Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Why hydroxy-Proline improves the catalytic power of peptidoglycan N-deacetylase enzyme: insight from theory

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Molecular modeling of the peptidoglycan N-acetylglucosamine deacetylase

Preparation of peptidoglycan N-acetylglucosamine deacetylase with and without 2-hydroxy proline post-translational mutation.

The crystallographic structure of the peptidoglycan N-acetylglucosamine deacetylase (PDA) BC1960 from *Bacillus cereus* (EC 3.5.1.33), was adopted as starting point of the present study (PDB code: 4L1G).[1] Due to the absence of Zn^{2+} cation in the crystal structure, we added manually in the position of the acetate ion (ACT), as shown in **Fig. S1**, thus generating the initial structures in the presence of natural proline and 2-hydroxy proline (2Hyp) post-translational mutation at position 171.

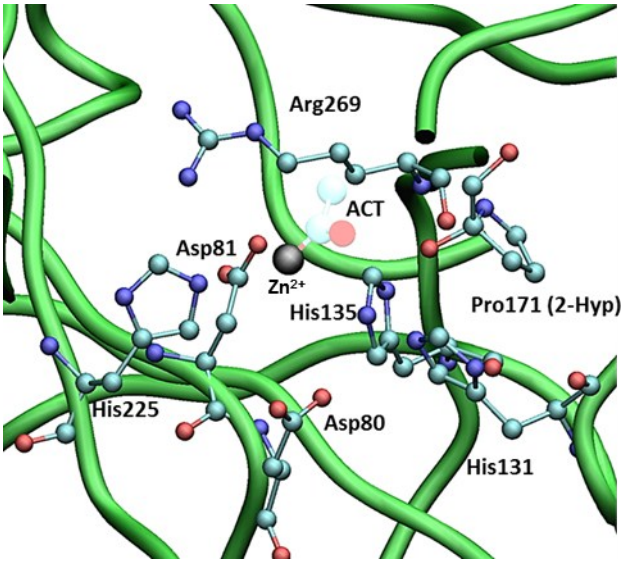

Fig. S1. 3D representation of PDA-2Hyp (PDB code: 4L1G) structure after replacing the acetate ion with Zn^{2+} cation (black sphere).

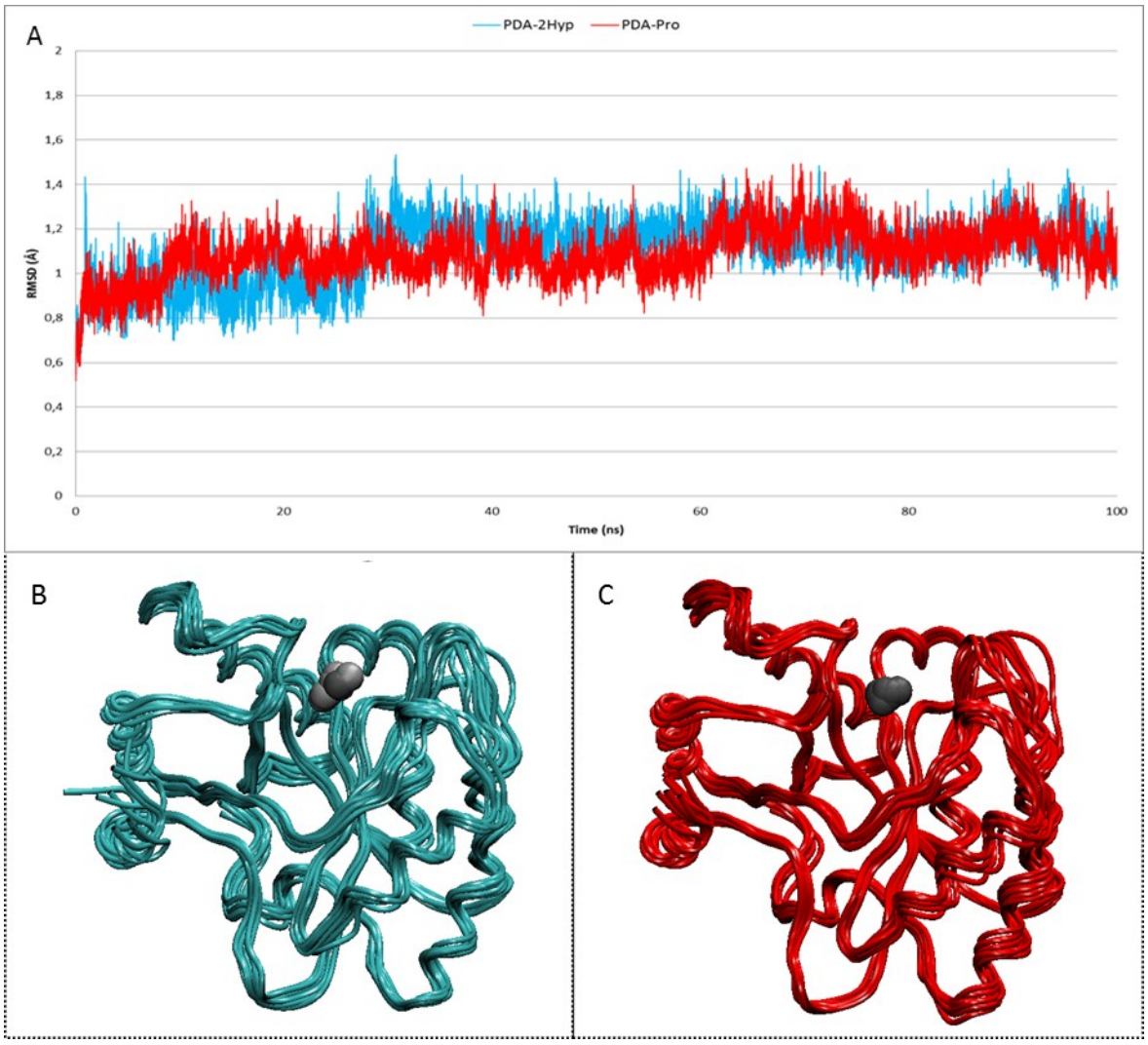

Fig. S2. (**A**) RMSD trends of PDA-Pro (blue line) and PDA-2Hyp (red line), calculated on backbone's atoms, expressed in Å. Superposition of 10 clusters extrapolated by 100 ns of MDs of (**B**) PDA-Pro and (**C**) PDA-2Hyp.

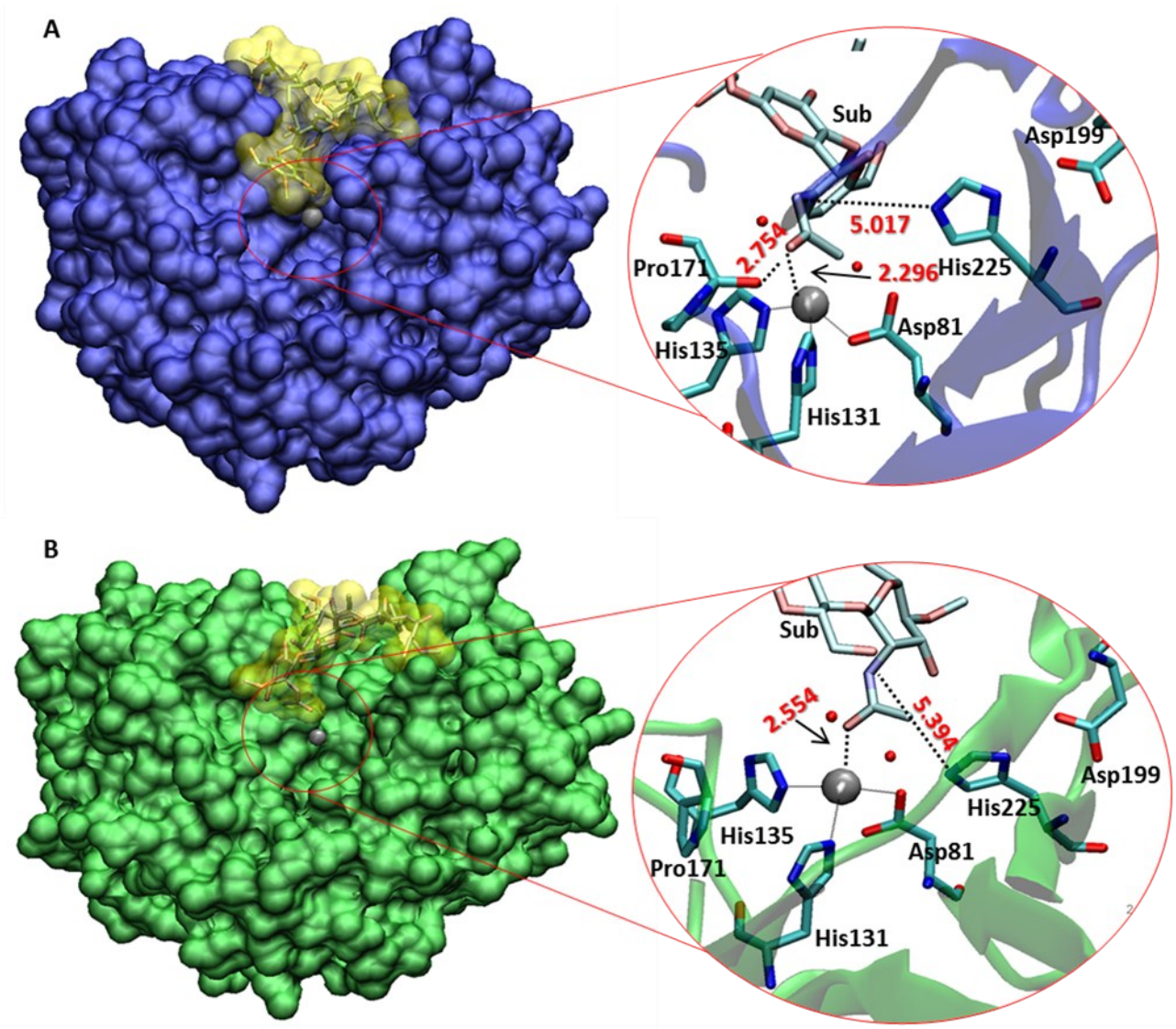

Fig. S3. Focus on the best docked poses of GlcNAc into the active site of (**A**) PDA-Pro and (**B**) PDA-2Hyp. GlcNAc is shown as cyan ball and stick and the enzymes are represented as blue and green cartoon, respectively, for the proline and 2-Hydroxy-proline at position 171. Relevant geometrical parameters of selected docked poses are also reported.

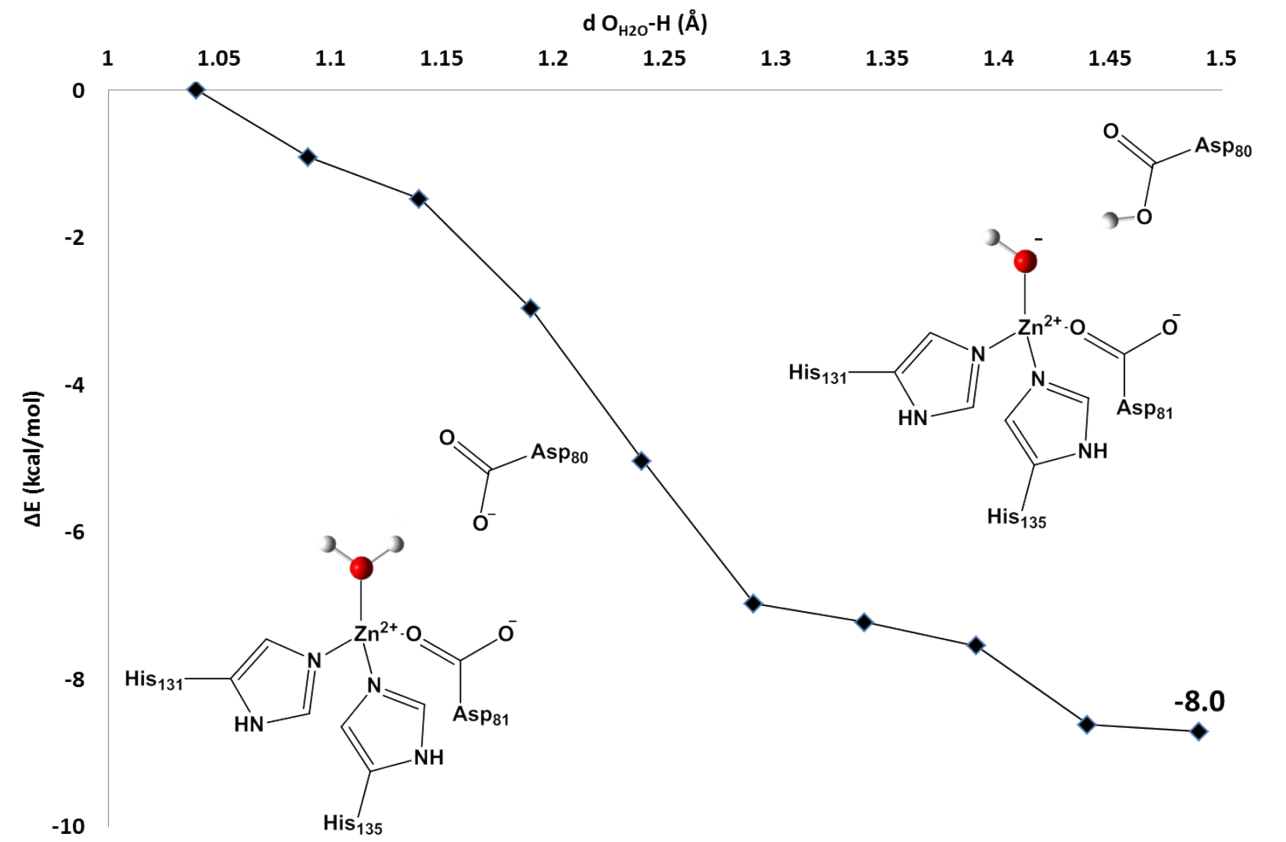

Fig. S4. Potential energy surface for the activation of water in presence of Asp80 base.

Computational details

In detail, the histidine residues (His131 and His135) participating in coordination metal-protein bonds were protonated in δ-position, while the His225 was considered fully protonated. Furthermore, the three glutamate residues, one bound to the Zn^{2+} (Asp81) and the others with catalytic function (Asp80 and Asp199), were deprotonated.

Both the structures were solvated using TIP3P water molecules within 12 Å from the macromolecules, in a rectangular water box (81 x 73 x 88 Å), meanwhile the counter ions (Cl^-) were added within 2 Å of the protein in order to neutralize the net charge. After this step, the PDA structures were minimized in four different step: (1) the water molecules were firstly minimized and the rest of the systems were restrained with a harmonic potential force of 50 kcal mol^{-1} $Å^{-2}$; (2) the hydrogens were minimized while the rest of the systems were submitted to a harmonic potential force of 50 kcal mol^{-1} $Å^{-2}$; (3) the protein's sidechains were relaxed while the remaining parts were restrained with a harmonic potential force of 50 kcal mol^{-1} $Å^{-2}$ and finally (4) the PDA structures were entirely minimized without restraints. After the minimization, the systems were undergone to molecular dynamics simulation (MDs). Initially, the solvated proteins were progressively heated from 0 to 310 K in 50 ps and additive 50 ps of MDs were performed in NVT ensemble at 310 K. Finally, 100 ns of MDs, in NPT ensemble, were executed at 310 K and 1 atm, as previously reported in similar works[5].

The Particle Mesh Ewald (PME)[6] summation method was employed to find the electrostatic potential and the long-range electrostatic interactions with 12 Å cut-off distance. The SHAKE[7] algorithm was adopted during all MDs, to constrain bonds involving hydrogen atoms, in order to use an integration step of 2 fs. The Zinc Amber Force Field (ZAFF)[8] was used to parametrize the Zn^{2+} coordinated to the His131, His135, Asp81 and one water molecule. In order to analyze the behavior of the coordination sphere of metal ion during MDs, we monitored the average values of distance between Zn^{2+} and donor atoms of above mentioned residues in comparison with those available related to the another member of CE4 family[9] (**Table S3**).

The ff14SB[10] force field was adopted to treat the other atoms, as implemented in AMBER16 package.[11] In particular, in the presence of PDA-2Hyp system, the non-canonical residue was parametrized by single geometry optimization at HF/6-31G(d) level of theory. The parameters have been derived by Antechamber tools as implemented in Amber 16,[11] adopting the General Amber

Force Field (GAFF),[12] to derive the Lennard-Jones parameters, the force field and the RESP method,[4] to obtain atomic charges.

The root-mean-square deviation (RMSD) analysis of the whole trajectories was performed to verify the stability of the systems during the MDs (**Fig. S2A**), calculated on the backbone atoms of the protein. In order to select different conformations of the enzyme both with and without the mutation, we performed RMSD-based clustering of the trajectory according to the relaxed complex scheme (RCS) docking protocol.[13,14] After removing overall rotation and translations by RMS-fitting the Cα atoms positions of the trajectory, we applied the average linkage clustering algorithm, implemented in *cpptraj*,[15] identifying 10 significant conformations for each one (**Fig. S2B** and **S2C**).

Docking of peptidoglycan N-acetylglucosamine

The substrate selected in the present study was the natural monomer of the PDA: the peptidoglycan N-acetylglucosamine (GlcNAc). Molecular docking experiments of GlcNAc to PDA were carried out by using AutoDock[16] and 10 output poses were generated for each generated structures. The AutoDock4$_{Zn}$ parameters[17] were chosen to treat Zn^{2+} cation. Box centroid was determined by the metal ion containing active center and a box of 20 Å size for X, Y and Z was used for grid point generation. For both structures, the best docking pose was selected according to the following geometric criteria: a distance cut-off equal to 3 Å for Zn^{2+}-$O_{sub,}$ 5 Å for both O_{sub}-OH_{2Hyp} and N_{sub}-$N_{\varepsilon His225}$. The obtained distances of the selected docked poses are reported in **Fig. S3A** and **S3B**.[1]

Molecular Dynamics of enzyme-substrate complex

To verify the stability of previous best docked poses, further 20 ns of MDs of enzyme-substrate complex have been performed, applying the same protocol above mentioned. The substrate GlcNAc has been fully parametrized adopting standard procedure previously reported for non-standard 2Hyp residue. RMSD analysis was performed to verify the structural behavior of the systems during the simulation (Fig. S5).

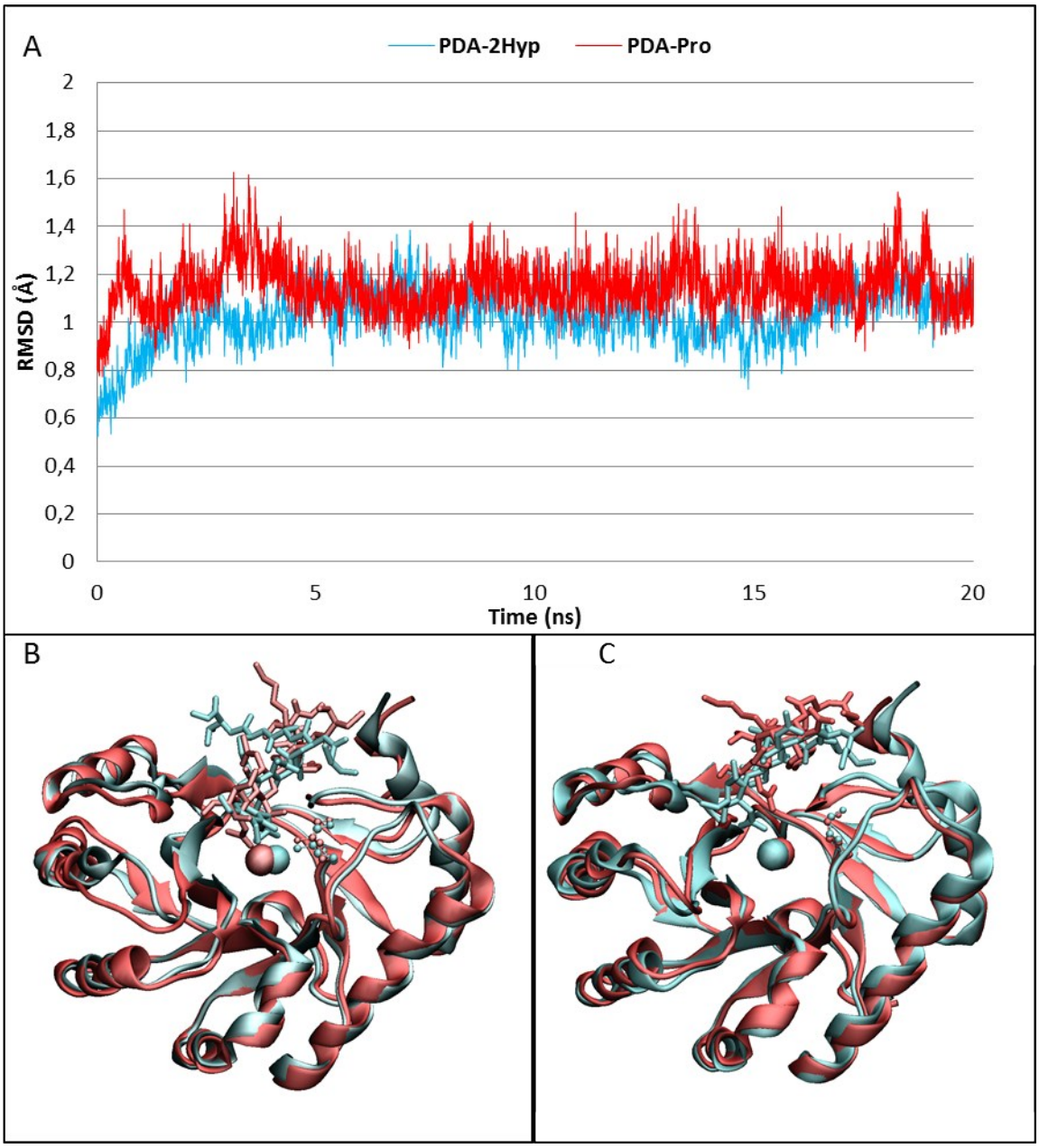

Fig. S5. (**A**) RMSD trends of PDA-Pro-GlcNAC (blue line) and PDA-2Hyp-GlcNAc (red line), calculated on backbone's atoms, expressed in Å. Superposition of docked pose and last frame of MDs of (B) PDA-2Hyp-GlcNAc and (C) PDA-Pro-GlcNAc.

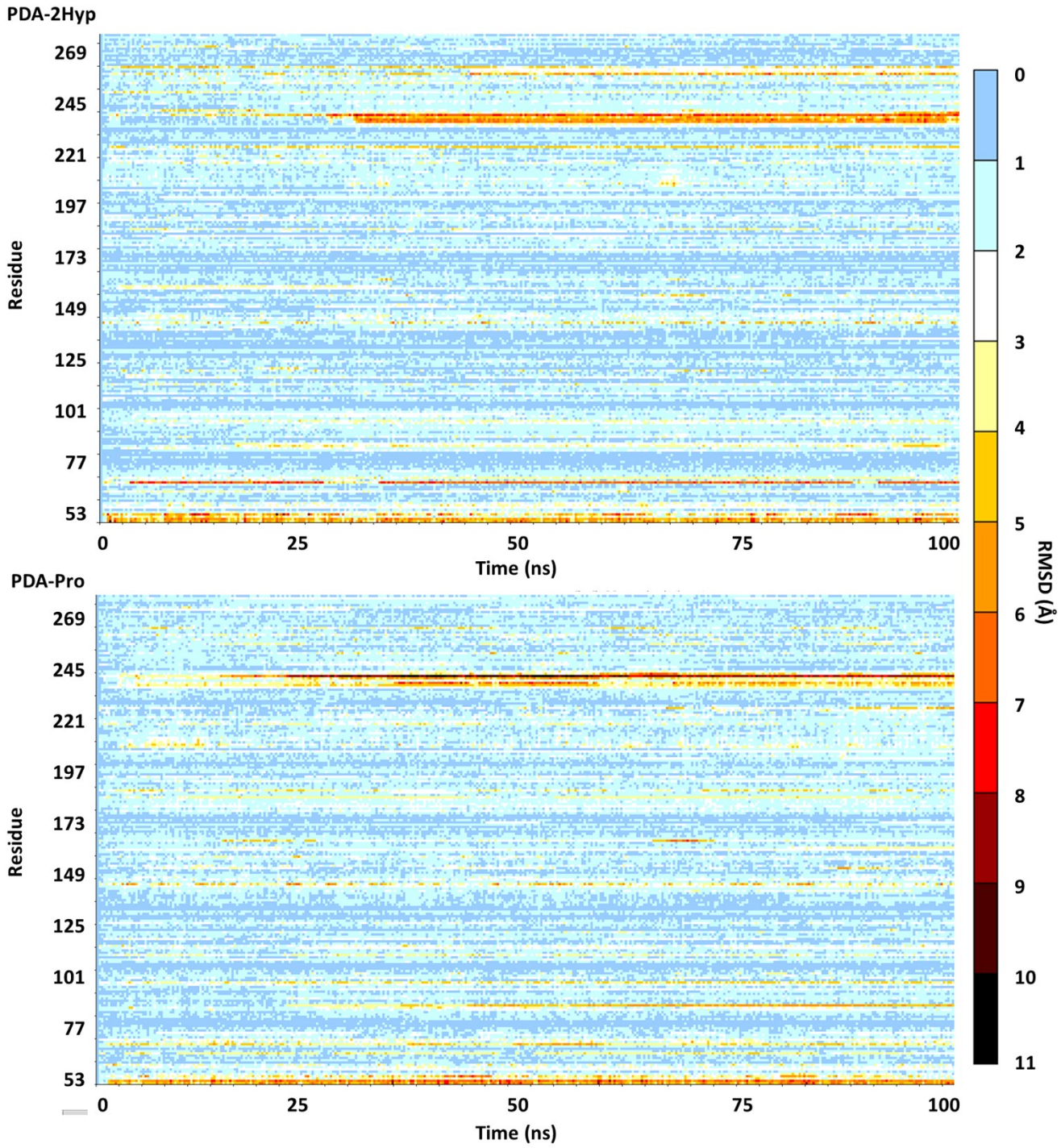

Fig. S6. RMSD heat maps for PDA-2Hyp e PDA-Pro systems along 100 ns of Molecular Dynamics.

Table S1. Extrapolated energy contributes for all stationary points isolated among mechanism. All values are in kcal mol^{-1}.

PDA-2Hyp	$\Delta E_{B3LYP-D3}$	Δ ZPE	-TΔS	ΔE_{tot}	
				No TΔS	TΔS
ES	0.0	0.0	0.0	0.0	0.0
TS1	20.6	1.1	-0.2	21.7	21.5
INT	18.0	0.5	0.2	18.5	18.7
TS2	26.2	-3.2	0.4	23.0	23.4
EP	-6.2	0.5	-0.2	-5.7	-5.5

PDA-Pro	$\Delta E_{B3LYP-D3}$	Δ ZPE	-TΔS	ΔE_{tot}	
				No TΔS	TΔS
ES	0.0	0.0	0.0	0.0	0.0
TS1	30.2	1.8	-0.1	32.0	31.9
INT	32.1	-1.0	0.4	31.1	31.5
TS2	32.2	-2.9	0.4	35.1	35.6
EP	-3.5	0.4	-0.2	-3.1	-3.3

Table S2. Calculated NBO values for selected atoms of ES complexes.

	$ES_{Clu\text{-}Hyp}$	$ES_{Clu\text{-}Pro}$
N_{Tyr172}	-0.605	-0.605
H_1	0.425	0.420
O_{Pro171}	-0.807	-
H_2	0.542	-
C_{sub}	0.702	0.693
O_{sub}	-0.722	-0.708

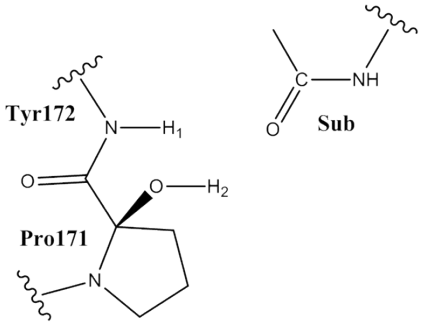

Table S3. The average values of the distance between Zn^{2+} and donor atoms of residues of the coordination sphere (His131, His135, Asp81, water molecule) in comparison with those available related to the another member of CE4 family[8].

	Distance in Å unit		Exp[8]
RESIDUE	**Zn^{2+}-PDA-2Hyp**	**Zn^{2+}-PDA-Pro**	**Zn^{2+}-PDA**
HIS131	2.799 ± 0.702	2.503 ± 0.540	2.153
HIS135	2.508 ± 0.310	2.286 ± 0.028	2.046
ASP81	2.340 ± 0.277	2.273 ± 0.092	2.022
WAT	2.304 ± 0.106	2.252 ± 0.102	2.104

The protonation state of titrable residues was evaluated at physiological pH according to the H++ server,[2] in comparison with the experimental suggestions.[1,3,4]

Table S4. Calculated pKa for ionizable residues of PDA retained in the QM model. Amino acids fully protonated (positively charged) or deprotonated (negatively charged) are highlighted in blue and red, respectively.

Residue	pKa
Asp80	2.675
Asp81	<0.000
His131	3.412
His135	3.339
Arg169	11.014
Asp199	3.924
His225	8.912

Table S5. Results for AutoDock Vina scoring using GlcNAc in presence of PDA-Pro and PDA-2Hyp structures.

Docking rank	Docking score (kcal/mol) PDA-Pro	Docking score (kcal/mol) PDA-2Hyp
1	-8.6	-11.9
2	-8.1	-10.2
3	-7.4	-10.0
4	-7.3	-9.9
5	-7.1	-9.8
6	-6.9	-9.1
7	-6.5	-9.0
8	-6.4	-8.8
9	-5.8	-8.7
10	-5.7	-8.7

List of parameters

2Hyp.prepc

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  3  DUMM  DU    M      -999.000    999.0      999.0         .00000
  4  N1    N     M        -1.001000   0.240000   0.056000  -0.123102
  5  C7    C     B      -0.742000   1.571000  -0.006000   0.682908
  6  O3    O     E       0.381000   1.999000   0.037000  -0.575176
  7  C8    CT    3      -1.932000   2.494000  -0.135000  -0.379667
  8  H12   HC    E       -1.563000   3.501000  -0.258000   0.107710
  9  H13   HC    E       -2.548000   2.228000  -0.987000   0.107710
 10  H14   HC    E       -2.552000   2.447000   0.754000   0.107710
 11  C1    CT    M        0.060000  -0.729000   0.188000   0.148813
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 13  H1    HO    E        1.145000  -1.407000   1.637000   0.433020
 14  C5    C     B       1.243000  -0.430000  -0.761000   0.714476
 15  O2    O     E        1.055000  -0.521000  -1.941000  -0.616448
 16  N2    N     B        2.505000  -0.292000  -0.250000  -0.722992
 17  H8    H     E        3.142000  -0.271000  -1.021000   0.384001
 18  C6    CT    3        2.921000   0.613000   0.821000   0.053156
 19  H9    H1    E        3.849000   0.239000   1.239000   0.052499
 20  H10   H1    E        3.079000   1.615000   0.441000   0.052499
 21  H11   H1    E        2.176000   0.664000   1.593000   0.052499
 22  C2    CT    M       -0.634000  -2.036000  -0.231000  -0.307912
 23  H2    HC    E       -0.126000  -2.901000   0.180000   0.125574
 24  H3    HC    E       -0.635000  -2.111000  -1.309000   0.125574
 25  C3    CT    M       -2.051000  -1.845000   0.304000   0.036362
 26  H4    HC    E       -2.077000  -2.015000   1.373000   0.036966
 27  H5    HC    E       -2.774000  -2.502000  -0.165000   0.036966
 28  C4    CT    M       -2.328000  -0.373000  -0.001000  -0.040982
 29  H6    H1    E       -3.001000   0.075000   0.718000   0.049921
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LOOP
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IMPROPER
  C7   C1   N1   C4
  C8   N1   C7   O3
  C1   N2   C5   O2
  C5   C6   N2   H8

DONE
STOP
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2Hyp.frcmod

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remark goes here
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CT 12.010       0.878
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OH 16.000       0.465
HO 1.008        0.135
H  1.008        0.161
H1 1.008        0.135

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CT-OH  320.00   1.410
CT-CT  310.00   1.526
OH-HO  553.00   0.960
N -H   434.00   1.010
CT-H1  340.00   1.090
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C -CT-HC 50.000 109.500

O -C -CT 80.000 120.400

HC-CT-HC 35.000 109.500

CT-N -CT 50.000 118.000

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CT-CT-HC 50.000 109.500

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OH-CT-C 80.000 120.400

OH-CT-CT 50.000 109.500

C -CT-CT 63.000 111.100

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H1-CT-H1 35.000 109.500

CT-CT-H1 50.000 109.500

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OH-CT-CT-HC 1 0.250 0.000 1.000

OH-CT-CT-CT 1 0.156 0.000 3.000

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HO-OH-CT-CT 1 0.250 0.000 1.000

C -CT-N -CT 1 0.000 0.000 2.000

C -CT-CT-HC 1 0.156 0.000 3.000

C -CT-CT-CT 1 0.156 0.000 3.000

O -C -CT-CT 1 0.000 0.000 2.000

O -C -N -H 1 2.500 180.000 -2.000

O -C -N -H 1 2.000 0.000 1.000

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H -N -CT-H1 1 0.000 0.000 2.000

CT-CT-CT-H1 1 0.156 0.000 3.000

HC-CT-CT-HC 1 0.150 0.000 3.000

HC-CT-CT-H1 1 0.156 0.000 3.000

IMPROPER

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CT-N -C -O 10.5 180.0 2.0 General improper torsional angle (2 general atom types)

C -CT-N -H 1.1 180.0 2.0

NONBON

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Glycan.prepc

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MOL XYZ 0

CHANGE OMIT DU BEG

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13	H3	h1	E	-1.748000	9.689000	0.588000	0.187596
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15	S1	sh	S	-1.432000	7.996000	2.268000	-0.368776
16	H5	hs	E	-2.528000	8.459000	2.854000	0.245837
17	C3	c	M	-0.938000	6.562000	-0.593000	0.487073
18	O1	o	E	-1.986000	6.120000	-0.990000	-0.547012
19	N2	ns	M	0.120000	5.777000	-0.315000	-0.408734
20	H6	hn	E	0.992000	6.162000	-0.028000	0.290967
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25	N3	ns	B	0.835000	2.606000	1.072000	-0.705547
26	H10	hn	E	-0.029000	2.161000	0.855000	0.274625
27	C8	c3	3	1.808000	1.826000	1.816000	0.297546
28	H11	h1	E	2.694000	2.435000	1.901000	0.055417
29	C9	c3	3	1.275000	1.484000	3.218000	-0.140355
30	H12	hc	E	1.033000	2.422000	3.706000	0.070412
31	H13	hc	E	0.348000	0.932000	3.111000	0.070412
32	C11	ca	S	2.253000	0.688000	4.056000	0.055763
33	C12	ca	B	2.083000	-0.671000	4.265000	-0.189731
34	H14	ha	E	1.236000	-1.175000	3.833000	0.167769
35	C14	ca	B	2.983000	-1.404000	5.026000	-0.309019
36	H16	ha	E	2.824000	-2.458000	5.181000	0.188281
37	C16	ca	B	4.077000	-0.774000	5.592000	0.427707
38	C15	ca	B	4.268000	0.588000	5.395000	-0.309019
39	C13	ca	S	3.362000	1.301000	4.639000	-0.189731
40	H15	ha	E	3.514000	2.360000	4.510000	0.167769
41	H17	ha	E	5.116000	1.067000	5.848000	0.188281
42	O6	oh	S	4.990000	-1.429000	6.341000	-0.560874
43	H18	ho	E	4.715000	-2.320000	6.508000	0.386961
44	C10	c	B	2.102000	0.556000	1.018000	0.642566
45	O5	o	E	1.198000	-0.180000	0.687000	-0.624653
46	N4	ns	B	3.383000	0.325000	0.708000	-0.609692
47	H19	hn	E	4.097000	0.967000	0.973000	0.338653
48	C17	c3	3	3.780000	-0.778000	-0.141000	-0.017583
49	H20	h1	E	3.126000	-1.611000	0.076000	0.098125
50	C18	c3	3	3.652000	-0.375000	-1.623000	-0.107309
51	H21	hc	E	2.735000	0.189000	-1.709000	0.072499
52	H22	hc	E	4.465000	0.302000	-1.866000	0.072499
53	C20	c3	3	3.611000	-1.539000	-2.615000	0.092141
54	H23	hc	E	4.548000	-2.084000	-2.628000	-0.018307
55	H24	hc	E	2.834000	-2.239000	-2.307000	-0.018307
56	C21	c3	3	3.280000	-1.018000	-4.019000	0.007585
57	H25	hc	E	2.420000	-0.357000	-3.959000	0.017353
58	H26	hc	E	4.105000	-0.420000	-4.394000	0.017353
59	C22	c3	3	2.972000	-2.139000	-5.005000	0.035196
60	H27	hx	E	3.862000	-2.655000	-5.336000	0.077778
61	H28	hx	E	2.283000	-2.861000	-4.593000	0.077778
62	N5	nz	3	2.286000	-1.572000	-6.217000	-0.370399
63	H29	hn	E	2.826000	-0.831000	-6.638000	0.320620
64	H30	hn	E	2.128000	-2.272000	-6.925000	0.320620
65	H31	hn	E	1.364000	-1.189000	-5.945000	0.320620
66	C19	c	B	5.227000	-1.116000	0.195000	0.577343
67	O7	o	E	6.023000	-0.237000	0.395000	-0.547964
68	N6	ns	B	5.538000	-2.425000	0.231000	-0.276792
69	H32	hn	E	4.857000	-3.102000	-0.031000	0.264077
70	C23	c3	3	6.897000	-2.887000	0.310000	-0.337401
71	H33	h1	E	7.488000	-2.122000	0.791000	0.163897
72	C24	c3	3	6.980000	-4.179000	1.129000	0.419948
73	H34	h1	E	8.002000	-4.536000	1.082000	-0.013231
74	C26	c3	3	6.581000	-3.982000	2.585000	-0.183610
75	H35	hc	E	5.567000	-3.611000	2.666000	0.046326
76	H36	hc	E	6.644000	-4.927000	3.118000	0.046326
77	H37	hc	E	7.247000	-3.281000	3.077000	0.046326
78	O8	oh	S	6.124000	-5.089000	0.471000	-0.716792
79	H38	ho	E	6.164000	-5.937000	0.891000	0.452173
80	C25	c	B	7.476000	-3.088000	-1.089000	0.896195
81	O9	o	E	6.877000	-2.925000	-2.104000	-0.596966
82	O10	os	S	8.742000	-3.443000	-1.030000	-0.404778
83	C28	c3	3	9.428000	-3.647000	-2.257000	0.021216
84	H42	h1	E	10.434000	-3.923000	-1.988000	0.076972
85	H43	h1	E	8.957000	-4.438000	-2.822000	0.076972
86	H44	h1	E	9.430000	-2.737000	-2.839000	0.076972
87	C5	c3	M	0.274000	3.925000	-1.924000	-0.441195
88	H8	hc	E	-0.420000	4.489000	-2.529000	0.162939
89	H9	hc	E	1.292000	4.148000	-2.214000	0.162939
90	C7	c	M	0.025000	2.452000	-2.106000	0.860251
91	O4	o	E	0.865000	1.615000	-2.050000	-0.574723
92	O3	os	M	-1.271000	2.189000	-2.326000	-0.503686
93	C29	c3	M	-1.934000	1.062000	-1.825000	0.364425

94 O11 os S -2.089000 1.274000 -0.456000 -0.404417
95 C31 c3 B -2.340000 0.158000 0.406000 0.171337
96 C34 c3 3 -3.092000 0.721000 1.596000 0.150747
97 H45 h1 E -3.210000 -0.038000 2.352000 0.054400
98 H46 h1 E -2.509000 1.529000 2.027000 0.054400
99 O12 oh S -4.375000 1.168000 1.245000 -0.646086
100 H47 ho E -4.305000 1.990000 0.778000 0.439443
101 H65 h1 E -1.395000 -0.244000 0.751000 0.092329
102 H61 h2 E -2.894000 1.109000 -2.313000 0.129034
103 C30 c3 M -1.275000 -0.306000 -2.018000 -0.043651
104 N7 ns B -0.641000 -0.577000 -3.296000 -0.587124
105 H48 hn E 0.300000 -0.882000 -3.197000 0.360560
106 C35 c B -0.974000 -0.387000 -4.578000 0.914757
107 O13 o E -0.170000 -0.696000 -5.452000 -0.763523
108 C36 c3 3 -2.282000 0.247000 -4.961000 -0.532446
109 H49 hc E -2.209000 1.318000 -4.806000 0.167530
110 H50 hc E -2.448000 0.062000 -6.012000 0.167530
111 H51 hc E -3.102000 -0.143000 -4.380000 0.167530
112 H62 h1 E -0.459000 -0.334000 -1.316000 0.196056
113 C32 c3 M -2.283000 -1.388000 -1.592000 0.095890
114 O14 oh S -3.108000 -1.682000 -2.679000 -0.697202
115 H52 ho E -3.774000 -2.291000 -2.375000 0.482030
116 H63 h1 E -1.724000 -2.269000 -1.292000 0.116481
117 C33 c3 M -3.103000 -0.915000 -0.371000 -0.031066
118 H64 h1 E -4.028000 -0.485000 -0.729000 0.111364
119 O15 os M -3.346000 -1.988000 0.505000 -0.415661
120 C37 c3 M -4.523000 -2.716000 0.439000 0.281689
121 O16 os S -4.790000 -3.051000 -0.896000 -0.300729
122 C39 c3 B -5.833000 -3.988000 -1.138000 -0.052282
123 C42 c3 3 -5.233000 -5.316000 -1.557000 0.211474
124 H53 h1 E -6.038000 -5.992000 -1.825000 0.038452
125 H54 h1 E -4.608000 -5.160000 -2.432000 0.038452
126 O17 oh S -4.474000 -5.818000 -0.489000 -0.712734
127 H55 ho E -4.162000 -6.689000 -0.692000 0.452266
128 H69 h1 E -6.406000 -3.595000 -1.968000 0.080637
129 H70 h2 E -4.316000 -3.610000 1.001000 0.132126
130 C38 c3 M -5.750000 -1.959000 0.961000 -0.013376
131 N8 ns B -5.622000 -1.413000 2.298000 -0.606986
132 H57 hn E -5.535000 -0.418000 2.312000 0.329572
133 C43 c B -5.071000 -1.958000 3.433000 0.776912
134 O20 o E -4.683000 -1.230000 4.304000 -0.622469
135 C44 c3 3 -4.974000 -3.459000 3.585000 -0.310019
136 H58 hc E -3.977000 -3.779000 3.298000 0.088586
137 H59 hc E -5.099000 -3.686000 4.634000 0.088586
138 H60 hc E -5.709000 -3.997000 3.009000 0.088586
139 H66 h1 E -5.831000 -1.085000 0.331000 0.110413
140 C40 c3 M -7.060000 -2.788000 0.730000 0.237934
141 O19 oh S -7.733000 -3.070000 1.920000 -0.622362
142 H56 ho E -7.814000 -2.275000 2.431000 0.416748
143 H67 h1 E -7.710000 -2.218000 0.072000 0.042508
144 C41 c3 M -6.791000 -4.130000 0.050000 0.177601
145 H68 h1 E -6.367000 -4.806000 0.784000 0.116168
146 O18 os M -7.951000 -4.683000 -0.494000 -0.419785
147 C45 c3 M -8.719000 -5.519000 0.335000 0.118148
148 H71 h1 E -9.161000 -4.971000 1.154000 0.037656
149 H72 h1 E -9.498000 -5.937000 -0.287000 0.037656
150 H73 h1 E -8.113000 -6.329000 0.733000 0.037656

LOOP
C13 C11
C33 C31
C41 C39

IMPROPER
C1 N2 C3 O1
C3 C4 N2 H6
C4 N3 C6 O2
C6 C8 N3 H10
C9 C12 C11 C13
C11 C14 C12 H14
C12 C16 C14 H16
C14 C15 C16 O6
C16 C13 C15 H17
C11 C15 C13 H15
C8 N4 C10 O5
C17 C10 N4 H19
C17 N6 C19 O7
C23 C19 N6 H32
C23 O9 C25 O10
C5 O4 C7 O3
C35 C30 N7 H48
C36 N7 C35 O13
C43 C38 N8 H57
C44 N8 C43 O20

DONE
STOP

Glycan.frcmod

remark goes here
MASS
n7 14.010 0.530
hn 1.008 0.161
c3 12.010 0.878
h1 1.008 0.135
sh 32.060 2.900
hs 1.008 0.135
c 12.010 0.616
o 16.000 0.434
ns 14.010 0.530

hc 1.008 0.135
ca 12.010 0.360
ha 1.008 0.135
oh 16.000 0.465
ho 1.008 0.135
hx 1.008 0.135
nz 14.010 0.530
os 16.000 0.465
h2 1.008 0.135

BOND
n7-hn 511.28 1.019 same as hn-n3
n7-c3 261.19 1.465 same as c3-n3
c3-h1 375.92 1.097
c3-c3 232.52 1.538
c3-c 243.22 1.524
c3-sh 180.78 1.843
sh-hs 294.59 1.347
c -o 652.57 1.218
c -ns 356.21 1.379 same as c -n
ns-hn 527.31 1.013 same as hn-n
ns-c3 263.77 1.462 same as c3-n
c3-hc 375.92 1.097
c3-ca 250.32 1.516
ca-ca 378.57 1.398
ca-ha 395.72 1.086
ca-oh 365.55 1.364
oh-ho 563.51 0.973
c3-hx 386.49 1.091
c3-nz 222.58 1.511 same as c3-n4
nz-hn 482.87 1.030 same as hn-n4
c3-oh 293.40 1.423
c -os 372.94 1.358
os-c3 284.76 1.432
c3-h2 377.33 1.096

ANGLE
n7-c3-h1 61.163 109.880 same as h1-c3-n3
n7-c3-c3 83.305 111.040 same as c3-c3-n3
n7-c3-c 83.673 111.140 same as c -c3-n3
hn-n7-c3 47.782 109.290 same as c3-n3-hn
c3-n7-c3 65.697 112.350 same as c3-n3-c3
h1-c3-h1 38.802 108.460
c3-c3-h1 46.868 109.560
c3-c3-sh 62.313 113.130
c3-c -o 84.552 123.200
c3-c -ns 84.266 115.180 same as c3-c -n
h1-c3-c 47.531 108.220
c3-c3-c 65.307 111.040
c3-sh-hs 51.361 96.400
h1-c3-sh 42.420 108.420
c -ns-hn 48.691 117.550 same as c -n -hn
c -ns-c3 65.252 120.690 same as c -n -c3
o -c -ns 113.811 123.050 same as n -c -o
ns-c3-h1 61.544 108.880 same as h1-c3-n
ns-c3-c 84.540 109.060 same as c -c3-n
ns-c3-c3 83.161 111.610 same as c3-c3-n
hn-ns-c3 46.147 117.680 same as c3-n -hn
c3-c3-hc 46.816 109.800
c3-c3-ca 65.183 112.070
c3-ca-ca 65.583 120.770
hc-c3-hc 38.960 107.580
hc-c3-ca 47.281 110.470
ca-ca-ha 48.680 119.880
ca-ca-ca 68.767 120.020
ca-ca-oh 87.211 119.900
ca-oh-ho 50.712 108.580
c3-c3-c3 64.888 111.510
c3-c3-hx 46.677 110.560
c3-c3-nz 80.976 114.210 same as c3-c3-n4
c3-nz-hn 46.193 110.110 same as c3-n4-hn
hx-c3-hx 38.782 109.750
hx-c3-nz 60.076 108.010 same as hx-c3-n4
hn-nz-hn 40.020 108.300 same as hn-n4-hn
c3-c3-oh 84.642 110.190
c3-c -os 86.419 110.720
c3-oh-ho 49.027 107.260
h1-c3-oh 62.540 110.260
c -os-c3 66.906 115.980
o -c -os 114.822 123.250
os-c3-h1 62.377 109.780
hc-c3-c 47.411 108.770
os-c3-os 110.893 108.290
os-c3-h2 62.442 109.580
os-c3-c3 85.306 107.970
c3-os-c3 66.293 112.480
h2-c3-c3 46.730 110.220

DIHE
n7-c3-c3-h1 1 0.156 0.000 3.000
n7-c3-c3-sh 1 0.156 0.000 3.000
n7-c3-c -o 1 0.000 180.000 2.000
n7-c3-c -ns 1 0.000 180.000 2.000
hn-n7-c3-h1 1 0.300 0.000 3.000 same as X -c3-n3-X
hn-n7-c3-c3 1 0.217 0.000 3.000 same as hn-n3-c3-c3
hn-n7-c3-c 1 0.300 0.000 3.000 same as X -c3-n3-X
c3-n7-c3-h1 1 0.225 0.000 3.000 same as h1-c3-n3-c3
c3-n7-c3-c3 1 0.020 180.000 -3.000
c3-n7-c3-c3 1 0.050 0.000 2.000
c3-n7-c3-c 1 0.300 0.000 3.000 same as X -c3-n3-X
c3-c3-sh-hs 1 0.250 0.000 3.000
c3-c -ns-hn 1 2.500 180.000 2.000 same as X -c -n -X

c3-c -ns-c3 1 0.260 180.000 -2.000 same as c3-n -c -c3
c3-c -ns-c3 1 0.500 0.000 1.000 same as c3-n -c -c3
h1-c3-c3-h1 1 0.156 0.000 3.000
h1-c3-c3-sh 1 0.156 0.000 3.000
h1-c3-c -o 1 0.800 0.000 -1.000
h1-c3-c -o 1 0.080 180.000 3.000
h1-c3-c -ns 1 0.000 180.000 2.000
c3-c3-c -o 1 0.270 180.000 2.000
c3-c3-c -ns 1 0.000 180.000 2.000
h1-c3-c3-c 1 0.156 0.000 3.000
h1-c3-sh-hs 1 0.143 0.000 3.000
sh-c3-c3-c 1 0.156 0.000 3.000
c -ns-c3-h1 1 0.000 180.000 2.000 same as h1-c3-n -c
c -ns-c3-c 1 0.390 180.000 -2.000 same as c -c3-n -c
c -ns-c3-c 1 0.640 0.000 1.000 same as c -c3-n -c
c -ns-c3-c3 1 0.100 180.000 -4.000 same as c -n -c3-c3
c -ns-c3-c3 1 0.170 0.000 -3.000 same as c -n -c3-c3
c -ns-c3-c3 1 1.020 180.000 1.000 same as c -n -c3-c3
o -c -ns-hn 1 2.500 180.000 -2.000 same as hn-n -c -o
o -c -ns-hn 1 2.000 0.000 1.000 same as hn-n -c -o
o -c -ns-c3 1 2.500 180.000 2.000 same as X -c -n -X
ns-c3-c -o 1 0.000 180.000 2.000
ns-c3-c -ns 1 0.000 180.000 2.000
ns-c3-c3-hc 1 0.156 0.000 3.000
ns-c3-c3-c 1 0.156 0.000 3.000
hn-ns-c3-h1 1 0.000 0.000 2.000 same as X -c3-n -X
hn-ns-c3-c 1 0.000 0.000 2.000 same as X -c3-n -X
hn-ns-c3-c3 1 0.000 0.000 2.000 same as X -c3-n -X
c3-c3-c -os 1 0.000 180.000 2.000
h1-c3-c3-hc 1 0.156 0.000 3.000
c -c3-c3-hc 1 0.156 0.000 3.000
c -c3-c3-c 1 0.156 0.000 3.000
ns-c3-c3-ca 1 0.156 0.000 3.000
c3-c3-ca-ca 1 0.245 180.000 2.000
h1-c3-c3-ca 1 0.156 0.000 3.000
c3-ca-ca-ha 1 3.625 180.000 2.000
c3-ca-ca-ca 1 3.625 180.000 2.000
hc-c3-ca-ca 1 0.000 180.000 2.000
ca-c3-c3-c 1 0.100 0.000 3.000
ca-ca-ca-ha 1 3.625 180.000 2.000
ca-ca-ca-ca 1 3.625 180.000 2.000
ca-ca-ca-oh 1 3.625 180.000 2.000
ha-ca-ca-ha 1 3.625 180.000 2.000
ca-ca-oh-ho 1 0.835 180.000 2.000
ha-ca-ca-oh 1 3.625 180.000 2.000
ns-c3-c3-c3 1 0.156 0.000 3.000
c3-c3-c3-hc 1 0.080 0.000 3.000
c3-c3-c3-c3 1 0.130 0.000 -3.000
c3-c3-c3-c3 1 0.290 180.000 -2.000
c3-c3-c3-c3 1 0.110 0.000 1.000
h1-c3-c3-c3 1 0.156 0.000 3.000
hc-c3-c3-hc 1 0.120 0.000 3.000
c3-c3-c3-c 1 0.100 0.000 3.000
c3-c3-c3-hx 1 0.156 0.000 3.000
c3-c3-c3-nz 1 0.156 0.000 3.000
c3-c3-nz-hn 1 0.156 0.000 3.000 same as X -c3-n4-X
hc-c3-c3-hx 1 0.156 0.000 3.000
hc-c3-c3-nz 1 0.156 0.000 3.000
hx-c3-nz-hn 1 0.109 0.000 3.000 same as hn-n4-c3-hx
ns-c3-c3-h1 1 0.156 0.000 3.000
ns-c3-c3-oh 1 0.156 0.000 3.000
ns-c3-c -os 1 0.000 180.000 2.000
c3-c3-oh-ho 1 0.000 0.000 3.000
c3-c -os-c3 1 1.580 180.000 -1.000
c3-c -os-c3 1 3.180 180.000 -2.000
c3-c -os-c3 1 0.730 0.000 3.000
h1-c3-c3-oh 1 0.000 0.000 -3.000
h1-c3-c3-oh 1 0.250 0.000 1.000
h1-c3-c -os 1 0.000 180.000 2.000
h1-c3-oh-ho 1 0.113 0.000 3.000
hc-c3-c3-oh 1 0.180 0.000 -3.000
hc-c3-c3-oh 1 0.510 0.000 1.000
oh-c3-c3-c 1 0.210 0.000 3.000
c -os-c3-h1 1 0.383 0.000 3.000
o -c -os-c3 1 2.700 180.000 -2.000
o -c -os-c3 1 1.400 180.000 1.000
hc-c3-c -o 1 0.830 0.000 -1.000
hc-c3-c -o 1 0.040 180.000 3.000
hc-c3-c -os 1 0.000 180.000 2.000
c -os-c3-os 1 0.383 0.000 3.000
c -os-c3-h2 1 0.383 0.000 3.000
c -os-c3-c3 1 0.383 0.000 -3.000
c -os-c3-c3 1 0.800 180.000 1.000
os-c3-os-c3 1 0.000 180.000 -3.000
os-c3-os-c3 1 1.240 0.000 -2.000
os-c3-os-c3 1 0.970 180.000 1.000
os-c3-c3-ns 1 0.156 0.000 3.000
os-c3-c3-h1 1 0.000 0.000 -3.000
os-c3-c3-h1 1 0.250 0.000 1.000
os-c3-c3-c3 1 0.156 0.000 3.000
c3-os-c3-c3 1 0.240 0.000 -3.000
c3-os-c3-c3 1 0.160 0.000 2.000
c3-os-c3-h1 1 0.337 0.000 3.000
c3-c3-c3-oh 1 0.210 0.000 3.000
os-c3-c3-oh 1 1.010 0.000 -3.000
os-c3-c3-oh 1 0.000 0.000 -2.000
os-c3-c3-oh 1 0.020 180.000 1.000
os-c3-c3-os 1 0.000 0.000 -3.000
os-c3-c3-os 1 0.000 180.000 -2.000
os-c3-c3-os 1 0.170 180.000 1.000
c3-os-c3-h2 1 0.383 0.000 3.000
h2-c3-c3-ns 1 0.156 0.000 3.000

h2-c3-c3-h1 1 0.156 0.000 3.000

h2-c3-c3-c3 1 0.156 0.000 3.000

ns-c -c3-hc 1 0.000 180.000 2.000

IMPROPER

c3-ns-c -o 10.5 180.0 2.0 General improper torsional angle (2 general atom types)

c -c3-ns-hn 1.1 180.0 2.0 Using default value

c3-ca-ca-ca 1.1 180.0 2.0

ca-ca-ca-ha 1.1 180.0 2.0 General improper torsional angle (2 general atom types)

ca-ca-ca-oh 1.1 180.0 2.0 Using default value

c3-o -c -os 10.5 180.0 2.0 General improper torsional angle (2 general atom types)

NONBON

n7 1.9686 0.0522

hn 0.6210 0.0100

c3 1.9069 0.1078

h1 1.3593 0.0208

sh 1.9825 0.2824

hs 0.6112 0.0124

c 1.8606 0.0988

o 1.7107 0.1463

ns 1.8352 0.1174

hc 1.4593 0.0208

ca 1.8606 0.0988

ha 1.4735 0.0161

oh 1.8200 0.0930

ho 0.3019 0.0047

hx 1.0593 0.0208

nz 1.5528 1.1450

os 1.7713 0.0726

h2 1.2593 0.0208

References

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Cartesian Coordinates

ES PDA-2Hyp

C	-0.278	3.029	1.918	H	-1.954	-6.034	1.556	H	-4.053	-4.043	-0.308
H	0.090	4.053	2.045	C	-1.016	-4.283	0.849	C	-5.429	-2.493	0.479
C	0.426	2.398	0.744	H	-0.739	-4.561	-0.157	H	-5.517	-2.726	1.543
O	0.199	2.719	-0.417	N	-0.788	-3.097	1.392	H	-6.268	-2.932	-0.064
O	1.314	1.472	1.078	C	-1.314	-3.147	2.675	C	-5.354	-0.987	0.222
C	3.385	-2.008	3.510	H	-1.215	-2.313	3.351	H	-4.758	-0.508	0.999
H	4.119	-2.802	3.361	C	-3.412	4.464	-1.759	H	-6.322	-0.486	0.166
C	2.398	-1.952	2.358	H	-2.533	4.891	-1.263	C	9.723	3.642	0.691
O	1.280	-1.365	2.586	H	-3.820	3.645	-1.161	H	10.183	2.756	1.140
O	2.732	-2.423	1.236	N	-3.090	3.973	-3.099	C	8.418	3.260	0.018
C	-4.149	1.756	3.005	H	-3.473	4.449	-3.901	O	7.365	3.835	0.611
H	-4.093	2.847	2.924	C	-2.285	2.920	-3.311	O	8.335	2.495	-0.927
H	-3.980	1.487	4.049	N	-1.547	2.417	-2.344	C	4.655	2.202	2.221
C	-3.136	1.089	2.137	H	-1.230	2.940	-1.527	H	3.935	3.020	2.341
N	-3.131	1.220	0.752	H	-1.069	1.500	-2.468	H	5.644	2.592	2.481
H	-3.921	1.506	0.167	N	-2.231	2.359	-4.545	C	4.657	1.697	0.818
C	-2.099	0.493	0.264	H	-3.017	2.418	-5.173	N	5.195	2.464	-0.200
H	-1.875	0.377	-0.781	H	-1.561	1.617	-4.695	H	5.971	3.050	0.032
N	-1.414	-0.064	1.250	N	-4.692	-0.912	-1.103	C	5.083	1.751	-1.307
C	-2.052	0.300	2.426	C	-3.989	-2.154	-1.432	H	5.457	2.037	-2.279
H	-1.660	0.017	3.391	O	-2.630	-1.883	-1.799	N	4.458	0.574	-1.061
C	-2.566	-4.952	4.098	H	-2.008	-2.488	-1.359	H	4.364	-0.243	-1.657
H	-2.607	-4.210	4.899	C	-4.717	-2.936	-2.551	C	4.199	0.513	0.296
H	-2.035	-5.831	4.483	O	-5.937	-3.051	-2.516	H	3.734	-0.354	0.737
C	-1.880	-4.373	2.907	C	-4.106	-2.968	-0.120	Zn	0.225	-1.292	0.881
N	-1.679	-5.077	1.727	H	-3.273	-2.681	0.530	C	4.223	-4.947	-0.050

O	5.511	-5.484	-0.342	O	5.766	-6.378	2.296	C	11.761	3.054	-3.064
C	6.413	-4.564	-1.003	H	1.621	-7.631	1.935	H	12.706	3.542	-2.946
C	6.920	-3.501	-0.007	O	1.816	-7.410	4.063	H	11.302	3.382	-3.973
H	6.116	-2.798	0.288	C	0.810	-5.615	2.618	H	11.129	3.298	-2.236
H	7.702	-2.892	-0.483	H	4.119	-6.346	4.392	N	10.698	1.596	-1.000
O	7.487	-4.129	1.123	C	3.107	-8.234	4.226	H	9.750	1.347	-0.805
H	6.904	-4.883	1.330	N	5.493	-7.886	4.705	C	10.682	4.267	-0.339
H	7.280	-5.194	-1.253	H	5.823	-6.135	1.369	H	11.058	5.194	0.040
H	4.267	-4.115	0.668	H	0.753	-5.223	1.624	C	11.243	2.667	-0.410
C	3.506	-4.504	-1.351	H	-0.166	-5.913	2.939	O	12.483	2.427	0.260
N	2.157	-3.995	-1.079	O	1.315	-4.608	3.499	N	9.920	4.696	-1.521
H	2.044	-3.454	-0.214	H	3.144	-8.648	5.212	H	9.177	5.302	-1.236
C	1.132	-3.995	-1.964	H	3.118	-9.025	3.505	H	10.525	5.184	-2.149
O	0.034	-3.451	-1.712	H	5.897	-7.188	5.296	C	-0.060	2.241	3.223
C	1.319	-4.752	-3.265	C	6.594	-8.915	4.142	H	0.974	2.282	3.496
H	1.417	-5.829	-3.073	H	0.696	-3.876	3.538	H	-0.652	2.673	4.003
H	2.214	-4.438	-3.811	C	7.925	-9.243	4.845	H	-0.351	1.222	3.077
H	0.440	-4.580	-3.886	O	6.248	-9.597	3.143	C	2.646	-2.198	4.848
H	3.454	-5.393	-1.989	H	8.741	-8.983	4.203	H	3.354	-2.432	5.616
C	4.364	-3.472	-2.109	H	7.995	-8.686	5.755	H	2.130	-1.296	5.102
O	4.358	-2.172	-1.529	H	7.964	-10.290	5.064	H	1.942	-2.999	4.756
H	4.324	-2.188	-0.534	C	-4.702	-5.791	-4.006	C	-4.482	5.564	-1.893
H	3.957	-3.324	-3.112	H	-5.686	-5.821	-3.588	H	-4.730	5.940	-0.923
C	5.802	-4.021	-2.301	H	-4.636	-6.489	-4.814	H	-4.101	6.360	-2.498
H	6.433	-3.199	-2.685	C	-3.673	-6.163	-2.922	C	-5.598	5.402	-2.584
O	5.655	-5.052	-3.276	C	-4.104	-6.662	-1.692	H	-6.412	6.031	-2.286
C	6.847	-5.392	-3.976	C	-2.310	-6.003	-3.170	H	-5.466	5.468	-3.644
H	6.574	-6.156	-4.712	C	-3.173	-7.000	-0.711	C	-5.973	-0.370	-4.048
H	7.622	-5.809	-3.317	H	-5.179	-6.788	-1.497	H	-4.971	-0.265	-4.410
H	7.269	-4.518	-4.499	C	-1.378	-6.340	-2.188	H	-6.192	-1.407	-3.901
O	-0.524	-0.068	-2.715	H	-1.969	-5.610	-4.139	C	-6.952	0.355	-5.027
H	0.157	-0.288	-2.003	C	-1.809	-6.838	-0.959	H	-6.589	0.312	-6.032
H	-1.216	-0.737	-2.620	H	-3.513	-7.393	0.258	C	-6.920	1.931	-4.446
O	1.100	-0.582	-0.670	H	-0.303	-6.214	-2.384	H	-7.914	2.328	-4.413
H	1.348	0.767	0.370	O	-0.854	-7.184	0.048	N	-6.315	1.881	-2.991
H	1.752	-1.255	-0.911	H	-0.581	-8.097	-0.070	C	-6.310	2.746	-1.743
H	9.530	4.351	1.502	C	7.548	0.339	-4.606	O	-6.119	2.252	-0.464
H	-3.594	-5.256	3.867	C	8.599	-0.550	-4.162	C	-6.677	4.121	-1.959
H	-5.169	1.456	2.738	C	8.685	-1.834	-4.659	H	-7.261	4.274	-1.062
H	3.918	-1.048	3.557	C	7.731	-2.252	-5.602	N	-7.419	4.164	-3.227
H	-1.345	3.099	1.696	C	6.720	-1.398	-6.029	H	-8.398	4.070	-3.043
H	4.386	1.410	2.924	C	6.619	-0.088	-5.533	H	-7.249	5.038	-3.683
C	-4.851	0.205	-1.884	C	9.403	0.189	-3.197	H	-7.937	-0.057	-4.956
C	-6.116	0.380	-2.711	H	9.477	-2.521	-4.332	H	-6.306	2.540	-5.076
H	-6.997	-0.001	-2.194	H	7.789	-3.274	-6.006	C	1.926	7.246	-2.917
O	-4.024	1.128	-1.819	H	5.985	-1.749	-6.769	H	2.802	7.754	-2.571
N	-3.903	-3.527	-3.456	H	5.814	0.575	-5.881	H	1.463	6.737	-2.098
H	-2.918	-3.307	-3.404	H	7.096	2.476	-4.024	C	2.320	6.223	-3.999
C	-4.408	-4.372	-4.527	H	9.208	2.243	-2.372	C	2.091	4.787	-3.908
H	-3.688	-4.440	-5.350	N	7.732	1.602	-3.904	C	2.952	6.490	-5.229
H	-5.330	-3.926	-4.901	C	8.838	1.469	-3.043	C	2.605	4.198	-5.124
O	3.539	-6.561	0.450	C	10.635	-0.375	-2.466	C	1.516	3.993	-2.936
C	3.258	-6.652	1.849	H	10.316	-0.986	-1.648	H	3.250	7.477	-5.581
C	4.632	-7.224	2.500	H	11.215	-0.964	-3.146	C	2.528	2.835	-5.326
H	3.048	-5.676	2.235	C	11.494	0.787	-1.934	C	1.445	2.608	-3.158
C	1.751	-6.833	2.637	H	12.350	0.395	-1.426	H	1.120	4.426	-2.006
C	4.329	-7.322	4.006	C	11.954	1.667	-3.111	H	3.598	5.163	-6.911
H	4.841	-8.200	2.114	O	12.520	1.119	-4.147	C	1.940	2.041	-4.327

H	2.915	2.372	-6.245	H	7.310	6.792	-1.375	H	4.092	3.552	-1.022
H	0.990	1.965	-2.390	H	6.627	8.352	-0.983	H	3.634	4.916	-0.031
H	1.873	0.954	-4.477	H	6.566	7.759	-2.626	H	6.038	5.009	-0.531
N	3.139	5.286	-5.933	C	5.163	6.813	-1.302	C	5.854	4.813	-2.662
C	0.940	8.268	-3.511	H	4.803	7.139	-0.349	H	5.348	5.351	-3.437
H	0.516	8.854	-2.723	H	4.461	7.086	-2.062	H	6.906	4.997	-2.728
H	1.458	8.909	-4.194	C	5.336	5.282	-1.290	H	5.667	3.766	-2.775
H	0.159	7.751	-4.029	C	3.979	4.615	-0.998				
C	6.520	7.480	-1.594	H	3.267	4.915	-1.739				

TS1 PDA-2Hyp

C	-0.278	2.883	1.857	C	-4.566	-2.976	-2.891	H	0.382	-2.020	-3.260
H	0.123	3.819	2.261	O	-5.789	-3.006	-2.789	H	2.689	-4.913	-1.580
C	0.683	2.359	0.833	C	-3.819	-3.192	-0.538	C	4.193	-3.733	-2.554
O	0.516	2.382	-0.381	H	-2.913	-3.045	0.055	O	5.015	-2.581	-2.367
O	1.767	1.880	1.424	H	-3.883	-4.248	-0.810	H	5.730	-2.787	-1.751
C	2.595	-2.193	4.110	C	-5.043	-2.661	0.206	H	3.562	-3.490	-3.407
H	2.875	-3.164	4.521	H	-5.045	-2.953	1.260	C	5.003	-4.975	-2.977
C	1.904	-2.361	2.770	H	-5.961	-3.004	-0.274	H	5.722	-4.658	-3.749
O	1.192	-1.350	2.381	C	-4.870	-1.154	0.030	O	4.037	-5.864	-3.530
O	2.078	-3.397	2.099	H	-4.138	-0.791	0.749	C	4.557	-6.814	-4.445
C	-3.891	1.698	3.244	H	-5.785	-0.569	0.132	H	3.711	-7.401	-4.806
H	-3.733	2.779	3.335	C	9.722	3.721	0.758	H	5.278	-7.499	-3.977
H	-3.729	1.252	4.227	H	10.376	3.192	1.450	H	5.047	-6.323	-5.299
C	-2.963	1.090	2.247	H	9.224	4.551	1.270	O	-0.704	0.070	-2.741
N	-2.997	1.410	0.894	C	8.687	2.765	0.201	H	0.050	-0.128	-2.149
H	-3.791	1.793	0.383	O	7.438	3.155	0.500	H	-1.327	-0.673	-2.610
C	-2.040	0.684	0.262	O	8.945	1.764	-0.440	O	1.133	-0.974	-0.866
H	-1.850	0.722	-0.798	C	4.666	2.132	2.178	H	2.427	1.530	0.786
N	-1.370	-0.055	1.129	H	4.261	3.097	1.857	H	1.977	-0.496	-0.792
C	-1.933	0.193	2.374	H	5.690	2.312	2.518	H	-3.666	-5.860	3.990
H	-1.522	-0.261	3.263	C	4.670	1.143	1.047	H	-4.938	1.537	2.967
C	-3.006	-5.075	4.373	N	5.511	1.284	-0.040	H	3.510	-1.608	3.959
H	-3.631	-4.303	4.829	H	6.242	1.958	0.064	H	-1.250	3.077	1.408
H	-2.388	-5.513	5.164	C	5.277	0.251	-0.835	H	4.064	1.769	3.013
C	-2.171	-4.475	3.291	H	5.774	0.044	-1.771	C	-4.710	0.059	-2.114
N	-1.280	-5.212	2.523	N	4.311	-0.555	-0.324	C	-6.170	0.394	-2.411
H	-1.080	-6.195	2.631	H	3.945	-1.435	-0.713	H	-6.681	0.540	-1.455
C	-0.678	-4.384	1.636	C	3.914	-0.001	0.883	O	-3.827	0.852	-2.504
H	0.074	-4.671	0.922	H	3.165	-0.462	1.510	N	-3.851	-3.544	-3.886
N	-1.135	-3.149	1.780	Zn	0.022	-1.599	0.782	H	-2.850	-3.418	-3.858
C	-2.062	-3.195	2.812	C	4.312	-4.577	-0.215	C	-4.465	-4.321	-4.953
H	-2.600	-2.318	3.131	O	4.965	-5.766	-0.635	H	-3.766	-4.468	-5.782
C	-3.402	4.408	-1.791	C	5.768	-5.640	-1.819	H	-5.335	-3.771	-5.311
H	-2.669	5.153	-2.110	C	7.121	-5.012	-1.461	O	3.717	-5.639	0.536
H	-3.202	4.141	-0.745	H	7.014	-3.952	-1.162	C	3.927	-6.015	2.132
N	-3.348	3.255	-2.676	H	7.777	-5.022	-2.338	C	5.055	-6.202	3.287
H	-4.157	2.633	-2.655	O	7.750	-5.753	-0.442	C	2.537	-7.009	2.069
C	-2.200	2.719	-3.113	H	7.061	-5.957	0.208	C	4.311	-6.905	4.437
N	-1.018	3.085	-2.599	H	5.982	-6.676	-2.097	H	5.842	-6.834	2.932
H	-0.902	3.234	-1.598	H	4.525	-3.765	0.499	O	5.610	-4.971	3.760
H	-0.199	2.651	-3.001	C	3.337	-4.068	-1.310	H	3.085	-7.511	1.299
N	-2.220	1.845	-4.129	N	2.567	-2.913	-0.788	O	2.349	-7.957	3.268
H	-3.071	1.710	-4.651	H	2.372	-3.085	0.208	C	1.202	-6.311	1.752
H	-1.522	1.102	-4.088	C	1.281	-2.535	-1.383	H	3.524	-6.272	4.792
N	-4.366	-1.031	-1.363	O	0.171	-3.039	-0.844	C	3.714	-8.229	3.927
C	-3.726	-2.295	-1.793	C	1.309	-2.463	-2.900	N	5.251	-7.181	5.533
O	-2.374	-2.091	-2.218	H	1.378	-3.481	-3.292	H	5.875	-4.430	3.013
H	-1.703	-2.568	-1.671	H	2.154	-1.879	-3.270	H	1.330	-5.663	0.910

H	0.460	-7.048	1.524	H	11.333	-0.700	-3.244	H	-8.368	3.978	-3.141
O	0.783	-5.545	2.884	C	11.569	1.005	-1.960	H	-7.231	4.991	-3.730
H	3.585	-8.902	4.749	H	12.427	0.609	-1.460	H	-7.814	-0.060	-5.212
H	4.376	-8.666	3.209	C	12.024	1.940	-3.097	H	-6.229	2.568	-5.212
H	5.010	-6.622	6.327	O	12.610	1.444	-4.148	C	1.895	7.328	-2.783
C	6.833	-7.459	5.447	C	11.805	3.320	-2.996	H	2.759	7.838	-2.408
H	-0.080	-5.163	2.711	H	12.740	3.820	-2.849	H	1.434	6.779	-1.989
C	7.788	-7.470	6.655	H	11.349	3.676	-3.896	C	2.318	6.357	-3.901
O	7.261	-7.845	4.328	H	11.161	3.520	-2.166	C	2.114	4.914	-3.869
H	8.539	-6.719	6.522	N	10.749	1.762	-1.003	C	2.957	6.684	-5.112
H	7.234	-7.266	7.548	H	9.804	1.489	-0.828	C	2.650	4.384	-5.103
H	8.252	-8.429	6.734	C	10.679	4.404	-0.236	C	1.544	4.072	-2.936
H	3.540	-5.086	2.496	H	11.034	5.321	0.183	H	3.240	7.689	-5.422
C	-4.914	-5.700	-4.434	C	11.269	2.818	-0.365	C	2.600	3.029	-5.360
H	-5.893	-5.621	-4.011	O	12.507	2.573	0.307	C	1.501	2.696	-3.213
H	-4.930	-6.398	-5.245	N	9.921	4.866	-1.408	H	1.132	4.460	-1.993
C	-3.928	-6.188	-3.356	H	9.164	5.447	-1.107	H	3.643	5.437	-6.839
C	-4.409	-6.674	-2.140	H	10.523	5.390	-2.010	C	2.017	2.185	-4.399
C	-2.554	-6.146	-3.597	C	-0.058	2.047	3.132	H	3.004	2.610	-6.292
C	-3.516	-7.118	-1.164	H	0.972	2.095	3.417	H	1.050	2.015	-2.476
H	-5.492	-6.707	-1.951	H	-0.665	2.437	3.923	H	1.971	1.104	-4.593
C	-1.661	-6.590	-2.620	H	-0.329	1.030	2.943	N	3.172	5.513	-5.862
H	-2.175	-5.765	-4.556	C	2.712	-2.405	4.606	C	0.897	8.356	-3.346
C	-2.142	-7.075	-1.404	H	3.417	-2.657	5.372	H	0.455	8.902	-2.539
H	-3.895	-7.500	-0.206	H	2.177	-1.523	4.891	H	1.410	9.033	-3.997
H	-0.578	-6.557	-2.810	H	2.024	-3.214	4.475	H	0.130	7.846	-3.892
O	-1.228	-7.529	-0.403	C	-4.491	5.494	-1.892	C	6.472	7.590	-1.405
H	-1.038	-8.460	-0.541	H	-4.755	5.826	-0.911	H	7.272	6.908	-1.205
C	7.657	0.595	-4.688	H	-4.118	6.320	-2.461	H	6.557	8.439	-0.758
C	8.720	-0.292	-4.269	C	-5.597	5.340	-2.601	H	6.522	7.911	-2.424
C	8.834	-1.554	-4.816	H	-6.425	5.942	-2.286	C	5.124	6.888	-1.153
C	7.896	-1.950	-5.785	H	-5.456	5.451	-3.656	H	4.749	7.170	-0.192
C	6.874	-1.098	-6.188	C	-5.854	-0.375	-4.297	H	4.425	7.179	-1.909
C	6.745	0.189	-5.641	H	-4.850	-0.237	-4.645	C	5.325	5.361	-1.201
C	9.501	0.422	-3.268	H	-6.055	-1.420	-4.194	C	3.977	4.659	-0.949
H	9.635	-2.239	-4.509	C	-6.836	0.372	-5.257	H	3.267	4.976	-1.685
H	7.977	-2.954	-6.229	H	-6.463	0.375	-6.259	H	4.110	3.600	-1.015
H	6.153	-1.432	-6.949	C	-6.838	1.923	-4.613	H	3.618	4.915	0.025
H	5.931	0.851	-5.971	H	-7.839	2.301	-4.574	H	6.024	5.071	-0.446
H	7.161	2.699	-4.026	N	-6.246	1.826	-3.155	C	5.864	4.957	-2.585
H	9.261	2.437	-2.363	C	-6.269	2.640	-1.874	H	5.356	5.517	-3.343
N	7.812	1.832	-3.935	O	-6.081	2.099	-0.613	H	6.913	5.162	-2.633
C	8.912	1.684	-3.068	C	-6.658	4.016	-2.038	H	5.697	3.912	-2.741
C	10.736	-0.149	-2.547	H	-7.254	4.123	-1.142				
H	10.420	-0.798	-1.757	N	-7.389	4.097	-3.311				

INT PDA-2Hyp

C	0.023	3.347	1.902	H	-3.304	1.912	4.285	C	-2.099	-4.882	3.628
H	0.437	4.357	1.818	C	-2.560	1.233	2.408	N	-1.533	-5.545	2.548
C	0.757	2.498	0.907	N	-2.576	1.241	1.018	H	-1.636	-6.528	2.343
O	0.500	2.397	-0.283	H	-3.324	1.614	0.431	C	-0.781	-4.666	1.839
O	1.812	1.933	1.490	C	-1.711	0.297	0.580	H	-0.230	-4.885	0.937
C	3.267	-0.785	4.266	H	-1.541	0.065	-0.454	N	-0.839	-3.472	2.403
H	4.277	-1.183	4.355	N	-1.117	-0.296	1.600	C	-1.649	-3.591	3.515
C	2.532	-1.435	3.110	C	-1.631	0.283	2.751	H	-1.851	-2.748	4.160
O	1.261	-1.194	3.065	H	-1.262	-0.003	3.724	C	-3.557	4.388	-1.575
O	3.150	-2.105	2.261	C	-2.979	-5.555	4.626	H	-2.701	4.778	-1.013
C	-3.408	2.148	3.223	H	-3.323	-4.830	5.367	H	-4.073	3.614	-1.001
H	-3.120	3.197	3.082	H	-2.448	-6.351	5.161	N	-3.140	3.846	-2.871

H	-3.553	4.226	-3.708	H	0.038	-2.765	-2.670	H	9.760	-8.208	2.693
C	-2.367	2.757	-2.990	H	2.810	-4.699	-1.091	H	9.063	-9.273	3.890
N	-1.659	2.295	-1.967	C	4.299	-3.633	-2.201	H	9.296	-9.834	2.252
H	-1.262	2.881	-1.240	O	5.181	-2.509	-2.109	C	-5.043	-6.061	-2.841
H	-1.161	1.406	-2.131	H	5.903	-2.709	-1.497	H	-5.960	-5.970	-2.297
N	-2.303	2.096	-4.164	H	3.647	-3.405	-3.043	H	-5.133	-6.846	-3.561
H	-3.049	2.167	-4.838	C	5.048	-4.930	-2.562	C	-3.899	-6.390	-1.864
H	-1.675	1.299	-4.221	H	5.758	-4.702	-3.374	C	-4.185	-6.728	-0.541
N	-4.383	-0.936	-0.505	O	4.031	-5.815	-3.023	C	-2.575	-6.350	-2.303
C	-3.748	-2.223	-0.838	C	4.488	-6.844	-3.885	C	-3.148	-7.026	0.343
O	-2.464	-2.062	-1.455	H	3.610	-7.419	-4.185	H	-5.229	-6.759	-0.196
H	-1.729	-2.339	-0.865	H	5.196	-7.525	-3.393	C	-1.537	-6.648	-1.417
C	-4.677	-3.082	-1.734	H	4.970	-6.432	-4.785	H	-2.348	-6.084	-3.345
O	-5.885	-3.099	-1.518	O	-0.792	-0.162	-2.792	C	-1.825	-6.986	-0.096
C	-3.646	-2.912	0.540	H	0.036	-0.408	-2.302	H	-3.374	-7.293	1.385
H	-2.721	-2.574	1.018	H	-1.452	-0.821	-2.509	H	-0.494	-6.617	-1.763
H	-3.603	-4.000	0.445	O	1.255	-0.912	-1.169	O	-0.762	-7.291	0.812
C	-4.859	-2.388	1.305	H	2.382	1.481	0.830	H	-0.557	-8.228	0.762
H	-4.750	-2.510	2.386	H	2.160	-0.590	-1.304	C	7.234	0.371	-5.135
H	-5.765	-2.894	0.970	H	-3.863	-5.999	4.154	C	8.350	-0.455	-4.731
C	-4.883	-0.914	0.893	H	-4.467	2.055	2.958	C	8.434	-1.768	-5.144
H	-4.234	-0.330	1.544	H	3.318	0.293	4.073	C	7.413	-2.278	-5.964
H	-5.878	-0.464	0.906	H	-1.052	3.383	1.731	C	6.340	-1.485	-6.353
C	9.766	4.102	-0.301	H	4.680	2.102	2.712	C	6.240	-0.146	-5.941
C	8.535	3.349	-0.763	C	-4.668	0.123	-1.331	C	9.213	0.373	-3.897
O	7.408	3.893	-0.279	C	-5.995	0.195	-2.077	H	9.275	-2.408	-4.846
O	8.557	2.368	-1.484	H	-6.798	-0.301	-1.531	H	7.469	-3.324	-6.301
C	4.909	2.637	1.786	O	-3.847	1.049	-1.439	H	5.553	-1.907	-6.996
H	4.192	3.457	1.684	N	-4.040	-3.817	-2.673	H	5.385	0.468	-6.258
H	5.907	3.078	1.863	H	-3.050	-3.656	-2.783	H	6.765	2.531	-4.662
C	4.858	1.715	0.603	C	-4.739	-4.734	-3.561	H	9.024	2.475	-3.200
N	5.378	2.116	-0.614	H	-4.145	-4.947	-4.456	N	7.438	1.686	-4.542
H	6.102	2.805	-0.582	H	-5.676	-4.265	-3.860	C	8.621	1.645	-3.780
C	5.258	1.085	-1.430	O	3.760	-4.512	1.427	C	10.524	-0.103	-3.247
H	5.616	1.049	-2.449	C	3.807	-5.884	2.236	H	10.301	-0.663	-2.363
N	4.647	0.039	-0.820	C	5.301	-6.503	2.401	H	11.060	-0.723	-3.935
H	4.540	-0.906	-1.202	H	3.440	-5.557	3.186	C	11.388	1.117	-2.877
C	4.390	0.420	0.491	C	2.410	-6.838	2.490	H	12.299	0.785	-2.425
H	4.016	-0.291	1.213	C	5.109	-7.720	3.324	C	11.710	1.923	-4.149
Zn	0.231	-1.871	1.567	H	5.668	-6.830	1.451	O	12.198	1.318	-5.193
C	4.452	-4.299	0.194	O	6.241	-5.601	2.989	C	11.475	3.304	-4.180
O	5.043	-5.544	-0.162	H	2.393	-6.875	1.421	H	12.410	3.824	-4.184
C	5.814	-5.542	-1.374	O	2.667	-8.250	3.049	H	10.925	3.553	-5.063
C	7.206	-4.955	-1.101	C	1.256	-6.178	3.269	H	10.913	3.589	-3.316
H	7.158	-3.869	-0.887	H	4.743	-7.392	4.274	N	10.653	1.968	-1.931
H	7.837	-5.066	-1.989	C	4.098	-8.693	2.690	H	9.735	1.708	-1.633
O	7.826	-5.640	-0.039	N	6.398	-8.404	3.507	C	10.699	4.405	-1.430
H	7.142	-5.761	0.638	H	6.196	-4.753	2.541	C	11.213	3.093	-1.469
H	5.974	-6.606	-1.580	H	1.069	-5.203	2.871	O	12.516	2.935	-0.902
H	5.203	-3.519	0.391	H	0.375	-6.777	3.173	N	9.727	5.001	-2.589
C	3.468	-3.840	-0.914	O	1.613	-6.071	4.649	H	8.993	5.605	-2.279
N	2.725	-2.621	-0.558	H	4.269	-9.680	3.063	H	10.256	5.459	-3.302
H	2.761	-2.451	0.452	H	4.216	-8.687	1.627	C	0.306	2.619	3.216
C	1.357	-2.386	-1.027	H	6.697	-8.305	4.456	H	1.358	2.707	3.388
O	0.351	-2.733	-0.153	C	7.640	-8.485	2.486	H	-0.228	3.089	4.016
C	1.069	-3.000	-2.400	H	0.870	-5.721	5.145	H	0.037	1.584	3.167
H	1.181	-4.085	-2.385	C	9.047	-8.988	2.858	C	-4.671	5.446	-1.684
H	1.726	-2.587	-3.169	O	7.370	-8.266	1.277	H	-4.843	5.883	-0.724

H	-4.373	6.207	-2.375	H	1.188	6.763	-2.519	H	6.185	7.884	-3.586
C	-5.839	5.205	-2.256	C	1.887	6.139	-4.451	C	4.941	6.997	-2.076
H	-6.643	5.831	-1.928	C	1.715	4.707	-4.241	H	4.657	7.380	-1.119
H	-5.805	5.199	-3.326	C	2.395	6.335	-5.750	H	4.164	7.196	-2.785
C	-6.150	-0.665	-3.280	C	2.137	4.047	-5.457	C	5.165	5.476	-1.975
H	-5.189	-0.559	-3.740	C	1.258	3.969	-3.168	C	3.864	4.795	-1.514
H	-6.319	-1.694	-3.043	H	2.627	7.302	-6.195	H	3.078	5.022	-2.205
C	-7.237	-0.039	-4.212	C	2.088	2.672	-5.557	H	4.010	3.736	-1.475
H	-6.965	-0.143	-5.241	C	1.214	2.570	-3.287	H	3.598	5.155	-0.542
C	-7.206	1.575	-3.746	H	0.933	4.456	-2.237	H	5.942	5.277	-1.268
H	-8.206	1.946	-3.648	H	2.931	4.909	-7.390	C	5.573	4.925	-3.354
N	-6.470	1.646	-2.353	C	1.620	1.935	-4.456	H	4.981	5.392	-4.114
C	-6.382	2.597	-1.173	H	2.406	2.155	-6.474	H	6.608	5.132	-3.530
O	-6.059	2.201	0.114	H	0.852	1.972	-2.438	H	5.412	3.868	-3.377
C	-6.813	3.943	-1.448	H	1.576	0.839	-4.524	C	2.656	-0.642	5.650
H	-7.318	4.143	-0.513	N	2.559	5.089	-6.384	H	2.983	-1.623	5.920
N	-7.667	3.875	-2.642	C	0.488	8.175	-3.979	H	3.221	0.086	6.194
H	-8.622	3.768	-2.362	H	0.118	8.804	-3.197	H	1.618	-0.534	5.886
H	-7.569	4.718	-3.170	H	0.920	8.779	-4.749	H	10.186	3.611	0.552
H	-8.197	-0.471	-4.022	H	-0.318	7.601	-4.386	H	9.495	5.104	-0.040
H	-6.672	2.154	-4.470	C	6.242	7.678	-2.538	H	11.236	5.331	-1.446
C	1.558	7.225	-3.410	H	7.072	7.030	-2.346				
H	2.444	7.780	-3.183	H	6.375	8.594	-2.000				

TS2 PDA-2Hyp

C	-0.326	3.275	1.816	H	-4.136	3.396	-1.404	C	4.557	1.687	1.070
H	0.054	4.175	2.303	N	-3.058	3.761	-3.167	N	5.430	1.581	0.005
C	0.626	2.806	0.754	H	-3.340	4.222	-4.017	H	6.192	2.228	0.021
O	0.290	2.342	-0.330	C	-2.260	2.688	-3.256	C	5.034	0.500	-0.667
O	1.874	2.922	1.164	N	-1.702	2.160	-2.175	H	5.512	0.148	-1.572
C	3.457	-1.374	4.088	H	-1.399	2.708	-1.375	N	3.949	-0.126	-0.129
H	3.992	-2.218	4.472	H	-1.153	1.297	-2.329	H	3.431	-1.538	-0.256
C	2.414	-1.846	3.103	N	-2.031	2.108	-4.452	C	3.648	0.641	0.992
O	1.457	-1.020	2.841	H	-2.656	2.244	-5.229	H	2.838	0.380	1.657
O	2.520	-2.961	2.539	H	-1.368	1.341	-4.489	Zn	0.112	-1.765	1.618
C	-3.938	2.007	2.849	N	-4.312	-1.129	-0.873	C	4.589	-4.144	0.473
H	-3.697	3.071	2.743	C	-3.593	-2.382	-1.159	O	5.249	-5.347	0.125
H	-3.968	1.776	3.916	O	-2.277	-2.152	-1.677	C	6.032	-5.297	-1.083
C	-2.928	1.148	2.165	H	-1.582	-2.400	-1.028	C	7.355	-4.565	-0.828
N	-2.762	1.150	0.785	C	-4.418	-3.289	-2.111	H	7.194	-3.491	-0.644
H	-3.458	1.473	0.107	O	-5.633	-3.361	-1.975	H	7.986	-4.635	-1.720
C	-1.788	0.268	0.473	C	-3.552	-3.072	0.223	O	8.053	-5.174	0.238
H	-1.464	0.046	-0.526	H	-2.683	-2.688	0.766	H	7.401	-5.328	0.938
N	-1.299	-0.287	1.569	H	-3.445	-4.154	0.130	H	6.288	-6.346	-1.264
C	-2.000	0.257	2.638	C	-4.849	-2.617	0.892	H	5.296	-3.324	0.676
H	-1.767	-0.016	3.656	H	-4.826	-2.737	1.978	C	3.598	-3.732	-0.649
C	-3.281	-5.014	4.900	H	-5.694	-3.177	0.488	N	2.793	-2.530	-0.239
H	-4.126	-4.322	4.901	C	-4.932	-1.146	0.475	H	2.567	-2.672	0.764
H	-2.975	-5.172	5.940	H	-4.381	-0.521	1.176	C	1.401	-2.225	-0.906
C	-2.169	-4.453	4.078	H	-5.952	-0.762	0.403	O	0.383	-2.625	-0.112
N	-0.959	-5.105	3.890	C	9.590	4.461	0.341	C	1.283	-2.852	-2.297
H	-0.701	-5.997	4.290	H	10.260	4.165	1.146	H	1.443	-3.931	-2.272
C	-0.165	-4.342	3.104	H	8.986	5.321	0.649	H	1.976	-2.390	-3.000
H	0.854	-4.570	2.828	C	8.682	3.292	-0.020	H	0.269	-2.670	-2.653
N	-0.802	-3.231	2.767	O	7.397	3.545	0.273	H	2.927	-4.582	-0.799
C	-2.047	-3.286	3.370	O	9.074	2.256	-0.520	C	4.394	-3.505	-1.949
H	-2.759	-2.483	3.262	C	4.656	2.804	2.077	O	5.186	-2.332	-1.926
C	-3.607	4.220	-1.891	H	4.431	3.773	1.620	H	5.643	-2.231	-1.080
H	-2.823	4.615	-1.236	H	5.674	2.870	2.471	H	3.722	-3.377	-2.794

C	5.206	-4.780	-2.268	C	-3.394	-6.554	-2.188	H	-4.882	-0.787	-4.156
H	5.877	-4.539	-3.106	C	-3.712	-6.914	-0.878	H	-6.015	-1.967	-3.539
O	4.223	-5.733	-2.665	C	-2.060	-6.427	-2.573	C	-6.910	-0.348	-4.775
C	4.708	-6.780	-3.489	C	-2.694	-7.144	0.048	H	-6.561	-0.441	-5.782
H	3.849	-7.405	-3.746	H	-4.764	-7.014	-0.574	C	-6.977	1.266	-4.312
H	5.451	-7.408	-2.978	C	-1.042	-6.657	-1.647	H	-7.995	1.597	-4.288
H	5.157	-6.390	-4.414	H	-1.810	-6.145	-3.606	N	-6.347	1.365	-2.870
O	-0.576	-0.188	-2.899	C	-1.359	-7.015	-0.336	C	-6.381	2.318	-1.689
H	0.212	-0.342	-2.322	H	-2.944	-7.426	1.081	O	-6.137	1.935	-0.382
H	-1.219	-0.873	-2.646	H	0.010	-6.556	-1.951	C	-6.844	3.646	-1.998
O	1.353	-0.792	-1.032	O	-0.316	-7.251	0.613	H	-7.423	3.826	-1.103
H	2.506	2.398	0.615	H	-0.047	-8.172	0.572	N	-7.607	3.545	-3.250
H	2.248	-0.378	-0.957	C	7.562	0.635	-4.653	H	-8.575	3.400	-3.040
H	-3.633	-5.973	4.503	C	8.678	-0.147	-4.167	H	-7.504	4.392	-3.772
H	-4.940	1.848	2.436	C	8.843	-1.455	-4.570	H	-7.864	-0.818	-4.654
H	4.140	-0.714	3.595	C	7.905	-2.005	-5.460	H	-6.415	1.865	-4.998
H	-1.316	3.455	1.398	C	6.832	-1.255	-5.928	C	1.510	7.258	-3.359
H	3.960	2.646	2.903	C	6.650	0.079	-5.527	H	2.355	7.848	-3.070
C	-4.574	-0.073	-1.710	C	9.445	0.714	-3.276	H	1.096	6.782	-2.496
C	-5.928	0.076	-2.390	H	9.685	-2.062	-4.210	C	1.956	6.186	-4.371
H	-6.732	-0.411	-1.838	H	8.026	-3.048	-5.789	C	1.827	4.748	-4.171
O	-3.696	0.789	-1.892	H	6.111	-1.708	-6.625	C	2.549	6.402	-5.630
N	-3.685	-3.992	-3.003	H	5.796	0.659	-5.906	C	2.360	4.106	-5.351
H	-2.696	-3.793	-3.040	H	6.975	2.774	-4.220	C	1.322	3.992	-3.132
C	-4.274	-4.957	-3.920	H	9.123	2.806	-2.599	H	2.773	7.378	-6.060
H	-3.623	-5.127	-4.784	N	7.671	1.956	-4.050	C	2.373	2.730	-5.451
H	-5.226	-4.554	-4.266	C	8.796	1.962	-3.204	C	1.342	2.593	-3.250
O	3.740	-4.606	1.829	C	10.723	0.290	-2.531	H	0.912	4.466	-2.228
C	3.417	-5.965	2.135	H	10.460	-0.279	-1.664	H	3.257	4.999	-7.224
C	4.843	-6.742	2.071	H	11.332	-0.308	-3.178	C	1.856	1.975	-4.384
H	3.014	-6.022	3.124	C	11.510	1.543	-2.103	H	2.776	2.226	-6.341
C	1.937	-6.796	1.931	H	12.398	1.248	-1.586	H	0.944	1.980	-2.428
C	4.497	-8.205	2.401	C	11.890	2.361	-3.351	H	1.861	0.878	-4.453
H	5.247	-6.684	1.082	O	12.476	1.777	-4.355	N	2.806	5.164	-6.248
O	5.809	-6.258	3.008	C	11.604	3.732	-3.402	C	0.448	8.165	-4.006
H	1.988	-6.389	0.942	H	12.515	4.289	-3.339	H	-0.003	8.778	-3.255
O	2.043	-8.330	1.861	H	11.110	3.960	-4.322	H	0.910	8.786	-4.745
C	0.787	-6.404	2.879	H	10.970	3.994	-2.581	H	-0.304	7.560	-4.469
H	4.093	-8.262	3.390	N	10.675	2.364	-1.215	C	6.098	7.896	-2.152
C	3.456	-8.726	1.392	H	9.749	2.068	-0.983	H	6.936	7.280	-1.900
N	5.712	-9.028	2.319	C	10.488	5.070	-0.751	H	6.155	8.816	-1.609
H	5.862	-5.301	2.951	H	10.806	6.046	-0.449	H	6.108	8.100	-3.202
H	1.123	-5.641	3.550	C	11.155	3.510	-0.716	C	4.794	7.163	-1.784
H	-0.038	-6.036	2.306	O	12.419	3.404	-0.056	H	4.427	7.535	-0.850
O	0.375	-7.551	3.628	N	9.680	5.358	-1.945	H	4.063	7.332	-2.547
H	3.525	-9.791	1.326	H	8.902	5.933	-1.690	C	5.071	5.652	-1.664
H	3.646	-8.296	0.430	H	10.240	5.837	-2.620	C	3.767	4.920	-1.296
H	5.953	-9.356	3.232	C	-0.035	2.603	3.170	H	3.025	5.116	-2.042
C	7.009	-8.805	1.394	H	0.998	2.733	3.418	H	3.952	3.868	-1.244
H	0.152	-8.264	3.025	H	-0.642	3.051	3.929	H	3.418	5.269	-0.346
C	8.345	-9.552	1.565	H	-0.258	1.559	3.106	H	5.802	5.484	-0.901
O	6.839	-8.083	0.377	C	-4.752	5.233	-2.083	C	5.598	5.118	-3.008
H	9.126	-8.847	1.757	H	-5.010	5.663	-1.138	H	5.045	5.562	-3.810
H	8.270	-10.235	2.384	H	-4.435	6.005	-2.752	H	6.634	5.366	-3.109
H	8.567	-10.094	0.669	C	-5.865	4.946	-2.737	H	5.481	4.056	-3.040
C	-4.519	-6.301	-3.210	H	-6.715	5.540	-2.469	C	2.770	-0.629	5.247
H	-5.461	-6.271	-2.704	H	-5.754	4.942	-3.802	H	2.447	0.334	4.911
H	-4.528	-7.090	-3.933	C	-5.869	-0.931	-3.766	H	1.923	-1.193	5.582

H	3.461	-0.511	6.055

EP PDA-2Hyp

C	-0.019	2.707	2.011	H	-4.766	-1.005	1.444	H	1.534	-0.298	-1.589
C	0.615	3.264	0.774	H	-6.333	-1.405	0.722	H	10.458	3.010	0.285
O	0.076	3.359	-0.323	C	9.798	3.812	-0.060	H	-3.743	-5.705	4.534
O	1.879	3.636	0.986	H	9.974	4.719	0.518	H	-5.501	1.598	3.177
C	3.475	-0.843	3.320	C	8.348	3.383	0.093	H	4.168	-0.537	2.531
H	3.279	0.027	3.949	O	8.077	2.274	-0.600	H	-0.897	3.272	2.247
C	2.214	-1.336	2.653	O	7.532	3.983	0.772	H	4.077	2.416	2.467
O	1.289	-0.450	2.422	C	4.956	2.123	1.889	C	-5.005	-0.321	-1.353
O	2.094	-2.527	2.307	H	5.586	2.998	1.704	C	-6.292	-0.257	-2.150
C	-4.480	1.946	3.367	H	5.550	1.428	2.496	H	-7.099	-0.857	-1.727
H	-4.450	3.019	3.147	C	4.550	1.500	0.590	O	-4.214	0.640	-1.371
H	-4.269	1.816	4.431	N	5.437	1.362	-0.467	N	-3.724	-3.931	-3.079
C	-3.487	1.191	2.551	H	6.369	1.723	-0.482	H	-2.769	-3.605	-3.090
N	-3.550	1.122	1.166	C	4.772	0.757	-1.437	C	-4.177	-4.891	-4.075
H	-4.374	1.301	0.580	H	5.176	0.455	-2.391	H	-3.557	-4.822	-4.944
C	-2.530	0.349	0.731	N	3.487	0.507	-1.067	H	-5.191	-4.677	-4.342
H	-2.371	0.085	-0.299	H	3.971	-1.788	-0.126	O	3.549	-5.061	0.753
N	-1.794	-0.064	1.750	C	3.333	0.968	0.226	C	3.975	-5.654	2.146
C	-2.378	0.459	2.896	H	2.412	0.845	0.772	C	5.458	-6.011	2.704
H	-1.950	0.287	3.871	Zn	-0.221	-1.379	1.611	C	2.602	-6.565	2.606
C	-3.418	-4.740	4.938	C	4.331	-4.569	-0.339	C	5.197	-6.785	4.011
H	-4.281	-4.070	4.944	O	4.635	-5.702	-1.152	H	5.968	-6.647	2.010
H	-3.110	-4.898	5.978	C	5.394	-5.410	-2.337	O	6.265	-4.864	2.982
C	-2.320	-4.143	4.123	C	6.873	-5.224	-1.975	H	2.734	-7.017	1.646
N	-1.091	-4.759	3.936	H	7.035	-4.290	-1.410	O	2.844	-7.614	3.706
H	-0.808	-5.643	4.334	H	7.469	-5.139	-2.890	C	1.457	-5.964	3.234
C	-0.315	-3.970	3.156	O	7.344	-6.337	-1.251	H	4.688	-6.149	4.705
H	0.707	-4.170	2.876	H	6.633	-6.573	-0.633	C	4.329	-8.020	3.712
N	-0.983	-2.877	2.821	H	5.336	-6.340	-2.913	N	6.479	-7.215	4.590
C	-2.229	-2.971	3.419	H	5.242	-4.128	0.102	H	6.243	-4.267	2.230
H	-2.966	-2.189	3.310	C	3.549	-3.510	-1.119	H	1.801	-5.028	3.619
C	-3.522	3.990	-1.378	N	3.151	-2.359	-0.320	H	0.691	-5.791	2.507
H	-2.672	4.148	-0.709	H	2.774	-2.640	0.584	O	0.929	-6.754	4.304
H	-4.190	3.228	-0.963	C	0.272	-1.745	-1.311	H	4.494	-8.763	4.465
N	-3.065	3.596	-2.713	O	-0.289	-2.146	-0.204	H	4.593	-8.419	2.755
H	-3.530	4.016	-3.504	C	0.481	-2.838	-2.340	H	6.638	-6.724	5.446
C	-2.331	2.496	-2.956	H	0.620	-3.803	-1.857	C	7.852	-7.565	3.828
N	-1.648	1.915	-1.959	H	1.337	-2.606	-2.972	H	1.640	-7.255	4.711
H	-1.243	2.492	-1.211	H	-0.407	-2.895	-2.978	C	9.216	-7.743	4.520
H	-1.089	1.099	-2.181	H	2.660	-4.015	-1.514	O	7.743	-7.861	2.610
N	-2.295	1.971	-4.189	C	4.359	-3.053	-2.338	H	9.908	-7.023	4.135
H	-3.007	2.220	-4.858	O	5.462	-2.218	-1.992	H	9.102	-7.600	5.574
H	-1.820	1.064	-4.299	H	6.051	-2.681	-1.380	H	9.585	-8.729	4.332
N	-4.725	-1.444	-0.639	H	3.729	-2.426	-2.975	C	-4.089	-6.314	-3.492
C	-3.835	-2.541	-1.065	C	4.773	-4.277	-3.178	H	-4.970	-6.520	-2.921
O	-2.617	-2.040	-1.589	H	5.507	-3.942	-3.929	H	-4.008	-7.021	-4.291
H	-1.891	-2.155	-0.932	O	3.570	-4.708	-3.809	C	-2.851	-6.422	-2.583
C	-4.527	-3.464	-2.094	C	3.760	-5.470	-4.990	C	-2.973	-6.953	-1.299
O	-5.706	-3.762	-1.943	H	2.766	-5.692	-5.385	C	-1.607	-5.989	-3.043
C	-3.647	-3.340	0.244	H	4.276	-6.422	-4.801	C	-1.852	-7.051	-0.476
H	-2.814	-2.898	0.800	H	4.330	-4.909	-5.745	H	-3.953	-7.295	-0.937
H	-3.406	-4.387	0.048	O	-1.225	-0.543	-3.797	C	-0.486	-6.086	-2.219
C	-4.966	-3.127	0.993	H	-0.385	-0.526	-3.294	H	-1.511	-5.569	-4.056
H	-4.878	-3.341	2.060	H	-1.825	-1.051	-3.224	C	-0.608	-6.618	-0.935
H	-5.744	-3.758	0.560	O	0.462	-0.546	-1.599	H	-1.948	-7.471	0.537
C	-5.269	-1.651	0.716	H	2.295	3.865	0.138	H	0.494	-5.745	-2.582

O	0.541	-6.718	-0.090	C	0.499	2.367	3.292	C	1.283	2.376	-3.195
H	0.980	-7.558	-0.246	H	0.634	2.989	4.038	H	0.969	4.175	-2.010
C	7.343	0.411	-5.169	H	-0.102	1.726	3.920	H	2.980	5.037	-7.105
C	8.471	-0.426	-4.821	H	1.635	2.499	2.862	C	1.703	1.835	-4.405
C	8.577	-1.703	-5.330	C	-4.652	5.036	-1.415	H	2.494	2.216	-6.397
C	7.567	-2.167	-6.191	H	-4.835	5.399	-0.425	H	0.927	1.711	-2.395
C	6.483	-1.363	-6.526	H	-4.363	5.851	-2.046	H	1.677	0.746	-4.554
C	6.361	-0.060	-6.016	C	-5.814	4.820	-2.009	N	2.601	5.137	-6.091
C	9.317	0.351	-3.924	H	-6.629	5.408	-1.640	C	0.473	8.005	-3.475
H	9.426	-2.351	-5.075	H	-5.776	4.894	-3.076	H	0.090	8.569	-2.650
H	7.640	-3.184	-6.603	C	-6.030	-0.962	-3.466	H	0.899	8.671	-4.196
H	5.706	-1.749	-7.202	H	-5.069	-0.807	-3.911	H	-0.323	7.451	-3.927
H	5.498	0.563	-6.291	H	-6.185	-2.008	-3.306	C	6.228	7.490	-2.044
H	6.839	2.523	-4.540	C	-7.123	-0.285	-4.354	H	7.067	6.842	-1.897
H	9.093	2.392	-3.075	H	-6.845	-0.309	-5.386	H	6.344	8.366	-1.440
N	7.525	1.681	-4.479	C	-7.119	1.290	-3.770	H	6.173	7.772	-3.075
C	8.705	1.602	-3.716	H	-8.124	1.638	-3.650	C	4.936	6.757	-1.641
C	10.633	-0.152	-3.304	N	-6.390	1.269	-2.372	H	4.643	7.064	-0.659
H	10.415	-0.779	-2.465	C	-6.321	2.132	-1.124	H	4.159	6.996	-2.337
H	11.181	-0.712	-4.034	O	-5.997	1.646	0.131	C	5.184	5.236	-1.652
C	11.476	1.050	-2.841	C	-6.772	3.487	-1.301	C	3.891	4.503	-1.248
H	12.391	0.700	-2.410	H	-7.284	3.610	-0.357	H	3.104	4.769	-1.925
C	11.791	1.952	-4.048	N	-7.620	3.495	-2.501	H	4.053	3.447	-1.288
O	12.292	1.434	-5.131	H	-8.574	3.353	-2.235	H	3.615	4.786	-0.254
C	11.535	3.328	-3.978	H	-7.533	4.377	-2.965	H	5.960	4.997	-0.957
H	12.462	3.862	-3.938	H	-8.077	-0.745	-4.201	C	5.605	4.795	-3.065
H	10.985	3.634	-4.843	H	-6.591	1.929	-4.446	H	5.009	5.308	-3.791
H	10.965	3.540	-3.098	C	1.555	7.032	-2.972	H	6.637	5.030	-3.219
N	10.724	1.818	-1.838	H	2.432	7.582	-2.699	H	5.460	3.740	-3.167
H	9.810	1.522	-1.565	H	1.189	6.500	-2.119	H	-0.287	1.685	1.845
C	10.634	4.484	-1.165	C	1.905	6.031	-4.089	C	3.916	-1.826	4.422
H	10.996	5.428	-0.814	C	1.755	4.585	-3.986	H	4.227	-2.746	3.974
C	11.265	2.914	-1.291	C	2.416	6.330	-5.367	H	4.730	-1.403	4.971
O	12.568	2.734	-0.731	C	2.192	4.023	-5.245	H	3.096	-2.010	5.084
N	9.754	4.876	-2.275	C	1.305	3.763	-2.973	H	3.465	-5.017	2.626
H	9.010	5.445	-1.925	H	2.634	7.330	-5.738				
H	10.279	5.394	-2.950	C	2.164	2.658	-5.446				

ES PDA-Pro

C	0.177	-4.964	-0.132	H	1.984	-2.985	2.802	H	1.572	-0.409	-3.055
H	-0.631	-5.616	-0.477	C	3.450	2.778	5.061	N	2.473	-0.414	-5.414
C	0.112	-3.653	-0.877	H	3.223	2.067	5.857	H	3.266	-0.393	-6.034
O	0.683	-3.471	-1.955	H	3.079	3.761	5.369	H	2.114	0.479	-5.109
O	-0.583	-2.735	-0.246	C	2.818	2.327	3.786	N	5.398	-0.520	-0.584
C	-2.666	0.050	3.740	N	2.928	3.031	2.595	C	4.742	0.600	0.130
H	-3.211	0.987	3.868	H	3.451	3.884	2.457	C	5.382	1.976	-0.113
C	-1.512	0.202	2.782	C	2.259	2.366	1.624	O	6.513	2.254	0.266
O	-0.625	-0.724	2.758	H	2.166	2.716	0.605	C	4.912	0.200	1.614
O	-1.446	1.197	2.001	N	1.719	1.268	2.129	H	4.064	-0.420	1.916
C	3.770	-5.038	1.394	C	2.054	1.234	3.473	H	4.948	1.072	2.267
H	3.364	-5.848	0.781	H	1.711	0.434	4.111	C	6.213	-0.613	1.617
H	3.588	-5.284	2.442	C	2.910	-3.866	-4.220	H	6.328	-1.235	2.508
C	3.135	-3.730	1.062	H	2.023	-4.134	-3.648	H	7.064	0.067	1.536
N	3.248	-3.136	-0.188	H	3.743	-3.648	-3.544	C	6.076	-1.445	0.342
H	3.900	-3.372	-0.931	N	2.662	-2.696	-5.074	H	5.475	-2.341	0.521
C	2.582	-1.964	-0.165	H	2.981	-2.737	-6.031	H	7.030	-1.762	-0.092
H	2.527	-1.285	-0.998	C	2.258	-1.499	-4.626	C	-9.825	-3.594	-0.105
N	2.005	-1.781	1.014	N	1.633	-1.346	-3.471	H	-10.507	-2.802	0.202
C	2.346	-2.877	1.791	H	1.225	-2.136	-2.945	H	-9.656	-4.286	0.726

C	-8.506	-3.002	-0.547	C	5.142	-0.894	-1.872	H	-1.087	-4.548	1.555
O	-7.521	-3.901	-0.481	C	6.042	-0.341	-2.969	H	0.290	-5.556	1.930
O	-8.355	-1.846	-0.911	H	7.016	-0.061	-2.558	H	0.507	-3.841	1.670
C	-4.542	-4.068	1.297	O	4.258	-1.726	-2.133	C	-10.444	-4.410	-1.255
H	-4.311	-4.977	0.730	N	4.552	2.866	-0.727	H	-10.962	-5.256	-0.854
H	-5.583	-4.152	1.621	H	3.675	2.534	-1.107	C	-11.434	-3.526	-2.036
C	-4.363	-2.845	0.457	C	4.962	4.223	-1.049	N	-9.380	-4.869	-2.159
N	-5.234	-2.578	-0.578	H	4.167	4.782	-1.555	H	-8.488	-4.663	-1.756
H	-6.093	-3.087	-0.634	H	5.822	4.181	-1.722	H	-9.463	-5.856	-2.296
C	-4.863	-1.427	-1.101	H	3.687	0.634	-0.155	O	-12.713	-3.641	-1.825
H	-5.368	-0.916	-1.907	O	-1.876	5.297	1.799	N	-10.976	-2.642	-2.929
N	-3.766	-0.940	-0.467	C	-1.715	5.137	3.210	H	-10.169	-2.090	-2.719
H	-3.300	-0.052	-0.638	H	-1.454	4.122	3.427	C	-11.600	-2.495	-4.104
C	-3.438	-1.833	0.539	C	-0.597	6.072	3.709	H	-12.349	-1.736	-4.018
H	-2.572	-1.705	1.167	H	-0.658	7.007	3.192	C	-12.261	-3.826	-4.506
Zn	0.636	-0.257	1.292	C	-3.035	5.490	3.921	C	-12.318	-4.882	-3.585
C	-2.487	4.125	1.252	H	-3.668	6.029	3.249	H	-11.763	-4.622	-2.708
O	-3.890	4.365	1.272	C	5.339	4.950	0.255	H	-13.338	-5.068	-3.320
C	-4.704	3.317	0.716	H	5.597	4.230	1.003	H	-11.898	-5.762	-4.025
C	-4.755	2.102	1.653	H	6.175	5.594	0.076	O	-12.764	-3.968	-5.697
H	-3.832	1.513	1.594	C	4.141	5.788	0.741	C	-10.577	-2.085	-5.180
H	-5.574	1.445	1.342	C	3.062	6.021	-0.112	H	-10.214	-2.959	-5.678
O	-4.993	2.510	2.990	C	4.134	6.311	2.033	H	-11.047	-1.439	-5.891
H	-4.574	3.378	3.084	C	1.977	6.779	0.327	C	-9.400	-1.346	-4.516
H	-5.702	3.762	0.699	H	3.068	5.608	-1.132	C	-8.957	-0.004	-4.867
H	-2.213	3.270	1.883	C	3.049	7.069	2.473	C	-8.571	-1.826	-3.484
C	-1.998	3.917	-0.191	H	4.985	6.126	2.706	C	-7.835	0.309	-4.012
N	-0.561	3.656	-0.210	C	1.970	7.303	1.620	C	-9.406	0.914	-5.795
H	-0.253	2.883	0.373	H	1.127	6.963	-0.345	H	-8.658	-2.805	-3.011
C	0.333	4.084	-1.129	H	3.044	7.482	3.492	C	-7.196	1.530	-4.114
O	1.486	3.604	-1.177	O	0.858	8.081	2.070	C	-8.745	2.151	-5.887
C	-0.088	5.174	-2.090	H	0.228	7.510	2.518	H	-10.258	0.692	-6.452
H	-0.422	6.067	-1.553	C	-2.736	6.360	5.156	C	-7.666	2.452	-5.066
H	-0.915	4.843	-2.726	H	-2.297	7.284	4.843	H	-6.341	1.783	-3.473
H	0.769	5.427	-2.715	O	-3.691	4.287	4.333	H	-9.094	2.890	-6.623
H	-2.222	4.829	-0.745	H	-4.221	4.463	5.113	H	-7.165	3.428	-5.156
C	-2.763	2.770	-0.881	N	-3.987	6.631	5.879	N	-7.613	-0.849	-3.156
O	-2.326	1.490	-0.429	H	-4.384	5.931	6.472	H	-6.903	-0.934	-2.456
H	-2.142	1.459	0.546	C	-4.595	7.815	5.743	C	-2.281	-2.695	-6.275
H	-2.550	2.796	-1.955	C	-5.910	7.989	6.193	C	-1.999	-3.479	-5.092
C	-4.283	2.982	-0.727	H	-6.591	7.606	5.462	C	-1.781	-2.858	-3.879
H	-4.797	2.059	-1.045	H	-6.044	7.463	7.116	C	-1.839	-1.456	-3.824
O	-4.565	4.051	-1.619	H	-6.100	9.031	6.346	C	-2.110	-0.703	-4.961
C	-5.926	4.168	-2.008	O	-3.899	8.908	5.136	C	-2.335	-1.318	-6.203
H	-5.973	4.969	-2.750	O	-0.378	5.976	5.290	C	-2.293	-4.937	-6.873
H	-6.583	4.434	-1.169	C	-1.600	6.041	6.029	C	-2.013	-4.879	-5.495
H	-6.296	3.237	-2.462	H	-1.618	6.938	6.612	H	-1.565	-3.440	-2.972
O	1.832	0.941	-1.894	H	-1.670	5.193	6.678	H	-1.666	-0.950	-2.863
H	1.096	0.514	-1.341	C	0.773	5.424	3.438	H	-2.150	0.395	-4.892
H	1.649	1.898	-1.859	H	1.068	5.622	2.428	H	-2.548	-0.709	-7.093
O	-0.018	-0.240	-0.553	H	1.500	5.833	4.108	H	-2.369	-5.852	-7.461
H	-0.434	-1.789	-0.595	O	0.681	4.011	3.639	N	-2.461	-3.634	-7.376
H	-0.799	0.328	-0.674	H	1.526	3.675	3.944	H	-2.667	-3.481	-8.342
H	4.540	2.842	4.967	C	-2.172	-0.504	5.089	C	-1.760	-6.067	-4.548
H	4.854	-5.011	1.238	H	-2.991	-0.551	5.777	H	-0.950	-5.832	-3.890
H	-3.357	-0.688	3.314	H	-1.771	-1.485	4.947	H	-2.642	-6.260	-3.974
H	1.137	-5.447	-0.307	H	-1.413	0.139	5.483	C	-1.403	-7.316	-5.375
H	-3.897	-4.041	2.179	C	-0.045	-4.708	1.370	H	-1.227	-8.142	-4.718

H	-2.213	-7.551	-6.034	H	-4.568	-5.181	-3.714	N	6.230	-1.468	-4.001
H	-0.521	-7.124	-5.950	C	-6.108	-5.057	-6.749	C	5.750	-2.857	-3.983
C	-7.344	-7.398	-5.695	H	-6.816	-5.724	-7.195	O	5.243	-3.354	-2.892
H	-8.202	-7.464	-5.060	H	-6.383	-4.046	-6.968	C	5.840	-3.642	-5.140
H	-7.572	-6.787	-6.543	H	-5.133	-5.255	-7.145	H	5.955	-4.670	-4.866
H	-7.068	-8.378	-6.025	C	5.459	0.892	-3.684	C	4.669	-3.774	-6.171
C	-6.174	-6.773	-4.912	H	4.403	0.768	-3.805	H	4.887	-4.358	-7.041
H	-6.332	-6.912	-3.863	H	5.650	1.768	-3.099	H	4.506	-2.756	-6.457
H	-5.258	-7.245	-5.201	C	6.249	0.841	-5.005	C	3.363	-4.675	-5.484
C	-6.094	-5.267	-5.224	H	6.605	1.820	-5.246	H	2.573	-4.667	-6.205
H	-6.934	-4.767	-4.788	H	5.610	0.491	-5.789	H	3.978	-5.537	-5.639
C	-4.793	-4.689	-4.638	C	7.225	-0.652	-4.847	N	7.000	-3.214	-5.934
H	-3.991	-4.844	-5.329	H	7.601	-1.262	-5.642	H	7.803	-3.747	-5.666
H	-4.915	-3.641	-4.462	H	8.037	-0.330	-4.230	H	6.812	-3.360	-6.905

TS1 PDA-Pro

C	1.052	-4.266	1.721	C	4.410	1.411	-1.172	C	-1.185	0.373	-0.861
H	0.944	-5.353	1.800	C	5.508	2.399	-1.589	O	0.117	0.781	-0.702
C	0.301	-3.776	0.520	O	6.656	2.288	-1.173	C	-1.543	0.059	-2.312
O	0.788	-3.615	-0.596	C	3.496	1.981	-0.073	H	-1.472	0.974	-2.906
O	-0.969	-3.508	0.793	H	2.575	1.395	-0.041	H	-2.557	-0.337	-2.381
C	-2.222	-0.917	4.513	H	3.231	3.025	-0.256	H	-0.838	-0.663	-2.723
H	-3.046	-0.303	4.880	C	4.326	1.780	1.205	H	-2.754	3.251	-1.147
C	-1.630	-0.323	3.246	H	3.694	1.726	2.094	C	-4.287	1.967	-0.380
O	-0.464	-0.771	2.917	H	5.034	2.603	1.330	O	-4.494	0.871	0.518
O	-2.283	0.509	2.585	C	5.088	0.462	0.960	H	-4.135	1.094	1.387
C	4.284	-3.259	3.735	H	4.642	-0.366	1.499	H	-4.528	1.567	-1.367
H	4.212	-4.352	3.734	H	6.142	0.530	1.238	C	-5.270	3.124	-0.113
H	3.966	-2.902	4.716	C	-8.959	-4.072	-0.621	H	-6.273	2.696	0.035
C	3.431	-2.652	2.672	H	-9.068	-2.989	-0.498	O	-5.229	3.914	-1.299
N	3.638	-2.885	1.315	C	-7.538	-4.394	-1.030	C	-6.405	4.668	-1.543
H	4.517	-3.172	0.894	O	-7.155	-5.600	-0.586	H	-6.251	5.198	-2.485
C	2.721	-2.174	0.614	O	-6.822	-3.650	-1.676	H	-6.603	5.408	-0.755
H	2.676	-2.104	-0.460	C	-3.931	-3.844	1.397	H	-7.288	4.017	-1.638
N	1.895	-1.555	1.437	H	-3.241	-4.583	0.983	O	1.421	-1.107	-1.962
C	2.330	-1.839	2.727	H	-4.874	-4.363	1.603	H	0.925	-1.850	-1.579
H	1.774	-1.483	3.579	C	-4.175	-2.724	0.436	H	0.986	-0.289	-1.552
C	3.729	3.394	3.898	N	-4.593	-2.993	-0.852	O	-1.204	-0.879	-0.047
H	3.841	2.785	4.798	H	-5.166	-3.805	-0.964	H	-1.371	-3.056	0.027
H	3.338	4.371	4.204	C	-4.851	-1.821	-1.412	H	-2.111	-1.028	0.298
C	2.815	2.712	2.937	H	-5.253	-1.682	-2.404	H	-9.184	-4.532	0.344
N	2.475	3.254	1.704	N	-4.595	-0.804	-0.560	H	4.727	3.551	3.472
H	2.769	4.153	1.354	H	-4.629	0.196	-0.773	H	5.340	-2.994	3.605
C	1.617	2.406	1.078	C	-4.153	-1.357	0.631	H	2.102	-3.999	1.646
H	1.157	2.564	0.118	H	-3.925	-0.746	1.494	H	4.978	-6.048	-2.228
N	1.399	1.347	1.837	Zn	0.282	-0.091	1.182	H	-3.516	-3.478	2.339
C	2.131	1.525	2.996	C	-2.603	3.208	0.980	C	5.640	-0.742	-1.149
H	2.088	0.803	3.796	O	-3.494	4.306	1.151	C	6.078	-0.493	-2.584
C	3.923	-6.061	-2.504	C	-4.896	3.968	1.119	H	6.926	0.197	-2.543
H	3.435	-6.896	-1.985	C	-5.321	3.387	2.472	O	5.925	-1.823	-0.590
N	3.335	-4.780	-2.139	H	-5.338	4.160	3.257	N	5.093	3.384	-2.428
C	2.184	-4.329	-2.638	H	-4.588	2.637	2.794	H	4.122	3.410	-2.704
N	1.219	-5.192	-3.010	O	-6.573	2.747	2.360	C	5.971	4.453	-2.888
H	0.998	-5.950	-2.373	H	-7.125	3.335	1.822	H	5.970	4.509	-3.981
H	0.400	-4.777	-3.433	H	-5.390	4.942	1.032	H	6.979	4.227	-2.540
N	1.974	-3.015	-2.842	H	-2.751	2.512	1.779	H	3.820	1.093	-2.038
H	2.767	-2.400	-2.756	C	-2.837	2.493	-0.356	O	-1.254	3.601	1.410
H	1.069	-2.671	-2.480	N	-2.206	1.194	-0.230	C	-1.205	3.945	2.798
N	5.000	0.254	-0.506	H	-2.110	1.145	0.788	H	-1.034	3.061	3.377

C	-0.060	4.947	3.039	H	-10.169	-2.090	-2.719	C	-7.344	-7.398	-5.695
H	0.203	5.415	2.113	C	-11.600	-2.495	-4.104	H	-8.202	-7.464	-5.060
C	-2.543	4.581	3.217	H	-12.349	-1.736	-4.018	H	-7.572	-6.787	-6.543
H	-3.086	4.875	2.344	C	-12.261	-3.826	-4.506	H	-7.068	-8.378	-6.025
C	5.704	5.896	-2.089	C	-12.318	-4.882	-3.585	C	-6.174	-6.773	-4.912
H	6.354	5.450	-1.366	H	-11.763	-4.622	-2.708	H	-6.332	-6.912	-3.863
H	6.237	6.647	-2.634	H	-13.338	-5.068	-3.320	H	-5.258	-7.245	-5.201
C	4.502	6.539	-1.371	H	-11.898	-5.762	-4.025	C	-6.094	-5.267	-5.224
C	3.208	6.317	-1.843	O	-12.764	-3.968	-5.697	H	-6.934	-4.767	-4.788
C	4.707	7.340	-0.249	C	-10.577	-2.085	-5.180	C	-4.793	-4.689	-4.638
C	2.119	6.898	-1.193	H	-10.214	-2.959	-5.678	H	-3.991	-4.844	-5.329
H	3.047	5.684	-2.729	H	-11.047	-1.439	-5.891	H	-4.915	-3.641	-4.462
C	3.618	7.921	0.402	C	-9.400	-1.346	-4.516	H	-4.568	-5.181	-3.714
H	5.727	7.514	0.124	C	-8.957	-0.004	-4.867	C	-6.108	-5.057	-6.749
C	2.324	7.700	-0.071	C	-8.571	-1.826	-3.484	H	-6.816	-5.724	-7.195
H	1.100	6.723	-1.565	C	-7.835	0.309	-4.012	H	-6.383	-4.046	-6.968
H	3.780	8.553	1.287	C	-9.406	0.914	-5.795	H	-5.133	-5.255	-7.145
O	1.208	8.297	0.595	H	-8.658	-2.805	-3.011	C	5.459	0.892	-3.684
H	0.918	7.724	1.310	C	-7.196	1.530	-4.114	H	4.403	0.768	-3.805
C	-2.271	5.818	4.092	C	-8.745	2.151	-5.887	H	5.650	1.768	-3.099
H	-1.744	6.553	3.518	H	-10.258	0.692	-6.452	C	6.249	0.841	-5.005
O	-3.311	3.631	3.960	C	-7.666	2.452	-5.066	H	6.605	1.820	-5.246
H	-3.881	4.093	4.577	H	-6.341	1.783	-3.473	H	5.610	0.491	-5.789
N	-3.546	6.379	4.558	H	-9.094	2.890	-6.623	C	7.225	-0.652	-4.847
H	-4.033	5.951	5.317	H	-7.165	3.428	-5.156	H	7.601	-1.262	-5.642
C	-4.058	7.464	3.963	N	-7.613	-0.849	-3.156	H	8.037	-0.330	-4.230
C	-5.384	7.841	4.201	H	-6.903	-0.934	-2.456	N	6.230	-1.468	-4.001
H	-6.037	7.254	3.591	C	-2.281	-2.695	-6.275	C	5.750	-2.857	-3.983
H	-5.620	7.681	5.234	C	-1.999	-3.479	-5.092	O	5.243	-3.354	-2.892
H	-5.509	8.877	3.963	C	-1.781	-2.858	-3.879	C	5.840	-3.642	-5.140
O	-3.242	8.242	3.079	C	-1.839	-1.456	-3.824	H	6.825	-4.052	-5.218
O	0.038	5.406	4.568	C	-2.110	-0.703	-4.961	C	4.996	-4.944	-5.352
C	-1.225	5.780	5.121	C	-2.335	-1.318	-6.203	H	5.636	-5.799	-5.284
H	-1.220	6.825	5.351	C	-2.293	-4.937	-6.873	H	4.537	-4.917	-6.318
H	-1.401	5.220	6.017	C	-2.013	-4.879	-5.495	C	3.883	-5.714	-4.252
C	1.163	4.203	3.604	H	-1.565	-3.440	-2.972	H	3.272	-6.333	-4.876
H	1.721	3.771	2.798	H	-1.666	-0.950	-2.863	N	5.561	-2.811	-6.319
H	1.783	4.891	4.138	H	-2.150	0.395	-4.892	H	6.417	-2.429	-6.668
O	0.726	3.168	4.489	H	-2.548	-0.709	-7.093	H	5.133	-3.371	-7.028
H	1.384	3.033	5.173	H	-2.369	-5.852	-7.461	C	-2.760	-2.324	4.191
H	-1.771	-1.485	4.947	N	-2.461	-3.634	-7.376	H	-1.939	-2.999	4.065
C	-10.444	-4.410	-1.255	H	-2.667	-3.481	-8.342	H	-3.379	-2.661	4.996
H	-10.749	-4.469	-0.231	C	-1.760	-6.067	-4.548	H	-3.334	-2.288	3.290
C	-11.434	-3.526	-2.036	H	-0.950	-5.832	-3.890	C	0.418	-3.652	2.983
N	-10.426	-5.758	-1.839	H	-2.642	-6.260	-3.974	H	-0.480	-4.182	3.225
H	-9.482	-6.024	-2.036	C	-1.403	-7.316	-5.375	H	1.106	-3.725	3.799
H	-10.826	-6.407	-1.192	H	-1.227	-8.142	-4.718	H	0.187	-2.623	2.802
O	-12.713	-3.641	-1.825	H	-2.213	-7.551	-6.034	H	3.318	-4.863	-3.932
N	-10.976	-2.642	-2.929	H	-0.521	-7.124	-5.950	H	3.951	-4.123	-1.703

INT PDA-Pro

C	6.088	1.110	6.587	C	4.237	5.016	9.746	H	9.246	2.676	6.027
H	5.559	0.184	6.347	O	5.483	5.239	9.476	C	7.678	3.944	6.597
C	5.411	2.267	5.894	O	3.292	5.317	8.999	H	7.396	4.400	5.670
O	5.543	2.488	4.694	C	9.521	1.478	8.533	N	7.228	4.310	7.783
O	4.663	3.013	6.700	H	9.135	0.492	8.248	C	7.799	3.454	8.712
C	3.975	4.319	11.069	H	9.606	1.503	9.622	H	7.560	3.534	9.761
H	2.970	4.548	11.427	C	8.628	2.574	8.059	C	9.956	9.342	10.436
H	4.724	4.594	11.814	N	8.515	2.895	6.709	H	10.029	8.738	11.344

H	9.564	10.327	10.717	H	2.878	7.552	9.368	H	-6.456	0.071	2.380
C	9.060	8.667	9.451	C	2.468	8.136	7.292	O	-7.322	1.865	0.708
N	8.760	9.206	8.208	N	3.346	6.939	6.668	C	-5.135	3.748	1.225
H	9.054	10.115	7.876	H	3.588	6.436	7.527	H	-4.772	2.874	0.727
C	7.896	8.385	7.571	C	4.265	6.588	5.603	H	-5.605	4.394	0.514
H	7.439	8.575	6.611	O	5.595	6.530	5.934	C	-3.958	4.487	1.889
N	7.624	7.337	8.335	C	4.020	7.478	4.375	C	-4.044	5.805	2.502
C	8.353	7.493	9.501	H	4.279	8.516	4.600	C	-2.632	4.030	2.015
H	8.270	6.778	10.306	H	2.966	7.441	4.088	C	-2.727	6.126	3.002
N	8.768	1.735	1.692	H	4.614	7.142	3.526	C	-5.088	6.694	2.660
H	8.823	1.737	0.686	H	2.586	9.072	6.734	H	-2.260	3.072	1.650
C	7.816	2.484	2.270	C	0.955	7.850	7.358	C	-2.495	7.329	3.643
N	7.514	2.338	3.554	O	0.647	6.598	7.977	C	-4.836	7.913	3.314
H	7.632	1.436	3.997	H	1.252	6.454	8.719	H	-6.095	6.465	2.287
H	6.761	2.912	3.979	H	0.549	7.777	6.344	C	-3.570	8.223	3.794
N	7.155	3.407	1.542	C	0.229	9.027	8.045	H	-1.500	7.589	4.027
H	7.508	3.745	0.661	H	-0.814	8.731	8.227	H	-5.660	8.629	3.445
H	6.338	3.851	1.938	O	0.291	10.095	7.097	H	-3.397	9.183	4.303
N	10.343	5.629	5.032	C	-0.764	11.037	7.215	N	-1.861	4.999	2.683
C	9.854	6.954	4.687	H	-0.620	11.780	6.424	H	-0.887	4.926	2.902
C	11.031	7.914	4.457	H	-0.758	11.556	8.185	C	3.161	3.138	0.130
O	12.183	7.563	4.676	H	-1.748	10.563	7.082	C	3.443	2.354	1.313
C	9.072	7.361	5.948	O	6.074	5.151	3.467	C	3.661	2.975	2.526
H	8.078	6.912	5.929	H	5.229	4.814	3.845	C	3.603	4.377	2.581
H	8.942	8.442	6.021	H	6.288	5.804	4.163	C	3.332	5.130	1.444
C	9.932	6.792	7.093	O	3.898	5.193	5.220	C	3.107	4.515	0.202
H	9.312	6.493	7.941	H	4.326	3.812	6.195	C	3.149	0.896	-0.468
H	10.642	7.548	7.443	H	2.932	5.154	5.108	C	3.429	0.954	0.910
C	10.698	5.597	6.472	H	-4.312	2.282	6.247	H	3.877	2.393	3.433
H	10.429	4.646	6.919	H	10.970	9.476	10.039	H	3.776	4.883	3.542
H	11.781	5.722	6.555	H	10.524	1.582	8.107	H	3.292	6.228	1.513
C	-4.018	2.252	5.180	H	7.122	1.029	6.246	H	2.894	5.124	-0.688
H	-4.610	2.993	4.664	H	1.494	2.142	7.856	H	3.073	-0.019	-1.056
C	-2.669	2.115	4.873	C	10.242	4.684	4.018	N	2.981	2.199	-0.971
O	-2.209	0.864	4.741	C	10.921	5.067	2.695	H	2.775	2.352	-1.937
O	-1.971	3.111	4.768	H	9.983	5.299	2.182	C	3.682	-0.234	1.857
C	1.174	2.058	6.813	O	9.360	3.833	4.243	H	4.492	0.001	2.515
H	1.960	1.535	6.255	N	10.689	9.151	4.003	H	2.800	-0.427	2.431
H	0.274	1.438	6.763	H	9.714	9.366	3.861	C	4.039	-1.483	1.030
C	0.913	3.409	6.233	C	11.673	10.199	3.759	H	4.215	-2.309	1.687
N	-0.035	3.614	5.247	H	11.522	10.639	2.768	H	3.229	-1.718	0.371
H	-0.830	3.007	5.266	H	12.664	9.745	3.806	H	4.921	-1.291	0.455
C	-0.027	4.908	4.979	H	9.217	6.915	3.795	C	-1.902	-1.565	0.710
H	-0.695	5.409	4.294	C	-5.134	1.312	5.146	H	-2.760	-1.631	1.345
N	0.919	5.549	5.717	H	-5.307	1.364	6.174	H	-2.130	-0.954	-0.138
H	1.170	6.535	5.714	C	-5.992	2.307	4.369	H	-1.626	-2.545	0.380
C	1.516	4.603	6.536	N	-4.984	0.075	4.566	C	-0.732	-0.940	1.493
H	2.303	4.842	7.232	H	-4.040	-0.191	4.369	H	-0.890	-1.079	2.542
Zn	6.067	5.926	7.741	H	-5.384	-0.574	5.213	H	0.184	-1.412	1.204
C	2.978	8.436	8.717	O	-7.271	2.192	4.580	C	-0.652	0.566	1.181
O	2.312	9.578	9.261	N	-5.534	3.191	3.476	H	-1.492	1.066	1.617
C	0.877	9.452	9.376	H	-4.727	3.743	3.686	C	0.649	1.144	1.767
C	0.514	8.594	10.595	C	-6.158	3.338	2.301	H	1.451	0.989	1.076
H	1.199	8.777	11.437	H	-6.907	4.097	2.387	H	0.527	2.192	1.943
H	0.622	7.534	10.334	C	-6.819	2.007	1.899	H	0.874	0.652	2.691
O	-0.833	8.817	10.966	C	-6.876	0.951	2.820	C	-0.666	0.776	-0.344
H	-0.972	9.774	10.910	H	-6.321	1.211	3.697	H	-1.374	0.109	-0.790
H	0.551	10.471	9.614	H	-7.896	0.765	3.085	H	-0.941	1.787	-0.563

H	0.309	0.578	-0.740	C	6.042	1.298	8.115	C	2.984	10.406	11.344
C	11.194	6.663	2.575	H	5.055	1.088	8.471	H	2.868	10.496	10.284
H	10.237	7.135	2.489	H	6.738	0.629	8.577	C	4.172	11.273	11.805
H	11.701	7.040	3.439	H	6.302	2.307	8.358	H	4.102	12.241	11.354
C	12.035	6.717	1.286	C	11.587	11.312	4.821	H	4.146	11.373	12.871
H	12.392	7.714	1.135	H	12.071	12.193	4.454	O	5.210	11.053	10.729
H	11.430	6.425	0.453	H	12.071	10.986	5.718	O	3.962	7.926	12.161
C	12.667	5.181	1.558	C	10.109	11.624	5.119	H	3.507	8.264	12.936
H	13.043	4.571	0.763	C	9.638	11.578	6.431	N	1.756	10.859	12.012
H	13.479	5.503	2.175	C	9.242	11.953	4.077	H	1.973	11.153	12.944
N	11.672	4.365	2.404	C	8.299	11.862	6.702	C	1.180	11.987	11.266
C	11.192	2.976	2.422	H	10.322	11.319	7.252	C	0.092	12.693	11.796
O	10.685	2.479	3.513	C	7.903	12.237	4.348	H	-0.739	12.623	11.127
C	11.282	2.191	1.265	H	9.613	11.990	3.043	H	-0.176	12.276	12.745
H	12.262	2.284	0.846	C	7.431	12.191	5.660	H	0.362	13.722	11.923
C	11.150	0.631	1.283	H	7.927	11.826	7.736	O	1.683	12.327	10.114
H	11.522	0.252	2.212	H	7.219	12.497	3.526	C	6.920	9.322	11.367
H	11.715	0.215	0.476	O	6.059	12.481	5.937	H	6.388	8.829	12.154
C	9.212	0.641	2.239	H	5.958	13.421	6.106	H	7.637	8.649	10.944
N	10.286	2.646	0.286	O	4.371	8.759	8.713	O	7.594	10.468	11.895
H	10.307	3.645	0.228	C	4.890	8.655	10.042	H	8.293	10.183	12.488
H	10.498	2.258	-0.610	H	5.355	7.700	10.169	C	9.781	0.140	0.852
C	4.069	2.799	10.843	C	5.928	9.768	10.277	H	9.734	-0.923	0.742
H	5.096	2.499	10.858	H	6.459	9.958	9.368	H	9.387	0.682	0.019
H	3.537	2.289	11.619	C	3.740	8.803	11.055	H	9.984	0.825	2.957
H	3.640	2.552	9.894	H	2.813	8.554	10.583	H	8.426	0.018	2.610

TS2 PDA-Pro

C	6.088	1.110	6.587	C	8.230	7.435	9.431	H	0.058	1.614	6.684
H	5.559	0.184	6.347	H	8.379	6.616	10.118	C	0.945	3.495	6.183
C	5.411	2.267	5.894	N	8.768	1.735	1.692	N	-0.108	3.908	5.388
O	5.543	2.488	4.694	H	8.823	1.737	0.686	H	-0.864	3.261	5.284
O	4.663	3.013	6.700	C	7.816	2.484	2.270	C	0.106	5.182	5.110
C	3.984	4.335	11.076	N	7.514	2.338	3.554	H	-0.563	5.823	4.557
H	2.979	4.564	11.434	H	7.632	1.436	3.997	N	1.294	5.621	5.659
H	4.733	4.610	11.821	H	6.761	2.912	3.979	H	2.306	6.674	5.984
C	4.246	5.032	9.753	N	7.155	3.407	1.542	C	1.818	4.539	6.358
O	5.497	5.261	9.470	H	7.508	3.745	0.661	H	2.750	4.600	6.893
O	3.301	5.333	9.006	H	6.338	3.851	1.938	Zn	6.076	5.942	7.748
C	9.570	1.410	8.535	N	10.343	5.629	5.032	C	2.818	8.525	8.531
H	9.184	0.424	8.250	C	9.854	6.954	4.687	O	2.024	9.625	8.982
H	9.655	1.435	9.624	C	11.031	7.914	4.457	C	0.599	9.390	8.983
C	8.677	2.506	8.061	O	12.183	7.563	4.676	C	0.201	8.537	10.195
N	8.564	2.827	6.711	C	9.072	7.361	5.948	H	0.797	8.794	11.084
H	9.295	2.608	6.029	H	8.078	6.912	5.929	H	0.410	7.483	9.978
C	7.727	3.876	6.599	H	8.942	8.442	6.021	O	-1.185	8.663	10.449
H	7.445	4.332	5.672	C	9.932	6.792	7.093	H	-1.392	9.605	10.351
N	7.277	4.242	7.785	H	9.312	6.493	7.941	H	0.177	10.386	9.162
C	7.848	3.386	8.714	H	10.642	7.548	7.443	H	2.732	7.653	9.198
H	7.609	3.466	9.763	C	10.698	5.597	6.472	C	2.454	8.152	7.079
C	9.758	9.350	10.359	H	10.429	4.646	6.919	N	3.250	6.943	6.648
H	10.065	8.648	11.139	H	11.781	5.722	6.555	H	3.597	6.452	7.534
H	9.315	10.225	10.850	C	-4.252	2.416	5.251	C	4.299	6.596	5.585
C	8.777	8.693	9.446	H	-4.844	3.157	4.735	O	5.610	6.538	5.965
N	8.194	9.344	8.368	C	-2.903	2.279	4.944	C	4.029	7.494	4.382
H	8.316	10.320	8.136	O	-2.443	1.028	4.812	H	4.288	8.532	4.607
C	7.326	8.501	7.764	O	-2.205	3.275	4.839	H	2.975	7.457	4.095
H	6.681	8.749	6.935	C	1.036	2.104	6.718	H	4.623	7.158	3.533
N	7.320	7.334	8.393	H	1.724	1.495	6.119	H	2.547	9.079	6.502

C	0.966	7.750	7.030	C	-2.120	7.507	2.780	C	11.192	2.976	2.422
O	0.703	6.493	7.661	C	-4.060	8.281	1.528	O	10.685	2.479	3.513
H	1.253	6.415	8.454	H	-5.448	6.773	0.797	C	11.282	2.191	1.265
H	0.653	7.619	5.989	C	-2.888	8.546	2.226	H	12.262	2.284	0.846
C	0.099	8.882	7.618	H	-1.196	7.733	3.328	C	11.150	0.631	1.283
H	-0.932	8.509	7.723	H	-4.643	9.112	1.106	H	11.522	0.252	2.212
O	0.157	9.928	6.645	H	-2.550	9.586	2.353	H	11.715	0.215	0.476
C	-0.972	10.787	6.647	N	-2.018	4.924	3.044	C	9.212	0.641	2.239
H	-0.820	11.518	5.848	H	-1.178	4.788	3.571	N	10.286	2.646	0.286
H	-1.087	11.329	7.598	C	3.161	3.138	0.130	H	10.307	3.645	0.228
H	-1.903	10.233	6.450	C	3.443	2.354	1.313	H	10.498	2.258	-0.610
O	6.074	5.151	3.467	C	3.661	2.975	2.526	C	4.078	2.815	10.850
H	5.229	4.814	3.845	C	3.603	4.377	2.581	H	5.105	2.515	10.865
H	6.288	5.804	4.163	C	3.332	5.130	1.444	H	3.546	2.305	11.626
O	3.949	5.358	5.266	C	3.107	4.515	0.202	H	3.649	2.568	9.901
H	4.326	3.812	6.195	C	3.149	0.896	-0.468	C	6.042	1.298	8.115
H	2.941	5.170	5.115	C	3.429	0.954	0.910	H	5.055	1.088	8.471
H	-4.546	2.446	6.318	H	3.877	2.393	3.433	H	6.738	0.629	8.577
H	10.659	9.675	9.825	H	3.776	4.883	3.542	H	6.302	2.307	8.358
H	10.573	1.514	8.109	H	3.292	6.228	1.513	C	11.587	11.312	4.821
H	7.122	1.029	6.246	H	2.894	5.124	-0.688	H	12.071	12.193	4.454
H	1.398	2.111	7.751	H	3.073	-0.019	-1.056	H	12.071	10.986	5.718
C	10.242	4.684	4.018	N	2.981	2.199	-0.971	C	10.109	11.624	5.119
C	10.921	5.067	2.695	H	2.775	2.352	-1.937	C	9.638	11.578	6.431
H	9.983	5.299	2.182	C	3.682	-0.234	1.857	C	9.242	11.953	4.077
O	9.360	3.833	4.243	H	4.492	0.001	2.515	C	8.299	11.862	6.702
N	10.689	9.151	4.003	H	2.800	-0.427	2.431	H	10.322	11.319	7.252
H	9.714	9.366	3.861	C	4.039	-1.483	1.030	C	7.903	12.237	4.348
C	11.673	10.199	3.759	H	4.215	-2.309	1.687	H	9.613	11.990	3.043
H	11.522	10.639	2.768	H	3.229	-1.718	0.371	C	7.431	12.191	5.660
H	12.664	9.745	3.806	H	4.921	-1.291	0.455	H	7.927	11.826	7.736
H	9.217	6.915	3.795	C	-1.902	-1.565	0.710	H	7.219	12.497	3.526
C	-5.134	1.312	5.146	H	-2.760	-1.631	1.345	O	6.059	12.481	5.937
H	-5.307	1.364	6.174	H	-2.130	-0.954	-0.138	H	5.958	13.421	6.106
C	-5.992	2.307	4.369	H	-1.626	-2.545	0.380	O	4.178	8.956	8.629
N	-4.984	0.075	4.566	C	-0.732	-0.940	1.493	C	4.590	8.926	9.999
H	-4.040	-0.191	4.369	H	-0.890	-1.079	2.542	H	5.115	8.014	10.193
H	-5.384	-0.574	5.213	H	0.184	-1.412	1.204	C	5.518	10.123	10.281
O	-7.271	2.192	4.580	C	-0.652	0.566	1.181	H	6.131	10.309	9.425
N	-5.534	3.191	3.476	H	-1.492	1.066	1.617	C	3.352	9.010	10.909
H	-4.727	3.743	3.686	C	0.649	1.144	1.767	H	2.489	8.677	10.371
C	-6.158	3.338	2.301	H	1.451	0.989	1.076	C	2.328	10.891	10.799
H	-6.907	4.097	2.387	H	0.527	2.192	1.943	H	1.830	11.614	10.188
C	-6.819	2.007	1.899	H	0.874	0.652	2.691	C	3.505	11.563	11.532
C	-6.876	0.951	2.820	C	-0.666	0.776	-0.344	H	3.587	12.582	11.215
H	-6.321	1.211	3.697	H	-1.374	0.109	-0.790	H	3.331	11.531	12.588
H	-7.896	0.765	3.085	H	-0.941	1.787	-0.563	O	4.668	11.370	10.585
H	-6.456	0.071	2.380	H	0.309	0.578	-0.740	O	3.547	8.181	12.057
O	-7.322	1.865	0.708	C	11.194	6.663	2.575	H	3.004	8.502	12.781
C	-5.135	3.748	1.225	H	10.237	7.135	2.489	N	1.383	10.346	11.784
H	-4.772	2.874	0.727	H	11.701	7.040	3.439	H	1.888	10.000	12.574
H	-5.605	4.394	0.514	C	12.035	6.717	1.286	C	0.463	11.408	12.218
C	-3.958	4.487	1.889	H	12.392	7.714	1.135	C	-0.428	11.171	13.274
C	-3.776	5.932	1.886	H	11.430	6.425	0.453	H	-1.433	11.289	12.926
C	-2.884	3.911	2.593	C	12.667	5.181	1.558	H	-0.292	10.174	13.638
C	-2.558	6.207	2.613	H	13.043	4.571	0.763	H	-0.240	11.868	14.063
C	-4.519	6.965	1.351	H	13.479	5.503	2.175	O	0.479	12.564	11.622
H	-2.744	2.842	2.764	N	11.672	4.365	2.404	C	6.412	9.803	11.494

H	5.832	9.308	12.245	H	7.592	10.814	12.706	H	9.387	0.682	0.019
H	7.215	9.166	11.187	C	9.781	0.140	0.852	H	9.984	0.825	2.957
O	6.945	11.018	12.027	H	9.734	-0.923	0.742	H	8.426	0.018	2.610

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C	6.088	1.110	6.587	H	11.781	5.722	6.555	H	4.326	3.812	6.195
H	5.559	0.184	6.347	C	-4.252	2.416	5.251	H	3.411	5.497	5.138
C	5.411	2.267	5.894	H	-4.844	3.157	4.735	H	-4.546	2.446	6.318
O	5.543	2.488	4.694	C	-2.903	2.279	4.944	H	10.731	9.808	9.807
O	4.663	3.013	6.700	O	-2.443	1.028	4.812	H	11.062	1.386	7.938
C	4.474	4.411	11.010	O	-2.205	3.275	4.839	H	7.122	1.029	6.246
H	3.510	4.760	11.382	C	0.976	1.872	6.579	H	1.444	1.852	7.569
H	5.266	4.616	11.734	H	1.490	1.142	5.943	C	10.242	4.684	4.018
C	4.784	5.044	9.666	H	-0.065	1.546	6.669	C	10.921	5.067	2.695
O	6.047	5.123	9.353	C	1.047	3.242	5.991	H	9.983	5.299	2.182
O	3.863	5.433	8.930	N	-0.007	3.795	5.289	O	9.360	3.833	4.243
C	10.059	1.282	8.364	H	-0.863	3.276	5.294	N	10.689	9.151	4.003
H	9.673	0.296	8.079	C	0.373	5.009	4.930	H	9.714	9.366	3.861
H	10.144	1.307	9.453	H	-0.243	5.732	4.418	C	11.673	10.199	3.759
C	9.166	2.378	7.890	N	1.668	5.267	5.333	H	11.522	10.639	2.768
N	9.053	2.699	6.540	H	2.133	6.826	6.268	H	12.664	9.745	3.806
H	9.784	2.480	5.858	C	2.088	4.136	6.026	H	9.217	6.915	3.795
C	8.216	3.748	6.428	H	3.070	4.062	6.459	C	-5.134	1.312	5.146
H	7.934	4.204	5.501	Zn	6.661	5.695	7.604	H	-5.307	1.364	6.174
N	7.766	4.114	7.614	C	2.599	8.664	8.783	C	-5.992	2.307	4.369
C	8.337	3.258	8.543	O	1.805	9.764	9.234	N	-4.984	0.075	4.566
H	8.098	3.338	9.592	C	0.380	9.529	9.235	H	-4.040	-0.191	4.369
C	9.830	9.483	10.341	C	-0.018	8.676	10.447	H	-5.384	-0.574	5.213
H	10.137	8.781	11.121	H	0.578	8.933	11.336	O	-7.271	2.192	4.580
H	9.387	10.358	10.832	H	0.191	7.622	10.230	N	-5.534	3.191	3.476
C	8.849	8.826	9.428	O	-1.404	8.802	10.701	H	-4.727	3.743	3.686
N	8.266	9.477	8.350	H	-1.611	9.744	10.603	C	-6.158	3.338	2.301
H	8.388	10.453	8.118	H	-0.042	10.525	9.414	H	-6.907	4.097	2.387
C	7.398	8.634	7.746	H	2.513	7.792	9.450	C	-6.819	2.007	1.899
H	6.753	8.882	6.917	C	2.235	8.291	7.331	C	-6.876	0.951	2.820
N	7.392	7.467	8.375	N	2.985	7.069	6.867	H	-6.321	1.211	3.697
C	8.302	7.568	9.413	H	3.378	6.591	7.786	H	-7.896	0.765	3.085
H	8.451	6.749	10.100	C	5.202	6.367	5.176	H	-6.456	0.071	2.380
N	8.768	1.735	1.692	O	6.218	6.311	5.783	O	-7.322	1.865	0.708
H	8.823	1.737	0.686	C	4.728	7.393	4.241	C	-5.135	3.748	1.225
C	7.816	2.484	2.270	H	5.108	8.400	4.435	H	-4.772	2.874	0.727
N	7.514	2.338	3.554	H	3.671	7.470	3.975	H	-5.605	4.394	0.514
H	7.632	1.436	3.997	H	5.262	6.973	3.389	C	-3.958	4.487	1.889
H	6.761	2.912	3.979	H	2.328	9.218	6.754	C	-3.776	5.932	1.886
N	7.155	3.407	1.542	C	0.747	7.889	7.282	C	-2.884	3.911	2.593
H	7.508	3.745	0.661	O	0.484	6.632	7.913	C	-2.558	6.207	2.613
H	6.338	3.851	1.938	H	1.034	6.554	8.706	C	-4.519	6.965	1.351
N	10.343	5.629	5.032	H	0.434	7.758	6.241	H	-2.744	2.842	2.764
C	9.854	6.954	4.687	C	-0.120	9.021	7.870	C	-2.120	7.507	2.780
C	11.031	7.914	4.457	H	-1.151	8.648	7.975	C	-4.060	8.281	1.528
O	12.183	7.563	4.676	O	-0.062	10.067	6.897	H	-5.448	6.773	0.797
C	9.072	7.361	5.948	C	-1.191	10.926	6.899	C	-2.888	8.546	2.226
H	8.078	6.912	5.929	H	-1.039	11.657	6.100	H	-1.196	7.733	3.328
H	8.942	8.442	6.021	H	-1.306	11.468	7.850	H	-4.643	9.112	1.106
C	9.932	6.792	7.093	H	-2.122	10.372	6.702	H	-2.550	9.586	2.353
H	9.312	6.493	7.941	O	6.114	5.127	3.401	N	-2.018	4.924	3.044
H	10.642	7.548	7.443	H	5.269	4.790	3.779	H	-1.178	4.788	3.571
C	10.698	5.597	6.472	H	6.328	5.780	4.097	C	3.161	3.138	0.130
H	10.429	4.646	6.919	O	4.427	5.300	5.179	C	3.443	2.354	1.313

C	3.661	2.975	2.526	H	11.701	7.040	3.439	H	7.219	12.497	3.526
C	3.603	4.377	2.581	C	12.035	6.717	1.286	O	6.059	12.481	5.937
C	3.332	5.130	1.444	H	12.392	7.714	1.135	H	5.958	13.421	6.106
C	3.107	4.515	0.202	H	11.430	6.425	0.453	O	3.959	9.095	8.881
C	3.149	0.896	-0.468	C	12.667	5.181	1.558	C	4.371	9.065	10.251
C	3.429	0.954	0.910	H	13.043	4.571	0.763	H	4.896	8.153	10.445
H	3.877	2.393	3.433	H	13.479	5.503	2.175	C	5.299	10.262	10.533
H	3.776	4.883	3.542	N	11.672	4.365	2.404	H	5.912	10.448	9.677
H	3.292	6.228	1.513	C	11.192	2.976	2.422	C	3.133	9.149	11.161
H	2.894	5.124	-0.688	O	10.685	2.479	3.513	H	2.270	8.816	10.623
H	3.073	-0.019	-1.056	C	11.282	2.191	1.265	C	2.109	11.030	11.051
N	2.981	2.199	-0.971	H	12.262	2.284	0.846	H	1.611	11.753	10.440
H	2.775	2.352	-1.937	C	11.150	0.631	1.283	C	3.286	11.702	11.784
C	3.682	-0.234	1.857	H	11.522	0.252	2.212	H	3.368	12.721	11.467
H	4.492	0.001	2.515	H	11.715	0.215	0.476	H	3.112	11.670	12.840
H	2.800	-0.427	2.431	C	9.212	0.641	2.239	O	4.449	11.509	10.837
C	4.039	-1.483	1.030	N	10.286	2.646	0.286	O	3.328	8.320	12.309
H	4.215	-2.309	1.687	H	10.307	3.645	0.228	H	2.785	8.641	13.033
H	3.229	-1.718	0.371	H	10.498	2.258	-0.610	N	1.164	10.485	12.036
H	4.921	-1.291	0.455	C	4.391	2.885	10.820	H	1.669	10.139	12.826
C	-1.902	-1.565	0.710	H	5.378	2.471	10.823	C	0.244	11.547	12.470
H	-2.760	-1.631	1.345	H	3.822	2.456	11.619	C	-0.647	11.310	13.526
H	-2.130	-0.954	-0.138	H	3.916	2.667	9.886	H	-1.652	11.428	13.178
H	-1.626	-2.545	0.380	C	6.042	1.298	8.115	H	-0.511	10.313	13.890
C	-0.732	-0.940	1.493	H	5.055	1.088	8.471	H	-0.459	12.007	14.315
H	-0.890	-1.079	2.542	H	6.738	0.629	8.577	O	0.260	12.703	11.874
H	0.184	-1.412	1.204	H	6.302	2.307	8.358	C	6.193	9.942	11.746
C	-0.652	0.566	1.181	C	11.587	11.312	4.821	H	5.613	9.447	12.497
H	-1.492	1.066	1.617	H	12.071	12.193	4.454	H	6.996	9.305	11.439
C	0.649	1.144	1.767	H	12.071	10.986	5.718	O	6.726	11.157	12.279
H	1.451	0.989	1.076	C	10.109	11.624	5.119	H	7.373	10.953	12.958
H	0.527	2.192	1.943	C	9.638	11.578	6.431	C	9.781	0.140	0.852
H	0.874	0.652	2.691	C	9.242	11.953	4.077	H	9.734	-0.923	0.742
C	-0.666	0.776	-0.344	C	8.299	11.862	6.702	H	9.387	0.682	0.019
H	-1.374	0.109	-0.790	H	10.322	11.319	7.252	H	9.984	0.825	2.957
H	-0.941	1.787	-0.563	C	7.903	12.237	4.348	H	8.426	0.018	2.610
H	0.309	0.578	-0.740	H	9.613	11.990	3.043				
C	11.194	6.663	2.575	C	7.431	12.191	5.660				
H	10.237	7.135	2.489	H	7.927	11.826	7.736				