.019673        -0.066731
C       -2.890899       0.253076        -0.529630
C       0.287269        0.666010        1.278053
C       1.537299        0.727360        0.391601
C       1.766536        -0.609840       -0.311878
O       2.663324        -1.346932       0.380138
N       1.456063        1.844857        -0.631191
O       1.243443        -1.007531       -1.335981
H       2.390217        2.027372        -1.052966
H       1.124701        2.725179        -0.177530
H       0.794256        1.623193        -1.400331
H       2.433814        0.947366        1.067858
H       0.113761        1.676698        1.743126
H       0.512152        0.014976        2.167433
H       -1.726423       2.031105        -0.213790
H       -1.066473       -2.034199       0.972945
H       -3.755381       0.619651        -1.099682
H       2.853866        -2.257668       -0.043117
H       -3.282662       -1.848418       -0.358376
###
22
his104 pm6_conformaciones E=0.168695895734 au
N       -2.738794       -0.831951       -0.218355
C       -1.635927       -0.958513       0.629728
C       -0.940083       0.252070        0.604716
N       -1.638651       1.110015        -0.265220
C       -2.728020       0.433418        -0.764192
C       0.267073        0.647116        1.362079
C       1.591033        0.526994        0.595857
C       1.689951        -0.812390       -0.126503
O       1.782393        -0.655980       -1.465915
N       1.804690        1.695243        -0.347276
O       1.697984        -1.909226       0.399888
H       2.755239        1.659691        -0.769399
H       1.714130        2.596498        0.170398
H       1.112589        1.702745        -1.120200
H       2.441677        0.547320        1.365854
H       0.157340        1.692574        1.764785
H       0.338166        0.025803        2.297206
H       -1.368068       2.074472        -0.502299
H       -1.420287       -1.865883       1.188467
H       -3.463114       0.834329        -1.475432
H       1.874033        -1.534166       -1.976763
H       -3.439586       -1.557062       -0.408538
###
22
his105 pm6_conformaciones E=0.169616904097 au
N       3.406876        0.515473        0.038110
C       2.181483        0.930165        0.567613
C       1.267745        -0.107578       0.381068
N       1.955609        -1.151519       -0.268686
C       3.257621        -0.756475       -0.472131
C       -0.151528       -0.199127       0.787148
C       -1.115198       0.134333        -0.361882
C       -2.492611       -0.446852       -0.050084
O       -3.422646       0.519300        0.118811
N       -1.178945       1.631638        -0.597558
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O       -2.761360       -1.629893       0.038352
H       -1.814861       1.854592        -1.390882
H       -0.233445       2.002632        -0.827057
H       -1.521384       2.133629        0.245707
H       -0.759111       -0.363026       -1.328304
H       -0.339653       0.467508        1.671577
H       -0.372506       -1.227412       1.183773
H       1.548088        -2.049494       -0.552373
H       2.031364        1.904263        1.027272
H       4.042412        -1.349637       -0.958493
H       -4.352735       0.152700        0.329993
H       4.274011        1.063044        0.028034
###
22
his106 pm6_conformaciones E=0.169643802837 au
N       3.395523        0.447313        -0.056356
C       2.182373        0.978748        0.389854
C       1.242942        -0.052788       0.391601
N       1.904502        -1.212742       -0.057177
C       3.214761        -0.891618       -0.328310
C       -0.176962       -0.041512       0.805052
C       -1.130919       0.231096        -0.368724
C       -2.531970       -0.250578       0.009909
O       -2.695563       -1.533498       -0.387289
N       -1.172748       1.708530        -0.709422
O       -3.405837       0.366435        0.587571
H       -1.812379       1.887744        -1.511944
H       -0.222412       2.044007        -0.975902
H       -1.491944       2.278072        0.099094
H       -0.783020       -0.336319       -1.295732
H       -0.328535       0.707958        1.628073
H       -0.441916       -1.019793       1.292962
H       1.479176        -2.139942       -0.161906
H       2.057182        2.022798        0.667300
H       3.981864        -1.582085       -0.701146
H       -3.593027       -1.932446       -0.111625
H       4.273932        0.964716        -0.167041
###
22
his107 pm6_conformaciones E=0.169824900781 au
N       -3.203468       0.491942        0.700345
C       -1.820782       0.703993        0.700230
C       -1.251144       -0.207892       -0.188852
N       -2.308124       -0.970716       -0.725991
C       -3.490919       -0.531109       -0.173082
C       0.153453        -0.467378       -0.580594
C       1.175195        0.416228        0.142340
C       2.532880        -0.290923       0.138411
O       2.689551        -0.976240       1.295147
N       1.302638        1.770077        -0.528740
O       3.378741        -0.284063       -0.734168
H       2.001052        2.365967        -0.037030
H       0.386319        2.267459        -0.510730
H       1.591539        1.679544        -1.523856
H       0.860490        0.587495        1.226988
H       0.264857        -0.375464       -1.696812
H       0.389436        -1.553729       -0.395395
H       -2.212906       -1.726171       -1.415171
H       -1.346071       1.472285        1.307439
H       -4.489013       -0.930246       -0.394900
H       3.565918        -1.496821       1.344562
H       -3.887376       1.015475        1.257057
###
22
his108 pm6_conformaciones E=0.169198104123 au
N       -2.993555       -0.168989       -0.702928
C       -1.794149       -0.881982       -0.785122
C       -1.021190       -0.538565       0.325442
N       -1.771041       0.383845        1.080181
C       -2.971087       0.600184        0.440079
C       0.319077        -1.017093       0.727428
C       1.396194        -0.621786       -0.296516
C       1.714332        0.868043        -0.166060
O       0.922449        1.577113        -1.003272
N       2.654253        -1.439637       -0.078057
O       2.534116        1.396603        0.559705
```

```
H       3.400124        -1.161774       -0.749021
H       2.449934        -2.452830       -0.223594
H       3.021821        -1.327109       0.887472
H       1.023015        -0.830333       -1.355346
H       0.594258        -0.661614       1.754996
H       0.288209        -2.137777       0.838017
H       -1.473306       0.822009        1.960507
H       -1.565969       -1.566710       -1.598174
H       -3.771561       1.268533        0.783329
H       1.056527        2.586808        -0.934084
H       -3.762231       -0.208271       -1.381450
###
22
his109 pm6_conformaciones E=0.169197665634 au
N       -2.993539       -0.169181       -0.703115
C       -1.793969       -0.881871       -0.785107
C       -1.021272       -0.538252       0.325597
N       -1.771441       0.384052        1.080143
C       -2.971387       0.600143        0.439823
C       0.318985        -1.016588       0.727824
C       1.396094        -0.621791       -0.296339
C       1.714678        0.867922        -0.166035
O       0.922759        1.577068        -1.003202
N       2.653931        -1.440066       -0.078125
O       2.534669        1.396444        0.559497
H       3.399320        -1.163220       -0.750121
H       2.448923        -2.453306       -0.222387
H       3.022480        -1.326685       0.886899
H       1.022696        -0.830351       -1.355106
H       0.594226        -0.660520       1.755181
H       0.288016        -2.137217       0.839014
H       -1.473879       0.822302        1.960488
H       -1.565508       -1.566622       -1.598059
H       -3.772113       1.268301        0.782828
H       1.057004        2.586711        -0.934139
H       -3.762029       -0.208496       -1.381853
###
21
his2010 pm6_conformaciones E=-0.840846399382E-02 au
N       3.333432        0.217869        -0.090139
C       2.332882        1.150868        0.206499
C       1.116581        0.469314        0.248544
N       1.395017        -0.883799       -0.025894
C       2.750753        -1.019955       -0.234275
C       -0.230422       0.994232        0.566572
C       -1.315217       0.533497        -0.415846
C       -1.898151       -0.832818       0.020348
O       -3.032398       -0.870183       0.552408
N       -2.423013       1.564891        -0.483754
O       -1.200694       -1.857385       -0.179556
H       -3.126903       1.298392        -1.198984
H       -2.041158       2.499517        -0.737064
H       -2.908429       1.654499        0.428629
H       -0.880476       0.421642        -1.456160
H       -0.504230       0.729002        1.620498
H       -0.179520       2.117569        0.594568
H       0.686394        -1.636964       -0.092369
H       2.537752        2.205282        0.366857
H       3.271198        -1.955027       -0.475370
H       4.333496        0.423068        -0.185955
###
21
his2011 pm6_conformaciones E=-0.127821718116E-01 au
N       -2.647359       -1.002705       -0.185504
C       -1.449706       -1.105751       0.530064
C       -0.896390       0.172627        0.619528
N       -1.776936       1.047457        -0.046651
C       -2.837214       0.315650        -0.533400
C       0.341349        0.614728        1.300519
C       1.593569        0.658398        0.418127
C       1.829955        -0.709594       -0.265122
O       1.316435        -0.940766       -1.385236
N       1.521982        1.769415        -0.609198
O       2.531139        -1.546829       0.354243
H       2.463524        1.968521        -0.999918
H       1.156266        2.644995        -0.178015
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H       0.894832        1.523080        -1.396046
H       2.482742        0.876466        1.090278
H       0.543582        -0.058389       2.175914
H       0.187836        1.618577        1.782169
H       -1.635599       2.059458        -0.168666
H       -1.080754       -2.045675       0.930048
H       -3.688843       0.716863        -1.099464
H       -3.277356       -1.778644       -0.417184
###
21
his2012 pm6_conformaciones E=-0.127822088606E-01 au
N       -2.647426       -1.002733       -0.185336
C       -1.449954       -1.105658       0.530478
C       -0.896469       0.172755        0.619463
N       -1.776955       1.047425        -0.046859
C       -2.837241       0.315531        -0.533513
C       0.341333        0.614586        1.300508
C       1.593617        0.658540        0.418238
C       1.830064        -0.709562       -0.265123
O       2.532369        -1.546422       0.353484
N       1.521955        1.769344        -0.609198
O       1.315589        -0.941045       -1.384735
H       2.463538        1.968778        -0.999650
H       1.155539        2.644788        -0.178414
H       0.895064        1.522613        -1.396166
H       2.482614        0.876568        1.090418
H       0.543647        -0.058763       2.175687
H       0.187768        1.618235        1.782455
H       -1.635240       2.059342        -0.169660
H       -1.081264       -2.045386       0.931091
H       -3.688941       0.716795        -1.099387
H       -3.277510       -1.778635       -0.416933
###
21
his2013 pm6_conformaciones E=-0.112230096746E-01 au
N       -2.420126       -0.702487       -0.995317
C       -1.103142       -0.227324       -1.007627
C       -0.920977       0.556256        0.132225
N       -2.147726       0.553880        0.826452
C       -3.051386       -0.215336       0.123637
C       0.248876        1.309649        0.641051
C       1.619449        0.719059        0.309156
C       1.656278        -0.822469       0.413098
O       1.243490        -1.360582       1.470145
N       2.094240        1.170053        -1.058514
O       2.124045        -1.480598       -0.546496
H       3.041628        0.797140        -1.257249
H       2.141202        2.208711        -1.103570
H       1.459372        0.846695        -1.809281
H       2.365636        1.116644        1.071989
H       0.177863        1.435245        1.756037
H       0.186441        2.374614        0.281985
H       -2.341671       1.051215        1.704802
H       -0.414660       -0.456946       -1.815543
H       -4.095135       -0.400680       0.409762
H       -2.840256       -1.312336       -1.705696
###
21
his2014 pm6_conformaciones E=-0.109986788107E-01 au
N       -3.185660       0.510508        0.678321
C       -1.798238       0.595129        0.837927
C       -1.210976       -0.284826       -0.071028
N       -2.261628       -0.900986       -0.780390
C       -3.458304       -0.405967       -0.309920
C       0.203249        -0.637993       -0.334208
C       1.213907        0.375941        0.204969
C       2.614689        -0.287635       0.230586
O       2.918441        -0.966209       1.241777
N       1.240470        1.625852        -0.650531
O       3.385678        -0.134913       -0.745751
H       1.929564        2.309591        -0.283279
H       0.307281        2.084700        -0.658994
H       1.495885        1.405020        -1.631086
H       0.948009        0.680671        1.263117
H       0.411108        -1.648236       0.113146
H       0.361206        -0.803622       -1.434301
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H       -2.155690       -1.605917       -1.519754
H       -1.331445       1.260259        1.560136
H       -4.455159       -0.694215       -0.667432
H       -3.881947       1.045220        1.208475
###
21
his201 pm6_conformaciones E=-0.122134383399E-01 au
N       -2.949571       -0.077368       -0.739671
C       -1.728778       -0.744036       -0.891876
C       -0.993476       -0.555462       0.279282
N       -1.784564       0.231485        1.138714
C       -2.975022       0.512747        0.503037
C       0.349520        -1.054063       0.647183
C       1.427326        -0.577253       -0.337725
C       1.627662        0.952598        -0.221355
O       0.895876        1.687106        -0.930703
N       2.726750        -1.305238       -0.064570
O       2.494779        1.410281        0.560435
H       3.480141        -0.961450       -0.689535
H       2.613528        -2.327196       -0.228119
H       3.033444        -1.172427       0.917321
H       1.109549        -0.817310       -1.398853
H       0.326053        -2.178256       0.669724
H       0.619496        -0.774272       1.697311
H       -1.528492       0.534315        2.086687
H       -1.467967       -1.300702       -1.788214
H       -3.801671       1.102753        0.920271
H       -3.701029       -0.033891       -1.437027
###
21
his202 pm6_conformaciones E=-0.120020423407E-01 au
N       -2.917797       0.023778        -0.751819
C       -1.686306       -0.600132       -0.978936
C       -0.976943       -0.589034       0.222849
N       -1.792772       0.051818        1.175293
C       -2.975828       0.412772        0.566300
C       0.362145        -1.131237       0.540360
C       1.447774        -0.552619       -0.378812
C       1.587749        0.972961        -0.158011
O       2.366358        1.406744        0.723925
N       2.765719        -1.249357       -0.114354
O       0.897220        1.728208        -0.886907
H       3.520042        -0.849930       -0.704429
H       2.690691        -2.264969       -0.332456
H       3.047729        -1.157738       0.879765
H       1.167684        -0.735654       -1.461746
H       0.334658        -2.250620       0.437899
H       0.625310        -0.969079       1.617034
H       -1.556483       0.209176        2.162552
H       -1.402867       -1.012139       -1.943668
H       -3.816470       0.925154        1.052180
H       -3.656519       0.166249        -1.449606
###
21
his203 pm6_conformaciones E=-0.127821063705E-01 au
N       -2.647455       -1.002689       -0.185300
C       -1.449873       -1.105695       0.530323
C       -0.896373       0.172704        0.619356
N       -1.776832       1.047446        -0.046878
C       -2.837200       0.315625        -0.533472
C       0.341319        0.614570        1.300548
C       1.593546        0.658359        0.418176
C       1.829981        -0.709585       -0.265186
O       2.531727        -1.546570       0.353865
N       1.521897        1.769511        -0.609007
O       1.316086        -0.941000       -1.385115
H       2.463332        1.968538        -0.999892
H       1.156393        2.645089        -0.177601
H       0.894464        1.523346        -1.395735
H       2.482694        0.876211        1.090271
H       0.187833        1.618359        1.782398
H       0.543473        -0.058732       2.175769
H       -1.635009       2.059284        -0.169712
H       -1.080750       -2.045535       0.930294
H       -3.688815       0.716799        -1.099528
H       -3.277783       -1.778527       -0.416446
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###
21
his204 pm6_conformaciones E=-0.127822189264E-01 au
N       -2.647726       -1.002471       -0.185338
C       -1.450261       -1.105709       0.530512
C       -0.896446       0.172472        0.619560
N       -1.776622       1.047431        -0.046987
C       -2.837069       0.315849        -0.533678
C       0.341271        0.614591        1.300560
C       1.593539        0.658240        0.418239
C       1.829980        -0.709662       -0.265248
O       1.315920        -0.941069       -1.385035
N       1.522141        1.769449        -0.608923
O       2.531985        -1.546584       0.353655
H       2.463738        1.968513        -0.999535
H       1.156524        2.644997        -0.177594
H       0.894975        1.523354        -1.395838
H       2.482657        0.876122        1.090461
H       0.187690        1.618502        1.782056
H       0.543495        -0.058430       2.175984
H       -1.634586       2.059273        -0.169702
H       -1.081703       -2.045641       0.930834
H       -3.688503       0.717172        -1.099936
H       -3.278156       -1.778189       -0.416618
###
21
his205 pm6_conformaciones E=-0.110509708918E-01 au
N       3.327790        0.520817        -0.030411
C       2.083204        0.977361        0.413229
C       1.203845        -0.105854       0.395855
N       1.933234        -1.220684       -0.060958
C       3.225369        -0.821899       -0.320113
C       -0.223166       -0.171913       0.782056
C       -1.165574       0.085127        -0.400001
C       -2.606657       -0.320903       0.004976
O       -3.262210       0.428594        0.767303
N       -1.134678       1.543525        -0.811291
O       -3.058632       -1.399088       -0.448674
H       -1.751641       1.710213        -1.630814
H       -0.168893       1.828929        -1.073828
H       -1.446709       2.160082        -0.038514
H       -0.846544       -0.536404       -1.290311
H       -0.421513       0.550203        1.616237
H       -0.455537       -1.172528       1.235108
H       1.564623        -2.170172       -0.178526
H       1.898423        2.008654        0.703978
H       4.033206        -1.461661       -0.697192
H       4.174773        1.089515        -0.132570
###
21
his206 pm6_conformaciones E=-0.110509765023E-01 au
N       3.327621        0.521011        -0.030157
C       2.082955        0.977260        0.413541
C       1.203768        -0.106129       0.395888
N       1.933326        -1.220702       -0.061208
C       3.225398        -0.821647       -0.320236
C       -0.223280       -0.172290       0.782004
C       -1.165576       0.084962        -0.400133
C       -2.606670       -0.320728       0.005029
O       -3.058756       -1.399039       -0.448219
N       -1.134273       1.543320        -0.811534
O       -3.262122       0.429120        0.767056
H       -1.751059       1.710086        -1.631131
H       -0.168382       1.828475        -1.073994
H       -1.446226       2.160059        -0.038874
H       -0.846782       -0.536795       -1.290313
H       -0.421858       0.549646        1.616224
H       -0.455758       -1.172905       1.234870
H       1.564832        -2.170224       -0.179032
H       1.898024        2.008416        0.704649
H       4.033332        -1.461142       -0.697566
H       4.174612        1.089766        -0.131796
###
21
his207 pm6_conformaciones E=-0.109322354999E-01 au
N       -3.183728       0.534884        0.664776
```

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C       -1.795047       0.643309        0.793573
C       -1.213604       -0.272443       -0.083428
N       -2.269340       -0.935419       -0.740507
C       -3.463428       -0.432185       -0.271825
C       0.199794        -0.629161       -0.347875
C       1.213774        0.384025        0.187265
C       2.607453        -0.291065       0.248293
O       2.912139        -0.908789       1.297607
N       1.272003        1.616528        -0.692998
O       3.370619        -0.212346       -0.742602
H       1.957459        2.301798        -0.322181
H       0.343130        2.082176        -0.733155
H       1.550066        1.372472        -1.661777
H       0.932078        0.713272        1.233440
H       0.356543        -0.802636       -1.447232
H       0.403976        -1.638669       0.104004
H       -2.167973       -1.671858       -1.448801
H       -1.323898       1.350030        1.471870
H       -4.463223       -0.749897       -0.594090
H       -3.876422       1.085560        1.182963
###
21
his208 pm6_conformaciones E=-0.122129865011E-01 au
N       -2.949613       -0.077272       -0.739432
C       -1.728885       -0.744017       -0.891930
C       -0.993355       -0.555602       0.279093
N       -1.784227       0.231309        1.138757
C       -2.974806       0.512697        0.503312
C       0.349584        -1.054525       0.646705
C       1.427490        -0.577255       -0.337831
C       1.627354        0.952680        -0.221363
O       0.895559        1.686967        -0.930915
N       2.727101        -1.304791       -0.064372
O       2.494153        1.410516        0.560666
H       3.480588        -0.960566       -0.688979
H       2.614341        -2.326767       -0.228213
H       3.033379        -1.172113       0.917687
H       1.110056        -0.817349       -1.399058
H       0.619529        -0.775424       1.697035
H       0.325979        -2.178792       0.668481
H       -1.528002       0.534044        2.086714
H       -1.468288       -1.300587       -1.788390
H       -3.801270       1.102770        0.920837
H       -3.701134       -0.033674       -1.436713
###
21
his209 pm6_conformaciones E=-0.840876959234E-02 au
N       3.333477        0.218983        -0.092053
C       2.332150        1.151194        0.204170
C       1.116766        0.468153        0.249451
N       1.396603        -0.885133       -0.022645
C       2.752290        -1.019930       -0.232717
C       -0.230403       0.992377        0.568465
C       -1.314867       0.533625        -0.415375
C       -1.899369       -0.832586       0.019002
O       -1.203040       -1.857458       -0.182222
N       -2.421803       1.566035        -0.482833
O       -3.033702       -0.869141       0.551047
H       -3.126925       1.299449        -1.196835
H       -2.039276       2.500002        -0.737676
H       -2.905869       1.656961        0.430074
H       -0.879431       0.422799        -1.455539
H       -0.504434       0.724832        1.621602
H       -0.179675       2.115651        0.598550
H       0.689483        -1.639579       -0.086603
H       2.535685        2.206259        0.361856
H       3.273754        -1.954851       -0.472168
H       4.333285        0.425064        -0.189115
###
20
his3010 pm6_conformaciones E=-0.167195655215 au
N       -2.914483       0.638939        0.328862
C       -1.692420       0.509377        0.993870
C       -1.008583       -0.539050       0.365011
N       -1.790416       -1.055177       -0.676788
C       -2.939995       -0.323896       -0.678459
```

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C       0.340034        -1.062095       0.691791
C       1.391497        -0.598897       -0.330632
C       1.556790        0.935219        -0.266430
O       2.422070        1.437337        0.490135
N       2.714590        -1.284555       -0.056979
O       0.796906        1.637066        -0.983617
H       3.439747        -0.972706       -0.730816
H       2.614686        -2.316804       -0.144865
H       3.053267        -1.078552       0.901044
H       1.063683        -0.882931       -1.374335
H       0.634735        -0.757537       1.724439
H       0.319619        -2.179993       0.729409
H       -1.411521       1.124268        1.833182
H       -3.774477       -0.461560       -1.358621
H       -3.643321       1.312198        0.551841
###
20
his3011 pm6_conformaciones E=-0.165158360285 au
N       -3.109490       -0.228421       -0.111758
C       -2.356223       0.779020        0.498395
C       -1.010365       0.454203        0.285304
N       -0.925829       -0.735118       -0.449765
C       -2.212219       -1.130331       -0.675478
C       0.156124        1.224424        0.786393
C       1.518046        0.853590        0.196974
C       1.827153        -0.649684       0.322454
O       2.242530        -1.275859       -0.686245
N       1.606887        1.289594        -1.253290
O       1.695525        -1.204473       1.444379
H       2.545660        1.084594        -1.643219
H       1.435329        2.312189        -1.337221
H       0.904409        0.799456        -1.833008
H       2.323256        1.408920        0.775262
H       0.210670        1.129520        1.900159
H       -0.027468       2.320076        0.634207
H       -2.796772       1.615151        1.016432
H       -2.511622       -2.019598       -1.221270
H       -4.123983       -0.277375       -0.136977
###
20
his3012 pm6_conformaciones E=-0.165158352615 au
N       -3.109529       -0.228388       -0.111765
C       -2.356245       0.779042        0.498375
C       -1.010402       0.454203        0.285262
N       -0.925879       -0.735080       -0.449853
C       -2.212276       -1.130286       -0.675535
C       0.156087        1.224377        0.786394
C       1.518058        0.853564        0.197035
C       1.827166        -0.649706       0.322462
O       1.695403        -1.204574       1.444323
N       1.607084        1.289661        -1.253190
O       2.242604        -1.275869       -0.686220
H       2.546053        1.085091        -1.642875
H       1.435108        2.312182        -1.337133
H       0.904970        0.799227        -1.833099
H       2.323167        1.408866        0.775469
H       0.210589        1.129362        1.900147
H       -0.027500       2.320028        0.634223
H       -2.796794       1.615159        1.016431
H       -2.511694       -2.019537       -1.221349
H       -4.124021       -0.277340       -0.136946
###
20
his3013 pm6_conformaciones E=-0.168076245419 au
N       -2.697647       0.339089        -0.662387
C       -1.590803       1.073977        -0.232089
C       -0.881966       0.246233        0.647789
N       -1.538390       -0.986898       0.765950
C       -2.635347       -0.905556       -0.038385
C       0.375559        0.552521        1.372830
C       1.624555        0.522908        0.479136
C       1.650138        -0.785484       -0.339084
O       2.145658        -1.799970       0.211718
N       1.676170        1.729684        -0.434717
O       1.155043        -0.811596       -1.492273
H       2.581488        1.767476        -0.943403
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H       1.575391        2.608490        0.114186
H       0.913645        1.707626        -1.135699
H       2.542633        0.554898        1.141477
H       0.527817        -0.157616       2.221258
H       0.293968        1.551049        1.872463
H       -1.391365       2.085111        -0.553701
H       -3.372583       -1.688324       -0.183599
H       -3.410349       0.663101        -1.311642
###
20
his3014 pm6_conformaciones E=-0.163711499557 au
N       3.219718        0.422409        -0.490682
C       1.966513        0.971328        -0.207929
C       1.223637        -0.039612       0.413334
N       2.001837        -1.200693       0.523036
C       3.208230        -0.893471       -0.030160
C       -0.176681       0.025688        0.898263
C       -1.147313       0.413590        -0.229662
C       -2.356193       -0.551468       -0.220020
O       -2.393737       -1.424602       -1.123596
N       -1.597674       1.851961        -0.087636
O       -3.225713       -0.466398       0.678804
H       -2.222601       2.125070        -0.871183
H       -0.773474       2.489324        -0.093874
H       -2.108202       2.003956        0.801923
H       -0.632368       0.318433        -1.234041
H       -0.477225       -0.945383       1.358876
H       -0.245579       0.742115        1.755438
H       1.694169        1.985794        -0.453390
H       4.056018        -1.564905       -0.110380
H       3.988541        0.901527        -0.951014
###
20
his301 pm6_conformaciones E=-0.167526462013 au
N       2.912381        -0.130129       0.576474
C       1.780290        -0.928026       0.760992
C       0.925146        -0.655219       -0.313126
N       1.513843        0.297280        -1.157464
C       2.717374        0.599548        -0.594804
C       -0.423695       -1.219461       -0.563744
C       -1.467738       -0.571363       0.363314
C       -1.362174       0.967463        0.267930
O       -0.731002       1.566817        1.176158
N       -2.859747       -1.034117       -0.010660
O       -1.870102       1.568732        -0.709642
H       -3.570553       -0.620689       0.622655
H       -2.930246       -2.070169       0.061714
H       -3.098946       -0.768564       -0.984035
H       -1.270857       -0.886609       1.431826
H       -0.413643       -2.325305       -0.400507
H       -0.717213       -1.099631       -1.633103
H       1.664073        -1.607183       1.590448
H       3.440796        1.305664        -0.989971
H       3.724858        -0.100792       1.187018
###
20
his302 pm6_conformaciones E=-0.167540764106 au
N       2.975925        -0.182935       0.606755
C       1.820725        -0.964460       0.682298
C       0.993189        -0.548807       -0.368525
N       1.623179        0.473758        -1.091425
C       2.824212        0.676660        -0.480617
C       -0.356743       -1.060512       -0.708498
C       -1.395712       -0.595702       0.326783
C       -1.529145       0.941657        0.267684
O       -2.288829       1.467095        -0.581127
N       -2.733331       -1.253714       0.061795
O       -0.834357       1.621160        1.067095
H       -3.411700       -1.023866       0.814713
H       -2.629188       -2.288824       0.025095
H       -3.135116       -0.941870       -0.841295
H       -1.057985       -0.896829       1.363778
H       -0.337066       -2.178895       -0.746947
H       -0.661909       -0.756575       -1.736331
H       1.668882        -1.727003       1.429476
H       3.574878        1.398782        -0.783790
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H       3.775123        -0.243739       1.232932
###
20
his303 pm6_conformaciones E=-0.166256827770 au
N       -2.744070       -0.752293       -0.121506
C       -1.658592       -0.922846       0.740485
C       -0.887688       0.242926        0.642749
N       -1.480975       1.126661        -0.269172
C       -2.604445       0.499740        -0.718298
C       0.369033        0.547907        1.369826
C       1.626646        0.506775        0.491122
C       1.646833        -0.789283       -0.348332
O       2.195820        -1.796915       0.161958
N       1.711154        1.727525        -0.401342
O       1.107961        -0.812204       -1.482397
H       2.613780        1.748250        -0.915759
H       1.642484        2.598154        0.164605
H       0.943507        1.740433        -1.094661
H       2.535785        0.512052        1.166830
H       0.295774        1.542717        1.876311
H       0.502732        -0.170294       2.216512
H       -1.516455       -1.804925       1.343796
H       -3.308704       0.904400        -1.438548
H       -3.492647       -1.422401       -0.276756
###
20
his304 pm6_conformaciones E=-0.166256759788 au
N       -2.743587       -0.752551       -0.121777
C       -1.657972       -0.923118       0.740073
C       -0.887546       0.243001        0.642878
N       -1.481246       1.126995        -0.268535
C       -2.604603       0.499932        -0.717790
C       0.369284        0.547955        1.369749
C       1.626759        0.506918        0.490887
C       1.646703        -0.789291       -0.348330
O       1.107989        -0.812347       -1.482503
N       1.710946        1.727622        -0.401665
O       2.195006        -1.797031       0.162348
H       2.614088        1.749281        -0.915093
H       1.640627        2.598222        0.164027
H       0.944090        1.739571        -1.095875
H       2.536088        0.512220        1.166312
H       0.296094        1.542737        1.876350
H       0.503103        -0.170331       2.216425
H       -1.515372       -1.805483       1.342858
H       -3.309204       0.904759        -1.437608
H       -3.492021       -1.422800       -0.277107
###
20
his305 pm6_conformaciones E=-0.163730684673 au
N       3.327306        0.496331        -0.020895
C       2.082078        0.930895        0.436922
C       1.231281        -0.180297       0.382604
N       1.935273        -1.292401       -0.099894
C       3.202343        -0.855929       -0.339439
C       -0.198067       -0.246400       0.772175
C       -1.135914       0.071959        -0.401515
C       -2.581542       -0.313629       -0.008877
O       -3.264278       0.479261        0.683396
N       -1.066284       1.541907        -0.764484
O       -3.015665       -1.426111       -0.396562
H       -1.657552       1.747615        -1.593517
H       -0.089259       1.816379        -0.991221
H       -1.387655       2.138540        0.019726
H       -0.831998       -0.525971       -1.311087
H       -0.393624       0.443648        1.629128
H       -0.443121       -1.259540       1.175183
H       1.888325        1.942758        0.757089
H       4.017109        -1.457626       -0.726714
H       4.162176        1.068547        -0.107569
###
20
his306 pm6_conformaciones E=-0.163730615302 au
N       3.327429        0.496222        -0.020804
C       2.082217        0.930924        0.436909
C       1.231304        -0.180175       0.382548
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N       1.935225        -1.292368       -0.099854
C       3.202345        -0.856039       -0.339336
C       -0.198040       -0.246232       0.772129
C       -1.135960       0.071787        -0.401594
C       -2.581598       -0.313546       -0.008675
O       -3.016321       -1.425590       -0.396960
N       -1.066328       1.541589        -0.765109
O       -3.263741       0.479159        0.684390
H       -1.657719       1.747020        -1.594126
H       -0.089316       1.815941        -0.992111
H       -1.387544       2.138546        0.018926
H       -0.832123       -0.526498       -1.310969
H       -0.393622       0.443994        1.628934
H       -0.443048       -1.259317       1.175335
H       1.888485        1.942842        0.756909
H       4.017087        -1.457808       -0.726548
H       4.162402        1.068311        -0.107309
###
20
his307 pm6_conformaciones E=-0.163711525434 au
N       3.219256        0.422127        -0.491339
C       1.966180        0.971272        -0.208417
C       1.223519        -0.039271       0.413708
N       2.001685        -1.200315       0.523798
C       3.207902        -0.893427       -0.029926
C       -0.176703       0.026607        0.898842
C       -1.147236       0.413834        -0.229455
C       -2.355551       -0.551903       -0.220213
O       -2.392543       -1.425022       -1.123807
N       -1.598344       1.851966        -0.087657
O       -3.225309       -0.467229       0.678433
H       -2.224545       2.124193        -0.870543
H       -0.774503       2.489808        -0.095382
H       -2.107854       2.004205        0.802477
H       -0.631899       0.318881        -1.233643
H       -0.245332       0.743960        1.755268
H       -0.477398       -0.943925       1.360368
H       1.693785        1.985577        -0.454491
H       4.055646        -1.564920       -0.110104
H       3.988079        0.901107        -0.951812
###
20
his308 pm6_conformaciones E=-0.167525922733 au
N       2.912660        -0.130523       0.576101
C       1.780715        -0.928699       0.760326
C       0.925168        -0.655075       -0.313252
N       1.513493        0.298157        -1.157060
C       2.717154        0.600100        -0.594490
C       -0.423665       -1.219221       -0.563962
C       -1.467778       -0.571450       0.363237
C       -1.362318       0.967401        0.268161
O       -0.730579       1.566458        1.176222
N       -2.859694       -1.034442       -0.010782
O       -1.870692       1.569071        -0.708914
H       -3.570497       -0.621758       0.622962
H       -2.929798       -2.070558       0.060829
H       -3.099238       -0.768233       -0.983888
H       -1.270825       -0.886766       1.431717
H       -0.717190       -1.099097       -1.633320
H       -0.413610       -2.325126       -0.401069
H       1.664774        -1.608470       1.589303
H       3.440373        1.306584        -0.989405
H       3.725293        -0.101482       1.186472
###
20
his309 pm6_conformaciones E=-0.167195762021 au
N       -2.914889       0.638670        0.328733
C       -1.692943       0.509306        0.994040
C       -1.008646       -0.538755       0.365185
N       -1.790057       -1.054868       -0.677015
C       -2.939837       -0.323955       -0.678800
C       0.339955        -1.061742       0.692058
C       1.391411        -0.598887       -0.330527
C       1.557066        0.935219        -0.266402
O       0.797061        1.637218        -0.983309
N       2.714374        -1.284899       -0.057057
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O       2.422690        1.437165        0.489890
H       3.439310        -0.973767       -0.731476
H       2.614033        -2.317170       -0.144176
H       3.053606        -1.078388       0.900661
H       1.063389        -0.882808       -1.374173
H       0.634727        -0.756937       1.724619
H       0.319442        -2.179631       0.730023
H       -1.412420       1.124282        1.833425
H       -3.774118       -0.461684       -1.359218
H       -3.644013       1.311603        0.551708
###
19
his4010 pm6_conformaciones E=-0.312899951517 au
N       -2.778550       0.580864        0.439795
C       -1.568278       0.321223        1.089099
C       -0.903912       -0.643871       0.319834
N       -1.686683       -0.979998       -0.791871
C       -2.817633       -0.222950       -0.696016
C       0.437189        -1.224719       0.574438
C       1.510007        -0.623469       -0.359923
C       1.441030        0.906925        -0.268227
O       1.930943        1.533084        0.711520
N       2.898095        -1.052406       -0.053888
O       0.854217        1.539052        -1.197558
H       2.979436        -2.064908       -0.190704
H       3.108982        -0.889308       0.933879
H       1.286312        -0.929427       -1.418031
H       0.722649        -1.079099       1.640608
H       0.417907        -2.330898       0.444302
H       -1.279952       0.798994        2.010240
H       -3.646115       -0.236667       -1.396712
H       -3.490938       1.236174        0.751243
###
19
his4011 pm6_conformaciones E=-0.312899622523 au
N       -2.763188       0.195671        -0.589795
C       -1.719746       1.026408        -0.169570
C       -0.887190       0.241738        0.638621
N       -1.404865       -1.058373       0.722870
C       -2.540860       -1.060073       -0.032122
C       0.369656        0.644414        1.313202
C       1.581394        0.727324        0.357804
C       1.792883        -0.642750       -0.296542
O       1.261237        -0.956760       -1.398975
N       1.491149        1.774992        -0.689723
O       2.510476        -1.484186       0.321751
H       1.404371        2.692645        -0.240429
H       0.633029        1.656119        -1.233155
H       2.490721        0.957687        0.982598
H       0.605867        -0.047303       2.152851
H       0.233514        1.635353        1.807224
H       -1.647975       2.065702        -0.446052
H       -3.196611       -1.910730       -0.184812
H       -3.535124       0.469702        -1.192255
###
19
his4012 pm6_conformaciones E=-0.312857522741 au
N       -2.830388       0.151946        -0.526055
C       -1.808993       0.991098        -0.071402
C       -0.910232       0.178915        0.632366
N       -1.365518       -1.146674       0.618836
C       -2.529433       -1.136285       -0.092558
C       0.344761        0.594773        1.302637
C       1.522755        0.803495        0.323915
C       1.911887        -0.554403       -0.270459
O       2.720842        -1.277707       0.382842
N       1.271280        1.781532        -0.764205
O       1.427981        -0.976107       -1.358908
H       0.999840        2.679632        -0.350137
H       0.466357        1.488133        -1.323817
H       2.399829        1.187808        0.918181
H       0.636259        -0.135376       2.089966
H       0.172850        1.545250        1.861612
H       -1.791475       2.052514        -0.258940
H       -3.152621       -2.000414       -0.296595
H       -3.633706       0.439765        -1.078756
```

```
###
19
his4014 pm6_conformaciones E=-0.309413026119 au
N       3.172784        0.804200        0.091754
C       1.813817        1.057288        -0.115654
C       1.212823        -0.181754       -0.370132
N       2.182346        -1.193119       -0.325725
C       3.361366        -0.568284       -0.044142
C       -0.214006       -0.466902       -0.661002
C       -1.156897       0.332126        0.260743
C       -2.607651       0.073805        -0.170801
O       -3.245517       1.022144        -0.715280
N       -1.039777       0.009174        1.706588
O       -3.157899       -1.048521       0.000777
H       -0.095205       0.246444        2.027038
H       -1.137120       -0.998326       1.851664
H       -0.942368       1.430102        0.138794
H       -0.428407       -0.222628       -1.728252
H       -0.424503       -1.556276       -0.579534
H       1.388544        2.046008        -0.070167
H       4.324165        -1.055297       0.063170
H       3.878046        1.501521        0.310921
###
19
his401 pm6_conformaciones E=-0.313523121835 au
N       2.828959        -0.011364       0.621789
C       1.679019        -0.760599       0.890211
C       0.881424        -0.687583       -0.258205
N       1.522687        0.095033        -1.228666
C       2.703351        0.489741        -0.670893
C       -0.458199       -1.285477       -0.474770
C       -1.536155       -0.585265       0.381947
C       -1.396572       0.933696        0.214345
O       -0.840256       1.590023        1.144796
N       -2.929774       -0.970513       0.047065
O       -1.793897       1.523837        -0.828428
H       -3.058160       -1.971894       0.224885
H       -3.102261       -0.843505       -0.953240
H       -1.359763       -0.840989       1.463242
H       -0.438554       -2.370786       -0.220197
H       -0.737760       -1.261836       -1.550851
H       1.517470        -1.278241       1.821189
H       3.454845        1.105953        -1.153329
H       3.607103        0.131247        1.260232
###
19
his402 pm6_conformaciones E=-0.313525326803 au
N       2.829041        -0.011879       0.621735
C       1.679203        -0.761472       0.889628
C       0.881458        -0.687520       -0.258632
N       1.522575        0.095936        -1.228511
C       2.703135        0.490497        -0.670436
C       -0.458199       -1.285165       -0.475409
C       -1.536070       -0.585376       0.381815
C       -1.396643       0.933666        0.214627
O       -1.794171       1.524073        -0.827893
N       -2.929620       -0.970747       0.047074
O       -0.840185       1.589715        1.145232
H       -3.057876       -1.972128       0.224964
H       -3.102109       -0.843893       -0.953230
H       -1.359391       -0.841395       1.462986
H       -0.438619       -2.370646       -0.221543
H       -0.737955       -1.260754       -1.551462
H       1.517861        -1.280082       1.820119
H       3.454497        1.107195        -1.152444
H       3.607158        0.130456        1.260248
###
19
his403 pm6_conformaciones E=-0.311557308554 au
N       -2.591316       -1.003889       -0.146428
C       -1.404426       -1.051382       0.591157
C       -0.902494       0.257256        0.622347
N       -1.765376       1.107250        -0.080491
C       -2.780561       0.318571        -0.536361
C       0.348132        0.726425        1.266231
C       1.563847        0.773134        0.315168
```

```
C       1.820358        -0.627584       -0.254952
O       2.577467        -1.401171       0.402789
N       1.461794        1.748761        -0.798844
O       1.298299        -1.026997       -1.334599
H       1.387852        2.694736        -0.412590
H       0.596646        1.595441        -1.320223
H       2.463234        1.063804        0.930006
H       0.204548        1.739394        1.708702
H       0.587241        0.080014        2.141870
H       -1.026037       -1.954489       1.038459
H       -3.628766       0.658038        -1.122017
H       -3.195697       -1.794967       -0.350924
###
19
his404 pm6_conformaciones E=-0.311536806937 au
N       -2.601248       -0.986907       -0.141454
C       -1.424171       -1.043260       0.611011
C       -0.899455       0.256669        0.626840
N       -1.739061       1.110329        -0.099817
C       -2.763250       0.332372        -0.554315
C       0.353279        0.713040        1.275788
C       1.570399        0.760221        0.326010
C       1.808424        -0.635349       -0.264855
O       1.276684        -1.014685       -1.347075
N       1.482685        1.753226        -0.773993
O       2.560248        -1.426068       0.378799
H       1.427622        2.694983        -0.374537
H       0.613495        1.622648        -1.294767
H       2.472485        1.029255        0.946675
H       0.214596        1.722398        1.727793
H       0.588812        0.057638        2.145874
H       -1.065160       -1.945998       1.074928
H       -3.598887       0.677399        -1.154545
H       -3.216402       -1.770984       -0.341241
###
19
his405 pm6_conformaciones E=-0.310051934224 au
N       3.270847        0.533330        -0.136965
C       2.011561        0.959555        0.294939
C       1.219018        -0.190575       0.400413
N       1.972121        -1.316924       0.042576
C       3.212109        -0.850867       -0.278695
C       -0.207836       -0.276433       0.795361
C       -1.127939       0.092209        -0.386110
C       -2.584928       -0.246309       -0.037039
O       -3.154392       0.260590        0.967924
N       -1.106698       1.528005        -0.773785
O       -3.212895       -1.041174       -0.797447
H       -0.200868       1.748361        -1.200865
H       -1.161158       2.116327        0.062412
H       -0.825918       -0.513996       -1.283027
H       -0.403249       0.389652        1.665719
H       -0.452977       -1.298810       1.162502
H       1.775862        1.991492        0.495189
H       4.050495        -1.457293       -0.603051
H       4.070311        1.132584        -0.318700
###
19
his406 pm6_conformaciones E=-0.310052366711 au
N       3.270808        0.533451        -0.136954
C       2.011368        0.959499        0.294672
C       1.219001        -0.190757       0.400144
N       1.972348        -1.317020       0.042517
C       3.212304        -0.850767       -0.278626
C       -0.207833       -0.276848       0.795097
C       -1.127970       0.092476        -0.386092
C       -2.584933       -0.246338       -0.037168
O       -3.212939       -1.040564       -0.798222
N       -1.106883       1.528597        -0.772640
O       -3.154317       0.259612        0.968312
H       -0.201579       1.749033        -1.200774
H       -1.160113       2.116285        0.064080
H       -0.826007       -0.513078       -1.283439
H       -0.403199       0.388785        1.665857
H       -0.452971       -1.299384       1.161763
H       1.775346        1.991435        0.494570
```

```
H       4.050865        -1.457088       -0.602745
H       4.070176        1.132838        -0.318669
###
19
his407 pm6_conformaciones E=-0.309394704031 au
N       3.175120        0.814409        0.075577
C       1.824562        1.073311        -0.174663
C       1.214098        -0.169383       -0.386208
N       2.170027        -1.188290       -0.275617
C       3.350274        -0.564787       0.003852
C       -0.211313       -0.445865       -0.691912
C       -1.151666       0.313490        0.264611
C       -2.608118       0.080178        -0.162732
O       -3.292564       1.081666        -0.523818
N       -1.032767       -0.071744       1.695702
O       -3.120655       -1.072864       -0.155927
H       -0.091823       0.164871        2.027301
H       -1.113764       -1.086278       1.796603
H       -0.934136       1.415071        0.188092
H       -0.421926       -1.537214       -0.657518
H       -0.426761       -0.152828       -1.746524
H       1.410720        2.067728        -0.186411
H       4.304974        -1.056864       0.152784
H       3.884785        1.512801        0.276309
###
19
his408 pm6_conformaciones E=-0.313813733945 au
N       2.861691        -0.088423       0.592011
C       1.734136        -0.892775       0.784579
C       0.890785        -0.661483       -0.308609
N       1.481594        0.273013        -1.170965
C       2.675598        0.604181        -0.601314
C       -0.449389       -1.244497       -0.560093
C       -1.518924       -0.612762       0.358541
C       -1.414365       0.914847        0.261124
O       -0.865785       1.542149        1.215573
N       -2.913122       -1.008644       0.038573
O       -1.832808       1.541333        -0.752300
H       -3.021916       -2.017454       0.183959
H       -3.108158       -0.850345       -0.953141
H       -1.309791       -0.919551       1.420291
H       -0.739417       -1.137360       -1.628183
H       -0.425420       -2.345817       -0.388907
H       1.615353        -1.548210       1.631549
H       3.396610        1.305482        -1.008798
H       3.663297        -0.031278       1.214344
###
19
his409 pm6_conformaciones E=-0.312899973194 au
N       -2.778673       0.580550        0.439794
C       -1.568502       0.320875        1.089270
C       -0.903823       -0.643833       0.319815
N       -1.686377       -0.979826       -0.792083
C       -2.817439       -0.222933       -0.696248
C       0.437291        -1.224607       0.574494
C       1.510133        -0.623391       -0.359908
C       1.440962        0.906990        -0.268170
O       0.854295        1.539083        -1.197638
N       2.898237        -1.052298       -0.053938
O       1.930379        1.533154        0.711818
H       2.979638        -2.064764       -0.191019
H       3.109139        -0.889408       0.933859
H       1.286351        -0.929328       -1.418004
H       0.722754        -1.078880       1.640669
H       0.417982        -2.330805       0.444480
H       -1.280447       0.798370        2.010625
H       -3.645797       -0.236586       -1.397093
H       -3.491060       1.235922        0.751108
###
# Conformations of LYSINE optimized with pm6
# opt freq pm6 scf=(xqc,tight) scrf(smd,solvent=water)
###
26
lys100 pm6_conformaciones E=0.820167300859E-01 au
N       2.625698        -1.276421       -0.717260
H       3.269186        -1.312801       0.096870
```

```
H       3.132778        -0.853241       -1.520995
H       2.384443        -2.258428       -0.972924
C       1.364688        -0.496758       -0.398505
H       0.731602        -0.448647       -1.344417
C       0.572161        -1.193310       0.720996
C       1.733446        0.919977        0.031927
H       0.496724        -2.283671       0.496286
H       1.132405        -1.141724       1.681383
C       -0.826389       -0.600242       0.902657
O       2.704499        1.276452        0.675070
H       -1.250680       -0.978280       1.858810
H       -0.769021       0.500509        1.037645
C       -1.762016       -0.953670       -0.257335
H       -1.358794       -0.566774       -1.219189
H       -1.791620       -2.058275       -0.395111
C       -3.189487       -0.459531       -0.039077
H       -3.891914       -0.985475       -0.733108
H       -3.550472       -0.693994       0.992665
N       -3.308373       1.034405        -0.273347
H       -2.972384       1.288569        -1.219081
H       -4.295739       1.337254        -0.190711
H       -2.750555       1.565532        0.417165
O       0.790277        1.790451        -0.391432
H       0.950146        2.749552        -0.084116
###
26
lys101 pm6_conformaciones E=0.817614039289E-01 au
N       -0.492187       1.740951        0.165700
H       -0.076572       1.343785        1.035588
H       -1.220308       2.430739        0.435349
H       0.271413        2.245170        -0.339699
C       -1.068857       0.649790        -0.712655
H       -1.502537       1.155262        -1.643138
C       0.010599        -0.343545       -1.170510
C       -2.217152       -0.080875       -0.030882
H       -0.400953       -0.909871       -2.041559
H       0.861137        0.226667        -1.614454
C       0.504732        -1.342514       -0.124092
O       -2.979913       -0.868205       -0.562425
H       -0.353290       -1.777304       0.432301
H       0.945944        -2.213156       -0.662817
C       1.525952        -0.819031       0.888278
H       1.151116        0.086862        1.413778
H       1.620993        -1.571647       1.707799
C       2.921487        -0.577883       0.315265
H       3.694761        -0.713894       1.112491
H       3.173643        -1.323791       -0.477577
N       3.063665        0.818134        -0.258749
H       2.763970        1.536691        0.426751
H       4.045354        1.006956        -0.526332
H       2.468123        0.932989        -1.102028
O       -2.322371       0.237775        1.280608
H       -3.085439       -0.241258       1.757000
###
26
lys102 pm6_conformaciones E=0.833020853891E-01 au
N       2.635473        -0.778799       0.864646
H       1.955218        -0.947744       1.630781
H       3.334533        -0.085344       1.198176
H       3.134943        -1.673897       0.676254
C       1.946883        -0.293737       -0.397597
H       2.745823        -0.198182       -1.207372
C       0.886041        -1.300931       -0.868874
C       1.322679        1.082538        -0.205953
H       0.607488        -1.060382       -1.920923
H       1.360401        -2.308485       -0.945045
C       -0.356633       -1.380171       0.020256
O       1.136250        1.909446        -1.080203
H       -0.684253       -2.440196       0.094457
H       -0.113148       -1.100047       1.067431
C       -1.515462       -0.525451       -0.507332
H       -1.150907       0.444211        -0.907050
H       -1.990304       -1.030619       -1.376667
C       -2.543397       -0.281576       0.598318
H       -2.879076       -1.242857       1.059749
H       -2.104471       0.319205        1.432836
```

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N       -3.751963       0.450798        0.049405
H       -4.239036       -0.116820       -0.665959
H       -4.426906       0.665236        0.805609
H       -3.474126       1.344578        -0.393090
O       0.962365        1.305112        1.079057
H       0.509668        2.206852        1.228711
###
26
lys103 pm6_conformaciones E=0.820956211937E-01 au
N       -1.840673       1.894685        -0.309263
H       -2.275760       2.072448        0.616523
H       -2.588342       1.929376        -1.030644
H       -1.169112       2.667466        -0.502735
C       -1.122810       0.558538        -0.335847
H       -0.637777       0.439546        -1.362026
C       -0.040513       0.512980        0.756411
C       -2.095973       -0.598349       -0.146746
H       0.577874        1.441459        0.701510
H       -0.508934       0.543955        1.765441
C       0.866892        -0.713284       0.642777
O       -1.939931       -1.739108       -0.541970
H       1.483820        -0.782503       1.566201
H       0.263971        -1.646206       0.647824
C       1.768803        -0.701127       -0.593915
H       2.249904        -1.698195       -0.710140
H       1.155987        -0.577475       -1.516001
C       2.827539        0.398337        -0.573485
H       3.255854        0.546549        -1.595810
H       2.384114        1.384141        -0.284609
N       3.956647        0.067963        0.384383
H       4.384509        -0.846003       0.155376
H       4.696740        0.790215        0.337876
H       3.616137        0.021466        1.360487
O       -3.193411       -0.232941       0.557672
H       -3.857689       -0.990953       0.704104
###
26
lys104 pm6_conformaciones E=0.836041125087E-01 au
N       -2.704785       -0.481379       -0.498612
H       -2.250220       -0.737383       -1.395972
H       -3.397318       0.271005        -0.688083
H       -3.223369       -1.317153       -0.153133
C       -1.687129       -0.042753       0.536226
H       -2.259279       0.273830        1.474530
C       -0.747574       -1.195201       0.921923
C       -0.923682       1.176596        0.039675
H       -0.078678       -0.835423       1.740799
H       -1.358433       -1.998837       1.399809
C       0.083862        -1.812565       -0.202942
O       -1.012514       1.722112        -1.045972
H       0.530555        -2.757381       0.184069
H       -0.567759       -2.144292       -1.039503
C       1.197742        -0.925107       -0.764072
H       1.722452        -1.477627       -1.576500
H       0.774805        -0.035910       -1.276280
C       2.200456        -0.512609       0.314451
H       1.680358        -0.115035       1.222914
H       2.793419        -1.391043       0.667897
N       3.146388        0.547773        -0.212224
H       2.630016        1.406653        -0.475058
H       3.846549        0.803552        0.507385
H       3.653833        0.211859        -1.049544
O       -0.091715       1.633457        1.004534
H       0.503629        2.403726        0.692469
###
26
lys105 pm6_conformaciones E=0.831986311933E-01 au
N       -1.846043       1.701739        0.456109
H       -2.010042       1.570801        1.474403
H       -2.696192       2.133083        0.041233
H       -1.061602       2.377206        0.345010
C       -1.509303       0.388066        -0.223630
H       -1.358393       0.589461        -1.338276
C       -0.230621       -0.229058       0.360509
C       -2.680357       -0.584152       -0.095928
H       -0.266636       -0.232498       1.472527
```

```
H       -0.189418       -1.305478       0.071435
C       1.031236        0.485265        -0.133050
O       -2.664766       -1.713185       0.356835
H       0.971567        0.663081        -1.228326
H       1.106568        1.495826        0.321170
C       2.282270        -0.335633       0.196923
H       2.353326        -0.509382       1.292534
H       2.207507        -1.348941       -0.254406
C       3.534349        0.380722        -0.309758
H       3.463751        0.593789        -1.405193
H       3.661805        1.373623        0.187127
N       4.767861        -0.460909       -0.049838
H       4.711286        -1.367670       -0.546858
H       5.619972        0.028644        -0.374817
H       4.875983        -0.660947       0.960269
O       -3.809392       -0.043050       -0.614555
H       -4.614385       -0.667798       -0.570365
###
26
lys106 pm6_conformaciones E=0.830996961282E-01 au
N       -1.360380       -1.288133       1.316591
H       -2.068908       -1.936584       0.922270
H       -1.758523       -0.850108       2.171732
H       -0.532974       -1.853036       1.603750
C       -0.946453       -0.238381       0.303596
H       -0.132673       0.413928        0.782289
C       -0.399665       -0.893163       -0.974816
C       -2.139386       0.644202        -0.041386
H       -1.096564       -1.691233       -1.321302
H       -0.399539       -0.141682       -1.798532
C       1.005684        -1.476588       -0.811591
O       -3.322763       0.384168        0.067995
H       1.069461        -2.115551       0.094488
H       1.185011        -2.180576       -1.656102
C       2.121690        -0.427450       -0.807941
H       3.064769        -0.894680       -1.169601
H       1.902379        0.374921        -1.545385
C       2.341939        0.170489        0.581705
H       1.398136        0.636768        0.976404
H       2.620166        -0.616694       1.324538
N       3.431779        1.223086        0.543728
H       3.183773        1.994278        -0.101106
H       3.581231        1.627773        1.484974
H       4.327801        0.817454        0.219827
O       -1.711252       1.834349        -0.529398
H       -2.474067       2.447559        -0.816650
###
26
lys107 pm6_conformaciones E=0.816621087984E-01 au
N       -1.720891       1.937138        0.154952
H       -1.432043       1.847360        1.148089
H       -2.713406       2.249053        0.134139
H       -1.137723       2.683781        -0.279379
C       -1.545913       0.635611        -0.602140
H       -1.946352       0.795676        -1.659045
C       -0.067509       0.234370        -0.705846
C       -2.356359       -0.472253       0.061744
H       0.009107        -0.644761       -1.387233
H       0.487251        1.043955        -1.237346
C       0.606404        -0.071287       0.634097
O       -2.585516       -0.637214       1.244683
H       0.679590        0.847347        1.254889
H       -0.011180       -0.775768       1.230574
C       1.998349        -0.682320       0.444253
H       2.342486        -1.112338       1.411378
H       1.950619        -1.544496       -0.255508
C       3.004503        0.355135        -0.054722
H       2.695999        0.780662        -1.041463
H       3.068935        1.222046        0.647286
N       4.380168        -0.265633       -0.200033
H       4.373082        -1.016337       -0.912947
H       5.073040        0.446486        -0.491810
H       4.701524        -0.679298       0.693026
O       -2.818757       -1.329796       -0.883113
H       -3.358545       -2.103358       -0.495955
###
```

```
26
lys108 pm6_conformaciones E=0.824876827170E-01 au
N       2.187457        -1.167926       -1.142708
H       2.945430        -1.403808       -0.472975
H       2.589856        -0.584243       -1.903585
H       1.850985        -2.058273       -1.569178
C       1.035582        -0.457623       -0.458940
H       0.240287        -0.230513       -1.251141
C       0.433028        -1.356598       0.634047
C       1.518828        0.852959        0.155137
H       0.212834        -2.361159       0.201675
H       1.191717        -1.552602       1.425245
C       -0.831880       -0.771916       1.266405
O       2.585347        1.074194        0.701109
H       -0.949628       -1.220790       2.279726
H       -0.712469       0.313985        1.464112
C       -2.114089       -1.039551       0.474372
H       -2.171980       -2.117945       0.202387
H       -2.993539       -0.872948       1.137525
C       -2.266942       -0.216238       -0.801066
H       -1.354177       -0.284409       -1.450618
H       -3.106310       -0.618363       -1.422346
N       -2.542668       1.242789        -0.493213
H       -1.710633       1.695623        -0.071330
H       -2.785283       1.760822        -1.356649
H       -3.329965       1.340985        0.172256
O       0.556655        1.791870        0.042375
H       0.786165        2.674885        0.498742
###
26
lys109 pm6_conformaciones E=0.824940445598E-01 au
N       -2.842942       1.127886        0.463802
C       -2.544827       -0.328890       0.769132
C       -2.217947       -1.119898       -0.496658
C       -0.723044       -1.356714       -0.734813
C       0.049988        -0.101182       -1.147850
C       0.801198        0.534617        0.035326
N       1.070049        2.003384        -0.227544
C       2.114565        -0.211771       0.252084
O       3.109257        -0.205943       -0.449003
O       2.039930        -0.964488       1.376471
H       2.878861        -1.514337       1.555401
H       1.607445        2.142117        -1.104576
H       1.603239        2.432541        0.555060
H       0.164088        2.515439        -0.322317
H       0.757650        -0.337373       -1.972237
H       -0.648549       0.645035        -1.596807
H       -0.265731       -1.829140       0.159621
H       -0.616105       -2.119482       -1.538476
H       -2.724484       -2.110136       -0.432566
H       -2.676191       -0.642340       -1.391258
H       -3.436453       -0.767541       1.282958
H       -1.717072       -0.381136       1.518468
H       -3.172306       1.618103        1.313849
H       -3.580031       1.208417        -0.258603
H       -2.003780       1.623928        0.114933
H       0.166583        0.463504        0.979674
###
26
lys110 pm6_conformaciones E=0.834791203027E-01 au
N       -2.783382       -1.236484       0.498530
H       -3.247378       -1.210498       -0.430263
H       -3.410173       -0.779234       1.189774
H       -2.676983       -2.236945       0.772070
C       -1.426097       -0.556619       0.460924
H       -0.966312       -0.645736       1.500926
C       -0.512956       -1.236607       -0.573640
C       -1.574940       0.928398        0.149087
H       -0.782055       -2.317926       -0.654033
H       -0.702815       -0.833920       -1.592723
C       0.971739        -1.137885       -0.214341
O       -0.826038       1.819804        0.501591
H       1.117398        -1.305389       0.874125
H       1.506668        -1.983246       -0.701974
C       1.606319        0.187199        -0.646282
H       1.311402        0.427151        -1.693174
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H       1.208718        1.028580        -0.039117
C       3.131730        0.160658        -0.581337
H       3.543648        -0.746214       -1.088635
H       3.556777        1.036924        -1.131739
N       3.631463        0.196027        0.849767
H       3.322130        -0.641445       1.372200
H       4.665909        0.228413        0.876625
H       3.270428        1.029165        1.346105
O       -2.677877       1.180110        -0.597656
H       -2.797388       2.163354        -0.836193
###
26
lys111 pm6_conformaciones E=0.890225996914E-01 au
N       -2.683273       0.133664        -0.857009
H       -3.220498       0.016437        0.022173
H       -2.908976       -0.662895       -1.484948
H       -3.017099       1.005389        -1.317175
C       -1.186246       0.218793        -0.585766
H       -0.669924       0.352923        -1.587242
C       -0.909597       1.432680        0.308946
C       -0.720620       -1.123782       0.017397
H       -1.483470       2.314859        -0.059981
H       -1.292504       1.252709        1.336640
C       0.573750        1.795043        0.346271
O       0.670744        -1.418626       -0.115331
H       0.930776        2.061036        -0.672860
H       0.692043        2.735326        0.932213
C       1.456635        0.719555        0.975324
H       2.438497        1.175192        1.257833
H       1.026115        0.388259        1.948925
C       1.735490        -0.511895       0.132766
H       2.508357        -1.185525       0.612480
H       -1.158338       -2.029546       -0.483118
N       2.239791        -0.154233       -1.275964
H       3.243913        0.117908        -1.249710
H       2.140918        -0.970116       -1.913465
H       1.708618        0.634503        -1.695701
O       -1.025059       -1.117660       1.400307
H       -0.696003       -1.954557       1.835320
###
26
lys112 pm6_conformaciones E=0.836305077254E-01 au
N       -1.850414       1.504559        -1.034706
H       -2.628634       1.810433        -0.419029
H       -2.263923       1.108687        -1.902691
H       -1.295799       2.347030        -1.293466
C       -0.964823       0.487916        -0.340195
H       -0.104909       0.219680        -1.050604
C       -0.396049       1.089512        0.956071
C       -1.721622       -0.798902       -0.041202
H       -0.061042       2.136431        0.761280
H       -1.204608       1.192422        1.714668
C       0.763430        0.279958        1.541269
O       -1.240530       -1.844488       0.355231
H       0.910668        0.604586        2.596596
H       0.494961        -0.794445       1.618670
C       2.087792        0.451949        0.791227
H       2.199473        1.500811        0.439580
H       2.931277        0.297553        1.500657
C       2.215311        -0.520145       -0.382262
H       2.123076        -1.580524       -0.040998
H       1.391967        -0.360733       -1.129950
N       3.549324        -0.342319       -1.078494
H       4.334986        -0.509887       -0.425643
H       3.640973        -1.006770       -1.867822
H       3.646009        0.617780        -1.453467
O       -3.050838       -0.672889       -0.271166
H       -3.580137       -1.521440       -0.077351
###
26
lys113 pm6_conformaciones E=0.833168069790E-01 au
N       -0.915242       1.653004        -0.310321
H       -1.109759       2.085087        0.613662
H       -1.450353       2.170125        -1.037215
H       0.102396        1.779937        -0.510852
C       -1.258543       0.175204        -0.322127
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H       -1.039269       -0.225429       -1.366347
C       -0.433840       -0.599223       0.718982
C       -2.744737       -0.012724       -0.025420
H       -0.303491       0.004054        1.646506
H       -1.013185       -1.490780       1.058521
C       0.919119        -1.076279       0.186613
O       -3.443266       0.596189        0.762552
H       1.248036        -1.946638       0.797849
H       0.812319        -1.476198       -0.844144
C       1.997460        0.010580        0.221396
H       1.738120        0.840368        -0.474184
H       2.042952        0.475196        1.230895
C       3.358665        -0.578369       -0.151880
H       3.655999        -1.389768       0.556539
H       3.330565        -1.046090       -1.166666
N       4.422418        0.501814        -0.136108
H       4.489350        0.941615        0.798705
H       5.348831        0.105878        -0.373207
H       4.204998        1.246515        -0.822256
O       -3.234924       -1.024851       -0.782513
H       -4.210971       -1.243439       -0.588500
###
26
lys114 pm6_conformaciones E=0.812571014576E-01 au
N       -0.987183       1.892414        -0.058770
H       -1.477141       2.153041        0.818084
H       -1.544730       2.246736        -0.860176
H       -0.060805       2.375659        -0.066256
C       -0.788819       0.393381        -0.155713
H       -0.215147       0.185394        -1.128842
C       0.026262        -0.133448       1.039352
C       -2.109829       -0.355729       -0.238852
H       0.679878        0.675333        1.446896
H       -0.642898       -0.383378       1.892733
C       0.876593        -1.351385       0.670908
O       -2.251989       -1.522290       -0.560896
H       1.434227        -1.679973       1.575474
H       0.214215        -2.207675       0.420260
C       1.849399        -1.121513       -0.489213
H       2.207863        -2.110698       -0.856620
H       1.310866        -0.685152       -1.364600
C       3.071708        -0.277100       -0.139076
H       3.463700        -0.527870       0.877050
H       3.908308        -0.497353       -0.848637
N       2.770336        1.208022        -0.199173
H       2.108252        1.485890        0.551542
H       3.636100        1.763505        -0.086138
H       2.332440        1.464755        -1.103526
O       -3.164398       0.420180        0.104373
H       -4.057980       -0.069618       0.066104
###
26
lys115 pm6_conformaciones E=0.820320443282E-01 au
N       -1.591126       1.761156        -0.614589
H       -2.006773       2.239772        0.208318
H       -2.261426       1.828255        -1.406923
H       -0.728579       2.280764        -0.882741
C       -1.251606       0.315843        -0.303485
H       -0.777535       -0.143253       -1.232316
C       -0.278817       0.216237        0.882908
C       -2.525050       -0.447676       0.046044
H       -0.631024       0.856366        1.724584
H       -0.302638       -0.822113       1.290037
C       1.159043        0.590578        0.521152
O       -3.449953       -0.085005       0.749122
H       1.199376        1.590133        0.039797
H       1.734443        0.709018        1.466122
C       1.827109        -0.455759       -0.376456
H       1.781323        -1.461094       0.096249
H       1.254203        -0.564142       -1.325753
C       3.268041        -0.094549       -0.727198
H       3.620023        -0.701558       -1.598239
H       3.355164        0.973513        -1.045600
N       4.200757        -0.338567       0.443934
H       4.147354        -1.322452       0.761837
H       5.182029        -0.140107       0.180260
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H       3.958422        0.267582        1.246082
O       -2.509054       -1.671064       -0.536526
H       -3.312046       -2.248309       -0.285695
###
26
lys116 pm6_conformaciones E=0.823215863678E-01 au
N       2.236674        -1.678641       -0.053252
H       2.018940        -1.699730       0.961730
H       3.270080        -1.667129       -0.161902
H       1.873320        -2.558046       -0.477502
C       1.608485        -0.477438       -0.733424
H       1.973305        -0.463852       -1.818281
C       0.076940        -0.580733       -0.742448
C       2.062379        0.833441        -0.107542
H       -0.321348       0.182334        -1.450787
H       -0.216687       -1.556819       -1.196981
C       -0.575228       -0.419957       0.632974
O       1.691436        1.948790        -0.425281
H       -0.140569       -1.142456       1.357266
H       -0.355911       0.582792        1.055220
C       -2.089231       -0.646101       0.577644
H       -2.317024       -1.610104       0.073038
H       -2.475565       -0.764514       1.614972
C       -2.812577       0.504753        -0.122899
H       -2.560747       1.486190        0.348119
H       -2.500940       0.587967        -1.193000
N       -4.313876       0.301256        -0.064049
H       -4.642253       0.244030        0.916187
H       -4.807162       1.087599        -0.522969
H       -4.588187       -0.574174       -0.542950
O       2.983248        0.641189        0.866901
H       3.309091        1.503982        1.300155
###
26
lys117 pm6_conformaciones E=0.827927140801E-01 au
N       -2.557305       -1.471444       -0.461454
H       -2.441025       -1.295757       -1.478609
H       -3.539735       -1.251004       -0.204162
H       -2.399127       -2.487009       -0.292757
C       -1.578792       -0.647872       0.355435
H       -1.721159       -0.920061       1.453480
C       -0.137546       -0.962291       -0.076942
C       -1.857678       0.844100        0.211027
H       -0.003187       -2.069816       -0.121061
H       0.042331        -0.611889       -1.117525
C       0.889779        -0.354461       0.883072
O       -1.576484       1.709619        1.019429
H       0.869772        0.753680        0.823260
H       0.617646        -0.596560       1.933491
C       2.303317        -0.875348       0.608144
H       2.955922        -0.653710       1.482289
H       2.292688        -1.987196       0.546991
C       2.927186        -0.325788       -0.672223
H       3.763928        -0.984634       -1.013612
H       2.193443        -0.312994       -1.515382
N       3.466785        1.076482        -0.465792
H       4.185379        1.089707        0.279320
H       3.899626        1.435634        -1.335653
H       2.713011        1.728635        -0.189076
O       -2.472056       1.132434        -0.960437
H       -2.685138       2.121238        -1.083290
###
25
lys200 pm6_conformaciones E=-0.959934995063E-01 au
N       -2.797953       1.186915        0.315990
C       0.863204        0.505605        0.108396
C       0.055869        -0.148162       -1.024133
C       -0.722227       -1.380039       -0.548532
C       -2.233922       -1.156771       -0.434614
C       -2.654311       -0.264605       0.731549
N       1.179892        1.948462        -0.231439
C       2.166721        -0.292720       0.335491
O       2.295066        -0.924800       1.414084
O       3.043011        -0.314736       -0.564499
H       1.721278        2.021299        -1.111458
H       1.728733        2.396815        0.526132
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H       0.296592        2.489952        -0.355735
H       0.255172        0.505555        1.062984
H       -0.643105       0.593608        -1.475503
H       0.727418        -0.422626       -1.864792
H       -0.547268       -2.213275       -1.264159
H       -0.324825       -1.753630       0.417499
H       -2.640429       -0.772423       -1.395809
H       -2.728377       -2.147645       -0.309905
H       -3.634698       -0.606042       1.148922
H       -1.928990       -0.330394       1.579502
H       -1.899452       1.583804        -0.009047
H       -3.131662       1.760707        1.110690
H       -3.480575       1.283096        -0.456799
###
25
lys201 pm6_conformaciones E=-0.985528820015E-01 au
N       3.162822        1.146753        -0.402674
C       -0.994102       0.145335        -0.118922
C       -0.423037       -0.936868       0.807252
C       1.098561        -0.869950       0.967880
C       1.848857        -0.990081       -0.362814
C       3.241806        -0.365913       -0.318704
N       -0.722671       1.533254        0.425104
C       -2.508309       -0.056352       -0.312484
O       -2.918133       -1.141929       -0.796889
O       -3.290849       0.876113        0.000073
H       -1.016648       1.607414        1.415980
H       -1.237056       2.249905        -0.118196
H       0.292566        1.759209        0.373355
H       -0.496700       0.067495        -1.138303
H       -0.899685       -0.873902       1.810808
H       -0.713331       -1.933901       0.408449
H       1.381360        0.060348        1.504261
H       1.419881        -1.683918       1.653173
H       1.946373        -2.060845       -0.645697
H       1.257553        -0.538212       -1.193803
H       3.791750        -0.651644       0.610922
H       3.864808        -0.740389       -1.168357
H       4.108353        1.565184        -0.428140
H       2.657599        1.539656        0.412955
H       2.651309        1.443049        -1.253133
###
25
lys202 pm6_conformaciones E=-0.946471236668E-01 au
N       -2.387917       1.677670        0.059797
H       -2.144502       1.853811        1.051985
H       -3.398610       1.450381        0.010332
H       -2.230041       2.559876        -0.467733
C       -1.550343       0.554963        -0.522250
H       -1.859212       0.413379        -1.599991
C       -0.062161       0.928808        -0.456788
C       -1.809921       -0.758301       0.246596
H       0.089548        1.910816        -0.960683
H       0.240694        1.111489        0.597654
C       0.835813        -0.124756       -1.115889
O       -1.941110       -0.741974       1.493898
H       0.239877        -0.799891       -1.763393
H       1.522241        0.378235        -1.831520
C       1.640506        -0.957085       -0.110726
H       1.138262        -0.979874       0.879710
H       1.660306        -2.020536       -0.440907
C       3.089917        -0.498756       0.041928
H       3.664991        -1.230366       0.662451
H       3.610130        -0.469436       -0.947247
N       3.186314        0.869213        0.688310
H       2.716772        0.877734        1.611107
H       4.177593        1.136662        0.827414
H       2.738260        1.593357        0.101237
O       -1.886134       -1.818408       -0.426947
###
25
lys203 pm6_conformaciones E=-0.979626267398E-01 au
N       0.626443        1.228932        0.987514
H       0.590159        1.919856        0.214980
H       1.253895        1.590883        1.726788
H       -0.340711       1.153159        1.380819
```

```
C       1.093979        -0.124673       0.491506
H       1.183811        -0.811729       1.386913
C       0.098156        -0.707168       -0.521960
C       2.490770        -0.003732       -0.149517
H       -0.313080       0.098397        -1.174209
H       0.644509        -1.369236       -1.232686
C       -1.028415       -1.518015       0.123031
O       2.980440        1.130800        -0.369257
H       -1.458702       -2.198403       -0.645111
H       -0.604799       -2.199499       0.892995
C       -2.151709       -0.695437       0.758915
H       -2.728023       -1.355397       1.448754
H       -1.739269       0.093789        1.428303
C       -3.132568       -0.095822       -0.247153
H       -3.283392       -0.770681       -1.124984
H       -4.144585       0.021627        0.215478
N       -2.669021       1.260346        -0.741103
H       -1.718191       1.192749        -1.157645
H       -3.313756       1.632421        -1.459006
H       -2.614447       1.941052        0.038216
O       3.102479        -1.067655       -0.429920
###
25
lys204 pm6_conformaciones E=-0.961169620824E-01 au
C       2.627945        0.081206        0.684448
N       -0.496974       -1.468105       -0.379573
C       -0.969864       -0.140213       0.178785
C       -0.479686       1.034167        -0.679700
C       0.837287        1.650187        -0.196728
C       2.083694        0.825391        -0.537073
C       -2.511412       -0.124779       0.244941
O       -3.061512       0.707462        1.011255
N       3.504434        -1.080350       0.258158
O       -3.171048       -0.925578       -0.462747
H       -0.841392       -1.607920       -1.347043
H       -0.837063       -2.255834       0.202212
H       0.540930        -1.514921       -0.403655
H       -0.568425       -0.043237       1.233326
H       -0.397168       0.733345        -1.748457
H       -1.256680       1.832701        -0.688038
H       0.938601        2.656038        -0.661587
H       0.787861        1.854744        0.893658
H       1.868774        0.120064        -1.370227
H       2.872726        1.492068        -0.947131
H       1.802941        -0.312800       1.329210
H       3.219443        0.765512        1.339025
H       3.916335        -1.551072       1.083005
H       2.954341        -1.781337       -0.273239
H       4.279247        -0.758986       -0.347255
###
25
lys205 pm6_conformaciones E=-0.952749025819E-01 au
N       -2.127209       1.713101        -0.540604
H       -2.027700       2.099906        0.415305
H       -3.139021       1.645654        -0.758629
H       -1.701792       2.389407        -1.206081
C       -1.457246       0.356921        -0.657757
H       -1.679402       -0.054408       -1.686603
C       0.058720        0.514842        -0.475518
C       -2.037469       -0.603733       0.402071
H       0.425648        1.330044        -1.142869
H       0.288547        0.864456        0.556744
C       0.809566        -0.783518       -0.785222
O       -2.424292       -0.142253       1.503404
H       0.601144        -1.542757       -0.004039
H       0.427314        -1.221506       -1.733109
C       2.320631        -0.573950       -0.924568
H       2.750944        -1.441187       -1.477651
H       2.534284        0.300273        -1.578421
C       3.066739        -0.448585       0.401248
H       2.699052        -1.191687       1.149817
H       4.153292        -0.676273       0.259026
N       2.940988        0.944565        0.986253
H       1.945501        1.187100        1.156508
H       3.448176        1.010129        1.887365
H       3.333028        1.653806        0.342541
```

```
O       -2.115847       -1.823806       0.113975
###
25
lys206 pm6_conformaciones E=-0.971895378785E-01 au
N       -1.172024       1.631851        -0.193998
H       -1.367264       1.893692        0.789791
H       -1.807894       2.173791        -0.807882
H       -0.188752       1.912799        -0.408219
C       -1.350112       0.142035        -0.406694
H       -1.216478       -0.070086       -1.510301
C       -0.324889       -0.657681       0.407784
C       -2.776106       -0.280797       0.003343
H       -0.260130       -0.266743       1.447782
H       -0.699340       -1.700155       0.531453
C       1.064719        -0.713197       -0.233119
O       -3.429236       0.436544        0.800849
H       1.578164        -1.633854       0.121018
H       0.980644        -0.838918       -1.332838
C       1.922751        0.513505        0.091158
H       1.462051        1.433856        -0.340501
H       1.941387        0.697017        1.188304
C       3.342686        0.400340        -0.457889
H       3.346858        0.009659        -1.505036
H       3.817330        1.411910        -0.513758
N       4.206333        -0.496018       0.409056
H       3.860441        -1.471415       0.398012
H       5.185138        -0.499954       0.070848
H       4.206867        -0.171652       1.392391
O       -3.239948       -1.343545       -0.482595
###
25
lys208 pm6_conformaciones E=-0.971428501110E-01 au
N       -0.519485       1.714030        0.267314
H       -0.106966       1.295138        1.125367
H       -1.239122       2.401617        0.552272
H       0.247592        2.221293        -0.227606
C       -1.107747       0.647558        -0.631563
H       -1.515845       1.167744        -1.553829
C       -0.036331       -0.354862       -1.078698
C       -2.286862       -0.063766       0.059430
H       -0.457084       -0.946748       -1.924814
H       0.811430        0.199786        -1.545756
C       0.470417        -1.317930       -0.002982
O       -2.508123       0.132602        1.278206
H       -0.372590       -1.676839       0.624220
H       0.845108        -2.237480       -0.507709
C       1.568930        -0.777646       0.916782
H       1.242996        0.152418        1.433824
H       1.713348        -1.502882       1.752727
C       2.919349        -0.576742       0.231682
H       3.754369        -0.731451       0.960014
H       3.085479        -1.330147       -0.576918
N       3.048865        0.814116        -0.358102
H       2.959765        1.539669        0.375526
H       3.963731        0.929651        -0.827935
H       2.299514        0.989291        -1.058625
O       -3.004868       -0.821072       -0.644850
###
25
lys209 pm6_conformaciones E=-0.907747949446E-01 au
N       2.460296        -1.031351       0.097168
H       2.035926        -1.384671       0.975577
H       3.296369        -0.473571       0.346420
H       2.770899        -1.852755       -0.458924
C       1.468756        -0.201853       -0.693230
H       1.966066        0.091503        -1.672659
C       0.216023        -1.019257       -1.029804
C       1.157229        1.115278        0.042048
H       -0.466024       -0.381092       -1.637676
H       0.510112        -1.837107       -1.731206
C       -0.529144       -1.645427       0.150402
O       1.812224        1.403185        1.077936
H       -1.222679       -2.419007       -0.251080
H       0.176722        -2.227004       0.783290
C       -1.311531       -0.682702       1.045525
H       -1.527421       -1.200166       2.011741
```

```
H       -0.693506       0.185773        1.347181
C       -2.647561       -0.225223       0.465419
H       -3.210027       -1.080986       0.017003
H       -3.308137       0.172545        1.276051
N       -2.466514       0.851162        -0.586925
H       -1.917188       0.487377        -1.390962
H       -3.381837       1.186359        -0.940802
H       -1.949766       1.663144        -0.203136
O       0.292949        1.882576        -0.443521
###
25
lys210 pm6_conformaciones E=-0.977380470632E-01 au
N       1.541551        1.858305        -0.424535
H       1.388244        1.559432        -1.404222
H       2.498687        2.250873        -0.355582
H       0.863166        2.618202        -0.212900
C       1.358840        0.704516        0.539729
H       1.638592        1.076601        1.573839
C       -0.100152       0.234713        0.577348
C       2.301274        -0.463021       0.189979
H       -0.212625       -0.498068       1.408367
H       -0.746847       1.091544        0.880207
C       -0.600631       -0.371089       -0.736231
O       2.814003        -0.538354       -0.953337
H       -0.666222       0.411468        -1.521229
H       0.134039        -1.107141       -1.125158
C       -1.953773       -1.072028       -0.584157
H       -2.089851       -1.773343       -1.440039
H       -1.955339       -1.732686       0.310288
C       -3.151677       -0.126067       -0.559656
H       -3.001581       0.740029        -1.249040
H       -4.069283       -0.649611       -0.926942
N       -3.425606       0.399470        0.836581
H       -2.649150       0.999961        1.167885
H       -4.295859       0.961187        0.851793
H       -3.534006       -0.377662       1.511842
O       2.531389        -1.313815       1.088899
###
25
lys211 pm6_conformaciones E=-0.958101658583E-01 au
N       2.093669        -1.638322       -0.446201
H       1.961048        -1.869830       0.554631
H       3.112426        -1.615942       -0.638126
H       1.675198        -2.405038       -1.009958
C       1.452253        -0.309299       -0.794648
H       1.722950        -0.069602       -1.869721
C       -0.074874       -0.386651       -0.685879
C       2.026288        0.809290        0.096428
H       -0.504550       0.506157        -1.195991
H       -0.442617       -1.251632       -1.285830
C       -0.596692       -0.478567       0.750990
O       2.751232        0.503581        1.076047
H       -0.018227       -1.236767       1.321706
H       -0.428047       0.479609        1.284107
C       -2.078437       -0.862657       0.816626
H       -2.296325       -1.694398       0.110723
H       -2.288607       -1.297620       1.821620
C       -3.044768       0.298777        0.599298
H       -4.040996       0.065956        1.052732
H       -2.691781       1.226478        1.112424
N       -3.246526       0.596247        -0.873850
H       -3.586631       -0.241437       -1.378555
H       -3.941487       1.353507        -1.002874
H       -2.359341       0.894668        -1.317549
O       1.760564        1.999552        -0.203031
###
25
lys212 pm6_conformaciones E=-0.970298387400E-01 au
N       2.008428        1.730607        -0.204631
H       2.150401        1.640367        -1.227040
H       2.929943        1.910519        0.236735
H       1.407799        2.563003        -0.039015
C       1.366081        0.484717        0.371688
H       1.288300        0.621656        1.491947
C       -0.030637       0.257895        -0.221645
C       2.254906        -0.747895       0.090767
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H       -0.022678       0.431209        -1.320686
H       -0.307367       -0.816649       -0.109406
C       -1.088089       1.136806        0.453620
O       2.842244        -0.855127       -1.013150
H       -1.135897       0.911130        1.539788
H       -0.783996       2.204593        0.398894
C       -2.475733       0.990452        -0.178238
H       -3.068943       1.905901        0.051041
H       -2.403007       0.982639        -1.287586
C       -3.267235       -0.215210       0.322057
H       -3.108581       -0.380484       1.416221
H       -4.365550       -0.038772       0.202816
N       -2.897533       -1.480680       -0.426645
H       -1.878918       -1.669501       -0.356593
H       -3.404238       -2.297378       -0.041756
H       -3.133609       -1.398594       -1.432054
O       2.345796        -1.614839       0.996417
###
25
lys213 pm6_conformaciones E=-0.960439932088E-01 au
N       -2.005667       1.697405        -0.217265
H       -2.444717       1.805478        0.715218
H       -2.757721       1.694417        -0.932665
H       -1.411598       2.533954        -0.386601
C       -1.174099       0.431191        -0.293836
H       -0.716612       0.378048        -1.326972
C       -0.062208       0.434511        0.763104
C       -2.083594       -0.804785       -0.092044
H       -0.465905       0.764133        1.746754
H       0.280170        -0.610806       0.937270
C       1.131673        1.314858        0.383938
O       -2.736862       -0.935656       0.972009
H       0.780035        2.314858        0.052226
H       1.724500        1.523412        1.301350
C       2.033846        0.715441        -0.699603
H       1.447533        0.090288        -1.407614
H       2.433253        1.537390        -1.337061
C       3.222771        -0.067483       -0.146433
H       4.027842        -0.152625       -0.918800
H       3.694275        0.461394        0.717959
N       2.820455        -1.461758       0.290557
H       2.502914        -2.024639       -0.517288
H       3.617857        -1.951665       0.734261
H       2.042551        -1.426440       0.974585
O       -2.121667       -1.655486       -1.016561
###
25
lys214 pm6_conformaciones E=-0.976495059622E-01 au
N       -1.307771       1.920929        -0.047766
H       -1.064922       1.844761        0.956574
H       -2.208111       2.429555        -0.124235
H       -0.569877       2.491114        -0.509223
C       -1.403374       0.555665        -0.696916
H       -1.820865       0.702226        -1.740322
C       -0.023054       -0.102580       -0.816790
C       -2.373005       -0.357294       0.079495
H       -0.128217       -1.043363       -1.401320
H       0.634399        0.540967        -1.446529
C       0.655525        -0.384770       0.526208
O       -2.626159       -0.124953       1.284895
H       0.865496        0.564454        1.062718
H       -0.029121       -0.945802       1.196444
C       1.947918        -1.191423       0.366067
H       2.335786        -1.461611       1.373627
H       1.729723        -2.166893       -0.124637
C       3.037745        -0.490879       -0.442037
H       3.896098        -1.186517       -0.616803
H       2.672348        -0.204410       -1.458938
N       3.550343        0.748212        0.265833
H       3.861479        0.524150        1.227287
H       4.354188        1.155334        -0.244575
H       2.813167        1.471027        0.332263
O       -2.885105       -1.321460       -0.548014
###
25
lys215 pm6_conformaciones E=-0.970216802382E-01 au
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N       -1.879843       1.968593        -0.063096
H       -2.075887       2.025848        0.953139
H       -2.766979       2.138610        -0.574264
H       -1.220140       2.736776        -0.303101
C       -1.287677       0.623904        -0.437158
H       -1.142037       0.607206        -1.558334
C       0.069629        0.439018        0.255082
C       -2.261175       -0.510529       -0.046536
H       0.743671        1.278035        -0.042699
H       -0.036269       0.536301        1.357403
C       0.712214        -0.904729       -0.101310
O       -2.762802       -0.540563       1.103534
H       0.059744        -1.737563       0.236412
H       0.781827        -1.017856       -1.203572
C       2.094981        -1.080800       0.535722
H       2.106089        -0.675943       1.571722
H       2.294874        -2.168779       0.669600
C       3.235770        -0.489577       -0.289186
H       4.203179        -0.991766       -0.038586
H       3.081100        -0.664065       -1.382687
N       3.388008        0.998894        -0.043082
H       3.703870        1.181246        0.926269
H       4.081754        1.409515        -0.692645
H       2.483894        1.491675        -0.177110
O       -2.516984       -1.382608       -0.915782
###
25
lys216 pm6_conformaciones E=-0.974977781594E-01 au
N       -1.276838       2.001650        -0.058424
H       -1.877287       2.157540        0.771246
H       -1.801416       2.304808        -0.900501
H       -0.438784       2.613606        0.037382
C       -0.854630       0.551952        -0.172993
H       -0.227910       0.450011        -1.111776
C       -0.017945       0.143134        1.048417
C       -2.087813       -0.372212       -0.281175
H       0.719570        0.944752        1.288764
H       -0.660110       0.084650        1.954387
C       0.703736        -1.191039       0.846562
O       -2.994924       -0.301514       0.584496
H       1.196631        -1.473729       1.803056
H       -0.036446       -1.998884       0.665198
C       1.735172        -1.200004       -0.285057
H       2.057533        -2.251743       -0.463647
H       1.265559        -0.892281       -1.246428
C       2.980597        -0.362486       -0.004699
H       3.255376        -0.382779       1.078357
H       3.864585        -0.781621       -0.546930
N       2.791632        1.078453        -0.439329
H       2.035254        1.536106        0.103280
H       3.662215        1.621044        -0.299439
H       2.533313        1.132101        -1.441279
O       -2.118369       -1.203532       -1.223713
###
25
lys217 pm6_conformaciones E=-0.967301232366E-01 au
N       -2.340857       -1.472727       -0.435393
H       -1.861976       -1.444375       -1.353655
H       -3.343189       -1.255741       -0.588769
H       -2.272740       -2.443957       -0.070652
C       -1.720464       -0.495678       0.542080
H       -2.289756       -0.585066       1.518521
C       -0.248276       -0.833544       0.806820
C       -1.871273       0.955674        0.043941
H       0.125544        -0.174218       1.622063
H       -0.180568       -1.863170       1.227373
C       0.656168        -0.711475       -0.423974
O       -2.091684       1.189441        -1.168374
H       0.289533        -1.373366       -1.237565
H       0.613607        0.315081        -0.840958
C       2.103953        -1.094488       -0.099601
H       2.122844        -1.980482       0.574682
H       2.612037        -1.444881       -1.026020
C       2.906461        0.028558        0.552168
H       2.300854        0.580492        1.311248
H       3.781431        -0.387111       1.111037
```

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N       3.414550        1.009986        -0.487352
H       2.630448        1.445738        -1.002861
H       3.965632        1.765654        -0.043481
H       4.021050        0.535699        -1.179919
O       -1.782068       1.867385        0.907070
###
24
lys300 pm6_conformaciones E=-0.239153031210 au
N       -2.824722       1.172395        0.309016
C       0.880811        0.613407        0.002085
C       0.038235        -0.096865       -1.071354
C       -0.675228       -1.343660       -0.536476
C       -2.187607       -1.172732       -0.361046
C       -2.585447       -0.247304       0.787442
N       1.412106        1.940685        -0.416153
C       2.104584        -0.233056       0.381010
O       2.346206        -0.453279       1.602747
O       2.874830        -0.701097       -0.508077
H       1.816136        1.879760        -1.353739
H       0.633951        2.604095        -0.491006
H       0.249094        0.766930        0.920136
H       -0.696411       0.621332        -1.494850
H       0.671597        -0.368911       -1.939033
H       -0.501613       -2.189433       -1.236182
H       -0.225300       -1.677287       0.420929
H       -2.651463       -0.843764       -1.316509
H       -2.638108       -2.174279       -0.173918
H       -3.521209       -0.614796       1.278285
H       -1.811027       -0.234111       1.592695
H       -1.960476       1.589984        -0.077654
H       -3.150918       1.771564        1.087970
H       -3.546313       1.193626        -0.434491
###
24
lys301 pm6_conformaciones E=-0.239672312966 au
N       -3.696596       -1.122304       -0.014226
C       0.976254        -0.120648       0.240197
C       0.521702        1.092730        -0.590983
C       -0.906823       1.549093        -0.282522
C       -1.992580       0.564107        -0.733047
C       -2.552343       -0.237862       0.442524
N       1.013345        0.092775        1.712561
C       2.399116        -0.504001       -0.194734
O       2.586865        -1.622074       -0.757279
O       3.366855        0.288143        -0.011646
H       1.436791        0.999324        1.922860
H       0.051391        0.150856        2.065412
H       0.290366        -0.986321       0.033208
H       1.211339        1.946477        -0.424240
H       0.613414        0.854961        -1.671867
H       -1.011087       1.780145        0.798037
H       -1.076202       2.523955        -0.789780
H       -2.813445       1.124439        -1.232199
H       -1.604421       -0.119728       -1.517030
H       -1.766281       -0.877409       0.912406
H       -2.920298       0.436122        1.254661
H       -4.462304       -0.558615       -0.424159
H       -4.085754       -1.659912       0.781043
H       -3.382469       -1.796654       -0.733917
###
24
lys302 pm6_conformaciones E=-0.240663207070 au
N       2.985570        -1.193296       -0.174860
H       3.118457        -1.369528       0.824221
H       3.027791        -2.113762       -0.622835
C       1.642998        -0.591754       -0.414604
H       1.447231        -0.620805       -1.521347
C       0.491616        -1.302393       0.316007
C       1.757486        0.874854        0.022213
H       0.654891        -2.401341       0.255954
H       0.516620        -1.078594       1.400889
C       -0.885697       -0.981279       -0.271642
O       1.940594        1.191327        1.230376
H       -0.833286       -0.945537       -1.379412
H       -1.571263       -1.827928       -0.051103
C       -1.482385       0.321146        0.271189
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H       -1.581220       0.270190        1.377458
H       -0.791975       1.170880        0.084828
C       -2.828158       0.661723        -0.367532
H       -3.080757       1.737239        -0.192494
H       -2.795946       0.536943        -1.477988
N       -3.946414       -0.196519       0.191489
H       -4.020012       -0.087919       1.218238
H       -4.855851       0.069718        -0.226190
H       -3.783966       -1.198186       -0.011105
O       1.696910        1.770367        -0.871539
###
24
lys303 pm6_conformaciones E=-0.239460892471 au
N       0.630100        0.995121        1.256423
H       0.359986        1.752643        0.619892
H       -0.237359       0.758442        1.760830
C       1.065416        -0.189411       0.469972
H       1.148692        -1.057946       1.180449
C       0.127910        -0.576393       -0.690480
C       2.465095        0.089348        -0.092029
H       -0.274583       0.334676        -1.184220
H       0.705122        -1.089452       -1.490322
C       -1.012789       -1.500822       -0.254248
O       2.792910        1.210005        -0.572066
H       -1.483733       -1.936793       -1.161891
H       -0.592401       -2.373797       0.289866
C       -2.090231       -0.852195       0.619655
H       -2.636098       -1.655474       1.167429
H       -1.635131       -0.242531       1.432535
C       -3.119783       -0.035233       -0.157140
H       -3.407547       -0.541230       -1.111001
H       -4.067370       0.056130        0.430503
N       -2.610631       1.358366        -0.470750
H       -1.711473       1.313940        -0.991233
H       -3.294461       1.881009        -1.046364
H       -2.438728       1.894919        0.399315
O       3.308976        -0.857595       -0.074169
###
24
lys304 pm6_conformaciones E=-0.240152088170 au
C       0.429455        1.132283        -0.021504
C       -1.054208       1.119749        -0.404131
C       -1.978807       0.572586        0.691314
C       -2.733464       -0.689916       0.281831
N       -3.880504       -0.361962       -0.656784
C       1.095470        -0.247777       -0.140827
C       2.623055        -0.111281       -0.234653
O       3.247648        -0.855873       -1.049358
N       0.866859        -1.178344       1.000119
O       3.261780        0.699237        0.494177
H       0.925423        -0.666276       1.884713
H       -0.091482       -1.540001       0.957587
H       0.729477        -0.745031       -1.080267
H       0.559303        1.539990        1.001110
H       0.956593        1.849700        -0.687205
H       -1.363271       2.157488        -0.652988
H       -1.192187       0.560923        -1.353274
H       -1.408723       0.352890        1.620572
H       -2.698700       1.360687        1.004490
H       -2.062253       -1.433496       -0.213455
H       -3.143413       -1.211256       1.182201
H       -3.531177       0.050360        -1.539528
H       -4.419339       -1.214363       -0.891719
H       -4.529160       0.319754        -0.226306
###
24
lys305 pm6_conformaciones E=-0.238983859310 au
N       2.272986        -0.957600       -1.270238
H       2.917546        -1.435268       -0.635114
H       1.937592        -1.680439       -1.913768
C       1.120488        -0.402233       -0.507092
H       0.310859        -0.126806       -1.243275
C       0.534804        -1.360526       0.541026
C       1.635366        0.887299        0.148309
H       0.413372        -2.368267       0.087855
H       1.258194        -1.517138       1.366791
```

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C       -0.804696       -0.886484       1.114395
O       2.490068        0.850992        1.079537
H       -0.997609       -1.439838       2.059403
H       -0.744366       0.175525        1.424367
C       -1.989514       -1.109865       0.167249
H       -1.820063       -2.021108       -0.448490
H       -2.901285       -1.348241       0.759103
C       -2.266174       0.061415        -0.772385
H       -1.313790       0.487673        -1.179002
H       -2.845608       -0.280163       -1.666193
N       -3.050966       1.155821        -0.073838
H       -2.539262       1.516817        0.749786
H       -3.229162       1.949767        -0.714792
H       -3.965646       0.798765        0.258382
O       1.207862        1.994451        -0.285229
###
24
lys306 pm6_conformaciones E=-0.239393222641 au
N       -2.110736       1.839719        -0.416525
H       -1.785964       2.264748        0.455946
H       -1.802702       2.473148        -1.160801
C       -1.462599       0.511806        -0.606580
H       -1.679307       0.170437        -1.655297
C       0.060260        0.513006        -0.390778
C       -2.154572       -0.448785       0.371572
H       0.514890        1.295908        -1.035519
H       0.303810        0.821309        0.646084
C       0.681168        -0.851203       -0.704509
O       -2.001156       -0.340667       1.617614
H       0.407140        -1.584709       0.080815
H       0.249379        -1.255155       -1.645554
C       2.204131        -0.799823       -0.861548
H       2.547943        -1.767748       -1.293660
H       2.488821        -0.046170       -1.628284
C       2.963294        -0.563249       0.442468
H       2.404340        -0.962989       1.322778
H       3.937805        -1.111940       0.432282
N       3.247999        0.910224        0.667322
H       2.371844        1.448697        0.777461
H       3.818334        1.045928        1.521756
H       3.766439        1.312902        -0.133795
O       -2.905557       -1.349894       -0.110557
###
24
lys307 pm6_conformaciones E=-0.239588562539 au
N       1.478710        -0.171414       1.842199
H       1.268777        0.820980        1.979224
H       0.747931        -0.673594       2.357998
C       1.370007        -0.513849       0.397721
H       1.541726        -1.621539       0.302133
C       0.022130        -0.154055       -0.255298
C       2.496947        0.209924        -0.350452
H       -0.286888       0.871138        0.041623
H       0.131484        -0.109209       -1.359198
C       -1.061609       -1.171721       0.116198
O       2.716401        1.440035        -0.188594
H       -0.700875       -2.197180       -0.113817
H       -1.229647       -1.168860       1.213259
C       -2.383411       -0.939304       -0.623390
H       -2.198194       -0.600745       -1.666001
H       -2.906106       -1.915608       -0.744956
C       -3.336432       0.015661        0.090984
H       -4.382027       -0.123863       -0.280619
H       -3.377617       -0.193485       1.188210
N       -2.933652       1.461510        -0.121176
H       -3.028073       1.728405        -1.117692
H       -3.525454       2.097922        0.441370
H       -1.943597       1.610626        0.152764
O       3.212020        -0.469484       -1.148410
###
24
lys309 pm6_conformaciones E=-0.238983119552 au
N       -0.522214       1.651616        0.636651
H       -0.061122       1.062440        1.342082
H       0.231363        2.233512        0.248534
C       -1.073724       0.795122        -0.443835
```

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H       -1.455012       1.488665        -1.248189
C       -0.069117       -0.171346       -1.101549
C       -2.277626       -0.001391       0.069722
H       -0.547882       -0.624643       -1.996774
H       0.773706        0.420251        -1.521648
C       0.458675        -1.294735       -0.205969
O       -2.462326       -0.260692       1.290561
H       -0.376387       -1.754626       0.362055
H       0.833657        -2.115466       -0.856883
C       1.562066        -0.899099       0.780067
H       1.230447        -0.063019       1.436954
H       1.721486        -1.745674       1.488552
C       2.905048        -0.576647       0.128450
H       3.743730        -0.799164       0.834671
H       3.089702        -1.218114       -0.767668
N       2.996405        0.880834        -0.280331
H       2.835521        1.505125        0.530954
H       3.928523        1.093797        -0.678274
H       2.277026        1.108277        -0.996724
O       -3.109678       -0.418050       -0.794710
###
24
lys310 pm6_conformaciones E=-0.240043832902 au
N       1.534275        1.755914        -0.829663
H       1.236877        1.288849        -1.689734
H       0.899036        2.553656        -0.722365
C       1.355154        0.842215        0.329865
H       1.619894        1.431192        1.254512
C       -0.069213       0.288565        0.525636
C       2.347553        -0.319823       0.227634
H       -0.090893       -0.362115       1.425126
H       -0.741781       1.138676        0.782319
C       -0.618193       -0.467629       -0.686959
O       2.711591        -0.808334       -0.878520
H       -0.734728       0.220957        -1.549718
H       0.115186        -1.230126       -1.021776
C       -1.950298       -1.168555       -0.398398
H       -2.099972       -1.977175       -1.151035
H       -1.908958       -1.703479       0.575373
C       -3.168328       -0.250133       -0.455529
H       -3.107436       0.456560        -1.318780
H       -4.099291       -0.847743       -0.621310
N       -3.327452       0.549011        0.823414
H       -2.475576       1.112889        1.013190
H       -4.133896       1.195804        0.756723
H       -3.480809       -0.074886       1.635310
O       2.810226        -0.802337       1.306322
###
24
lys311 pm6_conformaciones E=-0.238011540129 au
N       -2.144547       1.628569        -0.569586
H       -1.816173       2.037638        0.309596
H       -1.844781       2.279874        -1.301719
C       -1.485971       0.312979        -0.792127
H       -1.785572       -0.035548       -1.821905
C       0.052246        0.317010        -0.745478
C       -2.060295       -0.686805       0.219354
H       0.425860        -0.695942       -1.015016
H       0.426598        0.977161        -1.558333
C       0.642957        0.758103        0.595688
O       -2.193157       -0.412642       1.443091
H       0.164835        1.705985        0.924924
H       0.399806        0.017554        1.383770
C       2.158640        0.978202        0.539565
H       2.432201        1.578216        -0.355625
H       2.458326        1.618308        1.401502
C       2.983989        -0.304893       0.602311
H       4.018505        -0.085867       0.967615
H       2.554867        -1.032387       1.333293
N       3.083416        -0.972199       -0.755962
H       3.551704        -0.353694       -1.441287
H       3.621945        -1.855241       -0.695507
H       2.138233        -1.195262       -1.124503
O       -2.440323       -1.812730       -0.223572
###
24
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lys312 pm6_conformaciones E=-0.241460273185 au
N 2.733681 -1.354617 -0.613603
H 3.068573 -1.678701 0.296970
H 2.530199 -2.202431 -1.150987
C 1.482856 -0.563859 -0.449991
H 1.016369 -0.445744 -1.466660
C 0.452822 -1.198268 0.499263
C 1.901343 0.823064 0.055918
H 0.171126 -2.198561 0.106595
H 0.916357 -1.404426 1.486305
C -0.802969 -0.345481 0.700968
O 2.511519 0.968194 1.152982
H -1.437492 -0.828161 1.476080
H -0.538513 0.641019 1.131210
C -1.608247 -0.159234 -0.588923
H -0.986219 0.338121 -1.364855
H -1.864374 -1.146845 -1.030923
C -2.869336 0.676723 -0.379416
H -2.669766 1.568518 0.263894
H -3.233224 1.084954 -1.355077
N -3.979240 -0.142711 0.249814
H -3.703198 -0.485550 1.186575
H -4.838349 0.425277 0.359053
H -4.210675 -0.965303 -0.333869
O 1.633391 1.829488 -0.663569
###
24
lys313 pm6_conformaciones E=-0.239314217873 au
N 2.268944 1.532777 -0.607734
H 1.632603 1.552478 -1.409701
H 2.278156 2.489657 -0.242556
C 1.739946 0.617937 0.437750
H 2.330163 0.811509 1.378882
C 0.249503 0.785264 0.787010
C 2.019724 -0.828499 0.015423
H -0.040926 0.025032 1.542092
H 0.119353 1.759763 1.305371
C -0.695151 0.711973 -0.416439
O 1.856819 -1.245275 -1.164313
H -0.368303 1.428879 -1.200509
H -0.642361 -0.287186 -0.891534
C -2.141198 1.040162 -0.028668
H -2.160569 1.904632 0.672692
H -2.693654 1.400636 -0.924756
C -2.886252 -0.123378 0.620816
H -2.236544 -0.675401 1.342280
H -3.751841 0.253008 1.220894
N -3.405734 -1.093455 -0.423673
H -2.628988 -1.513892 -0.961957
H -3.940008 -1.861564 0.019834
H -4.031743 -0.614294 -1.095351
O 2.439776 -1.625882 0.910415
###
24
lys314 pm6_conformaciones E=-0.239722470031 au
N -1.476835 1.932333 0.184645
H -1.203827 1.757755 1.155393
H -0.760590 2.568297 -0.182460
C -1.435633 0.664054 -0.590427
H -1.772235 0.914950 -1.636833
C -0.059129 -0.019294 -0.702198
C -2.450266 -0.322663 -0.003341
H -0.184199 -1.031041 -1.141735
H 0.548647 0.534186 -1.450649
C 0.716255 -0.108206 0.615279
O -2.595038 -0.486604 1.237809
H 1.044391 0.903074 0.934507
H 0.057432 -0.468626 1.430958
C 1.925672 -1.045115 0.519090
H 2.379760 -1.164144 1.528100
H 1.590419 -2.069209 0.240300
C 2.986962 -0.604296 -0.485847
H 3.700953 -1.441011 -0.688246
H 2.534856 -0.353085 -1.476741
N 3.770268 0.593640 0.015742
H 4.258561 0.374658 0.901777

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H       4.482657        0.880951        -0.679663
H       3.147995        1.401469        0.189309
O       -3.152715       -0.998011       -0.818067
###
24
lys315 pm6_conformaciones E=-0.240671489676 au
N       -1.369970       1.636861        -0.827156
H       -1.060375       2.102659        0.029888
H       -0.648372       1.851546        -1.524132
C       -1.408840       0.164518        -0.610997
H       -1.582310       -0.320689       -1.610537
C       -0.143517       -0.434464       0.029910
C       -2.608607       -0.146882       0.292649
H       0.115595        0.112200        0.960159
H       -0.343968       -1.476589       0.355516
C       1.044410        -0.409273       -0.937478
O       -2.838250       0.517110        1.341022
H       0.768095        -0.906160       -1.891407
H       1.287044        0.635676        -1.221625
C       2.281666        -1.104104       -0.361240
H       2.018054        -2.132223       -0.026142
H       3.027934        -1.259699       -1.171533
C       2.922085        -0.368869       0.813808
H       2.155756        -0.058702       1.565724
H       3.624568        -1.046046       1.360356
N       3.687926        0.857089        0.354439
H       3.058026        1.546905        -0.088752
H       4.153793        1.318077        1.157018
H       4.415234        0.601752        -0.336767
O       -3.378994       -1.096099       -0.042104
###
24
lys316 pm6_conformaciones E=-0.240671647537 au
N       -1.666859       1.986605        -0.212874
H       -2.018808       2.185888        0.726863
H       -0.979721       2.720075        -0.412923
C       -0.985328       0.662156        -0.233703
H       -0.429074       0.572974        -1.208257
C       0.007647        0.447575        0.919928
C       -2.100758       -0.391093       -0.212809
H       0.764781        1.264204        0.901243
H       -0.505091       0.567623        1.896448
C       0.700358        -0.916835       0.873688
O       -2.746132       -0.651314       0.841904
H       1.264052        -1.065321       1.820190
H       -0.059287       -1.725708       0.872989
C       1.637610        -1.113266       -0.322451
H       1.738168        -2.203773       -0.527500
H       1.186276        -0.699814       -1.250568
C       3.039795        -0.547814       -0.109519
H       3.420560        -0.779422       0.915721
H       3.765110        -1.023262       -0.815554
N       3.073514        0.953659        -0.318965
H       2.371467        1.424535        0.286747
H       4.008614        1.335927        -0.091442
H       2.856288        1.195206        -1.302159
O       -2.382101       -0.998101       -1.289370
###
24
lys317 pm6_conformaciones E=-0.241070677837 au
N       -1.966843       1.973594        0.021764
H       -2.001114       2.041048        1.042022
H       -1.390417       2.763077        -0.285682
C       -1.306906       0.701684        -0.386127
H       -1.167860       0.731850        -1.501451
C       0.062240        0.462229        0.272243
C       -2.293020       -0.425005       -0.048565
H       0.735052        1.309817        0.008202
H       -0.021658       0.503236        1.376688
C       0.687450        -0.865227       -0.166308
O       -2.549717       -0.742454       1.146024
H       0.017176        -1.707053       0.106005
H       0.762511        -0.905487       -1.272919
C       2.062863        -1.111409       0.463994
H       2.082657        -0.758177       1.517842
H       2.234569        -2.209305       0.541788
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C       3.221355        -0.510188       -0.328650
H       4.179562        -1.030962       -0.081084
H       3.078349        -0.651126       -1.428395
N       3.386861        0.968676        -0.037230
H       3.699289        1.118634        0.938758
H       4.087827        1.391960        -0.671003
H       2.487707        1.473058        -0.160157
O       -2.866240       -1.029917       -1.003759
###
23
lys400 pm6_conformaciones E=-0.321860394715 au
N       3.283203        -0.071940       -0.631024
H       3.733107        -0.977740       -0.475983
H       2.894539        -0.101140       -1.575509
C       2.203833        0.140392        0.369259
H       2.709482        0.326323        1.361279
C       1.369264        1.384838        -0.005485
C       1.288916        -1.065028       0.557397
H       1.890630        2.280492        0.394489
H       1.373025        1.532679        -1.106702
C       -0.076798       1.372194        0.505315
O       0.956400        -1.803081       -0.362929
H       -0.136465       0.890855        1.500048
H       -0.398625       2.418123        0.694460
C       -1.042175       0.719041        -0.490984
H       -1.294198       1.451006        -1.283823
H       -0.556482       -0.115228       -1.027986
C       -2.337289       0.220594        0.189472
H       0.922209        -1.250603       1.581825
H       -2.778834       1.026582        0.825383
N       -3.347184       -0.103738       -0.873600
H       -2.943061       -0.685602       -1.606457
H       -4.105890       -0.657041       -0.476112
O       -2.118410       -0.889561       0.985130
###
23
lys401 pm6_conformaciones E=-0.369206977810 au
N       3.029266        -1.108203       -0.041681
H       3.760792        -0.414567       -0.212168
H       3.039125        -1.289618       0.963957
C       1.707228        -0.564885       -0.457512
H       1.659091        -0.643050       -1.578406
C       0.568526        -1.394830       0.162200
C       1.537841        0.914144        -0.079800
H       0.745300        -2.466768       -0.071229
H       0.609943        -1.344350       1.269294
C       -0.821198       -0.993658       -0.346827
O       1.988325        1.356987        1.014837
H       -0.757297       -0.599216       -1.379926
H       -1.447470       -1.904369       -0.437347
C       -1.522370       0.015016        0.570852
H       -1.787715       -0.472498       1.532099
H       -0.826275       0.827407        0.857760
C       -2.769743       0.640277        -0.065738
H       -2.998345       1.598033        0.453238
H       -2.575779       0.917743        -1.124998
N       -3.938441       -0.296213       -0.054091
H       -4.014150       -0.736551       0.864979
H       -4.796607       0.247575        -0.167414
O       0.955663        1.694857        -0.889647
###
23
lys402 pm6_conformaciones E=-0.368852264191 au
N       -1.518137       -1.249600       1.336367
H       -2.215287       -0.957433       2.025230
H       -1.931941       -2.029030       0.822780
C       -1.206665       -0.125706       0.412304
H       -0.588303       0.618042        0.983771
C       -0.425903       -0.594718       -0.827979
C       -2.493336       0.572082        -0.069290
H       -0.943349       -1.458037       -1.296249
H       -0.442156       0.207596        -1.596521
C       1.025104        -0.986422       -0.533032
O       -3.368751       -0.083772       -0.706404
H       1.066318        -1.699202       0.313009
H       1.423297        -1.549824       -1.403393
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C       1.923761        0.221403        -0.245091
H       1.862568        0.950680        -1.076507
H       1.560223        0.765839        0.649545
C       3.377210        -0.225814       -0.040843
H       3.427867        -0.999256       0.756031
H       3.762782        -0.717166       -0.960733
N       4.252242        0.953734        0.250875
H       3.866744        1.476328        1.040241
H       5.162843        0.617222        0.571957
O       -2.675170       1.793815        0.191869
###
23
lys403 pm6_conformaciones E=-0.372604906940 au
C       0.584730        1.358862        -0.645183
C       -0.868042       1.803265        -0.438276
C       -1.901578       0.684451        -0.618494
C       -2.188576       -0.062778       0.690846
N       -2.790923       -1.404043       0.413949
C       1.093704        0.382790        0.434142
C       1.417129        -0.961812       -0.233187
O       0.459855        -1.711829       -0.599454
N       2.234010        0.961657        1.186897
O       2.610611        -1.323650       -0.424904
H       2.669808        0.244897        1.770421
H       2.955655        1.295499        0.546125
H       -3.605782       -1.295488       -0.193893
H       1.230520        2.264121        -0.674854
H       0.701174        0.922450        -1.658408
H       -0.983773       2.280405        0.554970
H       -1.086854       2.613109        -1.167522
H       -2.846184       1.112910        -1.012660
H       -1.570752       -0.015282       -1.409604
H       -1.244814       -0.224079       1.269830
H       -2.825943       0.566112        1.349463
H       0.270303        0.182493        1.189011
H       -3.152898       -1.795285       1.286981
###
23
lys404 pm6_conformaciones E=-0.371040463606 au
N       2.791639        0.691961        -0.552128
H       3.455327        -0.013627       -0.223962
H       2.662495        0.516882        -1.550543
C       1.497378        0.553900        0.173068
H       1.654276        0.963537        1.207682
C       0.392536        1.358277        -0.533119
C       1.087697        -0.923810       0.295435
H       0.838744        2.278001        -0.972701
H       -0.002700       0.800682        -1.404788
C       -0.750490       1.778999        0.395789
O       0.902438        -1.629629       -0.737236
H       -0.336090       2.236252        1.318453
H       -1.316561       2.600671        -0.093239
C       -1.722840       0.661477        0.785521
H       -1.183235       -0.147879       1.312671
H       -2.422411       1.058155        1.551820
C       -2.537377       0.101337        -0.393047
H       -3.623723       0.207564        -0.178513
H       -2.362183       0.696237        -1.315049
N       -2.275644       -1.332299       -0.710516
H       -1.288899       -1.455882       -0.944150
H       -2.433609       -1.900475       0.124275
O       0.965709        -1.437726       1.445319
###
23
lys405 pm6_conformaciones E=-0.373150221238 au
N       -1.886547       1.828546        0.148720
H       -2.856085       1.931486        -0.159868
H       -1.906351       1.823199        1.169181
C       -1.318547       0.556229        -0.367101
H       -1.228316       0.659235        -1.483496
C       0.069484        0.271548        0.234550
C       -2.228458       -0.651621       -0.080214
H       0.057566        0.440500        1.330346
H       0.317691        -0.806492       0.110547
C       1.158778        1.127676        -0.421830
O       -2.800091       -0.778022       1.039904
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H       1.191903        0.928969        -1.512254
H       0.893575        2.200446        -0.334625
C       2.545968        0.908269        0.192352
H       3.185247        1.781842        -0.055859
H       2.484366        0.912835        1.298668
C       3.249999        -0.366012       -0.295731
H       3.116529        -0.481996       -1.393202
H       4.346671        -0.262519       -0.137939
N       2.808461        -1.628600       0.362441
H       2.970096        -1.563076       1.369853
H       1.792462        -1.728713       0.260844
O       -2.410170       -1.510962       -0.991464
###
23
lys406 pm6_conformaciones E=-0.372118743689 au
N       -2.735620       1.011800        -0.404054
H       -3.370407       0.355590        -0.863198
H       -3.098650       1.146367        0.541837
C       -1.362425       0.443613        -0.357602
H       -0.926675       0.578907        -1.387454
C       -0.490599       1.172649        0.683796
C       -1.337970       -1.061884       -0.048738
H       -1.093278       1.938278        1.219919
H       -0.171252       0.476056        1.487915
C       0.740384        1.855050        0.077397
O       -2.288404       -1.617309       0.570302
H       0.425065        2.590383        -0.690423
H       1.234370        2.460366        0.866517
C       1.754415        0.886496        -0.541409
H       1.272926        0.295824        -1.345126
H       2.544927        1.466799        -1.060447
C       2.389160        -0.034647       0.507327
H       3.099664        0.544147        1.136258
H       1.621328        -0.415254       1.217854
N       3.028788        -1.219569       -0.146987
H       3.651480        -0.906900       -0.895218
H       3.635643        -1.688773       0.529544
O       -0.340984       -1.752075       -0.423467
###
23
lys407 pm6_conformaciones E=-0.364236033219 au
N       1.101752        -1.266929       1.308788
H       0.084712        -1.408275       1.377523
H       1.440252        -2.082749       0.797545
C       1.346802        -0.062005       0.521623
H       -2.590621       -0.334017       -1.895225
C       0.442048        1.095738        0.804703
C       2.385400        -0.014096       -0.377221
H       0.252241        1.171935        1.896211
H       0.943301        2.049587        0.547297
C       -0.903656       1.040025        0.055519
O       3.109400        -1.066984       -0.714139
H       -1.329877       2.062170        -0.000851
H       -0.742385       0.736906        -0.996094
C       -1.908783       0.103158        0.733395
H       -1.499555       -0.931648       0.787672
H       -2.045377       0.403748        1.796253
C       -3.280623       0.101393        0.062944
H       -4.050594       -0.326787       0.752234
H       -3.626302       1.139219        -0.164932
N       -3.276278       -0.708726       -1.218863
H       -3.030076       -1.696713       -1.031751
H       -4.210586       -0.689933       -1.666852
O       2.783027        1.085842        -0.990148
###
23
lys408 pm6_conformaciones E=-0.369262091325 au
N       -2.109500       1.755131        -0.601859
H       -3.127357       1.657339        -0.616101
H       -1.876813       2.202160        0.286641
C       -1.469392       0.415727        -0.692312
H       -1.766428       -0.039341       -1.675725
C       0.060476        0.563578        -0.641922
C       -1.941078       -0.518975       0.435320
H       0.380641        1.240938        -1.461512
H       0.369655        1.078925        0.293817
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C       0.780738        -0.782887       -0.768762
O       -1.929268       -0.129220       1.635657
H       0.534461        -1.434969       0.092966
H       0.407894        -1.323286       -1.663572
C       2.302844        -0.630386       -0.884799
H       2.718475        -1.558412       -1.332850
H       2.552305        0.170763        -1.608454
C       3.015934        -0.383358       0.449890
H       2.623707        -1.076263       1.225391
H       4.095145        -0.636605       0.346931
N       2.935214        1.051145        0.870495
H       1.955636        1.353978        0.867873
H       3.244457        1.131278        1.841492
O       -2.369345       -1.669859       0.131612
###
23
lys410 pm6_conformaciones E=-0.370585966819 au
N       -1.630907       1.991006        -0.403535
H       -2.380814       1.961921        -1.098868
H       -2.070247       2.238818        0.484255
C       -0.968708       0.663801        -0.311105
H       -0.397230       0.507188        -1.269121
C       0.018347        0.630059        0.866483
C       -1.981954       -0.486157       -0.178297
H       0.754416        1.458294        0.748423
H       -0.504453       0.854053        1.818346
C       0.758883        -0.706313       0.988629
O       -2.828563       -0.502821       0.759521
H       1.379938        -0.685132       1.909203
H       0.032085        -1.525061       1.165505
C       1.633785        -1.059429       -0.220645
H       1.717470        -2.164801       -0.293450
H       1.138728        -0.747691       -1.162332
C       3.051837        -0.479856       -0.156597
H       3.518620        -0.733331       0.820114
H       3.686463        -0.970131       -0.928706
N       3.071230        0.991794        -0.434021
H       2.358197        1.451183        0.144961
H       3.963434        1.375116        -0.112898
O       -1.965439       -1.406261       -1.046190
###
23
lys411 pm6_conformaciones E=-0.370675686594 au
N       2.509056        -1.198814       -0.135843
H       3.296382        -0.662144       0.232961
H       2.102790        -1.691388       0.664938
C       1.503110        -0.281457       -0.732770
H       1.906455        0.029703        -1.740121
C       0.159135        -0.997932       -0.956187
C       1.294153        1.013135        0.064340
H       -0.517119       -0.335396       -1.538403
H       0.336621        -1.864230       -1.630767
C       -0.540678       -1.499527       0.310904
O       1.837907        1.182142        1.191698
H       -1.178432       -2.368977       0.043933
H       0.209615        -1.918935       1.015950
C       -1.390415       -0.460116       1.049524
H       -1.592343       -0.842326       2.074967
H       -0.820660       0.471729        1.211830
C       -2.740400       -0.152823       0.388657
H       -3.205143       -1.091784       0.016753
H       -3.445708       0.240361        1.155187
N       -2.606871       0.886765        -0.679992
H       -1.979142       0.534152        -1.411423
H       -3.513471       1.023135        -1.132311
O       0.584022        1.934454        -0.441630
###
23
lys413 pm6_conformaciones E=-0.372443458977 au
N       1.516805        1.593592        -0.986266
H       2.497400        1.873159        -1.058557
H       1.284423        1.114407        -1.856856
C       1.330709        0.679940        0.169248
H       1.497851        1.283960        1.102700
C       -0.085021       0.074247        0.196429
C       2.336935        -0.483817       0.173107
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H       -0.297897       -0.448198       -0.760804
H       -0.128931       -0.713692       0.977666
C       -1.161713       1.131025        0.466945
O       2.766294        -0.968749       -0.913047
H       -0.845333       1.782150        1.308232
H       -1.252834       1.807172        -0.405584
C       -2.529123       0.525563        0.801926
H       -2.436177       -0.186475       1.646648
H       -3.187097       1.332793        1.188388
C       -3.228488       -0.151648       -0.385359
H       -4.327597       -0.154072       -0.209151
H       -3.076512       0.437996        -1.314384
N       -2.809571       -1.559107       -0.645184
H       -1.812379       -1.580815       -0.875921
H       -2.896139       -2.101975       0.216921
O       2.740055        -0.948708       1.278931
###
23
lys414 pm6_conformaciones E=-0.369439188117 au
N       -1.209542       1.787100        -0.530718
H       -2.096790       2.190727        -0.838025
H       -1.045555       2.134597        0.415456
C       -1.300868       0.304021        -0.526577
H       -1.327124       -0.028461       -1.601214
C       -0.094047       -0.332091       0.187759
C       -2.586005       -0.210676       0.144932
H       0.228497        0.302711        1.039933
H       -0.385610       -1.297074       0.652351
C       1.079606        -0.563505       -0.771018
O       -3.136337       0.439784        1.078096
H       0.769377        -1.251227       -1.584191
H       1.352537        0.381696        -1.280731
C       2.303708        -1.150533       -0.058277
H       1.994823        -1.991914       0.596113
H       2.977755        -1.610830       -0.808401
C       3.074947        -0.127197       0.783250
H       2.372437        0.430028        1.440683
H       3.768284        -0.657821       1.472804
N       3.899150        0.777728        -0.079413
H       3.300376        1.213456        -0.783433
H       4.256327        1.547289        0.490703
O       -3.095742       -1.294420       -0.265789
###
23
lys415 pm6_conformaciones E=-0.369757839463 au
N       0.646164        1.714538        0.538781
H       1.372967        2.369300        0.243676
H       -0.000385       1.630138        -0.256235
C       1.248399        0.390953        0.845193
H       1.745660        0.487100        1.854504
C       0.180961        -0.712145       0.937791
C       2.355796        -0.017187       -0.138082
H       0.643651        -1.609113       1.400798
H       -0.600449       -0.402809       1.665748
C       -0.474024       -1.109484       -0.390734
O       2.698211        0.762883        -1.073822
H       0.270599        -1.097567       -1.211195
H       -0.804434       -2.167786       -0.323137
C       -1.667259       -0.232457       -0.787033
H       -1.363527       0.836942        -0.809215
H       -1.962708       -0.461798       -1.831270
C       -2.864799       -0.431632       0.149634
H       -3.297806       -1.443899       0.002804
H       -2.536376       -0.403007       1.213955
N       -3.874932       0.658672        -0.033287
H       -4.009529       0.844425        -1.028782
H       -4.781532       0.332248        0.307742
O       2.958140        -1.119750       0.015264
###
23
lys416 pm6_conformaciones E=-0.369901951694 au
N       2.179735        -1.748072       -0.198413
H       3.180500        -1.667519       -0.007251
H       1.738376        -1.972534       0.696493
C       1.656977        -0.459759       -0.721363
H       2.069667        -0.338880       -1.763840
```

```
C       0.120330        -0.468096       -0.810309
C       2.116643        0.767672        0.080053
H       -0.214101       0.437418        -1.357978
H       -0.198177       -1.319009       -1.447477
C       -0.575980       -0.545386       0.552467
O       2.621725        0.644064        1.231568
H       -0.162920       -1.390215       1.143507
H       -0.356681       0.363644        1.146920
C       -2.091819       -0.733543       0.425959
H       -2.316293       -1.624435       -0.193222
H       -2.510027       -0.968297       1.427695
C       -2.789355       0.502059        -0.155843
H       -2.427123       1.420507        0.354427
H       -2.526906       0.630470        -1.228502
N       -4.277012       0.351935        -0.067101
H       -4.542142       0.130901        0.894723
H       -4.711519       1.254618        -0.269817
O       2.007965        1.910762        -0.451927
###
23
lys417 pm6_conformaciones E=-0.371140644266 au
N       1.267784        1.887510        -0.539791
H       2.220568        2.209076        -0.722487
H       0.902355        1.545419        -1.430443
C       1.285026        0.795143        0.465430
H       1.594805        1.258034        1.445756
C       -0.108702       0.168672        0.646133
C       2.298925        -0.315875       0.154965
H       -0.084356       -0.528023       1.509460
H       -0.825008       0.965606        0.949921
C       -0.628795       -0.556934       -0.598906
O       2.793483        -0.443067       -1.000581
H       -0.646582       0.132472        -1.467655
H       0.075437        -1.365007       -0.884222
C       -2.020442       -1.167913       -0.393542
H       -2.183805       -1.945030       -1.171225
H       -2.059218       -1.718282       0.567145
C       -3.169950       -0.156472       -0.479581
H       -2.993855       0.549621        -1.319630
H       -4.114155       -0.687257       -0.737254
N       -3.399562       0.546922        0.822106
H       -2.506040       0.904331        1.179160
H       -3.975920       1.374503        0.654678
O       2.654248        -1.098959       1.086030
###
# Conformations of TYROSINE optimized with pm6
# opt freq pm6 scf=(xqc,tight) scrf(smd,solvent=water)
###
25
tyr100 pm6_conformaciones E=-0.648361228234E-01 au
N       -2.238406       1.626159        0.684299
H       -3.033539       1.529706        1.348189
H       -2.313065       2.554412        0.215809
H       -1.357639       1.619906        1.233607
C       -2.258175       0.518273        -0.350794
H       -3.259737       0.577438        -0.899679
C       -1.126043       0.696021        -1.375020
C       -2.182742       -0.862403       0.288158
H       -1.341920       0.048456        -2.259576
H       -1.171901       1.731875        -1.795790
C       0.241012        0.407766        -0.827444
O       -2.362736       -1.923032       -0.282065
C       0.982553        1.424698        -0.204968
C       0.790692        -0.880352       -0.952223
H       0.566963        2.434398        -0.120000
C       2.251940        1.163056        0.308842
C       2.060100        -1.163481       -0.453976
H       0.219807        -1.672187       -1.446251
H       2.829900        1.945443        0.802393
C       2.770862        -0.130803       0.176209
H       2.495067        -2.157650       -0.549112
O       4.021971        -0.475847       0.654143
H       4.457399        0.287876        1.147664
O       -1.880051       -0.801932       1.605285
H       -1.837157       -1.712952       2.061030
###
```

```
25
tyr101 pm6_conformaciones E=-0.649746263560E-01 au
N       2.150966        1.721449        -0.762468
H       2.936439        1.670570        -1.443801
H       2.202780        2.641669        -0.273771
H       1.259418        1.699379        -1.293398
C       2.232068        0.593188        0.247814
H       3.243419        0.670143        0.771299
C       1.126023        0.708603        1.308974
C       2.149219        -0.755323       -0.461228
H       1.386039        0.035060        2.162333
H       1.161466        1.729735        1.764435
C       -0.251817       0.406151        0.797991
O       1.534155        -1.031900       -1.475494
C       -0.769124       -0.895140       0.908029
C       -1.036621       1.422524        0.226527
H       -0.166585       -1.686244       1.364379
C       -2.046757       -1.193268       0.437069
C       -2.314354       1.147717        -0.255182
H       -0.644437       2.442897        0.157124
H       -2.455143       -2.201116       0.519823
C       -2.798889       -0.164447       -0.143886
H       -2.925644       1.927457        -0.707774
O       -4.064816       -0.374642       -0.657714
H       -4.369905       -1.326418       -0.527333
O       2.872579        -1.676874       0.215119
H       2.841560        -2.605962       -0.207975
###
25
tyr102 pm6_conformaciones E=-0.648218531361E-01 au
N       3.351125        -1.222121       0.020532
H       4.007449        -1.033974       -0.764398
H       3.272963        -2.254645       0.139512
H       3.763931        -0.829731       0.889496
C       1.985758        -0.624218       -0.265259
H       1.606457        -1.077389       -1.241979
C       1.011193        -0.952073       0.879499
C       2.073774        0.884911        -0.466076
H       1.066856        -2.045815       1.112095
H       1.341384        -0.454741       1.821818
C       -0.402254       -0.584887       0.534095
O       1.231102        1.595106        -0.985638
C       -1.040562       0.465049        1.213109
C       -1.092913       -1.299625       -0.461052
H       -0.508331       1.018387        1.991960
C       -2.355835       0.810945        0.903618
C       -2.404868       -0.968803       -0.789623
H       -0.597353       -2.122631       -0.984844
H       -2.861725       1.624103        1.425808
C       -3.016343       0.087798        -0.096921
H       -2.947911       -1.512076       -1.561994
O       -4.317062       0.369599        -0.473762
H       -4.703417       1.130405        0.062589
O       3.237354        1.386168        0.007664
H       3.342955        2.391389        -0.128247
###
25
tyr103 pm6_conformaciones E=-0.632656902376E-01 au
N       1.686019        -1.462712       -0.852169
H       2.278589        -1.599975       -1.696601
H       0.707450        -1.717949       -1.099443
H       2.010394        -2.119229       -0.115353
C       1.746699        -0.024233       -0.373326
H       1.385218        0.646968        -1.223306
C       0.855165        0.173531        0.864802
C       3.174338        0.398635        -0.048552
H       1.103316        -0.584121       1.646302
H       1.102821        1.151194        1.346984
C       -0.604210       0.135713        0.515831
O       3.528082        1.508721        0.305957
C       -1.376365       -0.992942       0.833538
C       -1.202221       1.236748        -0.121708
H       -0.913779       -1.851346       1.329805
C       -2.734053       -1.032551       0.517203
C       -2.555517       1.218014        -0.450869
H       -0.601881       2.118496        -0.363965
```

```
H       -3.342005       -1.904956       0.759490
C       -3.300535       0.074574        -0.125591
H       -3.027648       2.063840        -0.948180
O       -4.634564       0.108224        -0.492183
H       -5.115570       -0.732504       -0.213787
O       4.053096        -0.617280       -0.204070
H       5.018240        -0.353686       -0.002362
###
25
tyr104 pm6_conformaciones E=-0.648365743162E-01 au
N       -2.236536       1.626384        0.685358
H       -3.031516       1.530417        1.349560
H       -2.310551       2.554975        0.217376
H       -1.355524       1.619016        1.234148
C       -2.257948       0.518983        -0.350237
H       -3.259745       0.579196        -0.898544
C       -1.126169       0.696186        -1.374978
C       -2.183267       -0.862000       0.288186
H       -1.342461       0.048422        -2.259263
H       -1.171971       1.731921        -1.795995
C       0.240962        0.407853        -0.827637
O       -2.365124       -1.922172       -0.282402
C       0.982856        1.424714        -0.205568
C       0.790305        -0.880493       -0.952165
H       0.567650        2.434586        -0.120857
C       2.252207        1.162812        0.308323
C       2.059600        -1.163859       -0.453885
H       0.219149        -1.672222       -1.446034
H       2.830313        1.945216        0.801682
C       2.770681        -0.131202       0.176080
H       2.494361        -2.158143       -0.548744
O       4.021745        -0.476572       0.653956
H       4.456844        0.286531        1.148575
O       -1.879092       -0.802388       1.604889
H       -1.836396       -1.713494       2.060333
###
25
tyr105 pm6_conformaciones E=-0.648212227176E-01 au
N       3.351083        -1.222159       0.020718
H       4.007623        -1.033703       -0.763957
H       3.272881        -2.254716       0.139264
H       3.763643        -0.830101       0.889941
C       1.985765        -0.624162       -0.265197
H       1.606497        -1.077358       -1.241888
C       1.011147        -0.951916       0.879570
C       2.073869        0.884954        -0.466031
H       1.066825        -2.045624       1.112294
H       1.341316        -0.454442       1.821814
C       -0.402303       -0.584839       0.534098
O       1.231125        1.595273        -0.985263
C       -1.041052       0.464383        1.213816
C       -1.092550       -1.298948       -0.461779
H       -0.509183       1.017181        1.993298
C       -2.356319       0.810224        0.904258
C       -2.404499       -0.968163       -0.790436
H       -0.596697       -2.121458       -0.986079
H       -2.862528       1.622861        1.426960
C       -3.016408       0.087730        -0.097042
H       -2.947205       -1.510952       -1.563392
O       -4.317108       0.369503        -0.473948
H       -4.703716       1.129913        0.062771
O       3.237711        1.386053        0.007314
H       3.343240        2.391312        -0.128416
###
25
tyr106 pm6_conformaciones E=-0.647732603798E-01 au
N       3.347319        -1.228970       0.012431
H       4.001358        -1.041996       -0.774764
H       3.266457        -2.261360       0.130571
H       3.764340        -0.838568       0.880241
C       1.982773        -0.626740       -0.268034
H       1.598953        -1.077557       -1.244085
C       1.010843        -0.953296       0.879456
C       2.074679        0.882273        -0.467562
H       1.065047        -2.047277       1.111321
H       1.344685        -0.456932       1.820940
```

```
C       -0.402893       -0.583586       0.537777
O       1.230813        1.596321        -0.979807
C       -1.095105       -1.291070       -0.459632
C       -1.039585       0.464337        1.224096
H       -0.603174       -2.112427       -0.989112
C       -2.407017       -0.952112       -0.784909
C       -2.353453       0.815986        0.920300
H       -0.504645       1.010608        2.006297
H       -2.951214       -1.489564       -1.562812
C       -3.015883       0.099473        -0.087257
H       -2.857642       1.624619        1.447792
O       -4.312637       0.503247        -0.350031
H       -4.730885       -0.046230       -1.084251
O       3.243902        1.378519        -0.002236
H       3.352707        2.383200        -0.137968
###
25
tyr107 pm6_conformaciones E=-0.647731815417E-01 au
N       3.347337        -1.229005       0.012653
H       4.001793        -1.041346       -0.773967
H       3.266573        -2.261508       0.129978
H       3.763794        -0.839234       0.881034
C       1.982853        -0.626740       -0.267952
H       1.599051        -1.077319       -1.244126
C       1.010777        -0.953390       0.879408
C       2.074691        0.882393        -0.467305
H       1.064736        -2.047393       1.111161
H       1.344579        -0.457292       1.821038
C       -0.402894       -0.583448       0.537775
O       1.230208        1.596489        -0.978521
C       -1.094962       -1.290733       -0.460014
C       -1.039713       0.464153        1.224252
H       -0.602695       -2.111751       -0.989712
C       -2.406815       -0.951897       -0.785242
C       -2.353613       0.815832        0.920331
H       -0.504996       1.010337        2.006662
H       -2.951007       -1.489162       -1.563279
C       -3.015874       0.099500        -0.087337
H       -2.857785       1.624425        1.447897
O       -4.312753       0.502861        -0.349938
H       -4.730390       -0.045932       -1.085100
O       3.244434        1.378390        -0.003384
H       3.353180        2.383274        -0.138903
###
25
tyr108 pm6_conformaciones E=-0.630622533206E-01 au
N       -1.907400       1.727863        -0.718683
H       -2.469412       1.834700        -1.589172
H       -0.974038       2.158947        -0.885798
H       -2.370262       2.265959        0.040854
C       -1.750640       0.265343        -0.347067
H       -1.268371       -0.272781       -1.227413
C       -0.872543       0.107474        0.907238
C       -3.125317       -0.346000       -0.084676
H       -1.060273       0.939072        1.628699
H       -1.181579       -0.803703       1.476351
C       0.583526        0.022083        0.552164
O       -4.054078       0.129277        0.540472
C       1.356315        1.187576        0.429075
C       1.176034        -1.235222       0.341702
H       0.900551        2.168657        0.598526
C       2.704991        1.109105        0.083911
C       2.523192        -1.338801       0.002631
H       0.576409        -2.144318       0.443815
H       3.310420        2.009813        -0.022666
C       3.266320        -0.156117       -0.127623
H       2.990980        -2.308533       -0.160328
O       4.592803        -0.322023       -0.484016
H       5.060432        0.562357        -0.600660
O       -3.196157       -1.574715       -0.650502
H       -4.074866       -2.058169       -0.463179
###
25
tyr109 pm6_conformaciones E=-0.632663460805E-01 au
N       1.792372        -1.580926       -0.733724
H       2.404176        -1.746176       -1.559051
```

```
H       0.837752        -1.927116       -0.963991
H       2.152035        -2.148672       0.058520
C       1.741091        -0.106791       -0.379490
H       1.312314        0.456287        -1.274710
C       0.857631        0.124149        0.859358
C       3.133215        0.458225        -0.119550
H       1.092035        -0.627087       1.651681
H       1.124348        1.100430        1.333895
C       -0.602258       0.105727        0.512399
O       3.419179        1.639317        -0.045921
C       -1.346016       -1.077454       0.644487
C       -1.229176       1.279905        0.060177
H       -0.860933       -1.993587       0.995623
C       -2.703791       -1.098615       0.327525
C       -2.584252       1.282642        -0.262300
H       -0.650416       2.202533        -0.040053
H       -3.288225       -2.014024       0.425292
C       -3.301140       0.084522        -0.123783
H       -3.079172       2.186769        -0.613384
O       -4.637933       0.146329        -0.474500
H       -5.096995       -0.741287       -0.346354
O       4.058516        -0.515417       0.037012
H       4.996551        -0.157275       0.222925
###
25
tyr110 pm6_conformaciones E=-0.648441972834E-01 au
N       -2.213472       1.631692        0.695605
H       -3.009918       1.546317        1.359481
H       -2.271226       2.563721        0.232089
H       -1.332632       1.605887        1.244048
C       -2.254176       0.529625        -0.345225
H       -3.257525       0.604846        -0.888730
C       -1.124717       0.697174        -1.374278
C       -2.193444       -0.855873       0.285076
H       -1.345486       0.044971        -2.254198
H       -1.167965       1.730516        -1.801099
C       0.242481        0.406763        -0.828183
O       -2.388247       -1.910602       -0.291289
C       0.989292        1.423961        -0.212563
C       0.786550        -0.884372       -0.946698
H       0.578291        2.435977        -0.133097
C       2.258068        1.159587        0.301475
C       2.055215        -1.170264       -0.448274
H       0.211609        -1.676342       -1.435778
H       2.839815        1.942212        0.790186
C       2.771104        -0.137246       0.175621
H       2.485843        -2.166788       -0.538416
O       4.021030        -0.485312       0.654480
H       4.459186        0.278225        1.145754
O       -1.885848       -0.807359       1.601438
H       -1.853408       -1.721338       2.051788
###
25
tyr111 pm6_conformaciones E=-0.647144959012E-01 au
N       -2.293047       1.597358        0.680731
H       -3.094208       1.474538        1.333063
H       -2.389056       2.525069        0.215406
H       -1.420131       1.614939        1.241649
C       -2.267171       0.494480        -0.359512
H       -3.263401       0.527714        -0.920089
C       -1.127996       0.708461        -1.368816
C       -2.160474       -0.884573       0.278390
H       -1.328658       0.076926        -2.268600
H       -1.183932       1.752051        -1.768784
C       0.239027        0.424754        -0.818582
O       -2.297888       -1.950079       -0.294514
C       0.800466        -0.854978       -0.961604
C       0.970910        1.439285        -0.177927
H       0.239421        -1.645562       -1.468377
C       2.072245        -1.131841       -0.462821
C       2.242166        1.185386        0.331973
H       0.543315        2.442687        -0.076164
H       2.515783        -2.122314       -0.571400
C       2.773009        -0.104523       0.181366
H       2.813217        1.964747        0.834974
O       4.031362        -0.296074       0.721142
```

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H       4.373282        -1.229483       0.553306
O       -1.883038       -0.815796       1.600863
H       -1.810873       -1.725932       2.055166
###
24
tyr200 pm6_conformaciones E=-0.243535943310 au
N       -1.668682       -1.180729       1.235106
H       -2.020510       -2.003861       0.713795
H       -2.197047       -1.110428       2.126458
H       -0.671012       -1.355988       1.468101
C       -1.809670       0.089382        0.419433
H       -1.501374       0.959404        1.071547
C       -0.924690       0.035322        -0.834013
C       -3.280507       0.275825        -0.017989
H       -1.182909       -0.856823       -1.451200
H       -1.171978       0.904676        -1.490501
C       0.540819        0.050569        -0.507794
O       -3.934287       -0.722619       -0.409760
C       1.156547        1.238546        -0.081178
C       1.302955        -1.122200       -0.642455
H       0.566544        2.153342        0.021606
C       2.518666        1.263205        0.214473
C       2.667669        -1.120247       -0.359788
H       0.824111        -2.049581       -0.970819
H       3.005230        2.179342        0.550567
C       3.253023        0.079563        0.068651
H       3.266145        -2.023911       -0.464916
O       4.610210        0.020779        0.333469
H       4.952118        0.886192        0.717184
O       -3.768101       1.432209        0.014591
###
24
tyr201 pm6_conformaciones E=-0.245766269916 au
N       2.113223        1.633958        -0.819148
H       1.316086        1.436864        -1.449939
H       2.972980        1.701286        -1.398001
H       1.946478        2.560820        -0.377338
C       2.260948        0.559104        0.238182
H       3.270848        0.701970        0.732207
C       1.172844        0.681471        1.314582
C       2.228274        -0.846199       -0.399932
H       1.433955        0.003889        2.161588
H       1.217228        1.700451        1.770579
C       -0.211765       0.389853        0.812982
O       1.602530        -1.031699       -1.472954
C       -0.727408       -0.913836       0.886793
C       -0.999607       1.421574        0.272670
H       -0.126833       -1.715949       1.323679
C       -2.003966       -1.201460       0.404518
C       -2.277040       1.158692        -0.215698
H       -0.607969       2.443570        0.230913
H       -2.410454       -2.212064       0.456249
C       -2.757888       -0.157948       -0.145908
H       -2.891057       1.950566        -0.643143
O       -4.022534       -0.355819       -0.668510
H       -4.322178       -1.313390       -0.575601
O       2.832754        -1.767886       0.203177
###
24
tyr202 pm6_conformaciones E=-0.245413627016 au
N       3.398778        -1.169782       -0.036628
H       3.847083        -0.743663       0.794871
H       4.017831        -1.012358       -0.855100
H       3.332588        -2.195375       0.127863
C       2.024058        -0.581185       -0.282401
H       1.619883        -1.034273       -1.236874
C       1.086257        -0.914009       0.889612
C       2.123408        0.949317        -0.456406
H       1.160289        -2.001913       1.135423
H       1.424083        -0.400227       1.817800
C       -0.336445       -0.565433       0.560363
O       2.993226        1.588904        0.184503
C       -1.066208       -1.372971       -0.328981
C       -0.938920       0.566512        1.133655
H       -0.601070       -2.259339       -0.769448
C       -2.381919       -1.052892       -0.657068
```

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C       -2.256036       0.902729        0.824880
H       -0.376106       1.191802        1.831724
H       -2.955621       -1.668931       -1.351101
C       -2.956560       0.083551        -0.072374
H       -2.734798       1.775996        1.266004
O       -4.256005       0.472385        -0.345114
H       -4.695206       -0.144656       -1.010496
O       1.310752        1.512174        -1.234633
###
24
tyr203 pm6_conformaciones E=-0.242104798802 au
N       -1.746381       1.508779        -0.839232
H       -2.068818       2.178232        -0.114738
H       -2.340729       1.626028        -1.680776
H       -0.772638       1.767617        -1.097863
C       -1.791446       0.082543        -0.325814
H       -1.409165       -0.602687       -1.145157
C       -0.897423       -0.061197       0.911741
C       -3.256347       -0.330031       -0.054162
H       -1.118474       0.743519        1.650084
H       -1.162224       -1.004021       1.446156
C       0.560272        -0.078787       0.547891
O       -4.072408       -0.246501       -1.009305
C       1.117083        -1.220822       -0.051760
C       1.368687        1.041385        0.801493
H       0.491499        -2.097117       -0.242922
C       2.463512        -1.248042       -0.410422
C       2.720282        1.034455        0.458749
H       0.937796        1.931961        1.268337
H       2.902924        -2.127029       -0.883031
C       3.243429        -0.114035       -0.151105
H       3.354781        1.898037        0.652236
O       4.587835        -0.060054       -0.478617
H       4.876981        -0.878432       -0.989949
O       -3.594873       -0.772242       1.069495
###
24
tyr204 pm6_conformaciones E=-0.245413675343 au
N       3.398608        -1.170143       -0.036747
H       3.847123        -0.744125       0.794682
H       4.017601        -1.012925       -0.855307
H       3.332178        -2.195709       0.127835
C       2.024035        -0.581234       -0.282383
H       1.619651        -1.034248       -1.236815
C       1.086203        -0.913736       0.889719
C       2.123635        0.949243        -0.456372
H       1.160196        -2.001564       1.135863
H       1.424040        -0.399767       1.817793
C       -0.336502       -0.565230       0.560385
O       2.993354        1.588772        0.184735
C       -1.066317       -1.373075       -0.328648
C       -0.938936       0.566903        1.133341
H       -0.601194       -2.259556       -0.768889
C       -2.382043       -1.053092       -0.656758
C       -2.256098       0.902985        0.824599
H       -0.376049       1.192480        1.831099
H       -2.955792       -1.669346       -1.350554
C       -2.956648       0.083532        -0.072369
H       -2.734857       1.776345        1.265541
O       -4.256052       0.472368        -0.345331
H       -4.695486       -0.145214       -1.009919
O       1.311243        1.512216        -1.234803
###
24
tyr205 pm6_conformaciones E=-0.245457138461 au
N       3.405778        -1.156288       -0.030375
H       3.847306        -0.729005       0.804258
H       4.027805        -0.992786       -0.845461
H       3.345781        -2.182700       0.131621
C       2.028332        -0.576413       -0.281568
H       1.631326        -1.030678       -1.238460
C       1.087856        -0.918050       0.885772
C       2.118344        0.954988        -0.452210
H       1.164992        -2.006886       1.126291
H       1.421372        -0.407777       1.817499
C       -0.334956       -0.571864       0.554766
```

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O       1.309791        1.513417        -1.237790
C       -0.939609       0.557901        1.126919
C       -1.063338       -1.381906       -0.335413
H       -0.379859       1.185975        1.824697
C       -2.258267       0.889177        0.814768
C       -2.379216       -1.068377       -0.664813
H       -0.594698       -2.267577       -0.773963
H       -2.739287       1.762953        1.256209
C       -2.956290       0.070063        -0.080627
H       -2.951782       -1.686548       -1.355309
O       -4.261578       0.332881        -0.455787
H       -4.628190       1.144768        0.016147
O       2.976493        1.600097        0.199019
###
24
tyr206 pm6_conformaciones E=-0.245778628438 au
N       2.104956        1.649443        -0.806933
H       1.243721        1.517363        -1.365857
H       2.913502        1.652389        -1.458426
H       2.048237        2.585142        -0.355002
C       2.259176        0.564555        0.238442
H       3.270538        0.705865        0.730385
C       1.173348        0.673411        1.318836
C       2.229147        -0.836109       -0.410356
H       1.439178        -0.010760       2.159088
H       1.214431        1.688372        1.783707
C       -0.211195       0.380403        0.817396
O       2.845429        -1.757415       0.181721
C       -1.001600       1.410851        0.282546
C       -0.722871       -0.927052       0.885133
H       -0.616465       2.435311        0.246353
C       -2.278348       1.142319        -0.208840
C       -1.997381       -1.219010       0.404237
H       -0.117728       -1.727994       1.318323
H       -2.893812       1.935659        -0.635374
C       -2.755207       -0.172874       -0.143202
H       -2.401779       -2.229384       0.451617
O       -4.007436       -0.527477       -0.611854
H       -4.471778       0.246405        -1.060639
O       1.595362        -1.020537       -1.478717
###
24
tyr207 pm6_conformaciones E=-0.243536329103 au
N       -1.668004       -1.181545       1.234054
H       -2.018210       -2.004567       0.711494
H       -2.197418       -1.112763       2.124881
H       -0.670413       -1.355773       1.468048
C       -1.809571       0.089227        0.419481
H       -1.501334       0.958773        1.072235
C       -0.924794       0.036391        -0.834152
C       -3.280524       0.275668        -0.017544
H       -1.183073       -0.855181       -1.452167
H       -1.172218       0.906299        -1.489801
C       0.540751        0.051272        -0.508070
O       -3.934346       -0.722703       -0.409409
C       1.156791        1.239015        -0.081302
C       1.302556        -1.121732       -0.642772
H       0.567120        2.154023        0.021440
C       2.518886        1.263202        0.214554
C       2.667215        -1.120241       -0.359912
H       0.823462        -2.048911       -0.971375
H       3.005665        2.179170        0.550799
C       3.252877        0.079343        0.068768
H       3.265456        -2.024059       -0.465065
O       4.609992        0.020112        0.333880
H       4.952137        0.885505        0.717415
O       -3.768179       1.432019        0.015456
###
24
tyr208 pm6_conformaciones E=-0.242980500027 au
N       2.378913        1.822002        0.211257
H       2.959226        1.965709        -0.636404
H       2.965517        2.027081        1.043340
H       1.604103        2.516989        0.184200
C       1.823954        0.413356        0.271055
H       1.233265        0.320073        1.231050
```

```
C       0.915928        0.123017        -0.934911
C       2.979320        -0.615312       0.305243
H       1.052636        0.889297        -1.735930
H       1.229369        -0.822528       -1.437163
C       -0.533353       0.047782        -0.547891
O       2.954379        -1.485095       1.211274
C       -1.209166       -1.181279       -0.600326
C       -1.219964       1.206454        -0.144699
H       -0.680649       -2.084783       -0.916883
C       -2.556983       -1.265443       -0.251293
C       -2.564617       1.146212        0.213225
H       -0.695543       2.166415        -0.110559
H       -3.090270       -2.215612       -0.291732
C       -3.212035       -0.097302       0.155370
H       -3.104355       2.037411        0.530098
O       -4.542119       -0.094172       0.537073
H       -4.953959       -1.009841       0.463214
O       3.873959        -0.571875       -0.572932
###
24
tyr209 pm6_conformaciones E=-0.245413646982 au
N       3.398807        -1.169767       -0.036606
H       3.847176        -0.743435       0.794776
H       4.017784        -1.012580       -0.855153
H       3.332568        -2.195296       0.128202
C       2.024076        -0.581180       -0.282429
H       1.619937        -1.034280       -1.236907
C       1.086258        -0.914146       0.889514
C       2.123381        0.949326        -0.456397
H       1.160287        -2.002090       1.135111
H       1.424038        -0.400461       1.817760
C       -0.336437       -0.565500       0.560226
O       1.311073        1.512074        -1.235002
C       -1.066343       -1.373130       -0.328865
C       -0.938736       0.566675        1.133341
H       -0.601362       -2.259608       -0.769275
C       -2.382098       -1.052994       -0.656851
C       -2.255827       0.902943        0.824651
H       -0.375754       1.192008        1.831252
H       -2.955937       -1.669161       -1.350662
C       -2.956577       0.083583        -0.072319
H       -2.734479       1.776392        1.265546
O       -4.256007       0.472472        -0.344920
H       -4.695413       -0.144731       -1.010022
O       2.992849        1.588973        0.184969
###
24
tyr210 pm6_conformaciones E=-0.245413725021 au
N       3.398750        -1.169980       -0.036568
H       3.847219        -0.743750       0.794770
H       4.017752        -1.012876       -0.855136
H       3.332421        -2.195527       0.128194
C       2.024128        -0.581190       -0.282357
H       1.619869        -1.034217       -1.236899
C       1.086163        -0.913953       0.889526
C       2.123624        0.949271        -0.456360
H       1.160159        -2.001839       1.135442
H       1.423881        -0.400215       1.817786
C       -0.336517       -0.565401       0.560240
O       1.311001        1.512273        -1.234533
C       -1.066369       -1.372996       -0.328964
C       -0.938930       0.566617        1.133453
H       -0.601291       -2.259396       -0.769414
C       -2.382102       -1.052923       -0.656983
C       -2.256067       0.902822        0.824774
H       -0.376040       1.191975        1.831395
H       -2.955881       -1.669031       -1.350872
C       -2.956677       0.083590        -0.072359
H       -2.734798       1.776087        1.265927
O       -4.256148       0.472413        -0.345034
H       -4.695298       -0.144446       -1.010524
O       2.993552        1.588824        0.184501
###
24
tyr211 pm6_conformaciones E=-0.245413557818 au
N       3.398718        -1.170010       -0.036956
```

```
H       3.847101        -0.744495       0.794813
H       4.017760        -1.011996       -0.855317
H       3.332451        -2.195698       0.126771
C       2.024001        -0.581170       -0.282274
H       1.619456        -1.034110       -1.236739
C       1.086306        -0.913848       0.889833
C       2.123326        0.949312        -0.456303
H       1.160380        -2.001650       1.136035
H       1.424079        -0.399882       1.817940
C       -0.336436       -0.565379       0.560501
O       1.310374        1.512177        -1.234216
C       -1.066191       -1.373126       -0.328669
C       -0.938852       0.566759        1.133452
H       -0.601036       -2.259533       -0.769024
C       -2.381878       -1.053065       -0.656854
C       -2.255993       0.902896        0.824659
H       -0.375968       1.192340        1.831204
H       -2.955561       -1.669181       -1.350825
C       -2.956506       0.083490        -0.072362
H       -2.734711       1.776329        1.265500
O       -4.255889       0.472352        -0.345384
H       -4.695312       -0.145280       -1.009899
O       2.993474        1.588972        0.184142
###
23
tyr300 pm6_conformaciones E=-0.386435860456 au
N       -1.585598       -0.956060       1.429413
H       -2.434920       -1.134865       1.968901
H       -1.353295       -1.829978       0.954120
C       -1.816083       0.130082        0.439738
H       -1.553284       1.096097        0.951909
C       -0.946007       -0.029252       -0.822066
C       -3.284387       0.212801        -0.017216
H       -1.208158       -0.971189       -1.352438
H       -1.195320       0.779996        -1.546283
C       0.522362        0.008690        -0.511615
O       -3.846231       1.343079        -0.065369
C       1.135681        1.217795        -0.144856
C       1.288575        -1.166727       -0.587734
H       0.545538        2.135973        -0.091970
C       2.496963        1.260232        0.153664
C       2.652952        -1.147244       -0.302565
H       0.814158        -2.109835       -0.872262
H       2.980819        2.193040        0.445081
C       3.234036        0.072807        0.069639
H       3.254644        -2.052836       -0.363657
O       4.591285        0.030401        0.344909
H       4.925884        0.912610        0.694491
O       -3.917735       -0.833692       -0.336505
###
23
tyr301 pm6_conformaciones E=-0.386435521258 au
N       -1.586006       -0.955679       1.429803
H       -2.435351       -1.133682       1.969542
H       -1.354389       -1.830017       0.954945
C       -1.816068       0.130072        0.439581
H       -1.552988       1.096246        0.951293
C       -0.945938       -0.030280       -0.822014
C       -3.284365       0.213043        -0.017378
H       -1.208020       -0.972700       -1.351567
H       -1.195268       0.778309        -1.546968
C       0.522418        0.008080        -0.511551
O       -3.917888       -0.833381       -0.336577
C       1.135430        1.217421        -0.145073
C       1.288952        -1.167142       -0.587436
H       0.545047        2.135457        -0.092380
C       2.496710        1.260298        0.153407
C       2.653327        -1.147231       -0.302298
H       0.814805        -2.110442       -0.871766
H       2.980312        2.193311        0.444585
C       3.234096        0.073055        0.069632
H       3.255260        -2.052676       -0.363190
O       4.591352        0.031045        0.344957
H       4.925841        0.913524        0.693801
O       -3.846036       1.343402        -0.065646
###
```

```
23
tyr302 pm6_conformaciones E=-0.386435840192 au
N       -1.586040       -0.956564       1.429204
H       -2.435246       -1.134726       1.969050
H       -1.354633       -1.830603       0.953678
C       -1.816199       0.129846        0.439748
H       -1.553233       1.095693        0.952135
C       -0.945920       -0.029482       -0.821952
C       -3.284397       0.213031        -0.017356
H       -1.207982       -0.971435       -1.352361
H       -1.195131       0.779710        -1.546196
C       0.522421        0.008528        -0.511297
O       -3.846083       1.343403        -0.065248
C       1.135693        1.217697        -0.144587
C       1.288678        -1.166835       -0.587380
H       0.545464        2.135800        -0.091599
C       2.496987        1.260242        0.153758
C       2.653117        -1.147239       -0.302389
H       0.814343        -2.110031       -0.871746
H       2.980809        2.193085        0.445122
C       3.234162        0.072866        0.069591
H       3.254801        -2.052830       -0.363458
O       4.591482        0.030642        0.344588
H       4.926234        0.913037        0.693230
O       -3.917948       -0.833257       -0.336976
###
23
tyr303 pm6_conformaciones E=-0.388810373580 au
N       2.229725        1.701420        -0.781346
H       2.807168        1.472837        -1.593607
H       1.277570        1.820051        -1.130270
C       2.291827        0.601168        0.213075
H       3.296222        0.681270        0.719082
C       1.202430        0.746429        1.293750
C       2.208026        -0.800936       -0.413338
H       1.464055        0.098448        2.159702
H       1.241522        1.779318        1.708054
C       -0.183062       0.433636        0.805514
O       2.810595        -1.754679       0.158473
C       -0.972646       1.433474        0.214617
C       -0.695550       -0.869108       0.936956
H       -0.592285       2.455416        0.129690
C       -2.247319       1.138682        -0.268448
C       -1.967243       -1.187251       0.465346
H       -0.092831       -1.645997       1.414228
H       -2.862947       1.908007        -0.736470
C       -2.723203       -0.171527       -0.138047
H       -2.370964       -2.194348       0.563139
O       -3.973363       -0.550318       -0.595358
H       -4.438012       0.203383        -1.076246
O       1.560626        -0.999468       -1.481168
###
23
tyr304 pm6_conformaciones E=-0.386242571822 au
N       -1.552415       -1.105218       1.299851
H       -2.389460       -1.362769       1.825679
H       -1.312706       -1.910227       0.718706
C       -1.815266       0.090154        0.455662
H       -1.571740       0.990141        1.084295
C       -0.950190       0.110250        -0.820157
C       -3.286486       0.196207        0.015285
H       -1.215299       -0.746283       -1.478434
H       -1.201269       1.013648        -1.421328
C       0.518820        0.096539        -0.510611
O       -3.845326       1.329255        0.013527
C       1.251114        -1.095666       -0.630219
C       1.165557        1.273866        -0.097157
H       0.752561        -2.014101       -0.951298
C       2.614736        -1.122987       -0.338709
C       2.526374        1.270258        0.202686
H       0.599419        2.204574        -0.010032
H       3.190377        -2.044581       -0.429744
C       3.229922        0.063405        0.077449
H       3.035603        2.176965        0.525578
O       4.574642        0.119542        0.404760
H       5.024277        -0.772431       0.279868
```

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O       -3.925859       -0.835118       -0.339240
###
23
tyr305 pm6_conformaciones E=-0.386242671601 au
N       -1.552437       -1.104893       1.300104
H       -2.390341       -1.364405       1.823568
H       -1.309425       -1.909218       0.719379
C       -1.815328       0.090299        0.455621
H       -1.571916       0.990356        1.084234
C       -0.950198       0.110465        -0.820151
C       -3.286531       0.196097        0.015218
H       -1.215284       -0.745985       -1.478493
H       -1.201153       1.013902        -1.421331
C       0.518791        0.096630        -0.510492
O       -3.925660       -0.835358       -0.339290
C       1.251001        -1.095618       -0.630092
C       1.165582        1.273917        -0.097000
H       0.752366        -2.014049       -0.951071
C       2.614645        -1.123006       -0.338685
C       2.526423        1.270240        0.202735
H       0.599480        2.204641        -0.009776
H       3.190241        -2.044622       -0.429738
C       3.229907        0.063374        0.077386
H       3.035673        2.176909        0.525705
O       4.574671        0.119420        0.404599
H       5.024305        -0.772498       0.279140
O       -3.845591       1.329041        0.013492
###
23
tyr306 pm6_conformaciones E=-0.388748207081 au
N       2.240498        1.687181        -0.791860
H       2.818743        1.449484        -1.600974
H       1.289752        1.807811        -1.143851
C       2.294598        0.594066        0.210810
H       3.298707        0.672027        0.717748
C       1.204282        0.753565        1.288557
C       2.203734        -0.812379       -0.404899
H       1.461513        0.111176        2.160034
H       1.247750        1.789234        1.695151
C       -0.181960       0.443080        0.800984
O       1.562181        -1.014317       -1.475566
C       -0.699668       -0.855169       0.939103
C       -0.968236       1.444033        0.204095
H       -0.102236       -1.633282       1.420603
C       -1.973745       -1.168271       0.466431
C       -2.243593       1.155592        -0.276842
H       -0.582100       2.463668        0.115052
H       -2.380638       -2.174872       0.569833
C       -2.724969       -0.155163       -0.141177
H       -2.856674       1.923949        -0.746365
O       -3.987201       -0.380440       -0.661311
H       -4.293145       -1.327784       -0.506343
O       2.794044        -1.766218       0.179346
###
23
tyr307 pm6_conformaciones E=-0.388132820756 au
N       -3.305331       1.393433        -0.172994
H       -3.995056       1.041653        -0.842249
H       -3.710296       1.249589        0.754218
C       -2.036588       0.632171        -0.309992
H       -1.556354       0.967911        -1.270513
C       -1.092282       0.936797        0.869807
C       -2.243830       -0.890129       -0.389074
H       -1.152031       2.019125        1.125448
H       -1.439372       0.423405        1.791819
C       0.326427        0.566291        0.544924
O       -3.102817       -1.463701       0.338946
C       0.856803        -0.661162       0.970476
C       1.127363        1.453962        -0.196194
H       0.242223        -1.351530       1.553049
C       2.170066        -1.012930       0.657320
C       2.440882        1.125007        -0.520947
H       0.718584        2.415062        -0.519414
H       2.592231        -1.964279       0.983624
C       2.941204        -0.111898       -0.086156
H       3.068546        1.804989        -1.095535
```

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O       4.247590        -0.387491       -0.450837
H       4.565081        -1.260874       -0.060527
O       -1.536838       -1.564775       -1.194352
###
23
tyr308 pm6_conformaciones E=-0.386242747581 au
N       -1.552467       -1.105130       1.299962
H       -2.390245       -1.364383       1.823846
H       -1.310190       -1.909613       0.719033
C       -1.815351       0.090198        0.455640
H       -1.571761       0.990077        1.084409
C       -0.950209       0.110194        -0.820118
C       -3.286487       0.196247        0.015257
H       -1.215368       -0.746370       -1.478297
H       -1.201113       1.013485        -1.421518
C       0.518763        0.096424        -0.510501
O       -3.845177       1.329395        0.012956
C       1.251178        -1.095676       -0.630320
C       1.165386        1.273717        -0.096855
H       0.752685        -2.014155       -0.951402
C       2.614811        -1.122915       -0.338864
C       2.526233        1.270203        0.202920
H       0.599175        2.204354        -0.009527
H       3.190506        -2.044473       -0.429914
C       3.229910        0.063496        0.077417
H       3.035314        2.176912        0.526070
O       4.574662        0.119689        0.404590
H       5.024183        -0.772328       0.279628
O       -3.925900       -0.835200       -0.338736
###
23
tyr309 pm6_conformaciones E=-0.386242525470 au
N       -1.552419       -1.104317       1.300647
H       -2.390233       -1.363320       1.824513
H       -1.309905       -1.909010       0.720205
C       -1.815288       0.090497        0.455602
H       -1.571792       0.990869        1.083681
C       -0.950207       0.109860        -0.820224
C       -3.286489       0.196111        0.015149
H       -1.215296       -0.747060       -1.477967
H       -1.201238       1.012880        -1.421989
C       0.518779        0.096303        -0.510577
O       -3.925481       -0.835396       -0.339418
C       1.251162        -1.095872       -0.629985
C       1.165403        1.273747        -0.097303
H       0.752630        -2.014397       -0.950853
C       2.614789        -1.123030       -0.338541
C       2.526243        1.270300        0.202503
H       0.599206        2.204433        -0.010312
H       3.190537        -2.044568       -0.429445
C       3.229872        0.063510        0.077380
H       3.035340        2.177104        0.525324
O       4.574626        0.119744        0.404639
H       5.024310        -0.772167       0.279558
O       -3.845671       1.329014        0.013371
###
23
tyr311 pm6_conformaciones E=-0.388810303687 au
N       2.229715        1.701295        -0.782040
H       2.806184        1.471923        -1.594735
H       1.277346        1.820756        -1.130105
C       2.291776        0.601463        0.212888
H       3.296158        0.681908        0.718917
C       1.202246        0.747018        1.293448
C       2.208283        -0.800981       -0.413015
H       1.463819        0.099412        2.159657
H       1.241239        1.780049        1.707469
C       -0.183201       0.433925        0.805282
O       1.560881        -1.000274       -1.480648
C       -0.973068       1.433625        0.214546
C       -0.695325       -0.868973       0.936626
H       -0.592943       2.455671        0.129596
C       -2.247769       1.138572        -0.268353
C       -1.966979       -1.187386       0.465139
H       -0.092265       -1.645737       1.413604
H       -2.863602       1.907821        -0.736260
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C       -2.723318       -0.171748       -0.137976
H       -2.370376       -2.194654       0.562673
O       -3.973528       -0.550724       -0.594989
H       -4.438033       0.202698        -1.076555
O       2.811221        -1.754252       0.159200
###
22
tyr400 pm6_conformaciones E=-0.548273400114 au
N       2.190037        1.693268        -0.788899
H       2.749763        1.447099        -1.608129
H       1.234898        1.828769        -1.122870
C       2.243853        0.598833        0.212560
H       3.250628        0.669969        0.713392
C       1.155027        0.761436        1.294148
C       2.138425        -0.805294       -0.402252
H       1.416831        0.122222        2.165098
H       1.197481        1.798215        1.693696
C       -0.228143       0.442987        0.806479
O       1.501355        -1.002302       -1.478117
C       -0.741781       -0.858281       0.940638
C       -1.023783       1.431738        0.202897
H       -0.141422       -1.626342       1.433179
C       -1.996939       -1.185366       0.449713
C       -2.284039       1.129970        -0.293421
H       -0.646843       2.454703        0.122438
H       -2.386767       -2.191721       0.552876
C       -2.791097       -0.194059       -0.190165
H       -2.891345       1.896178        -0.762029
O       -3.951583       -0.501875       -0.683695
O       2.707400        -1.768790       0.188197
###
22
tyr401 pm6_conformaciones E=-0.547462011102 au
N       -3.366732       1.234182        -0.135444
H       -4.030590       0.809420        -0.788307
H       -3.721462       1.029416        0.800772
C       -2.021309       0.631936        -0.321211
H       -1.612447       1.029834        -1.289841
C       -1.081720       1.038030        0.833729
C       -2.052630       -0.903096       -0.409009
H       -1.149233       2.136837        0.990995
H       -1.432656       0.600907        1.791609
C       0.335199        0.637741        0.543749
O       -1.332215       -1.485782       -1.274048
C       1.151471        1.459012        -0.254129
C       0.855988        -0.567167       1.043395
H       0.758646        2.407663        -0.627606
C       2.446827        1.081827        -0.573968
C       2.147644        -0.968832       0.734183
H       0.234746        -1.201358       1.679431
H       3.071901        1.718422        -1.189749
C       2.966806        -0.152468       -0.094112
H       2.545112        -1.900617       1.119708
O       4.164040        -0.532361       -0.414726
O       -2.780144       -1.583318       0.369441
###
22
tyr402 pm6_conformaciones E=-0.547461840754 au
N       -3.366527       1.234575        -0.135552
H       -4.030539       0.809686        -0.788152
H       -3.721234       1.030434        0.800796
C       -2.021241       0.631980        -0.321158
H       -1.612206       1.029757        -1.289780
C       -1.081610       1.037791        0.833809
C       -2.052947       -0.903065       -0.408956
H       -1.149076       2.136559        0.991380
H       -1.432508       0.600522        1.791655
C       0.335294        0.637567        0.543727
O       -2.780749       -1.583117       0.369348
C       1.151551        1.458952        -0.254048
C       0.856113        -0.567376       1.043263
H       0.758684        2.407621        -0.627448
C       2.446932        1.081854        -0.573895
C       2.147795        -0.968959       0.734043
H       0.234878        -1.201679       1.679199
H       3.071997        1.718524        -1.189612
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C       2.966942        -0.152467       -0.094135
H       2.545289        -1.900766       1.119495
O       4.164195        -0.532274       -0.414783
O       -1.332518       -1.485900       -1.273885
###
22
tyr403 pm6_conformaciones E=-0.544294395379 au
N       -1.513865       -1.128375       1.283095
H       -2.374358       -1.441636       1.735433
H       -1.196754       -1.901366       0.695348
C       -1.766042       0.083235        0.457486
H       -1.522929       0.969175        1.105071
C       -0.893521       0.129081        -0.814292
C       -3.233177       0.201376        0.013079
H       -1.158343       -0.712583       -1.489882
H       -1.142531       1.045467        -1.394283
C       0.573740        0.105203        -0.501977
O       -3.877917       -0.824177       -0.350016
C       1.306388        -1.087433       -0.623942
C       1.230921        1.271829        -0.077460
H       0.801637        -1.998852       -0.953474
C       2.662581        -1.125949       -0.330223
C       2.585312        1.257398        0.225371
H       0.668981        2.203726        0.014680
H       3.222943        -2.048308       -0.429376
C       3.328540        0.051868        0.104434
H       3.087529        2.159783        0.554204
O       4.594294        0.024380        0.394789
O       -3.786073       1.337742        0.013446
###
22
tyr404 pm6_conformaciones E=-0.544117510854 au
N       -2.235214       1.730504        -0.787241
H       -2.973269       1.663148        -1.492676
H       -2.642502       2.221989        0.010648
C       -1.775229       0.374138        -0.388393
H       -1.200148       -0.047827       -1.257020
C       -0.863020       0.431779        0.855078
C       -2.964312       -0.564034       -0.108826
H       -0.989875       1.402222        1.383351
H       -1.180737       -0.323995       1.605797
C       0.578903        0.213551        0.500092
O       -3.780783       -0.302404       0.819912
C       1.088079        -1.092706       0.396672
C       1.435721        1.301523        0.269881
H       0.426856        -1.943583       0.574662
C       2.418782        -1.316305       0.076589
C       2.771586        1.103542        -0.054429
H       1.049970        2.320087        0.350843
H       2.808288        -2.325243       0.002708
C       3.288886        -0.215426       -0.155832
H       3.428239        1.947849        -0.229078
O       4.536116        -0.420397       -0.452869
O       -3.124920       -1.582767       -0.839985
###
22
tyr405 pm6_conformaciones E=-0.547457293549 au
N       -3.343291       1.270731        -0.143772
H       -4.017582       0.849159        -0.787772
H       -3.702791       1.095332        0.796567
C       -2.012559       0.633564        -0.317271
H       -1.586823       1.019332        -1.283732
C       -1.071801       1.018124        0.844101
C       -2.081656       -0.900071       -0.405987
H       -1.137356       2.114378        1.020342
H       -1.423241       0.565411        1.794513
C       0.345226        0.622987        0.547859
O       -2.849830       -1.561213       0.349548
C       1.155171        1.450329        -0.250374
C       0.872388        -0.581423       1.041709
H       0.756513        2.397971        -0.620267
C       2.451273        1.080329        -0.575025
C       2.165349        -0.975703       0.727826
H       0.255554        -1.220792       1.676861
H       3.071331        1.721315        -1.191341
C       2.978596        -0.152541       -0.099470
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H       2.568335        -1.906904       1.108998
O       4.177452        -0.524454       -0.423227
O       -1.351724       -1.502319       -1.249817
###
22
tyr406 pm6_conformaciones E=-0.547457257083 au
N       -3.342986       1.270794        -0.144938
H       -4.017211       0.848496        -0.788474
H       -3.702679       1.096652        0.795562
C       -2.012163       0.633410        -0.317466
H       -1.585860       1.018824        -1.283825
C       -1.071926       1.018180        0.844237
C       -2.081408       -0.900222       -0.405842
H       -1.137684       2.114389        1.020447
H       -1.423474       0.565366        1.794545
C       0.345097        0.623021        0.548182
O       -1.351105       -1.502929       -1.248951
C       0.872292        -0.581285       1.041912
C       1.155152        1.450562        -0.249952
H       0.255626        -1.220738       1.677135
C       2.165296        -0.975658       0.727795
C       2.451099        1.080581        -0.574711
H       0.756375        2.398280        -0.619439
H       2.568123        -1.906834       1.109165
C       2.978389        -0.152610       -0.099551
H       3.071355        1.721635        -1.190774
O       4.177028        -0.524664       -0.423966
O       -2.850253       -1.560843       0.349492
###
22
tyr407 pm6_conformaciones E=-0.542741731668 au
N       -3.106905       1.449235        -0.685034
H       -3.885484       0.969686        -1.141125
H       -3.459948       1.792381        0.210960
C       -1.973212       0.506223        -0.473075
H       -1.569903       0.231222        -1.486863
C       -0.870745       1.199547        0.342283
C       -2.475485       -0.793089       0.187850
H       -0.864899       2.285001        0.086798
H       -1.124708       1.188659        1.424300
C       0.507355        0.633018        0.146212
O       -2.262177       -1.060068       1.400829
C       0.738758        -0.724804       -0.118401
C       1.614312        1.495114        0.269184
H       -0.096779       -1.418984       -0.216849
C       2.028794        -1.219402       -0.257052
C       2.913007        1.025355        0.140327
H       1.447804        2.556562        0.471573
H       2.195462        -2.270111       -0.465425
C       3.145591        -0.351728       -0.124580
H       3.756303        1.699023        0.240919
O       4.351943        -0.819246       -0.242479
O       -3.142237       -1.595622       -0.534042
###
22
tyr408 pm6_conformaciones E=-0.548273057294 au
N       2.190321        1.693411        -0.788311
H       2.750117        1.447455        -1.607569
H       1.235236        1.829076        -1.122348
C       2.243966        0.598644        0.212781
H       3.250739        0.669499        0.713681
C       1.155078        0.760974        1.294381
C       2.138313        -0.805254       -0.402462
H       1.416803        0.121497        2.165147
H       1.197536        1.797660        1.694210
C       -0.228080       0.442711        0.806556
O       1.501421        -1.001778       -1.478525
C       -1.023492       1.431597        0.202885
C       -0.741947       -0.858472       0.940626
H       -0.646379       2.454491        0.122429
C       -2.283758       1.130050        -0.293525
C       -1.997140       -1.185327       0.449627
H       -0.141731       -1.626669       1.433128
H       -2.890840       1.896351        -0.762276
C       -2.791111       -0.193865       -0.190230
H       -2.387126       -2.191631       0.552704
```

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O       -3.951736       -0.501384       -0.683640
O       2.706868        -1.769083       0.187820
###
22
tyr409 pm6_conformaciones E=-0.544294399048 au
N       -1.513774       -1.128196       1.283234
H       -2.374035       -1.440971       1.736332
H       -1.197317       -1.901457       0.695499
C       -1.766049       0.083310        0.457565
H       -1.523116       0.969304        1.105073
C       -0.893511       0.128970        -0.814261
C       -3.233148       0.201301        0.013013
H       -1.158326       -0.712906       -1.489580
H       -1.142594       1.045219        -1.394474
C       0.573750        0.105219        -0.501971
O       -3.877899       -0.824189       -0.350155
C       1.306431        -1.087529       -0.623837
C       1.230868        1.271806        -0.077498
H       0.801539        -1.998958       -0.953111
C       2.662592        -1.125939       -0.330241
C       2.585337        1.257440        0.225323
H       0.669032        2.203754        0.014716
H       3.223115        -2.048229       -0.429438
C       3.328544        0.051992        0.104357
H       3.087381        2.159861        0.554287
O       4.594274        0.024324        0.394724
O       -3.786143       1.337657        0.013351
###
22
tyr410 pm6_conformaciones E=-0.547461804592 au
N       -3.366060       1.235162        -0.135831
H       -4.030217       0.810367        -0.788349
H       -3.720911       1.031464        0.800560
C       -2.021023       0.631979        -0.321163
H       -1.611635       1.029521        -1.289739
C       -1.081466       1.037543        0.833980
C       -2.053342       -0.903041       -0.408912
H       -1.148946       2.136272        0.991754
H       -1.432439       0.600040        1.791684
C       0.335452        0.637405        0.543850
O       -2.781868       -1.582734       0.369077
C       1.151601        1.458862        -0.253951
C       0.856339        -0.567537       1.043320
H       0.758651        2.407528        -0.627284
C       2.446970        1.081835        -0.573923
C       2.148023        -0.969035       0.733985
H       0.235188        -1.201877       1.679295
H       3.071943        1.718566        -1.189670
C       2.967063        -0.152472       -0.094233
H       2.545596        -1.900835       1.119379
O       4.164297        -0.532240       -0.415006
O       -1.332744       -1.486328       -1.273388
```