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SUPPORTING INFORMATION

The effect of hydrogen bonding on the π depletion and the $\pi - \pi$ stacking interaction†

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Contents

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S1 Cartesian Coordinates

S1.1 Benzene probe

Benzene

```
12
Energy = -231.8361423087
C     1.2056126   -0.6960608   -0.0000051
H     2.1440920   -1.2378921    0.0000051
C     1.2056126    0.6960608   -0.0000051
H     2.1440920    1.2378921    0.0000051
C     0.0000000    1.3921216   -0.0000051
H     0.0000000    2.4757842    0.0000051
C    -1.2056126    0.6960608   -0.0000051
H    -2.1440920    1.2378921    0.0000051
C    -1.2056126   -0.6960608   -0.0000051
H    -2.1440920   -1.2378921    0.0000051
C    -0.0000000   -1.3921216   -0.0000051
H     0.0000000   -2.4757842    0.0000051
```

S1.2 Dimers with benzene probe

The DADA01 dimer with the benzene probe

```
50
Energy = -1584.1670920650
C          0.97944        4.27963        0.00000
N         -0.15844        3.57207        0.00000
C          2.22299        3.69493        0.00000
C         -0.03201        2.24043        0.00000
C          2.24927        2.28843        0.00000
N          1.11633        1.55968        0.00000
N          3.40640        1.55569        0.00000
C          4.70278        2.02843        0.00000
O          5.04750        3.19027        0.00000
N         -1.18990        1.49275        0.00000
C         -2.50226        1.96404        0.00000
O         -3.43426        1.17386        0.00000
H          5.41605        1.19113        0.00000
H          0.86737        5.35742        0.00000
H          3.13761        4.26312        0.00000
H         -1.09949        0.47056        0.00000
H          3.30899        0.52445        0.00000
O         -2.68114        3.26556        0.00000
H         -1.76794        3.70601        0.00000
O          3.43426       -1.17386        0.00000
C          2.50226       -1.96404        0.00000
N          1.18990       -1.49275        0.00000
O          2.68114       -3.26556        0.00000
C          0.03201       -2.24043        0.00000
N         -1.11633       -1.55968        0.00000
N          0.15844       -3.57207        0.00000
H          1.76794       -3.70601        0.00000
C         -2.24927       -2.28843        0.00000
N         -3.40640       -1.55569        0.00000
C         -0.97944       -4.27963        0.00000
C         -2.22299       -3.69493        0.00000
C         -4.70278       -2.02843        0.00000
H         -5.41605       -1.19113        0.00000
O         -5.04750       -3.19027        0.00000
H         -0.86737       -5.35742        0.00000
H         -3.13761       -4.26312        0.00000
```

```
H          1.09949        -0.47056        0.00000
H         -3.30899        -0.52445        0.00000
C          2.45404         2.09843        3.7999949
H          3.39252         1.55659        3.8000051
C          2.45404         3.49055        3.7999949
H          3.39252         4.03238        3.8000051
C          1.24842         4.18661        3.7999949
H          1.24842         5.27027        3.8000051
C          0.04281         3.49055        3.7999949
H         -0.89567         4.03238        3.8000051
C          0.04281         2.09843        3.7999949
H         -0.89567         1.55659        3.8000051
C          1.24842         1.40237        3.7999949
H          1.24842         0.31870        3.8000051
```

The DADA02 dimer with the benzene probe

```
46
Energy = -1350.1108413893
C          4.02811         1.51915        0.00000
N          3.31953         2.62903        0.00000
N          3.55464         0.26633        0.00000
C          1.96898         2.43917        0.00000
C          2.20862         0.17300        0.00000
N          1.37322         1.22028        0.00000
N          1.20311         3.52702        0.00000
N          1.62439        -1.06904        0.00000
C          2.22691        -2.33689        0.00000
O          1.51666        -3.34741        0.00000
N          3.57025        -2.38291        0.00000
H          5.11973         1.62295        0.00000
H          1.67928         4.42096        0.00000
H          0.16575         3.46724        0.00000
H          4.09060        -1.49607        0.00000
H          3.99934        -3.29944        0.00000
H          0.58463        -1.08849        0.00000
N         -1.37318        -1.22022        0.00000
C         -2.20861        -0.17297        0.00000
C         -1.96891        -2.43913        0.00000
N         -3.55464        -0.26636        0.00000
N         -3.31944        -2.62904        0.00000
C         -4.02807        -1.51920        0.00000
N         -1.20306        -3.52698        0.00000
N         -1.62442         1.06909        0.00000
C         -2.22698         2.33692        0.00000
O         -1.51678         3.34749        0.00000
N         -3.57032         2.38285        0.00000
H         -5.11969        -1.62304        0.00000
H         -0.58466         1.08856        0.00000
H         -0.16571        -3.46724        0.00000
H         -1.67925        -4.42091        0.00000
H         -4.09059         1.49596        0.00000
H         -3.99947         3.29936        0.00000
C          3.46824         0.10833        3.7999949
H          4.07840        -0.78643        3.8000051
C          4.07101         1.36308        3.7999949
H          5.15038         1.44506        3.8000051
C          3.28717         2.51252        3.7999949
H          3.75638         3.48926        3.8000051
C          1.90057         2.40721        3.7999949
H          1.29041         3.30197        3.8000051
C          1.29780         1.15246        3.7999949
H          0.21843         1.07048        3.8000051
C          2.08163         0.00302        3.7999949
```

```
H          1.61242        -0.97372        3.8000051
```

The DADA03 dimer with the benzene probe

```
48
Energy = -1318.0018755226
C          4.15495         1.49042        0.00000
C          3.39911         2.62877        0.00000
N          3.62757         0.25377        0.00000
C          1.99093         2.46276        0.00000
C          2.29171         0.19409        0.00000
N          1.44228         1.22970        0.00000
N          1.16807         3.51606        0.00000
N          1.68719        -1.04962        0.00000
C          2.26860        -2.31461        0.00000
O          1.54839        -3.31986        0.00000
N          3.60887        -2.38435        0.00000
H          5.23885         1.53999        0.00000
H          1.56043         4.44064        0.00000
H          0.14299         3.40400        0.00000
H          4.13877        -1.51248        0.00000
H          4.01887        -3.30126        0.00000
H          0.66224        -1.05572        0.00000
N         -1.44228        -1.22970        0.00000
C         -2.29171        -0.19409        0.00000
C         -1.99093        -2.46276        0.00000
N         -3.62757        -0.25377        0.00000
C         -3.39911        -2.62877        0.00000
C         -4.15495        -1.49042        0.00000
N         -1.16807        -3.51606        0.00000
N         -1.68719         1.04962        0.00000
C         -2.26860         2.31461        0.00000
O         -1.54839         3.31986        0.00000
N         -3.60887         2.38435        0.00000
H         -5.23885        -1.53999        0.00000
H         -0.66224         1.05572        0.00000
H         -0.14299        -3.40400        0.00000
H         -1.56043        -4.44064        0.00000
H         -4.13877         1.51248        0.00000
H         -4.01887         3.30126        0.00000
H          3.84733         3.61305        0.00000
H         -3.84733        -3.61305        0.00000
C          2.20378         0.09028        3.7999949
H          1.71014        -0.87442        3.8000051
C          3.59398         0.16086        3.7999949
H          4.18251        -0.74890        3.8000051
C          4.22813         1.40015        3.7999949
H          5.31030         1.45509        3.8000051
C          3.47207         2.56887        3.7999949
H          3.96571         3.53357        3.8000051
C          2.08187         2.49829        3.7999949
H          1.49334         3.40805        3.8000051
C          1.44772         1.25900        3.7999949
H          0.36555         1.20406        3.8000051
```

The DADA04 dimer with the benzene probe

```
48
Energy = -1433.7786563013
C          1.02833         4.23793        0.00000
N         -0.12201         3.55566        0.00000
C          2.27449         3.64333        0.00000
C          0.00878         2.23241        0.00000
C          2.28893         2.24211        0.00000
N          1.14483         1.53060        0.00000
```

```
H          0.93653        5.31882        0.00000
H          3.19254        4.20622        0.00000
N         -1.15730        1.47302        0.00000
C         -2.41111        1.99823        0.00000
O         -3.42118        1.30420        0.00000
H         -2.43865        3.09121        0.00000
N          3.43897        1.48731        0.00000
C          4.73975        1.94018        0.00000
H          5.44199        1.09273        0.00000
O          5.10243        3.09706        0.00000
N         -1.14483       -1.53060        0.00000
C         -2.28893       -2.24211        0.00000
C         -0.00878       -2.23241        0.00000
C         -2.27449       -3.64333        0.00000
N          0.12201       -3.55566        0.00000
C         -1.02833       -4.23793        0.00000
H         -0.93653       -5.31882        0.00000
H         -3.19254       -4.20622        0.00000
N         -3.43897       -1.48731        0.00000
C         -4.73975       -1.94018        0.00000
H         -5.44199       -1.09273        0.00000
O         -5.10243       -3.09706        0.00000
N          1.15730       -1.47302        0.00000
C          2.41111       -1.99823        0.00000
O          3.42118       -1.30420        0.00000
H          2.43865       -3.09121        0.00000
H         -3.32801       -0.46096        0.00000
H          1.07665       -0.44559        0.00000
H         -1.07665        0.44559        0.00000
H          3.32801        0.46096        0.00000
C          2.44139        2.01020        3.7999949
H          3.37987        1.46837        3.8000051
C          2.44139        3.40232        3.7999949
H          3.37987        3.94416        3.8000051
C          1.23578        4.09838        3.7999949
H          1.23578        5.18205        3.8000051
C          0.03017        3.40232        3.7999949
H         -0.90831        3.94416        3.8000051
C          0.03017        2.01020        3.7999949
H         -0.90831        1.46837        3.8000051
C          1.23578        1.31414        3.7999949
H          1.23578        0.23048        3.8000051
```

The DADA05-R dimer with the benzene probe

```
54
Energy = -1612.8900918941
C          1.17978        4.23058        0.00000
N         -0.03815        3.67666        0.00000
C          2.39058        3.55939        0.00000
C          0.01768        2.33751        0.00000
C          2.33018        2.14663        0.00000
N          1.11401        1.55598        0.00000
N          3.43383        1.40542        0.00000
N         -1.17698        1.63361        0.00000
C         -2.48322        2.10722        0.00000
O         -3.43008        1.31231        0.00000
N         -2.66799        3.43865        0.00000
N         -1.11401       -1.55598        0.00000
C         -2.33018       -2.14663        0.00000
C         -0.01768       -2.33751        0.00000
C         -2.39058       -3.55939        0.00000
N          0.03815       -3.67666        0.00000
C         -1.17978       -4.23058        0.00000
```

```
N          1.17698        -1.63361        0.00000
C          2.48322        -2.10722        0.00000
O          3.43008        -1.31231        0.00000
N          2.66799        -3.43865        0.00000
N         -3.43383        -1.40542        0.00000
N          1.51484         5.56179        0.00000
N          3.45622         4.44152        0.00000
C          2.89628         5.62240        0.00000
H          3.41883         6.56597        0.00000
N         -3.45622        -4.44152        0.00000
N         -1.51484        -5.56179        0.00000
C         -2.89628        -5.62240        0.00000
H         -3.41883        -6.56597        0.00000
H         -1.85232         4.04596        0.00000
H         -3.61782         3.76484        0.00000
H         -1.09569         0.61329        0.00000
H          0.87409         6.33854        0.00000
H          4.31784         1.88602        0.00000
H          3.40133         0.37529        0.00000
H          1.09569        -0.61329        0.00000
H         -3.40133        -0.37529        0.00000
H         -4.31784        -1.88602        0.00000
H         -0.87409        -6.33854        0.00000
H          1.85232        -4.04596        0.00000
H          3.61782        -3.76484        0.00000
C          2.25097         2.01795        3.7999949
H          3.17527         1.45253        3.8000051
C          2.28586         3.40953        3.7999949
H          3.23732         3.92735        3.8000051
C          1.09846         4.13590        3.7999949
H          1.12561         5.21914        3.8000051
C         -0.12384         3.47069        3.7999949
H         -1.04814         4.03611        3.8000051
C         -0.15873         2.07911        3.7999949
H         -1.11019         1.56129        3.8000051
C          1.02868         1.35274        3.7999949
H          1.00152         0.26950        3.8000051
```

The DADA05-L dimer with the benzene probe

```
54
Energy = -1612.8880350908
C          1.17978         4.23058        0.00000
N         -0.03815         3.67666        0.00000
C          2.39058         3.55939        0.00000
C          0.01768         2.33751        0.00000
C          2.33018         2.14663        0.00000
N          1.11401         1.55598        0.00000
N          3.43383         1.40542        0.00000
N         -1.17698         1.63361        0.00000
C         -2.48322         2.10722        0.00000
O         -3.43008         1.31231        0.00000
N         -2.66799         3.43865        0.00000
N         -1.11401        -1.55598        0.00000
C         -2.33018        -2.14663        0.00000
C         -0.01768        -2.33751        0.00000
C         -2.39058        -3.55939        0.00000
N          0.03815        -3.67666        0.00000
C         -1.17978        -4.23058        0.00000
N          1.17698        -1.63361        0.00000
C          2.48322        -2.10722        0.00000
O          3.43008        -1.31231        0.00000
N          2.66799        -3.43865        0.00000
N         -3.43383        -1.40542        0.00000
```

```
N          1.51484        5.56179        0.00000
N          3.45622        4.44152        0.00000
C          2.89628        5.62240        0.00000
H          3.41883        6.56597        0.00000
N         -3.45622       -4.44152        0.00000
N         -1.51484       -5.56179        0.00000
C         -2.89628       -5.62240        0.00000
H         -3.41883       -6.56597        0.00000
H         -1.85232        4.04596        0.00000
H         -3.61782        3.76484        0.00000
H         -1.09569        0.61329        0.00000
H          0.87409        6.33854        0.00000
H          4.31784        1.88602        0.00000
H          3.40133        0.37529        0.00000
H          1.09569       -0.61329        0.00000
H         -3.40133       -0.37529        0.00000
H         -4.31784       -1.88602        0.00000
H         -0.87409       -6.33854        0.00000
H          1.85232       -4.04596        0.00000
H          3.61782       -3.76484        0.00000
C          3.49856        3.82236        3.7999949
H          4.42286        3.25694        3.8000051
C          3.53345        5.21394        3.7999949
H          4.48491        5.73176        3.8000051
C          2.34605        5.94031        3.7999949
H          2.37320        7.02355        3.8000051
C          1.12375        5.27510        3.7999949
H          0.19945        5.84052        3.8000051
C          1.08886        3.88352        3.7999949
H          0.13740        3.36570        3.8000051
C          2.27627        3.15715        3.7999949
H          2.24911        2.07391        3.8000051
```

The DADA06-R dimer with the benzene probe

```
88
Energy = -2504.7891683260
C         -5.51368        1.74136       -2.73635
C         -6.83727        1.92793       -3.11575
C         -5.09548        0.50265       -2.24342
C         -7.75003        0.88350       -3.00058
C         -6.01223       -0.54533       -2.14030
C         -7.33535       -0.35302       -2.51238
C         -3.68937        0.23038       -1.84170
N         -2.99912        1.30135       -1.39601
N         -1.68682        1.21300       -1.00233
C         -1.13444        2.36964       -0.58707
C          0.27355        2.20022       -0.04964
N          0.68459        3.29555        0.58847
N          1.91370        3.39174        1.18644
C          2.24325        4.64487        1.63133
C          3.51740        4.80077        2.38024
C          4.00976        6.10204        2.51429
C          4.20555        3.73658        2.96753
C          5.18597        6.33482        3.21258
C          5.37975        3.97672        3.67220
C          5.87400        5.27184        3.79310
O         -3.18391       -0.89348       -1.89404
O         -1.71808        3.45207       -0.63989
O          0.92831        1.16336       -0.17808
O          1.49236        5.58751        1.38826
H         -7.15368        2.88577       -3.50947
H         -8.78148        1.03198       -3.29612
H         -4.80524        2.55244       -2.86008
```

H	-5.67387	-1.50064	-1.76207
H	-8.04336	-1.16763	-2.42135
H	3.45104	6.91234	2.06494
H	5.56548	7.34484	3.30828
H	6.78927	5.45393	4.34359
H	3.83159	2.72420	2.89091
H	5.90385	3.14794	4.13287
C	-3.51740	-4.80077	-2.38024
C	-4.20555	-3.73658	-2.96753
C	-4.00976	-6.10204	-2.51429
C	-5.37975	-3.97672	-3.67220
C	-5.18597	-6.33482	-3.21258
C	-5.87400	-5.27184	-3.79310
C	-2.24325	-4.64487	-1.63133
N	-1.91370	-3.39174	-1.18644
N	-0.68459	-3.29555	-0.58847
C	-0.27355	-2.20022	0.04964
C	1.13444	-2.36964	0.58707
N	1.68682	-1.21300	1.00233
N	2.99912	-1.30135	1.39601
C	3.68937	-0.23038	1.84170
O	-1.49236	-5.58751	-1.38826
O	-0.92831	-1.16336	0.17808
O	1.71808	-3.45207	0.63989
O	3.18391	0.89348	1.89404
C	5.09548	-0.50265	2.24342
C	6.01223	0.54533	2.14030
C	5.51368	-1.74136	2.73635
C	7.33535	0.35302	2.51238
C	6.83727	-1.92793	3.11575
C	7.75003	-0.88350	3.00058
H	-5.90385	-3.14794	-4.13287
H	-6.78927	-5.45393	-4.34359
H	-3.45104	-6.91234	-2.06494
H	-5.56548	-7.34484	-3.30828
H	-3.83159	-2.72420	-2.89091
H	5.67387	1.50064	1.76207
H	8.04336	1.16763	2.42135
H	8.78148	-1.03198	3.29612
H	4.80524	-2.55244	2.86008
H	7.15368	-2.88577	3.50947
H	-3.37835	2.23380	-1.27765
H	-1.33600	0.28123	-0.73106
H	0.15919	4.16779	0.58479
H	2.39549	2.50905	1.36820
H	-2.39549	-2.50905	-1.36820
H	-0.15919	-4.16779	-0.58479
H	1.33600	-0.28123	0.73106
H	3.37835	-2.23380	1.27765
C	-6.28487	1.60254	1.21514
H	-5.25412	1.44306	1.50916
C	-6.68674	2.84486	0.73228
H	-5.96880	3.65244	0.65043
C	-8.01088	3.04971	0.35456
H	-8.32371	4.01676	-0.02130
C	-8.93318	2.01225	0.45972
H	-9.96393	2.17171	0.16571
C	-8.53132	0.76993	0.94258
H	-9.24925	-0.03766	1.02445
C	-7.20718	0.56507	1.32029
H	-6.89435	-0.40198	1.69617

The DADA06-L dimer with the benzene probe

```
88
Energy = -2504.7884962994
C         -5.51368        1.74136       -2.73635
C         -6.83727        1.92793       -3.11575
C         -5.09548        0.50265       -2.24342
C         -7.75003        0.88350       -3.00058
C         -6.01223       -0.54533       -2.14030
C         -7.33535       -0.35302       -2.51238
C         -3.68937        0.23038       -1.84170
N         -2.99912        1.30135       -1.39601
N         -1.68682        1.21300       -1.00233
C         -1.13444        2.36964       -0.58707
C          0.27355        2.20022       -0.04964
N          0.68459        3.29555        0.58847
N          1.91370        3.39174        1.18644
C          2.24325        4.64487        1.63133
C          3.51740        4.80077        2.38024
C          4.00976        6.10204        2.51429
C          4.20555        3.73658        2.96753
C          5.18597        6.33482        3.21258
C          5.37975        3.97672        3.67220
C          5.87400        5.27184        3.79310
O         -3.18391       -0.89348       -1.89404
O         -1.71808        3.45207       -0.63989
O          0.92831        1.16336       -0.17808
O          1.49236        5.58751        1.38826
H         -7.15368        2.88577       -3.50947
H         -8.78148        1.03198       -3.29612
H         -4.80524        2.55244       -2.86008
H         -5.67387       -1.50064       -1.76207
H         -8.04336       -1.16763       -2.42135
H          3.45104        6.91234        2.06494
H          5.56548        7.34484        3.30828
H          6.78927        5.45393        4.34359
H          3.83159        2.72420        2.89091
H          5.90385        3.14794        4.13287
C         -3.51740       -4.80077       -2.38024
C         -4.20555       -3.73658       -2.96753
C         -4.00976       -6.10204       -2.51429
C         -5.37975       -3.97672       -3.67220
C         -5.18597       -6.33482       -3.21258
C         -5.87400       -5.27184       -3.79310
C         -2.24325       -4.64487       -1.63133
N         -1.91370       -3.39174       -1.18644
N         -0.68459       -3.29555       -0.58847
C         -0.27355       -2.20022        0.04964
C          1.13444       -2.36964        0.58707
N          1.68682       -1.21300        1.00233
N          2.99912       -1.30135        1.39601
C          3.68937       -0.23038        1.84170
O         -1.49236       -5.58751       -1.38826
O         -0.92831       -1.16336        0.17808
O          1.71808       -3.45207        0.63989
O          3.18391        0.89348        1.89404
C          5.09548       -0.50265        2.24342
C          6.01223        0.54533        2.14030
C          5.51368       -1.74136        2.73635
C          7.33535        0.35302        2.51238
C          6.83727       -1.92793        3.11575
C          7.75003       -0.88350        3.00058
H         -5.90385       -3.14794       -4.13287
H         -6.78927       -5.45393       -4.34359
```

```
H         -3.45104       -6.91234       -2.06494
H         -5.56548       -7.34484       -3.30828
H         -3.83159       -2.72420       -2.89091
H          5.67387        1.50064        1.76207
H          8.04336        1.16763        2.42135
H          8.78148       -1.03198        3.29612
H          4.80524       -2.55244        2.86008
H          7.15368       -2.88577        3.50947
H         -3.37835        2.23380       -1.27765
H         -1.33600        0.28123       -0.73106
H          0.15919        4.16779        0.58479
H          2.39549        2.50905        1.36820
H         -2.39549       -2.50905       -1.36820
H         -0.15919       -4.16779       -0.58479
H          1.33600       -0.28123        0.73106
H          3.37835       -2.23380        1.27765
C          4.12220        5.48708        7.14498
H          5.04572        5.61463        7.69740
C          3.48110        6.59401        6.59571
H          3.90557        7.58323        6.72056
C          2.29470        6.43014        5.88606
H          1.79564        7.29180        5.45850
C          1.74940        5.15934        5.72568
H          0.82587        5.03178        5.17328
C          2.39049        4.05241        6.27495
H          1.96602        3.06318        6.15012
C          3.57689        4.21628        6.98460
H          4.07594        3.35461        7.41217
```

The DADA07-R dimer with the benzene probe

```
84
Energy = -2542.7571823282
C         -2.79126        4.87350       -0.46473
C         -3.97296        4.05446       -0.31267
C         -1.52798        4.13181       -0.30023
C         -3.89298        2.71186       -0.05798
C         -1.52029        2.75161       -0.03743
N         -2.71188        2.06653        0.07957
C         -0.31627        4.81822       -0.39901
C          0.88682        4.16134       -0.23903
C          0.90561        2.75928        0.02161
C         -0.29866        2.08333        0.11184
C          2.13473        1.92859        0.21975
N          3.29027        2.60054        0.27938
N          4.49711        1.98675        0.47781
C          5.59595        2.79390        0.45679
C          6.91196        2.10137        0.69010
H          6.80419        1.02399        0.80212
H          7.36947        2.52070        1.58763
H          7.57204        2.32100       -0.15005
O          2.07937        0.69320        0.34677
O          5.47717        4.00005        0.26325
O         -2.82637        6.08339       -0.70053
C         -5.09841        1.85761        0.13799
O         -6.26562        2.33445       -0.31666
O         -5.05623        0.78023        0.68696
H         -4.92655        4.56629       -0.35905
H         -0.37459        5.87836       -0.60155
H         -0.28880        1.02174        0.31191
O          2.08370        4.80327       -0.32260
N          2.71188       -2.06653        0.07957
C          1.52029       -2.75161       -0.03743
C          3.89298       -2.71186       -0.05798
```

```
C          1.52798       -4.13181       -0.30023
C          3.97296       -4.05446       -0.31267
C          2.79126       -4.87350       -0.46473
C          5.09841       -1.85761        0.13799
O          6.26562       -2.33445       -0.31666
O          5.05623       -0.78023        0.68696
C          0.29866       -2.08333        0.11184
C         -0.90561       -2.75928        0.02161
C         -0.88682       -4.16134       -0.23903
C          0.31627       -4.81822       -0.39901
C         -2.13473       -1.92859        0.21975
N         -3.29027       -2.60054        0.27938
N         -4.49711       -1.98675        0.47781
C         -5.59595       -2.79390        0.45679
C         -6.91196       -2.10137        0.69010
O         -5.47717       -4.00005        0.26325
O         -2.07937       -0.69320        0.34677
H          4.92655       -4.56629       -0.35905
H          0.37459       -5.87836       -0.60155
H          0.28880       -1.02174        0.31191
O         -2.08370       -4.80327       -0.32260
C         -2.09488       -6.21171       -0.56446
H         -1.63227       -6.43715       -1.52758
H         -3.14552       -6.48795       -0.57526
H         -1.57104       -6.74078        0.23441
C          2.09488        6.21171       -0.56446
H          1.63227        6.43715       -1.52758
H          3.14552        6.48795       -0.57526
H          1.57104        6.74078        0.23441
H         -2.69419        1.05362        0.24718
H          3.35935        3.60774        0.14123
H          4.49800        0.98030        0.62124
H         -4.49800       -0.98030        0.62124
H         -3.35935       -3.60774        0.14123
H          2.69419       -1.05362        0.24718
H         -6.11808        3.16787       -0.78873
H          6.11808       -3.16787       -0.78873
H         -6.80419       -1.02399        0.80212
H         -7.36947       -2.52070        1.58763
H         -7.57204       -2.32100       -0.15005
O          2.82637       -6.08339       -0.70053
C         -1.36578        3.31730        3.65102
H         -0.42728        2.78130        3.73019
C         -1.36613        4.68832        3.40959
H         -0.42791        5.21958        3.30082
C         -2.57177        5.37687        3.30790
H         -2.57205        6.44411        3.11997
C         -3.77705        4.69440        3.44763
H         -4.71555        5.23039        3.36849
C         -3.77670        3.32338        3.68906
H         -4.71492        2.79211        3.79785
C         -2.57107        2.63482        3.79076
H         -2.57079        1.56758        3.97870
```

The DADA07-L dimer with the benzene probe

```
84
Energy = -2542.7560704818
C         -2.79126        4.87350       -0.46473
C         -3.97296        4.05446       -0.31267
C         -1.52798        4.13181       -0.30023
C         -3.89298        2.71186       -0.05798
C         -1.52029        2.75161       -0.03743
N         -2.71188        2.06653        0.07957
```

C	-0.31627	4.81822	-0.39901
C	0.88682	4.16134	-0.23903
C	0.90561	2.75928	0.02161
C	-0.29866	2.08333	0.11184
C	2.13473	1.92859	0.21975
N	3.29027	2.60054	0.27938
N	4.49711	1.98675	0.47781
C	5.59595	2.79390	0.45679
C	6.91196	2.10137	0.69010
H	6.80419	1.02399	0.80212
H	7.36947	2.52070	1.58763
H	7.57204	2.32100	-0.15005
O	2.07937	0.69320	0.34677
O	5.47717	4.00005	0.26325
O	-2.82637	6.08339	-0.70053
C	-5.09841	1.85761	0.13799
O	-6.26562	2.33445	-0.31666
O	-5.05623	0.78023	0.68696
H	-4.92655	4.56629	-0.35905
H	-0.37459	5.87836	-0.60155
H	-0.28880	1.02174	0.31191
O	2.08370	4.80327	-0.32260
N	2.71188	-2.06653	0.07957
C	1.52029	-2.75161	-0.03743
C	3.89298	-2.71186	-0.05798
C	1.52798	-4.13181	-0.30023
C	3.97296	-4.05446	-0.31267
C	2.79126	-4.87350	-0.46473
C	5.09841	-1.85761	0.13799
O	6.26562	-2.33445	-0.31666
O	5.05623	-0.78023	0.68696
C	0.29866	-2.08333	0.11184
C	-0.90561	-2.75928	0.02161
C	-0.88682	-4.16134	-0.23903
C	0.31627	-4.81822	-0.39901
C	-2.13473	-1.92859	0.21975
N	-3.29027	-2.60054	0.27938
N	-4.49711	-1.98675	0.47781
C	-5.59595	-2.79390	0.45679
C	-6.91196	-2.10137	0.69010
O	-5.47717	-4.00005	0.26325
O	-2.07937	-0.69320	0.34677
H	4.92655	-4.56629	-0.35905
H	0.37459	-5.87836	-0.60155
H	0.28880	-1.02174	0.31191
O	-2.08370	-4.80327	-0.32260
C	-2.09488	-6.21171	-0.56446
H	-1.63227	-6.43715	-1.52758
H	-3.14552	-6.48795	-0.57526
H	-1.57104	-6.74078	0.23441
C	2.09488	6.21171	-0.56446
H	1.63227	6.43715	-1.52758
H	3.14552	6.48795	-0.57526
H	1.57104	6.74078	0.23441
H	-2.69419	1.05362	0.24718
H	3.35935	3.60774	0.14123
H	4.49800	0.98030	0.62124
H	-4.49800	-0.98030	0.62124
H	-3.35935	-3.60774	0.14123
H	2.69419	-1.05362	0.24718
H	-6.11808	3.16787	-0.78873
H	6.11808	-3.16787	-0.78873

```
H         -6.80419       -1.02399        0.80212
H         -7.36947       -2.52070        1.58763
H         -7.57204       -2.32100       -0.15005
O          2.82637       -6.08339       -0.70053
C          0.59095        3.22790        3.82617
H          1.52945        2.69190        3.90534
C          0.59060        4.59892        3.58474
H          1.52882        5.13018        3.47597
C         -0.61504        5.28747        3.48305
H         -0.61532        6.35471        3.29512
C         -1.82032        4.60500        3.62278
H         -2.75882        5.14099        3.54364
C         -1.81997        3.23398        3.86421
H         -2.75819        2.70271        3.97300
C         -0.61434        2.54542        3.96591
H         -0.61406        1.47818        4.15385
```

The DADA08 dimer with the benzene probe

```
52
Energy = -1544.4184063595
C     1.0152836    4.3255086    0.0000000
N    -0.1406299    3.6501668    0.0000000
C     2.2488753    3.7191610    0.0000000
C    -0.0401174    2.3171815    0.0000000
C     2.2429087    2.3142826    0.0000000
N     1.0974774    1.6094095    0.0000000
N     3.3893313    1.5596491    0.0000000
C     4.6902465    2.0063334    0.0000000
O     5.0658438    3.1605825    0.0000000
N    -1.1997261    1.5662250    0.0000000
C    -2.5275576    1.9873385    0.0000000
O    -3.4299841    1.1417363    0.0000000
H     5.3863987    1.1539695    0.0000000
H     0.9299469    5.4067309    0.0000000
H     3.1752012    4.2680398    0.0000000
H    -1.0896542    0.5496190    0.0000000
H     3.2753227    0.5285757    0.0000000
N    -2.7667894    3.3055080    0.0000000
O     3.4299841   -1.1417363    0.0000000
C     2.5275576   -1.9873385    0.0000000
N     1.1997261   -1.5662250    0.0000000
N     2.7667894   -3.3055080    0.0000000
C     0.0401174   -2.3171815    0.0000000
N    -1.0974774   -1.6094095    0.0000000
N     0.1406299   -3.6501668    0.0000000
C    -2.2429087   -2.3142826    0.0000000
N    -3.3893313   -1.5596491    0.0000000
C    -1.0152836   -4.3255086    0.0000000
C    -2.2488753   -3.7191610    0.0000000
C    -4.6902465   -2.0063334    0.0000000
H    -5.3863987   -1.1539695    0.0000000
O    -5.0658438   -3.1605825    0.0000000
H    -0.9299469   -5.4067309    0.0000000
H    -3.1752012   -4.2680398    0.0000000
H     1.0896542   -0.5496190    0.0000000
H    -3.2753227   -0.5285757    0.0000000
H    -1.9737448    3.9449972    0.0000000
H    -3.7281267    3.5978583    0.0000000
H     3.7281267   -3.5978583    0.0000000
H     1.9737448   -3.9449972    0.0000000
C          2.45404        2.09843        3.7999949
H          3.39252        1.55659        3.8000051
C          2.45404        3.49055        3.7999949
```

```
H          3.39252        4.03238        3.8000051
C          1.24842        4.18661        3.7999949
H          1.24842        5.27027        3.8000051
C          0.04281        3.49055        3.7999949
H         -0.89567        4.03238        3.8000051
C          0.04281        2.09843        3.7999949
H         -0.89567        1.55659        3.8000051
C          1.24842        1.40237        3.7999949
H          1.24842        0.31870        3.8000051
```

The DADA09-R dimer with the benzene probe

```
152
Energy = -3590.3828100216
C         -4.95355        4.49483        0.89834
C         -6.13282        3.79583        0.67287
C         -3.72120        3.84860        0.92819
C         -3.66067        2.45504        0.71226
C         -6.09159        2.41403        0.47490
C         -4.85441        1.77317        0.49351
O         -2.55003        4.51684        1.15415
N         -7.22933        1.62299        0.25767
C         -8.49291        2.04342       -0.04687
C         -9.48884        0.91010       -0.23228
C        -10.41328        1.14433       -1.42543
C        -11.46472        0.04549       -1.55483
O         -8.82215        3.21791       -0.16284
C         -2.41327        1.63042        0.65821
N         -1.25340        2.23116        0.96110
C          0.01160        1.55286        0.89664
C          1.10719        2.56109        1.22666
N          2.35477        2.10256        0.95726
C          3.56319        2.79624        1.13045
C          3.69296        3.94140        1.91768
C          4.92976        4.56451        2.02933
C          6.05088        4.07273        1.36803
C          5.93789        2.91245        0.57583
C          4.68977        2.30283        0.47813
C          7.02797        2.26424       -0.22341
N          8.20687        2.91307       -0.31421
C          9.29035        2.47653       -1.17574
C          9.53419        3.41826       -2.36127
C          9.88184        4.83409       -1.90089
O          6.82541        1.18409       -0.79440
O         -2.45074        0.42825        0.34042
O          0.83941        3.66475        1.69042
O          7.27864        4.68152        1.45946
C         -2.59303        5.91822        1.39314
C          7.39254        5.85235        2.26183
C         10.64128        2.83676       -3.24064
H         -5.00814        5.56339        1.05199
H         -7.07998        4.31094        0.64269
H         -4.79875        0.70617        0.33087
H         -7.08762        0.61722        0.35106
H         -8.96589       -0.04270       -0.33143
H        -10.08781        0.85312        0.68420
H        -10.88738        2.12072       -1.31180
H         -9.81369        1.19455       -2.33939
H        -12.08217       -0.01329       -0.65386
H        -10.99776       -0.93301       -1.70155
H        -12.12779        0.22789       -2.40314
H         -1.23544        3.20798        1.23646
H          0.05756        0.72491        1.61267
H          0.18608        1.12303       -0.09110
```

H	2.42085	1.18678	0.50511
H	2.83260	4.34645	2.42595
H	5.00496	5.44950	2.64500
H	4.61139	1.42634	-0.15048
H	8.29033	3.77698	0.20263
H	10.20692	2.39029	-0.58192
H	9.02529	1.48487	-1.53604
H	8.60670	3.45725	-2.94265
H	10.06049	5.48822	-2.75688
H	10.78986	4.82940	-1.28905
H	9.07474	5.27790	-1.31266
H	-3.19106	6.14376	2.28008
H	-2.99988	6.44842	0.52793
H	-1.55927	6.21170	1.55713
H	7.14563	5.63468	3.30379
H	6.74465	6.64766	1.88489
H	8.43349	6.15753	2.18629
H	11.58080	2.76569	-2.68392
H	10.81875	3.46733	-4.11429
H	10.38251	1.83539	-3.59232
C	2.59303	-5.91822	-1.39314
C	-7.39254	-5.85235	-2.26183
C	-4.92976	-4.56451	-2.02933
O	2.55003	-4.51684	-1.15415
C	-3.69296	-3.94140	-1.91768
O	-0.83941	-3.66475	-1.69042
C	4.95355	-4.49483	-0.89834
O	-7.27864	-4.68152	-1.45946
C	3.72120	-3.84860	-0.92819
C	-6.05088	-4.07273	-1.36803
C	6.13282	-3.79583	-0.67287
C	-9.88184	-4.83409	1.90089
C	-1.10719	-2.56109	-1.22666
C	-3.56319	-2.79624	-1.13045
N	1.25340	-2.23116	-0.96110
C	3.66067	-2.45504	-0.71226
N	-2.35477	-2.10256	-0.95726
C	-5.93789	-2.91245	-0.57583
C	-0.01160	-1.55286	-0.89664
C	-4.68977	-2.30283	-0.47813
C	6.09159	-2.41403	-0.47490
C	2.41327	-1.63042	-0.65821
C	-9.53419	-3.41826	2.36127
O	8.82215	-3.21791	0.16284
C	4.85441	-1.77317	-0.49351
C	-7.02797	-2.26424	0.22341
C	8.49291	-2.04342	0.04687
N	7.22933	-1.62299	-0.25767
O	-6.82541	-1.18409	0.79440
N	-8.20687	-2.91307	0.31421
C	-10.64128	-2.83676	3.24064
O	2.45074	-0.42825	-0.34042
C	9.48884	-0.91010	0.23228
C	-9.29035	-2.47653	1.17574
C	10.41328	-1.14433	1.42543
C	11.46472	-0.04549	1.55483
H	2.99988	-6.44842	-0.52793
H	3.19106	-6.14376	-2.28008
H	1.55927	-6.21170	-1.55713
H	-6.74465	-6.64766	-1.88489
H	-7.14563	-5.63468	-3.30379
H	-8.43349	-6.15753	-2.18629

```
H         -5.00496       -5.44950       -2.64500
H         -2.83260       -4.34645       -2.42595
H          5.00814       -5.56339       -1.05199
H          7.07998       -4.31094       -0.64269
H         -9.07474       -5.27790        1.31266
H        -10.78986       -4.82940        1.28905
H        -10.06049       -5.48822        2.75688
H          1.23544       -3.20798       -1.23646
H         -2.42085       -1.18678       -0.50511
H         -0.05756       -0.72491       -1.61267
H         -0.18608       -1.12303        0.09110
H         -4.61139       -1.42634        0.15048
H         -8.60670       -3.45725        2.94265
H          4.79875       -0.70617       -0.33087
H          7.08762       -0.61722       -0.35106
H         -8.29033       -3.77698       -0.20263
H        -11.58080       -2.76569        2.68392
H        -10.38251       -1.83539        3.59232
H        -10.81875       -3.46733        4.11429
H          8.96589        0.04270        0.33143
H         10.08781       -0.85312       -0.68420
H        -10.20692       -2.39029        0.58192
H         -9.02529       -1.48487        1.53604
H         10.88738       -2.12072        1.31180
H          9.81369       -1.19455        2.33939
H         10.99776        0.93301        1.70155
H         12.08217        0.01329        0.65386
H         12.12779       -0.22789        2.40314
C          6.97713        0.93931        3.68589
H          7.90361        0.61935        3.22373
C          6.95646        2.07566        4.48982
H          7.86684        2.64025        4.65346
C          5.76628        2.48671        5.08354
H          5.75017        3.37126        5.70933
C          4.59676        1.76140        4.87333
H          3.67028        2.08138        5.33549
C          4.61744        0.62506        4.06939
H          3.70706        0.06047        3.90576
C          5.80763        0.21401        3.47568
H          5.82581       -0.69406        2.87979
```

The DADA09-L dimer with the benzene probe

```
152
Energy = -3590.3853075899
C         -4.95355        4.49483        0.89834
C         -6.13282        3.79583        0.67287
C         -3.72120        3.84860        0.92819
C         -3.66067        2.45504        0.71226
C         -6.09159        2.41403        0.47490
C         -4.85441        1.77317        0.49351
O         -2.55003        4.51684        1.15415
N         -7.22933        1.62299        0.25767
C         -8.49291        2.04342       -0.04687
C         -9.48884        0.91010       -0.23228
C        -10.41328        1.14433       -1.42543
C        -11.46472        0.04549       -1.55483
O         -8.82215        3.21791       -0.16284
C         -2.41327        1.63042        0.65821
N         -1.25340        2.23116        0.96110
C          0.01160        1.55286        0.89664
C          1.10719        2.56109        1.22666
N          2.35477        2.10256        0.95726
C          3.56319        2.79624        1.13045
```

C	3.69296	3.94140	1.91768
C	4.92976	4.56451	2.02933
C	6.05088	4.07273	1.36803
C	5.93789	2.91245	0.57583
C	4.68977	2.30283	0.47813
C	7.02797	2.26424	-0.22341
N	8.20687	2.91307	-0.31421
C	9.29035	2.47653	-1.17574
C	9.53419	3.41826	-2.36127
C	9.88184	4.83409	-1.90089
O	6.82541	1.18409	-0.79440
O	-2.45074	0.42825	0.34042
O	0.83941	3.66475	1.69042
O	7.27864	4.68152	1.45946
C	-2.59303	5.91822	1.39314
C	7.39254	5.85235	2.26183
C	10.64128	2.83676	-3.24064
H	-5.00814	5.56339	1.05199
H	-7.07998	4.31094	0.64269
H	-4.79875	0.70617	0.33087
H	-7.08762	0.61722	0.35106
H	-8.96589	-0.04270	-0.33143
H	-10.08781	0.85312	0.68420
H	-10.88738	2.12072	-1.31180
H	-9.81369	1.19455	-2.33939
H	-12.08217	-0.01329	-0.65386
H	-10.99776	-0.93301	-1.70155
H	-12.12779	0.22789	-2.40314
H	-1.23544	3.20798	1.23646
H	0.05756	0.72491	1.61267
H	0.18608	1.12303	-0.09110
H	2.42085	1.18678	0.50511
H	2.83260	4.34645	2.42595
H	5.00496	5.44950	2.64500
H	4.61139	1.42634	-0.15048
H	8.29033	3.77698	0.20263
H	10.20692	2.39029	-0.58192
H	9.02529	1.48487	-1.53604
H	8.60670	3.45725	-2.94265
H	10.06049	5.48822	-2.75688
H	10.78986	4.82940	-1.28905
H	9.07474	5.27790	-1.31266
H	-3.19106	6.14376	2.28008
H	-2.99988	6.44842	0.52793
H	-1.55927	6.21170	1.55713
H	7.14563	5.63468	3.30379
H	6.74465	6.64766	1.88489
H	8.43349	6.15753	2.18629
H	11.58080	2.76569	-2.68392
H	10.81875	3.46733	-4.11429
H	10.38251	1.83539	-3.59232
C	2.59303	-5.91822	-1.39314
C	-7.39254	-5.85235	-2.26183
C	-4.92976	-4.56451	-2.02933
O	2.55003	-4.51684	-1.15415
C	-3.69296	-3.94140	-1.91768
O	-0.83941	-3.66475	-1.69042
C	4.95355	-4.49483	-0.89834
O	-7.27864	-4.68152	-1.45946
C	3.72120	-3.84860	-0.92819
C	-6.05088	-4.07273	-1.36803
C	6.13282	-3.79583	-0.67287

C	-9.88184	-4.83409	1.90089
C	-1.10719	-2.56109	-1.22666
C	-3.56319	-2.79624	-1.13045
N	1.25340	-2.23116	-0.96110
C	3.66067	-2.45504	-0.71226
N	-2.35477	-2.10256	-0.95726
C	-5.93789	-2.91245	-0.57583
C	-0.01160	-1.55286	-0.89664
C	-4.68977	-2.30283	-0.47813
C	6.09159	-2.41403	-0.47490
C	2.41327	-1.63042	-0.65821
C	-9.53419	-3.41826	2.36127
O	8.82215	-3.21791	0.16284
C	4.85441	-1.77317	-0.49351
C	-7.02797	-2.26424	0.22341
C	8.49291	-2.04342	0.04687
N	7.22933	-1.62299	-0.25767
O	-6.82541	-1.18409	0.79440
N	-8.20687	-2.91307	0.31421
C	-10.64128	-2.83676	3.24064
O	2.45074	-0.42825	-0.34042
C	9.48884	-0.91010	0.23228
C	-9.29035	-2.47653	1.17574
C	10.41328	-1.14433	1.42543
C	11.46472	-0.04549	1.55483
H	2.99988	-6.44842	-0.52793
H	3.19106	-6.14376	-2.28008
H	1.55927	-6.21170	-1.55713
H	-6.74465	-6.64766	-1.88489
H	-7.14563	-5.63468	-3.30379
H	-8.43349	-6.15753	-2.18629
H	-5.00496	-5.44950	-2.64500
H	-2.83260	-4.34645	-2.42595
H	5.00814	-5.56339	-1.05199
H	7.07998	-4.31094	-0.64269
H	-9.07474	-5.27790	1.31266
H	-10.78986	-4.82940	1.28905
H	-10.06049	-5.48822	2.75688
H	1.23544	-3.20798	-1.23646
H	-2.42085	-1.18678	-0.50511
H	-0.05756	-0.72491	-1.61267
H	-0.18608	-1.12303	0.09110
H	-4.61139	-1.42634	0.15048
H	-8.60670	-3.45725	2.94265
H	4.79875	-0.70617	-0.33087
H	7.08762	-0.61722	-0.35106
H	-8.29033	-3.77698	-0.20263
H	-11.58080	-2.76569	2.68392
H	-10.38251	-1.83539	3.59232
H	-10.81875	-3.46733	4.11429
H	8.96589	0.04270	0.33143
H	10.08781	-0.85312	-0.68420
H	-10.20692	-2.39029	0.58192
H	-9.02529	-1.48487	1.53604
H	10.88738	-2.12072	1.31180
H	9.81369	-1.19455	2.33939
H	10.99776	0.93301	1.70155
H	12.08217	0.01329	0.65386
H	12.12779	-0.22789	2.40314
C	-3.99035	1.73846	4.52439
H	-3.05393	1.19435	4.56164
C	-4.00053	3.11931	4.70098

```
H         -3.07204        3.65007        4.87569
C         -5.20349        3.81831        4.65313
H         -5.21142        4.89318        4.79059
C         -6.39628        3.13646        4.42869
H         -7.33269        3.68058        4.39144
C         -6.38609        1.75562        4.25210
H         -7.31458        1.22486        4.07739
C         -5.18312        1.05662        4.29996
H         -5.17520       -0.01825        4.16249
```

The DADA10-R dimer with the benzene probe

```
50
Energy = -1327.4748148326
N          1.54069       -1.04796        0.00000
C          2.27442       -2.17683        0.00000
C          3.69846       -2.15050        0.00000
C          4.33838       -0.94303        0.00000
C          3.36219        2.66712        0.00000
C          1.92519        2.54946        0.00000
N          1.42648        1.25629        0.00000
C          2.18957        0.12228        0.00000
C          3.59615        0.25371        0.00000
C          4.15108        1.56056        0.00000
N          1.61285       -3.34475        0.00000
H          4.24885       -3.08267        0.00000
H          5.42166       -0.89427        0.00000
H          0.58217       -3.38582        0.00000
H          5.23176        1.66174        0.00000
H          3.76610        3.66928        0.00000
O          1.14883        3.51803        0.00000
H          2.13424       -4.20299        0.00000
H          0.39611        1.15276        0.00000
N         -1.54069        1.04796        0.00000
C         -2.27442        2.17683        0.00000
C         -3.69846        2.15050        0.00000
C         -4.33838        0.94303        0.00000
C         -3.36219       -2.66712        0.00000
C         -1.92519       -2.54946        0.00000
N         -1.42648       -1.25629        0.00000
C         -2.18957       -0.12228        0.00000
C         -3.59615       -0.25371        0.00000
C         -4.15108       -1.56056        0.00000
N         -1.61285        3.34475        0.00000
H         -4.24885        3.08267        0.00000
H         -5.42166        0.89427        0.00000
H         -0.58217        3.38582        0.00000
H         -5.23176       -1.66174        0.00000
H         -3.76610       -3.66928        0.00000
O         -1.14883       -3.51803        0.00000
H         -2.13424        4.20299        0.00000
H         -0.39611       -1.15276        0.00000
C          3.20775        0.37194        3.7999949
H          3.78056       -0.54767        3.8000051
C          3.86323        1.59977        3.7999949
H          4.94629        1.63593        3.8000051
C          3.12737        2.78113        3.7999949
H          3.63762        3.73690        3.8000051
C          1.73603        2.73467        3.7999949
H          1.16322        3.65427        3.8000051
C          1.08054        1.50684        3.7999949
H         -0.00251        1.47067        3.8000051
C          1.81640        0.32547        3.7999949
H          1.30616       -0.63029        3.8000051
```

The DADA10-L dimer with the benzene probe

```
50
Energy = -1327.4748984511
N          1.54069       -1.04796        0.00000
C          2.27442       -2.17683        0.00000
C          3.69846       -2.15050        0.00000
C          4.33838       -0.94303        0.00000
C          3.36219        2.66712        0.00000
C          1.92519        2.54946        0.00000
N          1.42648        1.25629        0.00000
C          2.18957        0.12228        0.00000
C          3.59615        0.25371        0.00000
C          4.15108        1.56056        0.00000
N          1.61285       -3.34475        0.00000
H          4.24885       -3.08267        0.00000
H          5.42166       -0.89427        0.00000
H          0.58217       -3.38582        0.00000
H          5.23176        1.66174        0.00000
H          3.76610        3.66928        0.00000
O          1.14883        3.51803        0.00000
H          2.13424       -4.20299        0.00000
H          0.39611        1.15276        0.00000
N         -1.54069        1.04796        0.00000
C         -2.27442        2.17683        0.00000
C         -3.69846        2.15050        0.00000
C         -4.33838        0.94303        0.00000
C         -3.36219       -2.66712        0.00000
C         -1.92519       -2.54946        0.00000
N         -1.42648       -1.25629        0.00000
C         -2.18957       -0.12228        0.00000
C         -3.59615       -0.25371        0.00000
C         -4.15108       -1.56056        0.00000
N         -1.61285        3.34475        0.00000
H         -4.24885        3.08267        0.00000
H         -5.42166        0.89427        0.00000
H         -0.58217        3.38582        0.00000
H         -5.23176       -1.66174        0.00000
H         -3.76610       -3.66928        0.00000
O         -1.14883       -3.51803        0.00000
H         -2.13424        4.20299        0.00000
H         -0.39611       -1.15276        0.00000
C          3.51088       -2.28351        3.7999949
H          4.08369       -3.20312        3.8000051
C          4.16636       -1.05568        3.7999949
H          5.24942       -1.01952        3.8000051
C          3.43050        0.12568        3.7999949
H          3.94075        1.08145        3.8000051
C          2.03916        0.07922        3.7999949
H          1.46635        0.99882        3.8000051
C          1.38367       -1.14861        3.7999949
H          0.30062       -1.18478        3.8000051
C          2.11953       -2.32998        3.7999949
H          1.60929       -3.28574        3.8000051
```

The DDAA01-R dimer with the benzene probe

```
146
Energy = -3511.9126274066
C         -4.43726        3.53041       -3.61104
C         -5.63659        2.85467       -3.40316
C         -3.27197        3.13395       -2.95399
C         -5.69955        1.77283       -2.50399
C         -3.29538        2.03866       -2.06515
```

C	-4.51783	1.41134	-1.86622
O	-2.09894	3.77951	-3.14073
O	-6.77949	3.21964	-4.04896
C	-6.90555	0.95829	-2.16066
N	-7.97749	1.05642	-2.97626
O	-6.88805	0.20224	-1.18251
C	-2.12468	1.45166	-1.33988
N	-0.90427	1.90270	-1.66000
O	-2.28976	0.55370	-0.49939
C	0.30833	1.32550	-1.14448
C	1.45700	1.80682	-2.03168
N	2.65203	1.26120	-1.71353
O	1.24863	2.61641	-2.93237
C	3.89502	1.46704	-2.34648
C	4.03845	2.18576	-3.53704
C	5.30556	2.29792	-4.09545
C	6.42963	1.72705	-3.51399
C	6.27929	1.01745	-2.31769
C	5.01252	0.89137	-1.74291
N	7.35049	0.41828	-1.63738
C	8.62932	0.22593	-2.08240
O	9.03942	0.55208	-3.18807
C	-2.01299	4.85670	-4.08960
C	-0.58522	5.35336	-4.07339
C	-6.75717	4.34136	-4.94408
C	-8.16049	4.51185	-5.48173
C	-9.21460	0.32342	-2.76591
C	9.54237	-0.43593	-1.05892
C	-10.39780	1.25824	-2.53670
C	10.47171	-1.45502	-1.71134
H	-4.40420	4.36778	-4.28794
H	-4.54831	0.57326	-1.18587
H	-7.92474	1.73382	-3.72251
H	-0.77901	2.59947	-2.38678
H	0.49492	1.62417	-0.10843
H	0.25705	0.23638	-1.15005
H	2.64707	0.60827	-0.92932
H	3.17771	2.63574	-4.00270
H	5.42071	2.85093	-5.02048
H	7.40459	1.81409	-3.96460
H	4.89952	0.33574	-0.81990
H	7.15037	0.10631	-0.68980
H	-2.29815	4.47776	-5.07608
H	-2.71614	5.64257	-3.79610
H	0.10777	4.54787	-4.31329
H	-0.32560	5.74412	-3.08897
H	-0.47190	6.15437	-4.80638
H	-6.43105	5.22843	-4.39301
H	-6.04214	4.14384	-5.74847
H	-8.86528	4.69413	-4.66937
H	-8.47671	3.62247	-6.02917
H	-8.19164	5.36288	-6.16394
H	-9.40040	-0.31575	-3.63460
H	-9.04944	-0.32331	-1.90669
H	8.95021	-0.88676	-0.26150
H	10.13470	0.36547	-0.60350
H	-10.55852	1.91111	-3.39874
H	-10.23064	1.88524	-1.65991
H	-11.31088	0.68094	-2.37846
H	11.00771	-0.99511	-2.54113
H	9.90539	-2.30160	-2.10523
H	11.19705	-1.83529	-0.98914

C	4.43726	-3.53041	3.61104
C	5.63659	-2.85467	3.40316
C	3.27197	-3.13395	2.95399
C	5.69955	-1.77283	2.50399
C	3.29538	-2.03866	2.06515
C	4.51783	-1.41134	1.86622
O	2.09894	-3.77951	3.14073
O	6.77949	-3.21964	4.04896
C	6.90555	-0.95829	2.16066
N	7.97749	-1.05642	2.97626
O	6.88805	-0.20224	1.18251
C	2.12468	-1.45166	1.33988
N	0.90427	-1.90270	1.66000
O	2.28976	-0.55370	0.49939
C	-0.30833	-1.32550	1.14448
C	-1.45700	-1.80682	2.03168
N	-2.65203	-1.26120	1.71353
O	-1.24863	-2.61641	2.93237
C	-3.89502	-1.46704	2.34648
C	-4.03845	-2.18576	3.53704
C	-5.30556	-2.29792	4.09545
C	-6.42963	-1.72705	3.51399
C	-6.27929	-1.01745	2.31769
C	-5.01252	-0.89137	1.74291
N	-7.35049	-0.41828	1.63738
C	-8.62932	-0.22593	2.08240
O	-9.03942	-0.55208	3.18807
C	2.01299	-4.85670	4.08960
C	0.58522	-5.35336	4.07339
C	6.75717	-4.34136	4.94408
C	8.16049	-4.51185	5.48173
C	9.21460	-0.32342	2.76591
C	-9.54237	0.43593	1.05892
C	10.39780	-1.25824	2.53670
C	-10.47171	1.45502	1.71134
H	4.40420	-4.36778	4.28794
H	4.54831	-0.57326	1.18587
H	7.92474	-1.73382	3.72251
H	0.77901	-2.59947	2.38678
H	-0.49492	-1.62417	0.10843
H	-0.25705	-0.23638	1.15005
H	-2.64707	-0.60827	0.92932
H	-3.17771	-2.63574	4.00270
H	-5.42071	-2.85093	5.02048
H	-7.40459	-1.81409	3.96460
H	-4.89952	-0.33574	0.81990
H	-7.15037	-0.10631	0.68980
H	2.29815	-4.47776	5.07608
H	2.71614	-5.64257	3.79610
H	0.32560	-5.74412	3.08897
H	-0.10777	-4.54787	4.31329
H	0.47190	-6.15437	4.80638
H	6.43105	-5.22843	4.39301
H	6.04214	-4.14384	5.74847
H	8.47671	-3.62247	6.02917
H	8.86528	-4.69413	4.66937
H	8.19164	-5.36288	6.16394
H	9.40040	0.31575	3.63460
H	9.04944	0.32331	1.90669
H	-8.95021	0.88676	0.26150
H	-10.13470	-0.36547	0.60350
H	10.23064	-1.88524	1.65991

```
H         10.55852       -1.91111        3.39874
H         11.31088       -0.68094        2.37846
H         -9.90539        2.30160        2.10523
H        -11.00771        0.99511        2.54113
H        -11.19705        1.83529        0.98914
C          5.85568       -2.15646       -4.39135
H          6.72535       -2.60348       -3.92426
C          5.99098       -1.45321       -5.58513
H          6.96597       -1.35278       -6.04733
C          4.87376       -0.87894       -6.18516
H          4.97908       -0.33150       -7.11445
C          3.62123       -1.00793       -5.59141
H          2.75156       -0.56090       -6.05849
C          3.48593       -1.71119       -4.39763
H          2.51094       -1.81159       -3.93544
C          4.60315       -2.28545       -3.79760
H          4.49783       -2.83288       -2.86831
```

The DDAA01-L dimer with the benzene probe

```
146
Energy = -3511.9166811399
C         -4.43726        3.53041       -3.61104
C         -5.63659        2.85467       -3.40316
C         -3.27197        3.13395       -2.95399
C         -5.69955        1.77283       -2.50399
C         -3.29538        2.03866       -2.06515
C         -4.51783        1.41134       -1.86622
O         -2.09894        3.77951       -3.14073
O         -6.77949        3.21964       -4.04896
C         -6.90555        0.95829       -2.16066
N         -7.97749        1.05642       -2.97626
O         -6.88805        0.20224       -1.18251
C         -2.12468        1.45166       -1.33988
N         -0.90427        1.90270       -1.66000
O         -2.28976        0.55370       -0.49939
C          0.30833        1.32550       -1.14448
C          1.45700        1.80682       -2.03168
N          2.65203        1.26120       -1.71353
O          1.24863        2.61641       -2.93237
C          3.89502        1.46704       -2.34648
C          4.03845        2.18576       -3.53704
C          5.30556        2.29792       -4.09545
C          6.42963        1.72705       -3.51399
C          6.27929        1.01745       -2.31769
C          5.01252        0.89137       -1.74291
N          7.35049        0.41828       -1.63738
C          8.62932        0.22593       -2.08240
O          9.03942        0.55208       -3.18807
C         -2.01299        4.85670       -4.08960
C         -0.58522        5.35336       -4.07339
C         -6.75717        4.34136       -4.94408
C         -8.16049        4.51185       -5.48173
C         -9.21460        0.32342       -2.76591
C          9.54237       -0.43593       -1.05892
C        -10.39780        1.25824       -2.53670
C         10.47171       -1.45502       -1.71134
H         -4.40420        4.36778       -4.28794
H         -4.54831        0.57326       -1.18587
H         -7.92474        1.73382       -3.72251
H         -0.77901        2.59947       -2.38678
H          0.49492        1.62417       -0.10843
H          0.25705        0.23638       -1.15005
H          2.64707        0.60827       -0.92932
```

H	3.17771	2.63574	-4.00270
H	5.42071	2.85093	-5.02048
H	7.40459	1.81409	-3.96460
H	4.89952	0.33574	-0.81990
H	7.15037	0.10631	-0.68980
H	-2.29815	4.47776	-5.07608
H	-2.71614	5.64257	-3.79610
H	0.10777	4.54787	-4.31329
H	-0.32560	5.74412	-3.08897
H	-0.47190	6.15437	-4.80638
H	-6.43105	5.22843	-4.39301
H	-6.04214	4.14384	-5.74847
H	-8.86528	4.69413	-4.66937
H	-8.47671	3.62247	-6.02917
H	-8.19164	5.36288	-6.16394
H	-9.40040	-0.31575	-3.63460
H	-9.04944	-0.32331	-1.90669
H	8.95021	-0.88676	-0.26150
H	10.13470	0.36547	-0.60350
H	-10.55852	1.91111	-3.39874
H	-10.23064	1.88524	-1.65991
H	-11.31088	0.68094	-2.37846
H	11.00771	-0.99511	-2.54113
H	9.90539	-2.30160	-2.10523
H	11.19705	-1.83529	-0.98914
C	4.43726	-3.53041	3.61104
C	5.63659	-2.85467	3.40316
C	3.27197	-3.13395	2.95399
C	5.69955	-1.77283	2.50399
C	3.29538	-2.03866	2.06515
C	4.51783	-1.41134	1.86622
O	2.09894	-3.77951	3.14073
O	6.77949	-3.21964	4.04896
C	6.90555	-0.95829	2.16066
N	7.97749	-1.05642	2.97626
O	6.88805	-0.20224	1.18251
C	2.12468	-1.45166	1.33988
N	0.90427	-1.90270	1.66000
O	2.28976	-0.55370	0.49939
C	-0.30833	-1.32550	1.14448
C	-1.45700	-1.80682	2.03168
N	-2.65203	-1.26120	1.71353
O	-1.24863	-2.61641	2.93237
C	-3.89502	-1.46704	2.34648
C	-4.03845	-2.18576	3.53704
C	-5.30556	-2.29792	4.09545
C	-6.42963	-1.72705	3.51399
C	-6.27929	-1.01745	2.31769
C	-5.01252	-0.89137	1.74291
N	-7.35049	-0.41828	1.63738
C	-8.62932	-0.22593	2.08240
O	-9.03942	-0.55208	3.18807
C	2.01299	-4.85670	4.08960
C	0.58522	-5.35336	4.07339
C	6.75717	-4.34136	4.94408
C	8.16049	-4.51185	5.48173
C	9.21460	-0.32342	2.76591
C	-9.54237	0.43593	1.05892
C	10.39780	-1.25824	2.53670
C	-10.47171	1.45502	1.71134
H	4.40420	-4.36778	4.28794
H	4.54831	-0.57326	1.18587

```
H          7.92474       -1.73382        3.72251
H          0.77901       -2.59947        2.38678
H         -0.49492       -1.62417        0.10843
H         -0.25705       -0.23638        1.15005
H         -2.64707       -0.60827        0.92932
H         -3.17771       -2.63574        4.00270
H         -5.42071       -2.85093        5.02048
H         -7.40459       -1.81409        3.96460
H         -4.89952       -0.33574        0.81990
H         -7.15037       -0.10631        0.68980
H          2.29815       -4.47776        5.07608
H          2.71614       -5.64257        3.79610
H          0.32560       -5.74412        3.08897
H         -0.10777       -4.54787        4.31329
H          0.47190       -6.15437        4.80638
H          6.43105       -5.22843        4.39301
H          6.04214       -4.14384        5.74847
H          8.47671       -3.62247        6.02917
H          8.86528       -4.69413        4.66937
H          8.19164       -5.36288        6.16394
H          9.40040        0.31575        3.63460
H          9.04944        0.32331        1.90669
H         -8.95021        0.88676        0.26150
H        -10.13470       -0.36547        0.60350
H         10.23064       -1.88524        1.65991
H         10.55852       -1.91111        3.39874
H         11.31088       -0.68094        2.37846
H         -9.90539        2.30160        2.10523
H        -11.00771        0.99511        2.54113
H        -11.19705        1.83529        0.98914
C         -3.74294       -1.15132       -4.52508
H         -3.82786       -1.98755       -3.84110
C         -2.51414       -0.52282       -4.70691
H         -1.64254       -0.86981       -4.16447
C         -2.40503        0.55143       -5.58558
H         -1.44852        1.04068       -5.72713
C         -3.52473        0.99720       -6.28243
H         -3.43980        1.83343       -6.96641
C         -4.75352        0.36870       -6.10061
H         -5.62511        0.71568       -6.64304
C         -4.86262       -0.70556       -5.22193
H         -5.81915       -1.19480       -5.08039
```

The DDAA02 dimer with the benzene probe

```
46
Energy = -1357.7470688689
C          1.10895        4.18756       -0.04205
N         -0.05934        3.47850       -0.03552
C          2.29956        3.53740       -0.02080
C         -0.03121        2.11687       -0.00600
C          2.31317        2.07865        0.00930
N          1.08947        1.41992        0.01408
N         -1.23268        1.46534        0.00505
C         -2.48553        2.10749        0.00557
N         -3.52951        1.27303        0.04496
O          3.37660        1.44083        0.03300
H         -1.18086        0.41585        0.01627
H         -3.44913        0.23061        0.01671
H         -4.44355        1.70976        0.02164
O         -2.58965        3.34557       -0.01915
N         -1.08864       -1.42001        0.00657
C         -2.31226       -2.07742       -0.03478
C          0.03147       -2.11787        0.02530
```

```
C         -2.29913        -3.53618        -0.06110
N          0.05875        -3.47990         0.01787
C         -1.10953        -4.18772        -0.02925
N          1.23258        -1.46643         0.05112
C          2.48573        -2.10820         0.05086
N          3.52927        -1.27269         0.03009
O          2.58994        -3.34635         0.06330
H          1.03120        -3.87193         0.03781
H          1.18072        -0.41699         0.04231
H          3.44830        -0.22992         0.03413
H          4.44382        -1.70866         0.04323
O         -3.37505        -1.43835        -0.05001
H         -3.24912        -4.06646        -0.10045
H         -1.00723        -5.27374        -0.03934
H         -1.03264         3.86943        -0.04222
H          1.00578         5.27332        -0.06404
H          3.24977         4.06871        -0.02448
C          2.59036         2.40281         3.7999949
H          3.52884         1.86097         3.8000051
C          2.59036         3.79493         3.7999949
H          3.52884         4.33676         3.8000051
C          1.38474         4.49099         3.7999949
H          1.38474         5.57465         3.8000051
C          0.17913         3.79493         3.7999949
H         -0.75935         4.33676         3.8000051
C          0.17913         2.40281         3.7999949
H         -0.75935         1.86097         3.8000051
C          1.38474         1.70674         3.7999949
H          1.38474         0.62308         3.8000051
```

The DDAA03-R dimer with the benzene probe

```
56
Energy = -1514.1471194513
C         -3.83268         3.70308         0.91688
C         -4.84046         2.78097         1.08491
C         -2.56977         3.27149         0.48268
C         -4.56207         1.43750         0.79194
C         -2.37175         1.88232         0.24129
N         -3.38534         0.99300         0.38609
C         -1.46623         4.13147         0.25819
C         -0.27488         3.62114        -0.15256
C         -0.16034         2.20544        -0.32903
N         -1.18170         1.37226        -0.15241
N          1.03301         1.61557        -0.64819
C          2.18028         2.27162        -1.12396
N          3.25482         1.44681        -1.17814
O          2.19240         3.44009        -1.48567
N          3.38534        -0.99300         0.38609
C          2.37175        -1.88232         0.24129
C          4.56207        -1.43750         0.79194
C          2.56977        -3.27149         0.48268
C          4.84046        -2.78097         1.08491
C          3.83268        -3.70308         0.91688
N          1.18170        -1.37226        -0.15241
C          0.16034        -2.20544        -0.32903
C          0.27488        -3.62114        -0.15256
C          1.46623        -4.13147         0.25819
N         -1.03301        -1.61557        -0.64819
C         -2.18028        -2.27162        -1.12396
N         -3.25482        -1.44681        -1.17814
H         -3.29504        -0.59027        -0.61207
H         -4.11539        -1.89257        -1.44771
```

```
O         -2.19240       -3.44009       -1.48567
H         -1.07091       -0.59262       -0.53064
H          4.11539        1.89257       -1.44771
H          3.29504        0.59027       -0.61207
H          1.07091        0.59262       -0.53064
H         -3.99672        4.75723        1.11216
H         -5.82696        3.07068        1.42054
H         -5.34283        0.68898        0.89061
H         -1.57973        5.19732        0.42214
H          0.58722        4.23782       -0.34706
H          5.34283       -0.68898        0.89061
H          5.82696       -3.07068        1.42054
H          3.99672       -4.75723        1.11216
H         -0.58722       -4.23782       -0.34706
H          1.57973       -5.19732        0.42214
C         -1.45952        1.39431        3.86884
H         -0.50371        1.01397        3.52812
C         -1.62241        2.75652        4.10517
H         -0.79339        3.43657        3.94839
C         -2.85028        3.24511        4.54290
H         -2.97707        4.30550        4.72686
C         -3.91528        2.37149        4.74431
H         -4.87108        2.75182        5.08506
C         -3.75240        1.00928        4.50799
H         -4.58142        0.32921        4.66478
C         -2.52453        0.52069        4.07027
H         -2.39774       -0.53970        3.88631
```

The DDAA03-L dimer with the benzene probe

```
56
Energy = -1514.1486844090
C         -3.83268        3.70308        0.91688
C         -4.84046        2.78097        1.08491
C         -2.56977        3.27149        0.48268
C         -4.56207        1.43750        0.79194
C         -2.37175        1.88232        0.24129
N         -3.38534        0.99300        0.38609
C         -1.46623        4.13147        0.25819
C         -0.27488        3.62114       -0.15256
C         -0.16034        2.20544       -0.32903
N         -1.18170        1.37226       -0.15241
N          1.03301        1.61557       -0.64819
C          2.18028        2.27162       -1.12396
N          3.25482        1.44681       -1.17814
O          2.19240        3.44009       -1.48567
N          3.38534       -0.99300        0.38609
C          2.37175       -1.88232        0.24129
C          4.56207       -1.43750        0.79194
C          2.56977       -3.27149        0.48268
C          4.84046       -2.78097        1.08491
C          3.83268       -3.70308        0.91688
N          1.18170       -1.37226       -0.15241
C          0.16034       -2.20544       -0.32903
C          0.27488       -3.62114       -0.15256
C          1.46623       -4.13147        0.25819
N         -1.03301       -1.61557       -0.64819
C         -2.18028       -2.27162       -1.12396
N         -3.25482       -1.44681       -1.17814
H         -3.29504       -0.59027       -0.61207
H         -4.11539       -1.89257       -1.44771
O         -2.19240       -3.44009       -1.48567
H         -1.07091       -0.59262       -0.53064
H          4.11539        1.89257       -1.44771
```

```
H          3.29504        0.59027       -0.61207
H          1.07091        0.59262       -0.53064
H         -3.99672        4.75723        1.11216
H         -5.82696        3.07068        1.42054
H         -5.34283        0.68898        0.89061
H         -1.57973        5.19732        0.42214
H          0.58722        4.23782       -0.34706
H          5.34283       -0.68898        0.89061
H          5.82696       -3.07068        1.42054
H          3.99672       -4.75723        1.11216
H         -0.58722       -4.23782       -0.34706
H          1.57973       -5.19732        0.42214
C          0.87205        2.14885        3.41094
H          1.84856        1.77680        3.12399
C          0.67294        3.51485        3.59097
H          1.49446        4.20613        3.44415
C         -0.58152        3.99279        3.95962
H         -0.73651        5.05612        4.09976
C         -1.63688        3.10474        4.14824
H         -2.61338        3.47678        4.43521
C         -1.43778        1.73874        3.96821
H         -2.25929        1.04744        4.11505
C         -0.18332        1.26080        3.59957
H         -0.02833        0.19746        3.45944
```

The DDAA04-R dimer with the benzene probe

```
52
Energy = -1470.1208529143
C         -4.00770        3.22906        0.00000
C         -3.50532        4.54190        0.00000
N         -3.22898        2.15429        0.00000
C         -2.14692        4.73903        0.00000
C         -1.91200        2.35536        0.00000
N         -1.33917        3.64993        0.00000
N         -0.95942        1.43872        0.00000
C          0.02816        3.49371        0.00000
C          0.22882        2.11917        0.00000
N          1.38063        1.39175        0.00000
C          2.65170        1.94671        0.00000
N          3.64432        1.01574        0.00000
O          2.84840        3.15587        0.00000
H         -5.07666        3.05042        0.00000
H         -4.17289        5.39112        0.00000
H          0.72388        4.31043        0.00000
C          4.00770       -3.22906        0.00000
N          3.22898       -2.15429        0.00000
C          3.50532       -4.54190        0.00000
C          1.91200       -2.35536        0.00000
C          2.14692       -4.73903        0.00000
N          1.33917       -3.64993        0.00000
N          0.95942       -1.43872        0.00000
C         -0.02816       -3.49371        0.00000
C         -0.22882       -2.11917        0.00000
N         -1.38063       -1.39175        0.00000
C         -2.65170       -1.94671        0.00000
N         -3.64432       -1.01574        0.00000
O         -2.84840       -3.15587        0.00000
H          5.07666       -3.05042        0.00000
H          4.17289       -5.39112        0.00000
H          1.66847       -5.70808        0.00000
H         -0.72388       -4.31043        0.00000
H         -1.66847        5.70808        0.00000
H          1.25822        0.36503        0.00000
```

```
H          3.49064        0.01186        0.00000
H          4.58542        1.36598        0.00000
H         -3.49064       -0.01186        0.00000
H         -4.58542       -1.36598        0.00000
H         -1.25822       -0.36503        0.00000
C         -1.56188        2.40233        3.7999949
H         -0.81801        1.61532        3.8000051
C         -1.16331        3.73571        3.7999949
H         -0.10917        3.98664        3.8000051
C         -2.11892        4.74673        3.7999949
H         -1.80866        5.78467        3.8000051
C         -3.47310        4.42437        3.7999949
H         -4.21697        5.21137        3.8000051
C         -3.87168        3.09099        3.7999949
H         -4.92581        2.84005        3.8000051
C         -2.91607        2.07997        3.7999949
H         -3.22634        1.04202        3.8000051
```

The DDAA04-L dimer with the benzene probe

```
52
Energy = -1470.1218556952
C         -4.00770        3.22906        0.00000
C         -3.50532        4.54190        0.00000
N         -3.22898        2.15429        0.00000
C         -2.14692        4.73903        0.00000
C         -1.91200        2.35536        0.00000
N         -1.33917        3.64993        0.00000
N         -0.95942        1.43872        0.00000
C          0.02816        3.49371        0.00000
C          0.22882        2.11917        0.00000
N          1.38063        1.39175        0.00000
C          2.65170        1.94671        0.00000
N          3.64432        1.01574        0.00000
O          2.84840        3.15587        0.00000
H         -5.07666        3.05042        0.00000
H         -4.17289        5.39112        0.00000
H          0.72388        4.31043        0.00000
C          4.00770       -3.22906        0.00000
N          3.22898       -2.15429        0.00000
C          3.50532       -4.54190        0.00000
C          1.91200       -2.35536        0.00000
C          2.14692       -4.73903        0.00000
N          1.33917       -3.64993        0.00000
N          0.95942       -1.43872        0.00000
C         -0.02816       -3.49371        0.00000
C         -0.22882       -2.11917        0.00000
N         -1.38063       -1.39175        0.00000
C         -2.65170       -1.94671        0.00000
N         -3.64432       -1.01574        0.00000
O         -2.84840       -3.15587        0.00000
H          5.07666       -3.05042        0.00000
H          4.17289       -5.39112        0.00000
H          1.66847       -5.70808        0.00000
H         -0.72388       -4.31043        0.00000
H         -1.66847        5.70808        0.00000
H          1.25822        0.36503        0.00000
H          3.49064        0.01186        0.00000
H          4.58542        1.36598        0.00000
H         -3.49064       -0.01186        0.00000
H         -4.58542       -1.36598        0.00000
H         -1.25822       -0.36503        0.00000
C          0.33920        2.16333        3.7999949
H          1.27768        1.62150        3.8000051
```

```
C          0.33920        3.55545        3.7999949
H          1.27768        4.09728        3.8000051
C         -0.86642        4.25151        3.7999949
H         -0.86642        5.33517        3.8000051
C         -2.07203        3.55545        3.7999949
H         -3.01051        4.09728        3.8000051
C         -2.07203        2.16333        3.7999949
H         -3.01051        1.62150        3.8000051
C         -0.86642        1.46727        3.7999949
H         -0.86642        0.38360        3.8000051
```

The DDAA06-R dimer with the benzene probe

```
50
Energy = -1327.4548540838
N          1.50635       -1.11038        0.00000
C          2.17221       -2.29114        0.00000
C          3.58674       -2.27342        0.00000
C          4.24175       -1.06801        0.00000
C          3.36262        2.54721        0.00000
C          1.91807        2.43546        0.00000
N          1.34046        1.18734        0.00000
C          2.12772        0.11695        0.00000
C          3.54421        0.15003        0.00000
C          4.14321        1.43791        0.00000
N          1.45315       -3.41143        0.00000
H          4.12003       -3.21381        0.00000
H          5.32643       -1.04724        0.00000
H          0.39771       -3.40978        0.00000
H          5.22561        1.51393        0.00000
H          3.77696        3.54614        0.00000
O          1.20087        3.46465        0.00000
H          1.94554       -4.28757        0.00000
H          0.45233       -1.12164        0.00000
N         -1.50635        1.11038        0.00000
C         -2.17221        2.29114        0.00000
C         -3.58674        2.27342        0.00000
C         -4.24175        1.06801        0.00000
C         -3.36262       -2.54721        0.00000
C         -1.91807       -2.43546        0.00000
N         -1.34046       -1.18734        0.00000
C         -2.12772       -0.11695        0.00000
C         -3.54421       -0.15003        0.00000
C         -4.14321       -1.43791        0.00000
N         -1.45315        3.41143        0.00000
H         -4.12003        3.21381        0.00000
H         -5.32643        1.04724        0.00000
H         -0.39771        3.40978        0.00000
H         -5.22561       -1.51393        0.00000
H         -3.77696       -3.54614        0.00000
O         -1.20087       -3.46465        0.00000
H         -1.94554        4.28757        0.00000
H         -0.45233        1.12164        0.00000
C          3.38228        0.12464        3.7999949
H          3.93770       -0.80582        3.8000051
C          4.05972        1.34012        3.7999949
H          5.14249        1.35582        3.8000051
C          3.34619        2.53542        3.7999949
H          3.87353        3.48158        3.8000051
C          1.95522        2.51524        3.7999949
H          1.39979        3.44569        3.8000051
C          1.27777        1.29976        3.7999949
H          0.19500        1.28404        3.8000051
C          1.99129        0.10445        3.7999949
```

```
H          1.46395       -0.84171        3.8000051
```

The DDAA06-L dimer with the benzene probe

```
50
Energy = -1327.4538985010
N          1.50635       -1.11038        0.00000
C          2.17221       -2.29114        0.00000
C          3.58674       -2.27342        0.00000
C          4.24175       -1.06801        0.00000
C          3.36262        2.54721        0.00000
C          1.91807        2.43546        0.00000
N          1.34046        1.18734        0.00000
C          2.12772        0.11695        0.00000
C          3.54421        0.15003        0.00000
C          4.14321        1.43791        0.00000
N          1.45315       -3.41143        0.00000
H          4.12003       -3.21381        0.00000
H          5.32643       -1.04724        0.00000
H          0.39771       -3.40978        0.00000
H          5.22561        1.51393        0.00000
H          3.77696        3.54614        0.00000
O          1.20087        3.46465        0.00000
H          1.94554       -4.28757        0.00000
H          0.45233       -1.12164        0.00000
N         -1.50635        1.11038        0.00000
C         -2.17221        2.29114        0.00000
C         -3.58674        2.27342        0.00000
C         -4.24175        1.06801        0.00000
C         -3.36262       -2.54721        0.00000
C         -1.91807       -2.43546        0.00000
N         -1.34046       -1.18734        0.00000
C         -2.12772       -0.11695        0.00000
C         -3.54421       -0.15003        0.00000
C         -4.14321       -1.43791        0.00000
N         -1.45315        3.41143        0.00000
H         -4.12003        3.21381        0.00000
H         -5.32643        1.04724        0.00000
H         -0.39771        3.40978        0.00000
H         -5.22561       -1.51393        0.00000
H         -3.77696       -3.54614        0.00000
O         -1.20087       -3.46465        0.00000
H         -1.94554        4.28757        0.00000
H         -0.45233        1.12164        0.00000
C          3.63481       -2.32958        3.7999949
H          4.11190       -3.28966        3.8000051
C          4.39044       -1.16121        3.7999949
H          5.45575       -1.21180        3.8000051
C          3.77753        0.07216        3.7999949
H          4.36574        0.98164        3.8000051
C          2.40900        0.13714        3.7999949
H          1.93190        1.09722        3.8000051
C          1.65336       -1.03123        3.7999949
H          0.58805       -0.98065        3.8000051
C          2.26626       -2.26460        3.7999949
H          1.67805       -3.17409        3.8000051
```

The DDAA07 dimer with the benzene probe

```
58
Energy = -1514.7161732778
H          4.80022       -3.00135        0.26849
C          3.87499       -3.37573        0.71130
N          2.78852       -2.43233        0.52643
C          2.40301       -2.08960       -0.70201
```

```
O          2.92504       -2.53748       -1.73782
N          1.34380       -1.16799       -0.73470
C          0.78010       -0.66729       -1.87010
N         -0.20894        0.19385       -1.76876
C         -0.77644        0.69860       -2.92699
O         -1.71211        1.51304       -2.85999
N          1.28155       -1.09417       -3.05528
C          0.76899       -0.63604       -4.24056
C         -0.25050        0.25220       -4.20010
C          1.40047       -1.17404       -5.48271
H          4.01538       -3.51147        1.78155
H          3.64224       -4.33787        0.25065
H          2.32747       -2.03643        1.36648
H          0.94056       -0.82212        0.15762
H          2.05894       -1.77258       -2.95428
H         -0.69044        0.64427       -5.10511
H          2.46607       -0.93161       -5.50713
H          0.92267       -0.75128       -6.36398
H          1.30977       -2.26276       -5.51864
H         -4.80022        3.00135       -0.26849
C         -3.87499        3.37573       -0.71130
N         -2.78852        2.43233       -0.52643
C         -2.40301        2.08960        0.70201
O         -2.92504        2.53748        1.73782
N         -1.34380        1.16799        0.73470
C         -0.78010        0.66729        1.87010
N          0.20894       -0.19385        1.76876
C          0.77644       -0.69860        2.92699
O          1.71211       -1.51304        2.85999
N         -1.28155        1.09417        3.05528
C         -0.76899        0.63604        4.24056
C          0.25050       -0.25220        4.20010
C         -1.40047        1.17404        5.48271
H         -4.01538        3.51147       -1.78155
H         -3.64224        4.33787       -0.25065
H         -2.32747        2.03643       -1.36648
H         -0.94056        0.82212       -0.15762
H         -2.05894        1.77258        2.95428
H          0.69044       -0.64427        5.10511
H         -2.46607        0.93161        5.50713
H         -0.92267        0.75128        6.36398
H         -1.30977        2.26276        5.51864
C          3.61335        1.98037       -3.20313
H          4.44868        1.29804       -3.30790
C          3.00489        2.51480       -4.33546
H          3.36658        2.24848       -5.32165
C          1.93179        3.39136       -4.20087
H          1.45815        3.80738       -5.08229
C          1.46716        3.73349       -2.93396
H          0.63184        4.41583       -2.82920
C          2.07562        3.19907       -1.80163
H          1.71394        3.46540       -0.81544
C          3.14872        2.32251       -1.93622
H          3.62237        1.90650       -1.05478
```

The DDAA08-R dimer with the benzene probe

```
62
Energy = -1775.0894982826
C         -2.37955        6.18735        0.00000
C         -3.63506        5.55276        0.00000
C         -3.67311        4.16063        0.00000
N         -1.21435        5.54068        0.00000
C         -1.27095        4.20510        0.00000
```

```
C         -2.46244        3.45563        0.00000
N         -0.08028        3.51362        0.00000
C         -2.38732        1.98100        0.00000
C         -0.05268        2.15553        0.00000
N         -1.14244        1.39519        0.00000
N          1.16775        1.54895        0.00000
C          2.40878        2.23467        0.00000
N          3.47811        1.42868        0.00000
O          2.48098        3.47027        0.00000
O         -3.42548        1.30542        0.00000
C          4.81215        1.99749        0.00000
H          4.97880        2.62580       -0.89296
H          5.53265        1.16577        0.00000
H          4.97880        2.62580        0.89296
C          2.46244       -3.45563        0.00000
C          1.27095       -4.20510        0.00000
C          3.67311       -4.16063        0.00000
N          1.21435       -5.54068        0.00000
C          3.63506       -5.55276        0.00000
C          2.37955       -6.18735        0.00000
C          2.38732       -1.98100        0.00000
N          0.08028       -3.51362        0.00000
C          0.05268       -2.15553        0.00000
N          1.14244       -1.39519        0.00000
N         -1.16775       -1.54895        0.00000
C         -2.40878       -2.23467        0.00000
N         -3.47811       -1.42868        0.00000
C         -4.81215       -1.99749        0.00000
H         -4.97880       -2.62580       -0.89296
H         -5.53265       -1.16577        0.00000
H         -4.97880       -2.62580        0.89296
O         -2.48098       -3.47027        0.00000
O          3.42548       -1.30542        0.00000
H         -4.55151        6.14832        0.00000
H         -4.60890        3.59574        0.00000
H         -2.31618        7.28233        0.00000
H          4.60890       -3.59574        0.00000
H          4.55151       -6.14832        0.00000
H          2.31618       -7.28233        0.00000
H         -0.84878       -3.98549        0.00000
H         -1.15000       -0.50057        0.00000
H         -3.37968       -0.39181        0.00000
H          1.15000        0.50057        0.00000
H          3.37968        0.39181        0.00000
H          0.84878        3.98549        0.00000
C         -1.42420        3.97432        3.7999949
H         -0.57278        3.30515        3.8000051
C         -1.22846        5.35231        3.7999949
H         -0.22468        5.75579        3.8000051
C         -2.32223        6.21197        3.7999949
H         -2.16988        7.28463        3.8000051
C         -3.61173        5.69364        3.7999949
H         -4.46314        6.36281        3.8000051
C         -3.80748        4.31565        3.7999949
H         -4.81125        3.91217        3.8000051
C         -2.71370        3.45600        3.7999949
H         -2.86607        2.38333       3.8000051
```

The DDAA08-L dimer with the benzene probe

```
62
Energy = -1775.0922026487
C         -2.37955        6.18735        0.00000
C         -3.63506        5.55276        0.00000
```

C	-3.67311	4.16063	0.00000
N	-1.21435	5.54068	0.00000
C	-1.27095	4.20510	0.00000
C	-2.46244	3.45563	0.00000
N	-0.08028	3.51362	0.00000
C	-2.38732	1.98100	0.00000
C	-0.05268	2.15553	0.00000
N	-1.14244	1.39519	0.00000
N	1.16775	1.54895	0.00000
C	2.40878	2.23467	0.00000
N	3.47811	1.42868	0.00000
O	2.48098	3.47027	0.00000
O	-3.42548	1.30542	0.00000
C	4.81215	1.99749	0.00000
H	4.97880	2.62580	-0.89296
H	5.53265	1.16577	0.00000
H	4.97880	2.62580	0.89296
C	2.46244	-3.45563	0.00000
C	1.27095	-4.20510	0.00000
C	3.67311	-4.16063	0.00000
N	1.21435	-5.54068	0.00000
C	3.63506	-5.55276	0.00000
C	2.37955	-6.18735	0.00000
C	2.38732	-1.98100	0.00000
N	0.08028	-3.51362	0.00000
C	0.05268	-2.15553	0.00000
N	1.14244	-1.39519	0.00000
N	-1.16775	-1.54895	0.00000
C	-2.40878	-2.23467	0.00000
N	-3.47811	-1.42868	0.00000
C	-4.81215	-1.99749	0.00000
H	-4.97880	-2.62580	-0.89296
H	-5.53265	-1.16577	0.00000
H	-4.97880	-2.62580	0.89296
O	-2.48098	-3.47027	0.00000
O	3.42548	-1.30542	0.00000
H	-4.55151	6.14832	0.00000
H	-4.60890	3.59574	0.00000
H	-2.31618	7.28233	0.00000
H	4.60890	-3.59574	0.00000
H	4.55151	-6.14832	0.00000
H	2.31618	-7.28233	0.00000
H	-0.84878	-3.98549	0.00000
H	-1.15000	-0.50057	0.00000
H	-3.37968	-0.39181	0.00000
H	1.15000	0.50057	0.00000
H	3.37968	0.39181	0.00000
H	0.84878	3.98549	0.00000
C	-0.08438	2.11478	3.7999949
H	0.90042	1.67946	3.8000051
C	-0.23928	3.49825	3.7999949
H	0.62494	4.13986	3.8000051
C	-1.50441	4.05749	3.7999949
H	-1.62500	5.13441	3.8000051
C	-2.61463	3.23325	3.7999949
H	-3.59943	3.66857	3.8000051
C	-2.45974	1.84978	3.7999949
H	-3.32396	1.20817	3.8000051
C	-1.19461	1.29055	3.7999949
H	-1.07403	0.21361	3.8000051

S1.3 Dimers

The DADA01 dimer

```
38
Energy = -1352.3175940848
C          0.97944        4.27963        0.00000
N         -0.15844        3.57207        0.00000
C          2.22299        3.69493        0.00000
C         -0.03201        2.24043        0.00000
C          2.24927        2.28843        0.00000
N          1.11633        1.55968        0.00000
N          3.40640        1.55569        0.00000
C          4.70278        2.02843        0.00000
O          5.04750        3.19027        0.00000
N         -1.18990        1.49275        0.00000
C         -2.50226        1.96404        0.00000
O         -3.43426        1.17386        0.00000
H          5.41605        1.19113        0.00000
H          0.86737        5.35742        0.00000
H          3.13761        4.26312        0.00000
H         -1.09949        0.47056        0.00000
H          3.30899        0.52445        0.00000
O         -2.68114        3.26556        0.00000
H         -1.76794        3.70601        0.00000
O          3.43426       -1.17386        0.00000
C          2.50226       -1.96404        0.00000
N          1.18990       -1.49275        0.00000
O          2.68114       -3.26556        0.00000
C          0.03201       -2.24043        0.00000
N         -1.11633       -1.55968        0.00000
N          0.15844       -3.57207        0.00000
H          1.76794       -3.70601        0.00000
C         -2.24927       -2.28843        0.00000
N         -3.40640       -1.55569        0.00000
C         -0.97944       -4.27963        0.00000
C         -2.22299       -3.69493        0.00000
C         -4.70278       -2.02843        0.00000
H         -5.41605       -1.19113        0.00000
O         -5.04750       -3.19027        0.00000
H         -0.86737       -5.35742        0.00000
H         -3.13761       -4.26312        0.00000
H          1.09949       -0.47056        0.00000
H         -3.30899       -0.52445        0.00000
```

The DADA02 dimer

```
34
Energy = -1118.2660891212
C          4.02811        1.51915        0.00000
N          3.31953        2.62903        0.00000
N          3.55464        0.26633        0.00000
C          1.96898        2.43917        0.00000
C          2.20862        0.17300        0.00000
N          1.37322        1.22028        0.00000
N          1.20311        3.52702        0.00000
N          1.62439       -1.06904        0.00000
C          2.22691       -2.33689        0.00000
O          1.51666       -3.34741        0.00000
N          3.57025       -2.38291        0.00000
H          5.11973        1.62295        0.00000
H          1.67928        4.42096        0.00000
H          0.16575        3.46724        0.00000
```

```
H          4.09060       -1.49607        0.00000
H          3.99934       -3.29944        0.00000
H          0.58463       -1.08849        0.00000
N         -1.37318       -1.22022        0.00000
C         -2.20861       -0.17297        0.00000
C         -1.96891       -2.43913        0.00000
N         -3.55464       -0.26636        0.00000
N         -3.31944       -2.62904        0.00000
C         -4.02807       -1.51920        0.00000
N         -1.20306       -3.52698        0.00000
N         -1.62442        1.06909        0.00000
C         -2.22698        2.33692        0.00000
O         -1.51678        3.34749        0.00000
N         -3.57032        2.38285        0.00000
H         -5.11969       -1.62304        0.00000
H         -0.58466        1.08856        0.00000
H         -0.16571       -3.46724        0.00000
H         -1.67925       -4.42091        0.00000
H         -4.09059        1.49596        0.00000
H         -3.99947        3.29936        0.00000
```

The DADA03 dimer

```
36
Energy = -1086.1554775277
C          4.15495        1.49042        0.00000
C          3.39911        2.62877        0.00000
N          3.62757        0.25377        0.00000
C          1.99093        2.46276        0.00000
C          2.29171        0.19409        0.00000
N          1.44228        1.22970        0.00000
N          1.16807        3.51606        0.00000
N          1.68719       -1.04962        0.00000
C          2.26860       -2.31461        0.00000
O          1.54839       -3.31986        0.00000
N          3.60887       -2.38435        0.00000
H          5.23885        1.53999        0.00000
H          1.56043        4.44064        0.00000
H          0.14299        3.40400        0.00000
H          4.13877       -1.51248        0.00000
H          4.01887       -3.30126        0.00000
H          0.66224       -1.05572        0.00000
N         -1.44228       -1.22970        0.00000
C         -2.29171       -0.19409        0.00000
C         -1.99093       -2.46276        0.00000
N         -3.62757       -0.25377        0.00000
C         -3.39911       -2.62877        0.00000
C         -4.15495       -1.49042        0.00000
N         -1.16807       -3.51606        0.00000
N         -1.68719        1.04962        0.00000
C         -2.26860        2.31461        0.00000
O         -1.54839        3.31986        0.00000
N         -3.60887        2.38435        0.00000
H         -5.23885       -1.53999        0.00000
H         -0.66224        1.05572        0.00000
H         -0.14299       -3.40400        0.00000
H         -1.56043       -4.44064        0.00000
H         -4.13877        1.51248        0.00000
H         -4.01887        3.30126        0.00000
H          3.84733        3.61305        0.00000
H         -3.84733       -3.61305        0.00000
```

The DADA04 dimer

36
Energy = -1201.9308748780
C 1.02833 4.23793 0.00000
N -0.12201 3.55566 0.00000
C 2.27449 3.64333 0.00000
C 0.00878 2.23241 0.00000
C 2.28893 2.24211 0.00000
N 1.14483 1.53060 0.00000
H 0.93653 5.31882 0.00000
H 3.19254 4.20622 0.00000
N -1.15730 1.47302 0.00000
C -2.41111 1.99823 0.00000
O -3.42118 1.30420 0.00000
H -2.43865 3.09121 0.00000
N 3.43897 1.48731 0.00000
C 4.73975 1.94018 0.00000
H 5.44199 1.09273 0.00000
O 5.10243 3.09706 0.00000
N -1.14483 -1.53060 0.00000
C -2.28893 -2.24211 0.00000
C -0.00878 -2.23241 0.00000
C -2.27449 -3.64333 0.00000
N 0.12201 -3.55566 0.00000
C -1.02833 -4.23793 0.00000
H -0.93653 -5.31882 0.00000
H -3.19254 -4.20622 0.00000
N -3.43897 -1.48731 0.00000
C -4.73975 -1.94018 0.00000
H -5.44199 -1.09273 0.00000
O -5.10243 -3.09706 0.00000
N 1.15730 -1.47302 0.00000
C 2.41111 -1.99823 0.00000
O 3.42118 -1.30420 0.00000
H 2.43865 -3.09121 0.00000
H -3.32801 -0.46096 0.00000
H 1.07665 -0.44559 0.00000
H -1.07665 0.44559 0.00000
H 3.32801 0.46096 0.00000

The DADA05 dimer

42
Energy = -1381.0415350056
C 1.17978 4.23058 0.00000
N -0.03815 3.67666 0.00000
C 2.39058 3.55939 0.00000
C 0.01768 2.33751 0.00000
C 2.33018 2.14663 0.00000
N 1.11401 1.55598 0.00000
N 3.43383 1.40542 0.00000
N -1.17698 1.63361 0.00000
C -2.48322 2.10722 0.00000
O -3.43008 1.31231 0.00000
N -2.66799 3.43865 0.00000
N -1.11401 -1.55598 0.00000
C -2.33018 -2.14663 0.00000
C -0.01768 -2.33751 0.00000
C -2.39058 -3.55939 0.00000
N 0.03815 -3.67666 0.00000
C -1.17978 -4.23058 0.00000
N 1.17698 -1.63361 0.00000
C 2.48322 -2.10722 0.00000
O 3.43008 -1.31231 0.00000

```
N          2.66799        -3.43865         0.00000
N         -3.43383        -1.40542         0.00000
N          1.51484         5.56179         0.00000
N          3.45622         4.44152         0.00000
C          2.89628         5.62240         0.00000
H          3.41883         6.56597         0.00000
N         -3.45622        -4.44152         0.00000
N         -1.51484        -5.56179         0.00000
C         -2.89628        -5.62240         0.00000
H         -3.41883        -6.56597         0.00000
H         -1.85232         4.04596         0.00000
H         -3.61782         3.76484         0.00000
H         -1.09569         0.61329         0.00000
H          0.87409         6.33854         0.00000
H          4.31784         1.88602         0.00000
H          3.40133         0.37529         0.00000
H          1.09569        -0.61329         0.00000
H         -3.40133        -0.37529         0.00000
H         -4.31784        -1.88602         0.00000
H         -0.87409        -6.33854         0.00000
H          1.85232        -4.04596         0.00000
H          3.61782        -3.76484         0.00000
```

The DADA06 dimer

```
76
Energy = -2272.9436677781
C         -5.51368         1.74136        -2.73635
C         -6.83727         1.92793        -3.11575
C         -5.09548         0.50265        -2.24342
C         -7.75003         0.88350        -3.00058
C         -6.01223        -0.54533        -2.14030
C         -7.33535        -0.35302        -2.51238
C         -3.68937         0.23038        -1.84170
N         -2.99912         1.30135        -1.39601
N         -1.68682         1.21300        -1.00233
C         -1.13444         2.36964        -0.58707
C          0.27355         2.20022        -0.04964
N          0.68459         3.29555         0.58847
N          1.91370         3.39174         1.18644
C          2.24325         4.64487         1.63133
C          3.51740         4.80077         2.38024
C          4.00976         6.10204         2.51429
C          4.20555         3.73658         2.96753
C          5.18597         6.33482         3.21258
C          5.37975         3.97672         3.67220
C          5.87400         5.27184         3.79310
O         -3.18391        -0.89348        -1.89404
O         -1.71808         3.45207        -0.63989
O          0.92831         1.16336        -0.17808
O          1.49236         5.58751         1.38826
H         -7.15368         2.88577        -3.50947
H         -8.78148         1.03198        -3.29612
H         -4.80524         2.55244        -2.86008
H         -5.67387        -1.50064        -1.76207
H         -8.04336        -1.16763        -2.42135
H          3.45104         6.91234         2.06494
H          5.56548         7.34484         3.30828
H          6.78927         5.45393         4.34359
H          3.83159         2.72420         2.89091
H          5.90385         3.14794         4.13287
C         -3.51740        -4.80077        -2.38024
C         -4.20555        -3.73658        -2.96753
```

C	-4.00976	-6.10204	-2.51429
C	-5.37975	-3.97672	-3.67220
C	-5.18597	-6.33482	-3.21258
C	-5.87400	-5.27184	-3.79310
C	-2.24325	-4.64487	-1.63133
N	-1.91370	-3.39174	-1.18644
N	-0.68459	-3.29555	-0.58847
C	-0.27355	-2.20022	0.04964
C	1.13444	-2.36964	0.58707
N	1.68682	-1.21300	1.00233
N	2.99912	-1.30135	1.39601
C	3.68937	-0.23038	1.84170
O	-1.49236	-5.58751	-1.38826
O	-0.92831	-1.16336	0.17808
O	1.71808	-3.45207	0.63989
O	3.18391	0.89348	1.89404
C	5.09548	-0.50265	2.24342
C	6.01223	0.54533	2.14030
C	5.51368	-1.74136	2.73635
C	7.33535	0.35302	2.51238
C	6.83727	-1.92793	3.11575
C	7.75003	-0.88350	3.00058
H	-5.90385	-3.14794	-4.13287
H	-6.78927	-5.45393	-4.34359
H	-3.45104	-6.91234	-2.06494
H	-5.56548	-7.34484	-3.30828
H	-3.83159	-2.72420	-2.89091
H	5.67387	1.50064	1.76207
H	8.04336	1.16763	2.42135
H	8.78148	-1.03198	3.29612
H	4.80524	-2.55244	2.86008
H	7.15368	-2.88577	3.50947
H	-3.37835	2.23380	-1.27765
H	-1.33600	0.28123	-0.73106
H	0.15919	4.16779	0.58479
H	2.39549	2.50905	1.36820
H	-2.39549	-2.50905	-1.36820
H	-0.15919	-4.16779	-0.58479
H	1.33600	-0.28123	0.73106
H	3.37835	-2.23380	1.27765

The DADA07 dimer

72
Energy = -2310.9065606417

C	-2.79126	4.87350	-0.46473
C	-3.97296	4.05446	-0.31267
C	-1.52798	4.13181	-0.30023
C	-3.89298	2.71186	-0.05798
C	-1.52029	2.75161	-0.03743
N	-2.71188	2.06653	0.07957
C	-0.31627	4.81822	-0.39901
C	0.88682	4.16134	-0.23903
C	0.90561	2.75928	0.02161
C	-0.29866	2.08333	0.11184
C	2.13473	1.92859	0.21975
N	3.29027	2.60054	0.27938
N	4.49711	1.98675	0.47781
C	5.59595	2.79390	0.45679
C	6.91196	2.10137	0.69010
H	6.80419	1.02399	0.80212
H	7.36947	2.52070	1.58763
H	7.57204	2.32100	-0.15005

```
O          2.07937        0.69320        0.34677
O          5.47717        4.00005        0.26325
O         -2.82637        6.08339       -0.70053
C         -5.09841        1.85761        0.13799
O         -6.26562        2.33445       -0.31666
O         -5.05623        0.78023        0.68696
H         -4.92655        4.56629       -0.35905
H         -0.37459        5.87836       -0.60155
H         -0.28880        1.02174        0.31191
O          2.08370        4.80327       -0.32260
N          2.71188       -2.06653        0.07957
C          1.52029       -2.75161       -0.03743
C          3.89298       -2.71186       -0.05798
C          1.52798       -4.13181       -0.30023
C          3.97296       -4.05446       -0.31267
C          2.79126       -4.87350       -0.46473
C          5.09841       -1.85761        0.13799
O          6.26562       -2.33445       -0.31666
O          5.05623       -0.78023        0.68696
C          0.29866       -2.08333        0.11184
C         -0.90561       -2.75928        0.02161
C         -0.88682       -4.16134       -0.23903
C          0.31627       -4.81822       -0.39901
C         -2.13473       -1.92859        0.21975
N         -3.29027       -2.60054        0.27938
N         -4.49711       -1.98675        0.47781
C         -5.59595       -2.79390        0.45679
C         -6.91196       -2.10137        0.69010
O         -5.47717       -4.00005        0.26325
O         -2.07937       -0.69320        0.34677
H          4.92655       -4.56629       -0.35905
H          0.37459       -5.87836       -0.60155
H          0.28880       -1.02174        0.31191
O         -2.08370       -4.80327       -0.32260
C         -2.09488       -6.21171       -0.56446
H         -1.63227       -6.43715       -1.52758
H         -3.14552       -6.48795       -0.57526
H         -1.57104       -6.74078        0.23441
C          2.09488        6.21171       -0.56446
H          1.63227        6.43715       -1.52758
H          3.14552        6.48795       -0.57526
H          1.57104        6.74078        0.23441
H         -2.69419        1.05362        0.24718
H          3.35935        3.60774        0.14123
H          4.49800        0.98030        0.62124
H         -4.49800       -0.98030        0.62124
H         -3.35935       -3.60774        0.14123
H          2.69419       -1.05362        0.24718
H         -6.11808        3.16787       -0.78873
H          6.11808       -3.16787       -0.78873
H         -6.80419       -1.02399        0.80212
H         -7.36947       -2.52070        1.58763
H         -7.57204       -2.32100       -0.15005
O          2.82637       -6.08339       -0.70053
```

The DADA08 dimer

```
40
Energy = -1312.5705111590
C     1.0152836     4.3255086     0.0000000
N    -0.1406299     3.6501668     0.0000000
C     2.2488753     3.7191610     0.0000000
C    -0.0401174     2.3171815     0.0000000
```

```
C     2.2429087    2.3142826    0.0000000
N     1.0974774    1.6094095    0.0000000
N     3.3893313    1.5596491    0.0000000
C     4.6902465    2.0063334    0.0000000
O     5.0658438    3.1605825    0.0000000
N    -1.1997261    1.5662250    0.0000000
C    -2.5275576    1.9873385    0.0000000
O    -3.4299841    1.1417363    0.0000000
H     5.3863987    1.1539695    0.0000000
H     0.9299469    5.4067309    0.0000000
H     3.1752012    4.2680398    0.0000000
H    -1.0896542    0.5496190    0.0000000
H     3.2753227    0.5285757    0.0000000
N    -2.7667894    3.3055080    0.0000000
O     3.4299841   -1.1417363    0.0000000
C     2.5275576   -1.9873385    0.0000000
N     1.1997261   -1.5662250    0.0000000
N     2.7667894   -3.3055080    0.0000000
C     0.0401174   -2.3171815    0.0000000
N    -1.0974774   -1.6094095    0.0000000
N     0.1406299   -3.6501668    0.0000000
C    -2.2429087   -2.3142826    0.0000000
N    -3.3893313   -1.5596491    0.0000000
C    -1.0152836   -4.3255086    0.0000000
C    -2.2488753   -3.7191610    0.0000000
C    -4.6902465   -2.0063334    0.0000000
H    -5.3863987   -1.1539695    0.0000000
O    -5.0658438   -3.1605825    0.0000000
H    -0.9299469   -5.4067309    0.0000000
H    -3.1752012   -4.2680398    0.0000000
H     1.0896542   -0.5496190    0.0000000
H    -3.2753227   -0.5285757    0.0000000
H    -1.9737448    3.9449972    0.0000000
H    -3.7281267    3.5978583    0.0000000
H     3.7281267   -3.5978583    0.0000000
H     1.9737448   -3.9449972    0.0000000
```

The DADA09 dimer

```
140
Energy = -3358.5375199446
C         -4.95355        4.49483        0.89834
C         -6.13282        3.79583        0.67287
C         -3.72120        3.84860        0.92819
C         -3.66067        2.45504        0.71226
C         -6.09159        2.41403        0.47490
C         -4.85441        1.77317        0.49351
O         -2.55003        4.51684        1.15415
N         -7.22933        1.62299        0.25767
C         -8.49291        2.04342       -0.04687
C         -9.48884        0.91010       -0.23228
C        -10.41328        1.14433       -1.42543
C        -11.46472        0.04549       -1.55483
O         -8.82215        3.21791       -0.16284
C         -2.41327        1.63042        0.65821
N         -1.25340        2.23116        0.96110
C          0.01160        1.55286        0.89664
C          1.10719        2.56109        1.22666
N          2.35477        2.10256        0.95726
C          3.56319        2.79624        1.13045
C          3.69296        3.94140        1.91768
C          4.92976        4.56451        2.02933
C          6.05088        4.07273        1.36803
```

C	5.93789	2.91245	0.57583
C	4.68977	2.30283	0.47813
C	7.02797	2.26424	-0.22341
N	8.20687	2.91307	-0.31421
C	9.29035	2.47653	-1.17574
C	9.53419	3.41826	-2.36127
C	9.88184	4.83409	-1.90089
O	6.82541	1.18409	-0.79440
O	-2.45074	0.42825	0.34042
O	0.83941	3.66475	1.69042
O	7.27864	4.68152	1.45946
C	-2.59303	5.91822	1.39314
C	7.39254	5.85235	2.26183
C	10.64128	2.83676	-3.24064
H	-5.00814	5.56339	1.05199
H	-7.07998	4.31094	0.64269
H	-4.79875	0.70617	0.33087
H	-7.08762	0.61722	0.35106
H	-8.96589	-0.04270	-0.33143
H	-10.08781	0.85312	0.68420
H	-10.88738	2.12072	-1.31180
H	-9.81369	1.19455	-2.33939
H	-12.08217	-0.01329	-0.65386
H	-10.99776	-0.93301	-1.70155
H	-12.12779	0.22789	-2.40314
H	-1.23544	3.20798	1.23646
H	0.05756	0.72491	1.61267
H	0.18608	1.12303	-0.09110
H	2.42085	1.18678	0.50511
H	2.83260	4.34645	2.42595
H	5.00496	5.44950	2.64500
H	4.61139	1.42634	-0.15048
H	8.29033	3.77698	0.20263
H	10.20692	2.39029	-0.58192
H	9.02529	1.48487	-1.53604
H	8.60670	3.45725	-2.94265
H	10.06049	5.48822	-2.75688
H	10.78986	4.82940	-1.28905
H	9.07474	5.27790	-1.31266
H	-3.19106	6.14376	2.28008
H	-2.99988	6.44842	0.52793
H	-1.55927	6.21170	1.55713
H	7.14563	5.63468	3.30379
H	6.74465	6.64766	1.88489
H	8.43349	6.15753	2.18629
H	11.58080	2.76569	-2.68392
H	10.81875	3.46733	-4.11429
H	10.38251	1.83539	-3.59232
C	2.59303	-5.91822	-1.39314
C	-7.39254	-5.85235	-2.26183
C	-4.92976	-4.56451	-2.02933
O	2.55003	-4.51684	-1.15415
C	-3.69296	-3.94140	-1.91768
O	-0.83941	-3.66475	-1.69042
C	4.95355	-4.49483	-0.89834
O	-7.27864	-4.68152	-1.45946
C	3.72120	-3.84860	-0.92819
C	-6.05088	-4.07273	-1.36803
C	6.13282	-3.79583	-0.67287
C	-9.88184	-4.83409	1.90089
C	-1.10719	-2.56109	-1.22666
C	-3.56319	-2.79624	-1.13045

```
N          1.25340       -2.23116       -0.96110
C          3.66067       -2.45504       -0.71226
N         -2.35477       -2.10256       -0.95726
C         -5.93789       -2.91245       -0.57583
C         -0.01160       -1.55286       -0.89664
C         -4.68977       -2.30283       -0.47813
C          6.09159       -2.41403       -0.47490
C          2.41327       -1.63042       -0.65821
C         -9.53419       -3.41826        2.36127
O          8.82215       -3.21791        0.16284
C          4.85441       -1.77317       -0.49351
C         -7.02797       -2.26424        0.22341
C          8.49291       -2.04342        0.04687
N          7.22933       -1.62299       -0.25767
O         -6.82541       -1.18409        0.79440
N         -8.20687       -2.91307        0.31421
C        -10.64128       -2.83676        3.24064
O          2.45074       -0.42825       -0.34042
C          9.48884       -0.91010        0.23228
C         -9.29035       -2.47653        1.17574
C         10.41328       -1.14433        1.42543
C         11.46472       -0.04549        1.55483
H          2.99988       -6.44842       -0.52793
H          3.19106       -6.14376       -2.28008
H          1.55927       -6.21170       -1.55713
H         -6.74465       -6.64766       -1.88489
H         -7.14563       -5.63468       -3.30379
H         -8.43349       -6.15753       -2.18629
H         -5.00496       -5.44950       -2.64500
H         -2.83260       -4.34645       -2.42595
H          5.00814       -5.56339       -1.05199
H          7.07998       -4.31094       -0.64269
H         -9.07474       -5.27790        1.31266
H        -10.78986       -4.82940        1.28905
H        -10.06049       -5.48822        2.75688
H          1.23544       -3.20798       -1.23646
H         -2.42085       -1.18678       -0.50511
H         -0.05756       -0.72491       -1.61267
H         -0.18608       -1.12303        0.09110
H         -4.61139       -1.42634        0.15048
H         -8.60670       -3.45725        2.94265
H          4.79875       -0.70617       -0.33087
H          7.08762       -0.61722       -0.35106
H         -8.29033       -3.77698       -0.20263
H        -11.58080       -2.76569        2.68392
H        -10.38251       -1.83539        3.59232
H        -10.81875       -3.46733        4.11429
H          8.96589        0.04270        0.33143
H         10.08781       -0.85312       -0.68420
H        -10.20692       -2.39029        0.58192
H         -9.02529       -1.48487        1.53604
H         10.88738       -2.12072        1.31180
H          9.81369       -1.19455        2.33939
H         10.99776        0.93301        1.70155
H         12.08217        0.01329        0.65386
H         12.12779       -0.22789        2.40314
```

The DADA10 dimer

```
38
Energy = -1095.6272018917
N          1.54069       -1.04796        0.00000
C          2.27442       -2.17683        0.00000
```

```
C          3.69846        -2.15050         0.00000
C          4.33838        -0.94303         0.00000
C          3.36219         2.66712         0.00000
C          1.92519         2.54946         0.00000
N          1.42648         1.25629         0.00000
C          2.18957         0.12228         0.00000
C          3.59615         0.25371         0.00000
C          4.15108         1.56056         0.00000
N          1.61285        -3.34475         0.00000
H          4.24885        -3.08267         0.00000
H          5.42166        -0.89427         0.00000
H          0.58217        -3.38582         0.00000
H          5.23176         1.66174         0.00000
H          3.76610         3.66928         0.00000
O          1.14883         3.51803         0.00000
H          2.13424        -4.20299         0.00000
H          0.39611         1.15276         0.00000
N         -1.54069         1.04796         0.00000
C         -2.27442         2.17683         0.00000
C         -3.69846         2.15050         0.00000
C         -4.33838         0.94303         0.00000
C         -3.36219        -2.66712         0.00000
C         -1.92519        -2.54946         0.00000
N         -1.42648        -1.25629         0.00000
C         -2.18957        -0.12228         0.00000
C         -3.59615        -0.25371         0.00000
C         -4.15108        -1.56056         0.00000
N         -1.61285         3.34475         0.00000
H         -4.24885         3.08267         0.00000
H         -5.42166         0.89427         0.00000
H         -0.58217         3.38582         0.00000
H         -5.23176        -1.66174         0.00000
H         -3.76610        -3.66928         0.00000
O         -1.14883        -3.51803         0.00000
H         -2.13424         4.20299         0.00000
H         -0.39611        -1.15276         0.00000
```

The DDAA01 dimer

```
134
Energy = -3280.0661456010
C          -4.43726         3.53041        -3.61104
C          -5.63659         2.85467        -3.40316
C          -3.27197         3.13395        -2.95399
C          -5.69955         1.77283        -2.50399
C          -3.29538         2.03866        -2.06515
C          -4.51783         1.41134        -1.86622
O          -2.09894         3.77951        -3.14073
O          -6.77949         3.21964        -4.04896
C          -6.90555         0.95829        -2.16066
N          -7.97749         1.05642        -2.97626
O          -6.88805         0.20224        -1.18251
C          -2.12468         1.45166        -1.33988
N          -0.90427         1.90270        -1.66000
O          -2.28976         0.55370        -0.49939
C           0.30833         1.32550        -1.14448
C           1.45700         1.80682        -2.03168
N           2.65203         1.26120        -1.71353
O           1.24863         2.61641        -2.93237
C           3.89502         1.46704        -2.34648
C           4.03845         2.18576        -3.53704
C           5.30556         2.29792        -4.09545
C           6.42963         1.72705        -3.51399
```

C	6.27929	1.01745	-2.31769
C	5.01252	0.89137	-1.74291
N	7.35049	0.41828	-1.63738
C	8.62932	0.22593	-2.08240
O	9.03942	0.55208	-3.18807
C	-2.01299	4.85670	-4.08960
C	-0.58522	5.35336	-4.07339
C	-6.75717	4.34136	-4.94408
C	-8.16049	4.51185	-5.48173
C	-9.21460	0.32342	-2.76591
C	9.54237	-0.43593	-1.05892
C	-10.39780	1.25824	-2.53670
C	10.47171	-1.45502	-1.71134
H	-4.40420	4.36778	-4.28794
H	-4.54831	0.57326	-1.18587
H	-7.92474	1.73382	-3.72251
H	-0.77901	2.59947	-2.38678
H	0.49492	1.62417	-0.10843
H	0.25705	0.23638	-1.15005
H	2.64707	0.60827	-0.92932
H	3.17771	2.63574	-4.00270
H	5.42071	2.85093	-5.02048
H	7.40459	1.81409	-3.96460
H	4.89952	0.33574	-0.81990
H	7.15037	0.10631	-0.68980
H	-2.29815	4.47776	-5.07608
H	-2.71614	5.64257	-3.79610
H	0.10777	4.54787	-4.31329
H	-0.32560	5.74412	-3.08897
H	-0.47190	6.15437	-4.80638
H	-6.43105	5.22843	-4.39301
H	-6.04214	4.14384	-5.74847
H	-8.86528	4.69413	-4.66937
H	-8.47671	3.62247	-6.02917
H	-8.19164	5.36288	-6.16394
H	-9.40040	-0.31575	-3.63460
H	-9.04944	-0.32331	-1.90669
H	8.95021	-0.88676	-0.26150
H	10.13470	0.36547	-0.60350
H	-10.55852	1.91111	-3.39874
H	-10.23064	1.88524	-1.65991
H	-11.31088	0.68094	-2.37846
H	11.00771	-0.99511	-2.54113
H	9.90539	-2.30160	-2.10523
H	11.19705	-1.83529	-0.98914
C	4.43726	-3.53041	3.61104
C	5.63659	-2.85467	3.40316
C	3.27197	-3.13395	2.95399
C	5.69955	-1.77283	2.50399
C	3.29538	-2.03866	2.06515
C	4.51783	-1.41134	1.86622
O	2.09894	-3.77951	3.14073
O	6.77949	-3.21964	4.04896
C	6.90555	-0.95829	2.16066
N	7.97749	-1.05642	2.97626
O	6.88805	-0.20224	1.18251
C	2.12468	-1.45166	1.33988
N	0.90427	-1.90270	1.66000
O	2.28976	-0.55370	0.49939
C	-0.30833	-1.32550	1.14448
C	-1.45700	-1.80682	2.03168
N	-2.65203	-1.26120	1.71353

```
O         -1.24863       -2.61641        2.93237
C         -3.89502       -1.46704        2.34648
C         -4.03845       -2.18576        3.53704
C         -5.30556       -2.29792        4.09545
C         -6.42963       -1.72705        3.51399
C         -6.27929       -1.01745        2.31769
C         -5.01252       -0.89137        1.74291
N         -7.35049       -0.41828        1.63738
C         -8.62932       -0.22593        2.08240
O         -9.03942       -0.55208        3.18807
C          2.01299       -4.85670        4.08960
C          0.58522       -5.35336        4.07339
C          6.75717       -4.34136        4.94408
C          8.16049       -4.51185        5.48173
C          9.21460       -0.32342        2.76591
C         -9.54237        0.43593        1.05892
C         10.39780       -1.25824        2.53670
C        -10.47171        1.45502        1.71134
H          4.40420       -4.36778        4.28794
H          4.54831       -0.57326        1.18587
H          7.92474       -1.73382        3.72251
H          0.77901       -2.59947        2.38678
H         -0.49492       -1.62417        0.10843
H         -0.25705       -0.23638        1.15005
H         -2.64707       -0.60827        0.92932
H         -3.17771       -2.63574        4.00270
H         -5.42071       -2.85093        5.02048
H         -7.40459       -1.81409        3.96460
H         -4.89952       -0.33574        0.81990
H         -7.15037       -0.10631        0.68980
H          2.29815       -4.47776        5.07608
H          2.71614       -5.64257        3.79610
H          0.32560       -5.74412        3.08897
H         -0.10777       -4.54787        4.31329
H          0.47190       -6.15437        4.80638
H          6.43105       -5.22843        4.39301
H          6.04214       -4.14384        5.74847
H          8.47671       -3.62247        6.02917
H          8.86528       -4.69413        4.66937
H          8.19164       -5.36288        6.16394
H          9.40040        0.31575        3.63460
H          9.04944        0.32331        1.90669
H         -8.95021        0.88676        0.26150
H        -10.13470       -0.36547        0.60350
H         10.23064       -1.88524        1.65991
H         10.55852       -1.91111        3.39874
H         11.31088       -0.68094        2.37846
H         -9.90539        2.30160        2.10523
H        -11.00771        0.99511        2.54113
H        -11.19705        1.83529        0.98914
```

The DDAA02 dimer

```
34
Energy = -1125.9004393937
C          1.10895        4.18756       -0.04205
N         -0.05934        3.47850       -0.03552
C          2.29956        3.53740       -0.02080
C         -0.03121        2.11687       -0.00600
C          2.31317        2.07865        0.00930
N          1.08947        1.41992        0.01408
N         -1.23268        1.46534        0.00505
C         -2.48553        2.10749        0.00557
```

```
N         -3.52951        1.27303        0.04496
O          3.37660        1.44083        0.03300
H         -1.18086        0.41585        0.01627
H         -3.44913        0.23061        0.01671
H         -4.44355        1.70976        0.02164
O         -2.58965        3.34557       -0.01915
N         -1.08864       -1.42001        0.00657
C         -2.31226       -2.07742       -0.03478
C          0.03147       -2.11787        0.02530
C         -2.29913       -3.53618       -0.06110
N          0.05875       -3.47990        0.01787
C         -1.10953       -4.18772       -0.02925
N          1.23258       -1.46643        0.05112
C          2.48573       -2.10820        0.05086
N          3.52927       -1.27269        0.03009
O          2.58994       -3.34635        0.06330
H          1.03120       -3.87193        0.03781
H          1.18072       -0.41699        0.04231
H          3.44830       -0.22992        0.03413
H          4.44382       -1.70866        0.04323
O         -3.37505       -1.43835       -0.05001
H         -3.24912       -4.06646       -0.10045
H         -1.00723       -5.27374       -0.03934
H         -1.03264        3.86943       -0.04222
H          1.00578        5.27332       -0.06404
H          3.24977        4.06871       -0.02448
```

The DDAA03 dimer

```
44
Energy = -1282.2999495597
C         -3.83268        3.70308        0.91688
C         -4.84046        2.78097        1.08491
C         -2.56977        3.27149        0.48268
C         -4.56207        1.43750        0.79194
C         -2.37175        1.88232        0.24129
N         -3.38534        0.99300        0.38609
C         -1.46623        4.13147        0.25819
C         -0.27488        3.62114       -0.15256
C         -0.16034        2.20544       -0.32903
N         -1.18170        1.37226       -0.15241
N          1.03301        1.61557       -0.64819
C          2.18028        2.27162       -1.12396
N          3.25482        1.44681       -1.17814
O          2.19240        3.44009       -1.48567
N          3.38534       -0.99300        0.38609
C          2.37175       -1.88232        0.24129
C          4.56207       -1.43750        0.79194
C          2.56977       -3.27149        0.48268
C          4.84046       -2.78097        1.08491
C          3.83268       -3.70308        0.91688
N          1.18170       -1.37226       -0.15241
C          0.16034       -2.20544       -0.32903
C          0.27488       -3.62114       -0.15256
C          1.46623       -4.13147        0.25819
N         -1.03301       -1.61557       -0.64819
C         -2.18028       -2.27162       -1.12396
N         -3.25482       -1.44681       -1.17814
H         -3.29504       -0.59027       -0.61207
H         -4.11539       -1.89257       -1.44771
O         -2.19240       -3.44009       -1.48567
H         -1.07091       -0.59262       -0.53064
```

```
H          4.11539        1.89257       -1.44771
H          3.29504        0.59027       -0.61207
H          1.07091        0.59262       -0.53064
H         -3.99672        4.75723        1.11216
H         -5.82696        3.07068        1.42054
H         -5.34283        0.68898        0.89061
H         -1.57973        5.19732        0.42214
H          0.58722        4.23782       -0.34706
H          5.34283       -0.68898        0.89061
H          5.82696       -3.07068        1.42054
H          3.99672       -4.75723        1.11216
H         -0.58722       -4.23782       -0.34706
H          1.57973       -5.19732        0.42214
```

The DDAA04 dimer

```
40
Energy = -1238.2726246954
C         -4.00770        3.22906        0.00000
C         -3.50532        4.54190        0.00000
N         -3.22898        2.15429        0.00000
C         -2.14692        4.73903        0.00000
C         -1.91200        2.35536        0.00000
N         -1.33917        3.64993        0.00000
N         -0.95942        1.43872        0.00000
C          0.02816        3.49371        0.00000
C          0.22882        2.11917        0.00000
N          1.38063        1.39175        0.00000
C          2.65170        1.94671        0.00000
N          3.64432        1.01574        0.00000
O          2.84840        3.15587        0.00000
H         -5.07666        3.05042        0.00000
H         -4.17289        5.39112        0.00000
H          0.72388        4.31043        0.00000
C          4.00770       -3.22906        0.00000
N          3.22898       -2.15429        0.00000
C          3.50532       -4.54190        0.00000
C          1.91200       -2.35536        0.00000
C          2.14692       -4.73903        0.00000
N          1.33917       -3.64993        0.00000
N          0.95942       -1.43872        0.00000
C         -0.02816       -3.49371        0.00000
C         -0.22882       -2.11917        0.00000
N         -1.38063       -1.39175        0.00000
C         -2.65170       -1.94671        0.00000
N         -3.64432       -1.01574        0.00000
O         -2.84840       -3.15587        0.00000
H          5.07666       -3.05042        0.00000
H          4.17289       -5.39112        0.00000
H          1.66847       -5.70808        0.00000
H         -0.72388       -4.31043        0.00000
H         -1.66847        5.70808        0.00000
H          1.25822        0.36503        0.00000
H          3.49064        0.01186        0.00000
H          4.58542        1.36598        0.00000
H         -3.49064       -0.01186        0.00000
H         -4.58542       -1.36598        0.00000
H         -1.25822       -0.36503        0.00000
```

The DDAA05 dimer

```
38
```

```
S    -2.3906043    2.2719308    0.6013863
O    -3.2901753    1.3733313    1.3007449
O    -2.3165679    3.6401578    1.0829363
N    -0.9531313    1.5241564    0.5439539
C     0.1509392    2.2280299    0.2906138
N     0.2195346    3.5407439    0.0889844
H    -0.5863392    4.0925016    0.3575179
H     1.1568008    3.9207482   -0.0501658
N     1.3076496    1.4964852    0.2213638
C     2.5874961    2.0393220    0.0253852
H     1.1973362    0.4889715    0.3899489
N     3.5848274    1.1334311    0.0999505
H     3.4744514    0.2398709    0.5853896
H     4.5100144    1.5290883    0.0588417
O     2.7752060    3.2270190   -0.2325869
N    -3.5848274   -1.1334311    0.0999505
C    -2.5874961   -2.0393220    0.0253852
H    -4.5100144   -1.5290883    0.0588417
H    -3.4744514   -0.2398709    0.5853896
N    -1.3076496   -1.4964852    0.2213638
C    -0.1509392   -2.2280299    0.2906138
H    -1.1973362   -0.4889715    0.3899489
N     0.9531313   -1.5241564    0.5439539
N    -0.2195346   -3.5407439    0.0889844
H     0.5863392   -4.0925016    0.3575179
H    -1.1568008   -3.9207482   -0.0501658
S     2.3906043   -2.2719308    0.6013863
O     3.2901753   -1.3733313    1.3007449
O     2.3165679   -3.6401578    1.0829363
O    -2.7752060   -3.2270190   -0.2325869
C     2.9215116   -2.3382055   -1.0994095
H     2.9925652   -1.3228068   -1.4849029
H     2.1979973   -2.9219116   -1.6670245
H     3.8957798   -2.8252151   -1.1113118
C    -2.9215116    2.3382055   -1.0994095
H    -3.8957798    2.8252151   -1.1113118
H    -2.9925652    1.3228068   -1.4849029
H    -2.1979973    2.9219116   -1.6670245
```

The DDAA06 dimer

```
38
Energy = -1095.6075045348
N          1.50635       -1.11038        0.00000
C          2.17221       -2.29114        0.00000
C          3.58674       -2.27342        0.00000
C          4.24175       -1.06801        0.00000
C          3.36262        2.54721        0.00000
C          1.91807        2.43546        0.00000
N          1.34046        1.18734        0.00000
C          2.12772        0.11695        0.00000
C          3.54421        0.15003        0.00000
C          4.14321        1.43791        0.00000
N          1.45315       -3.41143        0.00000
H          4.12003       -3.21381        0.00000
H          5.32643       -1.04724        0.00000
H          0.39771       -3.40978        0.00000
H          5.22561        1.51393        0.00000
H          3.77696        3.54614        0.00000
O          1.20087        3.46465        0.00000
H          1.94554       -4.28757        0.00000
H          0.45233       -1.12164        0.00000
N         -1.50635        1.11038        0.00000
C         -2.17221        2.29114        0.00000
```

```
C         -3.58674        2.27342        0.00000
C         -4.24175        1.06801        0.00000
C         -3.36262       -2.54721        0.00000
C         -1.91807       -2.43546        0.00000
N         -1.34046       -1.18734        0.00000
C         -2.12772       -0.11695        0.00000
C         -3.54421       -0.15003        0.00000
C         -4.14321       -1.43791        0.00000
N         -1.45315        3.41143        0.00000
H         -4.12003        3.21381        0.00000
H         -5.32643        1.04724        0.00000
H         -0.39771        3.40978        0.00000
H         -5.22561       -1.51393        0.00000
H         -3.77696       -3.54614        0.00000
O         -1.20087       -3.46465        0.00000
H         -1.94554        4.28757        0.00000
H         -0.45233        1.12164        0.00000
```

The DDAA07 dimer

```
46
Energy = -1282.8684698777
H          4.80022       -3.00135        0.26849
C          3.87499       -3.37573        0.71130
N          2.78852       -2.43233        0.52643
C          2.40301       -2.08960       -0.70201
O          2.92504       -2.53748       -1.73782
N          1.34380       -1.16799       -0.73470
C          0.78010       -0.66729       -1.87010
N         -0.20894        0.19385       -1.76876
C         -0.77644        0.69860       -2.92699
O         -1.71211        1.51304       -2.85999
N          1.28155       -1.09417       -3.05528
C          0.76899       -0.63604       -4.24056
C         -0.25050        0.25220       -4.20010
C          1.40047       -1.17404       -5.48271
H          4.01538       -3.51147        1.78155
H          3.64224       -4.33787        0.25065
H          2.32747       -2.03643        1.36648
H          0.94056       -0.82212        0.15762
H          2.05894       -1.77258       -2.95428
H         -0.69044        0.64427       -5.10511
H          2.46607       -0.93161       -5.50713
H          0.92267       -0.75128       -6.36398
H          1.30977       -2.26276       -5.51864
H         -4.80022        3.00135       -0.26849
C         -3.87499        3.37573       -0.71130
N         -2.78852        2.43233       -0.52643
C         -2.40301        2.08960        0.70201
O         -2.92504        2.53748        1.73782
N         -1.34380        1.16799        0.73470
C         -0.78010        0.66729        1.87010
N          0.20894       -0.19385        1.76876
C          0.77644       -0.69860        2.92699
O          1.71211       -1.51304        2.85999
N         -1.28155        1.09417        3.05528
C         -0.76899        0.63604        4.24056
C          0.25050       -0.25220        4.20010
C         -1.40047        1.17404        5.48271
H         -4.01538        3.51147       -1.78155
H         -3.64224        4.33787       -0.25065
H         -2.32747        2.03643       -1.36648
H         -0.94056        0.82212       -0.15762
```

```
H         -2.05894        1.77258        2.95428
H          0.69044       -0.64427        5.10511
H         -2.46607        0.93161        5.50713
H         -0.92267        0.75128        6.36398
H         -1.30977        2.26276        5.51864
```

The DDAA08 dimer

```
50
Energy = -1543.2427077421
C         -2.37955        6.18735        0.00000
C         -3.63506        5.55276        0.00000
C         -3.67311        4.16063        0.00000
N         -1.21435        5.54068        0.00000
C         -1.27095        4.20510        0.00000
C         -2.46244        3.45563        0.00000
N         -0.08028        3.51362        0.00000
C         -2.38732        1.98100        0.00000
C         -0.05268        2.15553        0.00000
N         -1.14244        1.39519        0.00000
N          1.16775        1.54895        0.00000
C          2.40878        2.23467        0.00000
N          3.47811        1.42868        0.00000
O          2.48098        3.47027        0.00000
O         -3.42548        1.30542        0.00000
C          4.81215        1.99749        0.00000
H          4.97880        2.62580       -0.89296
H          5.53265        1.16577        0.00000
H          4.97880        2.62580        0.89296
C          2.46244       -3.45563        0.00000
C          1.27095       -4.20510        0.00000
C          3.67311       -4.16063        0.00000
N          1.21435       -5.54068        0.00000
C          3.63506       -5.55276        0.00000
C          2.37955       -6.18735        0.00000
C          2.38732       -1.98100        0.00000
N          0.08028       -3.51362        0.00000
C          0.05268       -2.15553        0.00000
N          1.14244       -1.39519        0.00000
N         -1.16775       -1.54895        0.00000
C         -2.40878       -2.23467        0.00000
N         -3.47811       -1.42868        0.00000
C         -4.81215       -1.99749        0.00000
H         -4.97880       -2.62580       -0.89296
H         -5.53265       -1.16577        0.00000
H         -4.97880       -2.62580        0.89296
O         -2.48098       -3.47027        0.00000
O          3.42548       -1.30542        0.00000
H         -4.55151        6.14832        0.00000
H         -4.60890        3.59574        0.00000
H         -2.31618        7.28233        0.00000
H          4.60890       -3.59574        0.00000
H          4.55151       -6.14832        0.00000
H          2.31618       -7.28233        0.00000
H         -0.84878       -3.98549        0.00000
H         -1.15000       -0.50057        0.00000
H         -3.37968       -0.39181        0.00000
H          1.15000        0.50057        0.00000
H          3.37968        0.39181        0.00000
H          0.84878        3.98549        0.00000
```

S1.4 Monomers with benzene probe

Molecule DADA01 with the benzene probe

```
31
Energy = -907.9787827350
C          0.97944         4.27963         0.00000
N         -0.15844         3.57207         0.00000
C          2.22299         3.69493         0.00000
C         -0.03201         2.24043         0.00000
C          2.24927         2.28843         0.00000
N          1.11633         1.55968         0.00000
N          3.40640         1.55569         0.00000
C          4.70278         2.02843         0.00000
O          5.04750         3.19027         0.00000
N         -1.18990         1.49275         0.00000
C         -2.50226         1.96404         0.00000
O         -3.43426         1.17386         0.00000
H          5.41605         1.19113         0.00000
H          0.86737         5.35742         0.00000
H          3.13761         4.26312         0.00000
H         -1.09949         0.47056         0.00000
H          3.30899         0.52445         0.00000
O         -2.68114         3.26556         0.00000
H         -1.76794         3.70601         0.00000
C          2.45404         2.09843         3.79999
H          3.39252         1.55659         3.80001
C          2.45404         3.49055         3.79999
H          3.39252         4.03238         3.80001
C          1.24842         4.18661         3.79999
H          1.24842         5.27027         3.80001
C          0.04281         3.49055         3.79999
H         -0.89567         4.03238         3.80001
C          0.04281         2.09843         3.79999
H         -0.89567         1.55659         3.80001
C          1.24842         1.40237         3.79999
H          1.24842         0.31870         3.80001
```

Molecule DADA02 with the benzene probe

```
29
Energy = -790.9523543834
C          4.02811         1.51915         0.00000
N          3.31953         2.62903         0.00000
N          3.55464         0.26633         0.00000
C          1.96898         2.43917         0.00000
C          2.20862         0.17300         0.00000
N          1.37322         1.22028         0.00000
N          1.20311         3.52702         0.00000
N          1.62439        -1.06904         0.00000
C          2.22691        -2.33689         0.00000
O          1.51666        -3.34741         0.00000
N          3.57025        -2.38291         0.00000
H          5.11973         1.62295         0.00000
H          1.67928         4.42096         0.00000
H          0.16575         3.46724         0.00000
H          4.09060        -1.49607         0.00000
H          3.99934        -3.29944         0.00000
H          0.58463        -1.08849         0.00000
C          3.46824         0.10833         3.79999
H          4.07840        -0.78643         3.80001
C          4.07101         1.36308         3.79999
H          5.15038         1.44506         3.80001
C          3.28717         2.51252         3.79999
H          3.75638         3.48926         3.80001
```

```
C          1.90057        2.40721        3.79999
H          1.29041        3.30197        3.80001
C          1.29780        1.15246        3.79999
H          0.21843        1.07048        3.80001
C          2.08163        0.00302        3.79999
H          1.61242       -0.97372        3.80001
```

Molecule DADA03 with the benzene probe

```
30
Energy = -774.8988259432
C          4.15495        1.49042        0.00000
C          3.39911        2.62877        0.00000
N          3.62757        0.25377        0.00000
C          1.99093        2.46276        0.00000
C          2.29171        0.19409        0.00000
N          1.44228        1.22970        0.00000
N          1.16807        3.51606        0.00000
N          1.68719       -1.04962        0.00000
C          2.26860       -2.31461        0.00000
O          1.54839       -3.31986        0.00000
N          3.60887       -2.38435        0.00000
H          5.23885        1.53999        0.00000
H          1.56043        4.44064        0.00000
H          0.14299        3.40400        0.00000
H          4.13877       -1.51248        0.00000
H          4.01887       -3.30126        0.00000
H          0.66224       -1.05572        0.00000
H          3.84733        3.61305        0.00000
C          2.20378        0.09028        3.79999
H          1.71014       -0.87442        3.80001
C          3.59398        0.16086        3.79999
H          4.18251       -0.74890        3.80001
C          4.22813        1.40015        3.79999
H          5.31030        1.45509        3.80001
C          3.47207        2.56887        3.79999
H          3.96571        3.53357        3.80001
C          2.08187        2.49829        3.79999
H          1.49334        3.40805        3.80001
C          1.44772        1.25900        3.79999
H          0.36555        1.20406        3.80001
```

Molecule DADA04 with the benzene probe

```
30
Energy = -832.7885659783
C          1.02833        4.23793        0.00000
N         -0.12201        3.55566        0.00000
C          2.27449        3.64333        0.00000
C          0.00878        2.23241        0.00000
C          2.28893        2.24211        0.00000
N          1.14483        1.53060        0.00000
H          0.93653        5.31882        0.00000
H          3.19254        4.20622        0.00000
N         -1.15730        1.47302        0.00000
C         -2.41111        1.99823        0.00000
O         -3.42118        1.30420        0.00000
H         -2.43865        3.09121        0.00000
N          3.43897        1.48731        0.00000
C          4.73975        1.94018        0.00000
H          5.44199        1.09273        0.00000
O          5.10243        3.09706        0.00000
H         -1.07665        0.44559        0.00000
H          3.32801        0.46096        0.00000
C          2.44139        2.01020        3.79999
```

```
H          3.37987        1.46837        3.80001
C          2.44139        3.40232        3.79999
H          3.37987        3.94416        3.80001
C          1.23578        4.09838        3.79999
H          1.23578        5.18205        3.80001
C          0.03017        3.40232        3.79999
H         -0.90831        3.94416        3.80001
C          0.03017        2.01020        3.79999
H         -0.90831        1.46837        3.80001
C          1.23578        1.31414        3.79999
H          1.23578        0.23048        3.80001
```

Molecule DADA05-R with the benzene probe

```
33
Energy = -922.3445336616
C          1.17978        4.23058        0.00000
N         -0.03815        3.67666        0.00000
C          2.39058        3.55939        0.00000
C          0.01768        2.33751        0.00000
C          2.33018        2.14663        0.00000
N          1.11401        1.55598        0.00000
N          3.43383        1.40542        0.00000
N         -1.17698        1.63361        0.00000
C         -2.48322        2.10722        0.00000
O         -3.43008        1.31231        0.00000
N         -2.66799        3.43865        0.00000
N          1.51484        5.56179        0.00000
N          3.45622        4.44152        0.00000
C          2.89628        5.62240        0.00000
H          3.41883        6.56597        0.00000
H         -1.85232        4.04596        0.00000
H         -3.61782        3.76484        0.00000
H         -1.09569        0.61329        0.00000
H          0.87409        6.33854        0.00000
H          4.31784        1.88602        0.00000
H          3.40133        0.37529        0.00000
C          2.25097        2.01795        3.79999
H          3.17527        1.45253        3.80001
C          2.28586        3.40953        3.79999
H          3.23732        3.92735        3.80001
C          1.09846        4.13590        3.79999
H          1.12561        5.21914        3.80001
C         -0.12384        3.47069        3.79999
H         -1.04814        4.03611        3.80001
C         -0.15873        2.07911        3.79999
H         -1.11019        1.56129        3.80001
C          1.02868        1.35274        3.79999
H          1.00152        0.26950        3.80001
```

Molecule DADA05-L with the benzene probe

```
33
Energy = -922.3434173603
C          1.17978        4.23058        0.00000
N         -0.03815        3.67666        0.00000
C          2.39058        3.55939        0.00000
C          0.01768        2.33751        0.00000
C          2.33018        2.14663        0.00000
N          1.11401        1.55598        0.00000
N          3.43383        1.40542        0.00000
N         -1.17698        1.63361        0.00000
C         -2.48322        2.10722        0.00000
O         -3.43008        1.31231        0.00000
N         -2.66799        3.43865        0.00000
```

```
N          1.51484        5.56179        0.00000
N          3.45622        4.44152        0.00000
C          2.89628        5.62240        0.00000
H          3.41883        6.56597        0.00000
H         -1.85232        4.04596        0.00000
H         -3.61782        3.76484        0.00000
H         -1.09569        0.61329        0.00000
H          0.87409        6.33854        0.00000
H          4.31784        1.88602        0.00000
H          3.40133        0.37529        0.00000
C          3.49856        3.82236        3.79999
H          4.42286        3.25694        3.80001
C          3.53345        5.21394        3.79999
H          4.48491        5.73176        3.80001
C          2.34605        5.94031        3.79999
H          2.37320        7.02355        3.80001
C          1.12375        5.27510        3.79999
H          0.19945        5.84052        3.80001
C          1.08886        3.88352        3.79999
H          0.13740        3.36570        3.80001
C          2.27627        3.15715        3.79999
H          2.24911        2.07391        3.80001
```

Molecule DADA06-R with the benzene probe

```
50
Energy = -1368.2893346166
C         -5.51368        1.74136       -2.73635
C         -6.83727        1.92793       -3.11575
C         -5.09548        0.50265       -2.24342
C         -7.75003        0.88350       -3.00058
C         -6.01223       -0.54533       -2.14030
C         -7.33535       -0.35302       -2.51238
C         -3.68937        0.23038       -1.84170
N         -2.99912        1.30135       -1.39601
N         -1.68682        1.21300       -1.00233
C         -1.13444        2.36964       -0.58707
C          0.27355        2.20022       -0.04964
N          0.68459        3.29555        0.58847
N          1.91370        3.39174        1.18644
C          2.24325        4.64487        1.63133
C          3.51740        4.80077        2.38024
C          4.00976        6.10204        2.51429
C          4.20555        3.73658        2.96753
C          5.18597        6.33482        3.21258
C          5.37975        3.97672        3.67220
C          5.87400        5.27184        3.79310
O         -3.18391       -0.89348       -1.89404
O         -1.71808        3.45207       -0.63989
O          0.92831        1.16336       -0.17808
O          1.49236        5.58751        1.38826
H         -7.15368        2.88577       -3.50947
H         -8.78148        1.03198       -3.29612
H         -4.80524        2.55244       -2.86008
H         -5.67387       -1.50064       -1.76207
H         -8.04336       -1.16763       -2.42135
H          3.45104        6.91234        2.06494
H          5.56548        7.34484        3.30828
H          6.78927        5.45393        4.34359
H          3.83159        2.72420        2.89091
H          5.90385        3.14794        4.13287
H         -3.37835        2.23380       -1.27765
H         -1.33600        0.28123       -0.73106
H          0.15919        4.16779        0.58479
```

```
H          2.39549        2.50905        1.36820
C         -6.28487        1.60254        1.21514
H         -5.25412        1.44306        1.50916
C         -6.68674        2.84486        0.73228
H         -5.96880        3.65244        0.65043
C         -8.01088        3.04971        0.35456
H         -8.32371        4.01676       -0.02130
C         -8.93318        2.01225        0.45972
H         -9.96393        2.17171        0.16571
C         -8.53132        0.76993        0.94258
H         -9.24925       -0.03766        1.02445
C         -7.20718        0.56507        1.32029
H         -6.89435       -0.40198        1.69617
```

Molecule DADA06-L with the benzene probe

```
50
Energy = -1368.2893016540
C         -5.51368        1.74136       -2.73635
C         -6.83727        1.92793       -3.11575
C         -5.09548        0.50265       -2.24342
C         -7.75003        0.88350       -3.00058
C         -6.01223       -0.54533       -2.14030
C         -7.33535       -0.35302       -2.51238
C         -3.68937        0.23038       -1.84170
N         -2.99912        1.30135       -1.39601
N         -1.68682        1.21300       -1.00233
C         -1.13444        2.36964       -0.58707
C          0.27355        2.20022       -0.04964
N          0.68459        3.29555        0.58847
N          1.91370        3.39174        1.18644
C          2.24325        4.64487        1.63133
C          3.51740        4.80077        2.38024
C          4.00976        6.10204        2.51429
C          4.20555        3.73658        2.96753
C          5.18597        6.33482        3.21258
C          5.37975        3.97672        3.67220
C          5.87400        5.27184        3.79310
O         -3.18391       -0.89348       -1.89404
O         -1.71808        3.45207       -0.63989
O          0.92831        1.16336       -0.17808
O          1.49236        5.58751        1.38826
H         -7.15368        2.88577       -3.50947
H         -8.78148        1.03198       -3.29612
H         -4.80524        2.55244       -2.86008
H         -5.67387       -1.50064       -1.76207
H         -8.04336       -1.16763       -2.42135
H          3.45104        6.91234        2.06494
H          5.56548        7.34484        3.30828
H          6.78927        5.45393        4.34359
H          3.83159        2.72420        2.89091
H          5.90385        3.14794        4.13287
H         -3.37835        2.23380       -1.27765
H         -1.33600        0.28123       -0.73106
H          0.15919        4.16779        0.58479
H          2.39549        2.50905        1.36820
C          4.12220        5.48708        7.14498
H          5.04572        5.61463        7.69740
C          3.48110        6.59401        6.59571
H          3.90557        7.58323        6.72056
C          2.29470        6.43014        5.88606
H          1.79564        7.29180        5.45850
C          1.74940        5.15934        5.72568
H          0.82587        5.03178        5.17328
```

```
C          2.39049        4.05241        6.27495
H          1.96602        3.06318        6.15012
C          3.57689        4.21628        6.98460
H          4.07594        3.35461        7.41217
```

Molecule DADA07-R with the benzene probe

```
48
Energy = -1387.2764796096
C         -2.79126        4.87350       -0.46473
C         -3.97296        4.05446       -0.31267
C         -1.52798        4.13181       -0.30023
C         -3.89298        2.71186       -0.05798
C         -1.52029        2.75161       -0.03743
N         -2.71188        2.06653        0.07957
C         -0.31627        4.81822       -0.39901
C          0.88682        4.16134       -0.23903
C          0.90561        2.75928        0.02161
C         -0.29866        2.08333        0.11184
C          2.13473        1.92859        0.21975
N          3.29027        2.60054        0.27938
N          4.49711        1.98675        0.47781
C          5.59595        2.79390        0.45679
C          6.91196        2.10137        0.69010
H          6.80419        1.02399        0.80212
H          7.36947        2.52070        1.58763
H          7.57204        2.32100       -0.15005
O          2.07937        0.69320        0.34677
O          5.47717        4.00005        0.26325
O         -2.82637        6.08339       -0.70053
C         -5.09841        1.85761        0.13799
O         -6.26562        2.33445       -0.31666
O         -5.05623        0.78023        0.68696
H         -4.92655        4.56629       -0.35905
H         -0.37459        5.87836       -0.60155
H         -0.28880        1.02174        0.31191
O          2.08370        4.80327       -0.32260
C          2.09488        6.21171       -0.56446
H          1.63227        6.43715       -1.52758
H          3.14552        6.48795       -0.57526
H          1.57104        6.74078        0.23441
H         -2.69419        1.05362        0.24718
H          3.35935        3.60774        0.14123
H          4.49800        0.98030        0.62124
H         -6.11808        3.16787       -0.78873
C         -1.36578        3.31730        3.65102
H         -0.42728        2.78130        3.73019
C         -1.36613        4.68832        3.40959
H         -0.42791        5.21958        3.30082
C         -2.57177        5.37687        3.30790
H         -2.57205        6.44411        3.11997
C         -3.77705        4.69440        3.44763
H         -4.71555        5.23039        3.36849
C         -3.77670        3.32338        3.68906
H         -4.71492        2.79211        3.79785
C         -2.57107        2.63482        3.79076
H         -2.57079        1.56758        3.97870
```

Molecule DADA07-L with the benzene probe

```
48
Energy = -1387.2753051930
C         -2.79126        4.87350       -0.46473
C         -3.97296        4.05446       -0.31267
C         -1.52798        4.13181       -0.30023
```

```
C         -3.89298        2.71186       -0.05798
C         -1.52029        2.75161       -0.03743
N         -2.71188        2.06653        0.07957
C         -0.31627        4.81822       -0.39901
C          0.88682        4.16134       -0.23903
C          0.90561        2.75928        0.02161
C         -0.29866        2.08333        0.11184
C          2.13473        1.92859        0.21975
N          3.29027        2.60054        0.27938
N          4.49711        1.98675        0.47781
C          5.59595        2.79390        0.45679
C          6.91196        2.10137        0.69010
H          6.80419        1.02399        0.80212
H          7.36947        2.52070        1.58763
H          7.57204        2.32100       -0.15005
O          2.07937        0.69320        0.34677
O          5.47717        4.00005        0.26325
O         -2.82637        6.08339       -0.70053
C         -5.09841        1.85761        0.13799
O         -6.26562        2.33445       -0.31666
O         -5.05623        0.78023        0.68696
H         -4.92655        4.56629       -0.35905
H         -0.37459        5.87836       -0.60155
H         -0.28880        1.02174        0.31191
O          2.08370        4.80327       -0.32260
C          2.09488        6.21171       -0.56446
H          1.63227        6.43715       -1.52758
H          3.14552        6.48795       -0.57526
H          1.57104        6.74078        0.23441
H         -2.69419        1.05362        0.24718
H          3.35935        3.60774        0.14123
H          4.49800        0.98030        0.62124
H         -6.11808        3.16787       -0.78873
C          0.59095        3.22790        3.82617
H          1.52945        2.69190        3.90534
C          0.59060        4.59892        3.58474
H          1.52882        5.13018        3.47597
C         -0.61504        5.28747        3.48305
H         -0.61532        6.35471        3.29512
C         -1.82032        4.60500        3.62278
H         -2.75882        5.14099        3.54364
C         -1.81997        3.23398        3.86421
H         -2.75819        2.70271        3.97300
C         -0.61434        2.54542        3.96591
H         -0.61406        1.47818        4.15385
```

Molecule DADA08 with the benzene probe

```
32
Energy = -888.1058489655
C          1.01528        4.32551        0.00000
N         -0.14063        3.65017        0.00000
C          2.24888        3.71916        0.00000
C         -0.04012        2.31718        0.00000
C          2.24291        2.31428        0.00000
N          1.09748        1.60941        0.00000
N          3.38933        1.55965        0.00000
C          4.69025        2.00633        0.00000
O          5.06584        3.16058        0.00000
N         -1.19973        1.56622        0.00000
C         -2.52756        1.98734        0.00000
O         -3.42998        1.14174        0.00000
H          5.38640        1.15397        0.00000
H          0.92995        5.40673        0.00000
```

```
H          3.17520        4.26804        0.00000
H         -1.08965        0.54962        0.00000
H          3.27532        0.52858        0.00000
N         -2.76679        3.30551        0.00000
H         -1.97374        3.94500        0.00000
H         -3.72813        3.59786        0.00000
C          2.45404        2.09843        3.79999
H          3.39252        1.55659        3.80001
C          2.45404        3.49055        3.79999
H          3.39252        4.03238        3.80001
C          1.24842        4.18661        3.79999
H          1.24842        5.27027        3.80001
C          0.04281        3.49055        3.79999
H         -0.89567        4.03238        3.80001
C          0.04281        2.09843        3.79999
H         -0.89567        1.55659        3.80001
C          1.24842        1.40237        3.79999
H          1.24842        0.31870        3.80001
```

Molecule DADA09-R with the benzene probe

```
82
Energy = -1911.0752223752
C         -4.95355        4.49483        0.89834
C         -6.13282        3.79583        0.67287
C         -3.72120        3.84860        0.92819
C         -3.66067        2.45504        0.71226
C         -6.09159        2.41403        0.47490
C         -4.85441        1.77317        0.49351
O         -2.55003        4.51684        1.15415
N         -7.22933        1.62299        0.25767
C         -8.49291        2.04342       -0.04687
C         -9.48884        0.91010       -0.23228
C        -10.41328        1.14433       -1.42543
C        -11.46472        0.04549       -1.55483
O         -8.82215        3.21791       -0.16284
C         -2.41327        1.63042        0.65821
N         -1.25340        2.23116        0.96110
C          0.01160        1.55286        0.89664
C          1.10719        2.56109        1.22666
N          2.35477        2.10256        0.95726
C          3.56319        2.79624        1.13045
C          3.69296        3.94140        1.91768
C          4.92976        4.56451        2.02933
C          6.05088        4.07273        1.36803
C          5.93789        2.91245        0.57583
C          4.68977        2.30283        0.47813
C          7.02797        2.26424       -0.22341
N          8.20687        2.91307       -0.31421
C          9.29035        2.47653       -1.17574
C          9.53419        3.41826       -2.36127
C          9.88184        4.83409       -1.90089
O          6.82541        1.18409       -0.79440
O         -2.45074        0.42825        0.34042
O          0.83941        3.66475        1.69042
O          7.27864        4.68152        1.45946
C         -2.59303        5.91822        1.39314
C          7.39254        5.85235        2.26183
C         10.64128        2.83676       -3.24064
H         -5.00814        5.56339        1.05199
H         -7.07998        4.31094        0.64269
H         -4.79875        0.70617        0.33087
H         -7.08762        0.61722        0.35106
H         -8.96589       -0.04270       -0.33143
```

```
H        -10.08781         0.85312         0.68420
H        -10.88738         2.12072        -1.31180
H         -9.81369         1.19455        -2.33939
H        -12.08217        -0.01329        -0.65386
H        -10.99776        -0.93301        -1.70155
H        -12.12779         0.22789        -2.40314
H         -1.23544         3.20798         1.23646
H          0.05756         0.72491         1.61267
H          0.18608         1.12303        -0.09110
H          2.42085         1.18678         0.50511
H          2.83260         4.34645         2.42595
H          5.00496         5.44950         2.64500
H          4.61139         1.42634        -0.15048
H          8.29033         3.77698         0.20263
H         10.20692         2.39029        -0.58192
H          9.02529         1.48487        -1.53604
H          8.60670         3.45725        -2.94265
H         10.06049         5.48822        -2.75688
H         10.78986         4.82940        -1.28905
H          9.07474         5.27790        -1.31266
H         -3.19106         6.14376         2.28008
H         -2.99988         6.44842         0.52793
H         -1.55927         6.21170         1.55713
H          7.14563         5.63468         3.30379
H          6.74465         6.64766         1.88489
H          8.43349         6.15753         2.18629
H         11.58080         2.76569        -2.68392
H         10.81875         3.46733        -4.11429
H         10.38251         1.83539        -3.59232
C          6.97713         0.93931         3.68589
H          7.90361         0.61935         3.22373
C          6.95646         2.07566         4.48982
H          7.86684         2.64025         4.65346
C          5.76628         2.48671         5.08354
H          5.75017         3.37126         5.70933
C          4.59676         1.76140         4.87333
H          3.67028         2.08138         5.33549
C          4.61744         0.62506         4.06939
H          3.70706         0.06047         3.90576
C          5.80763         0.21401         3.47568
H          5.82581        -0.69406         2.87979
```

Molecule DADA09-L with the benzene probe

```
82
Energy = -1911.0777879151
C         -4.95355         4.49483         0.89834
C         -6.13282         3.79583         0.67287
C         -3.72120         3.84860         0.92819
C         -3.66067         2.45504         0.71226
C         -6.09159         2.41403         0.47490
C         -4.85441         1.77317         0.49351
O         -2.55003         4.51684         1.15415
N         -7.22933         1.62299         0.25767
C         -8.49291         2.04342        -0.04687
C         -9.48884         0.91010        -0.23228
C        -10.41328         1.14433        -1.42543
C        -11.46472         0.04549        -1.55483
O         -8.82215         3.21791        -0.16284
C         -2.41327         1.63042         0.65821
N         -1.25340         2.23116         0.96110
C          0.01160         1.55286         0.89664
C          1.10719         2.56109         1.22666
N          2.35477         2.10256         0.95726
```

C	3.56319	2.79624	1.13045
C	3.69296	3.94140	1.91768
C	4.92976	4.56451	2.02933
C	6.05088	4.07273	1.36803
C	5.93789	2.91245	0.57583
C	4.68977	2.30283	0.47813
C	7.02797	2.26424	-0.22341
N	8.20687	2.91307	-0.31421
C	9.29035	2.47653	-1.17574
C	9.53419	3.41826	-2.36127
C	9.88184	4.83409	-1.90089
O	6.82541	1.18409	-0.79440
O	-2.45074	0.42825	0.34042
O	0.83941	3.66475	1.69042
O	7.27864	4.68152	1.45946
C	-2.59303	5.91822	1.39314
C	7.39254	5.85235	2.26183
C	10.64128	2.83676	-3.24064
H	-5.00814	5.56339	1.05199
H	-7.07998	4.31094	0.64269
H	-4.79875	0.70617	0.33087
H	-7.08762	0.61722	0.35106
H	-8.96589	-0.04270	-0.33143
H	-10.08781	0.85312	0.68420
H	-10.88738	2.12072	-1.31180
H	-9.81369	1.19455	-2.33939
H	-12.08217	-0.01329	-0.65386
H	-10.99776	-0.93301	-1.70155
H	-12.12779	0.22789	-2.40314
H	-1.23544	3.20798	1.23646
H	0.05756	0.72491	1.61267
H	0.18608	1.12303	-0.09110
H	2.42085	1.18678	0.50511
H	2.83260	4.34645	2.42595
H	5.00496	5.44950	2.64500
H	4.61139	1.42634	-0.15048
H	8.29033	3.77698	0.20263
H	10.20692	2.39029	-0.58192
H	9.02529	1.48487	-1.53604
H	8.60670	3.45725	-2.94265
H	10.06049	5.48822	-2.75688
H	10.78986	4.82940	-1.28905
H	9.07474	5.27790	-1.31266
H	-3.19106	6.14376	2.28008
H	-2.99988	6.44842	0.52793
H	-1.55927	6.21170	1.55713
H	7.14563	5.63468	3.30379
H	6.74465	6.64766	1.88489
H	8.43349	6.15753	2.18629
H	11.58080	2.76569	-2.68392
H	10.81875	3.46733	-4.11429
H	10.38251	1.83539	-3.59232
C	-3.99035	1.73846	4.52439
H	-3.05393	1.19435	4.56164
C	-4.00053	3.11931	4.70098
H	-3.07204	3.65007	4.87569
C	-5.20349	3.81831	4.65313
H	-5.21142	4.89318	4.79059
C	-6.39628	3.13646	4.42869
H	-7.33269	3.68058	4.39144
C	-6.38609	1.75562	4.25210
H	-7.31458	1.22486	4.07739

```
C         -5.18312        1.05662        4.29996
H         -5.17520       -0.01825        4.16249
```

Molecule DADA10-R with the benzene probe

```
31
Energy = -779.6348666740
N          1.54069       -1.04796        0.00000
C          2.27442       -2.17683        0.00000
C          3.69846       -2.15050        0.00000
C          4.33838       -0.94303        0.00000
C          3.36219        2.66712        0.00000
C          1.92519        2.54946        0.00000
N          1.42648        1.25629        0.00000
C          2.18957        0.12228        0.00000
C          3.59615        0.25371        0.00000
C          4.15108        1.56056        0.00000
N          1.61285       -3.34475        0.00000
H          4.24885       -3.08267        0.00000
H          5.42166       -0.89427        0.00000
H          0.58217       -3.38582        0.00000
H          5.23176        1.66174        0.00000
H          3.76610        3.66928        0.00000
O          1.14883        3.51803        0.00000
H          2.13424       -4.20299        0.00000
H          0.39611        1.15276        0.00000
C          3.20775        0.37194        3.79999
H          3.78056       -0.54767        3.80001
C          3.86323        1.59977        3.79999
H          4.94629        1.63593        3.80001
C          3.12737        2.78113        3.79999
H          3.63762        3.73690        3.80001
C          1.73603        2.73467        3.79999
H          1.16322        3.65427        3.80001
C          1.08054        1.50684        3.79999
H         -0.00251        1.47067        3.80001
C          1.81640        0.32547        3.79999
H          1.30616       -0.63029        3.80001
```

Molecule DADA10-L with the benzene probe

```
31
Energy = -779.6349283856
N          1.54069       -1.04796        0.00000
C          2.27442       -2.17683        0.00000
C          3.69846       -2.15050        0.00000
C          4.33838       -0.94303        0.00000
C          3.36219        2.66712        0.00000
C          1.92519        2.54946        0.00000
N          1.42648        1.25629        0.00000
C          2.18957        0.12228        0.00000
C          3.59615        0.25371        0.00000
C          4.15108        1.56056        0.00000
N          1.61285       -3.34475        0.00000
H          4.24885       -3.08267        0.00000
H          5.42166       -0.89427        0.00000
H          0.58217       -3.38582        0.00000
H          5.23176        1.66174        0.00000
H          3.76610        3.66928        0.00000
O          1.14883        3.51803        0.00000
H          2.13424       -4.20299        0.00000
H          0.39611        1.15276        0.00000
C          3.51088       -2.28351        3.79999
H          4.08369       -3.20312        3.80001
C          4.16636       -1.05568        3.79999
```

```
H          5.24942       -1.01952        3.80001
C          3.43050        0.12568        3.79999
H          3.94075        1.08145        3.80001
C          2.03916        0.07922        3.79999
H          1.46635        0.99882        3.80001
C          1.38367       -1.14861        3.79999
H          0.30062       -1.18478        3.80001
C          2.11953       -2.32998        3.79999
H          1.60929       -3.28574        3.80001
```

Molecule DDAA01-R with the benzene probe

```
79
Energy = -1871.8393826992
C         -4.43726        3.53041       -3.61104
C         -5.63659        2.85467       -3.40316
C         -3.27197        3.13395       -2.95399
C         -5.69955        1.77283       -2.50399
C         -3.29538        2.03866       -2.06515
C         -4.51783        1.41134       -1.86622
O         -2.09894        3.77951       -3.14073
O         -6.77949        3.21964       -4.04896
C         -6.90555        0.95829       -2.16066
N         -7.97749        1.05642       -2.97626
O         -6.88805        0.20224       -1.18251
C         -2.12468        1.45166       -1.33988
N         -0.90427        1.90270       -1.66000
O         -2.28976        0.55370       -0.49939
C          0.30833        1.32550       -1.14448
C          1.45700        1.80682       -2.03168
N          2.65203        1.26120       -1.71353
O          1.24863        2.61641       -2.93237
C          3.89502        1.46704       -2.34648
C          4.03845        2.18576       -3.53704
C          5.30556        2.29792       -4.09545
C          6.42963        1.72705       -3.51399
C          6.27929        1.01745       -2.31769
C          5.01252        0.89137       -1.74291
N          7.35049        0.41828       -1.63738
C          8.62932        0.22593       -2.08240
O          9.03942        0.55208       -3.18807
C         -2.01299        4.85670       -4.08960
C         -0.58522        5.35336       -4.07339
C         -6.75717        4.34136       -4.94408
C         -8.16049        4.51185       -5.48173
C         -9.21460        0.32342       -2.76591
C          9.54237       -0.43593       -1.05892
C        -10.39780        1.25824       -2.53670
C         10.47171       -1.45502       -1.71134
H         -4.40420        4.36778       -4.28794
H         -4.54831        0.57326       -1.18587
H         -7.92474        1.73382       -3.72251
H         -0.77901        2.59947       -2.38678
H          0.49492        1.62417       -0.10843
H          0.25705        0.23638       -1.15005
H          2.64707        0.60827       -0.92932
H          3.17771        2.63574       -4.00270
H          5.42071        2.85093       -5.02048
H          7.40459        1.81409       -3.96460
H          4.89952        0.33574       -0.81990
H          7.15037        0.10631       -0.68980
H         -2.29815        4.47776       -5.07608
H         -2.71614        5.64257       -3.79610
H          0.10777        4.54787       -4.31329
```

```
H          -0.32560        5.74412       -3.08897
H          -0.47190        6.15437       -4.80638
H          -6.43105        5.22843       -4.39301
H          -6.04214        4.14384       -5.74847
H          -8.86528        4.69413       -4.66937
H          -8.47671        3.62247       -6.02917
H          -8.19164        5.36288       -6.16394
H          -9.40040       -0.31575       -3.63460
H          -9.04944       -0.32331       -1.90669
H           8.95021       -0.88676       -0.26150
H          10.13470        0.36547       -0.60350
H         -10.55852        1.91111       -3.39874
H         -10.23064        1.88524       -1.65991
H         -11.31088        0.68094       -2.37846
H          11.00771       -0.99511       -2.54113
H           9.90539       -2.30160       -2.10523
H          11.19705       -1.83529       -0.98914
C           5.85568       -2.15646       -4.39135
H           6.72535       -2.60348       -3.92426
C           5.99098       -1.45321       -5.58513
H           6.96597       -1.35278       -6.04733
C           4.87376       -0.87894       -6.18516
H           4.97908       -0.33150       -7.11445
C           3.62123       -1.00793       -5.59141
H           2.75156       -0.56090       -6.05849
C           3.48593       -1.71119       -4.39763
H           2.51094       -1.81159       -3.93544
C           4.60315       -2.28545       -3.79760
H           4.49783       -2.83288       -2.86831
```

Molecule DDAA01-L with the benzene probe

```
79
Energy = -1871.8427012548
C          -4.43726        3.53041       -3.61104
C          -5.63659        2.85467       -3.40316
C          -3.27197        3.13395       -2.95399
C          -5.69955        1.77283       -2.50399
C          -3.29538        2.03866       -2.06515
C          -4.51783        1.41134       -1.86622
O          -2.09894        3.77951       -3.14073
O          -6.77949        3.21964       -4.04896
C          -6.90555        0.95829       -2.16066
N          -7.97749        1.05642       -2.97626
O          -6.88805        0.20224       -1.18251
C          -2.12468        1.45166       -1.33988
N          -0.90427        1.90270       -1.66000
O          -2.28976        0.55370       -0.49939
C           0.30833        1.32550       -1.14448
C           1.45700        1.80682       -2.03168
N           2.65203        1.26120       -1.71353
O           1.24863        2.61641       -2.93237
C           3.89502        1.46704       -2.34648
C           4.03845        2.18576       -3.53704
C           5.30556        2.29792       -4.09545
C           6.42963        1.72705       -3.51399
C           6.27929        1.01745       -2.31769
C           5.01252        0.89137       -1.74291
N           7.35049        0.41828       -1.63738
C           8.62932        0.22593       -2.08240
O           9.03942        0.55208       -3.18807
C          -2.01299        4.85670       -4.08960
C          -0.58522        5.35336       -4.07339
C          -6.75717        4.34136       -4.94408
```

C	-8.16049	4.51185	-5.48173
C	-9.21460	0.32342	-2.76591
C	9.54237	-0.43593	-1.05892
C	-10.39780	1.25824	-2.53670
C	10.47171	-1.45502	-1.71134
H	-4.40420	4.36778	-4.28794
H	-4.54831	0.57326	-1.18587
H	-7.92474	1.73382	-3.72251
H	-0.77901	2.59947	-2.38678
H	0.49492	1.62417	-0.10843
H	0.25705	0.23638	-1.15005
H	2.64707	0.60827	-0.92932
H	3.17771	2.63574	-4.00270
H	5.42071	2.85093	-5.02048
H	7.40459	1.81409	-3.96460
H	4.89952	0.33574	-0.81990
H	7.15037	0.10631	-0.68980
H	-2.29815	4.47776	-5.07608
H	-2.71614	5.64257	-3.79610
H	0.10777	4.54787	-4.31329
H	-0.32560	5.74412	-3.08897
H	-0.47190	6.15437	-4.80638
H	-6.43105	5.22843	-4.39301
H	-6.04214	4.14384	-5.74847
H	-8.86528	4.69413	-4.66937
H	-8.47671	3.62247	-6.02917
H	-8.19164	5.36288	-6.16394
H	-9.40040	-0.31575	-3.63460
H	-9.04944	-0.32331	-1.90669
H	8.95021	-0.88676	-0.26150
H	10.13470	0.36547	-0.60350
H	-10.55852	1.91111	-3.39874
H	-10.23064	1.88524	-1.65991
H	-11.31088	0.68094	-2.37846
H	11.00771	-0.99511	-2.54113
H	9.90539	-2.30160	-2.10523
H	11.19705	-1.83529	-0.98914
C	-3.74294	-1.15132	-4.52508
H	-3.82786	-1.98755	-3.84110
C	-2.51414	-0.52282	-4.70691
H	-1.64254	-0.86981	-4.16447
C	-2.40503	0.55143	-5.58558
H	-1.44852	1.04068	-5.72713
C	-3.52473	0.99720	-6.28243
H	-3.43980	1.83343	-6.96641
C	-4.75352	0.36870	-6.10061
H	-5.62511	0.71568	-6.64304
C	-4.86262	-0.70556	-5.22193
H	-5.81915	-1.19480	-5.08039

Molecule DDAA02 with the benzene probe

29
Energy = -794.7500484841

C	1.10895	4.18756	-0.04205
N	-0.05934	3.47850	-0.03552
C	2.29956	3.53740	-0.02080
C	-0.03121	2.11687	-0.00600
C	2.31317	2.07865	0.00930
N	1.08947	1.41992	0.01408
N	-1.23268	1.46534	0.00505
C	-2.48553	2.10749	0.00557
N	-3.52951	1.27303	0.04496
O	3.37660	1.44083	0.03300

```
H         -1.18086        0.41585        0.01627
H         -3.44913        0.23061        0.01671
H         -4.44355        1.70976        0.02164
O         -2.58965        3.34557       -0.01915
H         -1.03264        3.86943       -0.04222
H          1.00578        5.27332       -0.06404
H          3.24977        4.06871       -0.02448
C          2.59036        2.40281        3.79999
H          3.52884        1.86097        3.80001
C          2.59036        3.79493        3.79999
H          3.52884        4.33676        3.80001
C          1.38474        4.49099        3.79999
H          1.38474        5.57465        3.80001
C          0.17913        3.79493        3.79999
H         -0.75935        4.33676        3.80001
C          0.17913        2.40281        3.79999
H         -0.75935        1.86097        3.80001
C          1.38474        1.70674        3.79999
H          1.38474        0.62308        3.80001
```

Molecule DDAA03-R with the benzene probe

```
34
Energy = -872.9666849266
C         -3.83268        3.70308        0.91688
C         -4.84046        2.78097        1.08491
C         -2.56977        3.27149        0.48268
C         -4.56207        1.43750        0.79194
C         -2.37175        1.88232        0.24129
N         -3.38534        0.99300        0.38609
C         -1.46623        4.13147        0.25819
C         -0.27488        3.62114       -0.15256
C         -0.16034        2.20544       -0.32903
N         -1.18170        1.37226       -0.15241
N          1.03301        1.61557       -0.64819
C          2.18028        2.27162       -1.12396
N          3.25482        1.44681       -1.17814
O          2.19240        3.44009       -1.48567
H          4.11539        1.89257       -1.44771
H          3.29504        0.59027       -0.61207
H          1.07091        0.59262       -0.53064
H         -3.99672        4.75723        1.11216
H         -5.82696        3.07068        1.42054
H         -5.34283        0.68898        0.89061
H         -1.57973        5.19732        0.42214
H          0.58722        4.23782       -0.34706
C         -1.45952        1.39431        3.86884
H         -0.50371        1.01397        3.52812
C         -1.62241        2.75652        4.10517
H         -0.79339        3.43657        3.94839
C         -2.85028        3.24511        4.54290
H         -2.97707        4.30550        4.72686
C         -3.91528        2.37149        4.74431
H         -4.87108        2.75182        5.08506
C         -3.75240        1.00928        4.50799
H         -4.58142        0.32921        4.66478
C         -2.52453        0.52069        4.07027
H         -2.39774       -0.53970        3.88631
```

Molecule DDAA03-L with the benzene probe

```
34
Energy = -872.9677364691
C         -3.83268        3.70308        0.91688
C         -4.84046        2.78097        1.08491
```

```
C         -2.56977        3.27149         0.48268
C         -4.56207        1.43750         0.79194
C         -2.37175        1.88232         0.24129
N         -3.38534        0.99300         0.38609
C         -1.46623        4.13147         0.25819
C         -0.27488        3.62114        -0.15256
C         -0.16034        2.20544        -0.32903
N         -1.18170        1.37226        -0.15241
N          1.03301        1.61557        -0.64819
C          2.18028        2.27162        -1.12396
N          3.25482        1.44681        -1.17814
O          2.19240        3.44009        -1.48567
H          4.11539        1.89257        -1.44771
H          3.29504        0.59027        -0.61207
H          1.07091        0.59262        -0.53064
H         -3.99672        4.75723         1.11216
H         -5.82696        3.07068         1.42054
H         -5.34283        0.68898         0.89061
H         -1.57973        5.19732         0.42214
H          0.58722        4.23782        -0.34706
C          0.87205        2.14885         3.41094
H          1.84856        1.77680         3.12399
C          0.67294        3.51485         3.59097
H          1.49446        4.20613         3.44415
C         -0.58152        3.99279         3.95962
H         -0.73651        5.05612         4.09976
C         -1.63688        3.10474         4.14824
H         -2.61338        3.47678         4.43521
C         -1.43778        1.73874         3.96821
H         -2.25929        1.04744         4.11505
C         -0.18332        1.26080         3.59957
H         -0.02833        0.19746         3.45944
```

Molecule DDAA04-R with the benzene probe

```
32
Energy = -850.9564581745
C         -4.00770        3.22906         0.00000
C         -3.50532        4.54190         0.00000
N         -3.22898        2.15429         0.00000
C         -2.14692        4.73903         0.00000
C         -1.91200        2.35536         0.00000
N         -1.33917        3.64993         0.00000
N         -0.95942        1.43872         0.00000
C          0.02816        3.49371         0.00000
C          0.22882        2.11917         0.00000
N          1.38063        1.39175         0.00000
C          2.65170        1.94671         0.00000
N          3.64432        1.01574         0.00000
O          2.84840        3.15587         0.00000
H         -5.07666        3.05042         0.00000
H         -4.17289        5.39112         0.00000
H          0.72388        4.31043         0.00000
H         -1.66847        5.70808         0.00000
H          1.25822        0.36503         0.00000
H          3.49064        0.01186         0.00000
H          4.58542        1.36598         0.00000
C         -1.56188        2.40233         3.79999
H         -0.81801        1.61532         3.80001
C         -1.16331        3.73571         3.79999
H         -0.10917        3.98664         3.80001
C         -2.11892        4.74673         3.79999
H         -1.80866        5.78467         3.80001
C         -3.47310        4.42437         3.79999
```

```
H          -4.21697         5.21137         3.80001
C          -3.87168         3.09099         3.79999
H          -4.92581         2.84005         3.80001
C          -2.91607         2.07997         3.79999
H          -3.22634         1.04202         3.80001
```

Molecule DDAA04-L with the benzene probe

```
32
Energy = -850.9569561228
C          -4.00770         3.22906         0.00000
C          -3.50532         4.54190         0.00000
N          -3.22898         2.15429         0.00000
C          -2.14692         4.73903         0.00000
C          -1.91200         2.35536         0.00000
N          -1.33917         3.64993         0.00000
N          -0.95942         1.43872         0.00000
C           0.02816         3.49371         0.00000
C           0.22882         2.11917         0.00000
N           1.38063         1.39175         0.00000
C           2.65170         1.94671         0.00000
N           3.64432         1.01574         0.00000
O           2.84840         3.15587         0.00000
H          -5.07666         3.05042         0.00000
H          -4.17289         5.39112         0.00000
H           0.72388         4.31043         0.00000
H          -1.66847         5.70808         0.00000
H           1.25822         0.36503         0.00000
H           3.49064         0.01186         0.00000
H           4.58542         1.36598         0.00000
C           0.33920         2.16333         3.79999
H           1.27768         1.62150         3.80001
C           0.33920         3.55545         3.79999
H           1.27768         4.09728         3.80001
C          -0.86642         4.25151         3.79999
H          -0.86642         5.33517         3.80001
C          -2.07203         3.55545         3.79999
H          -3.01051         4.09728         3.80001
C          -2.07203         2.16333         3.79999
H          -3.01051         1.62150         3.80001
C          -0.86642         1.46727         3.79999
H          -0.86642         0.38360         3.80001
```

Molecule DDAA06-R with the benzene probe

```
31
Energy = -779.5918995099
N           1.50635        -1.11038         0.00000
C           2.17221        -2.29114         0.00000
C           3.58674        -2.27342         0.00000
C           4.24175        -1.06801         0.00000
C           3.36262         2.54721         0.00000
C           1.91807         2.43546         0.00000
N           1.34046         1.18734         0.00000
C           2.12772         0.11695         0.00000
C           3.54421         0.15003         0.00000
C           4.14321         1.43791         0.00000
N           1.45315        -3.41143         0.00000
H           4.12003        -3.21381         0.00000
H           5.32643        -1.04724         0.00000
H           0.39771        -3.40978         0.00000
H           5.22561         1.51393         0.00000
H           3.77696         3.54614         0.00000
O           1.20087         3.46465         0.00000
H           1.94554        -4.28757         0.00000
```

```
H          0.45233       -1.12164        0.00000
C          3.38228        0.12464        3.79999
H          3.93770       -0.80582        3.80001
C          4.05972        1.34012        3.79999
H          5.14249        1.35582        3.80001
C          3.34619        2.53542        3.79999
H          3.87353        3.48158        3.80001
C          1.95522        2.51524        3.79999
H          1.39979        3.44569        3.80001
C          1.27777        1.29976        3.79999
H          0.19500        1.28404        3.80001
C          1.99129        0.10445        3.79999
H          1.46395       -0.84171        3.80001
```

Molecule DDAA06-L with the benzene probe

```
31
Energy = -779.5916504132
N          1.50635       -1.11038        0.00000
C          2.17221       -2.29114        0.00000
C          3.58674       -2.27342        0.00000
C          4.24175       -1.06801        0.00000
C          3.36262        2.54721        0.00000
C          1.91807        2.43546        0.00000
N          1.34046        1.18734        0.00000
C          2.12772        0.11695        0.00000
C          3.54421        0.15003        0.00000
C          4.14321        1.43791        0.00000
N          1.45315       -3.41143        0.00000
H          4.12003       -3.21381        0.00000
H          5.32643       -1.04724        0.00000
H          0.39771       -3.40978        0.00000
H          5.22561        1.51393        0.00000
H          3.77696        3.54614        0.00000
O          1.20087        3.46465        0.00000
H          1.94554       -4.28757        0.00000
H          0.45233       -1.12164        0.00000
C          3.63481       -2.32958        3.79999
H          4.11190       -3.28966        3.80001
C          4.39044       -1.16121        3.79999
H          5.45575       -1.21180        3.80001
C          3.77753        0.07216        3.79999
H          4.36574        0.98164        3.80001
C          2.40900        0.13714        3.79999
H          1.93190        1.09722        3.80001
C          1.65336       -1.03123        3.79999
H          0.58805       -0.98065        3.80001
C          2.26626       -2.26460        3.79999
H          1.67805       -3.17409        3.80001
```

Molecule DDAA07 with the benzene probe

```
35
Energy = -873.2349990235
H          4.80022       -3.00135        0.26849
C          3.87499       -3.37573        0.71130
N          2.78852       -2.43233        0.52643
C          2.40301       -2.08960       -0.70201
O          2.92504       -2.53748       -1.73782
N          1.34380       -1.16799       -0.73470
C          0.78010       -0.66729       -1.87010
N         -0.20894        0.19385       -1.76876
C         -0.77644        0.69860       -2.92699
O         -1.71211        1.51304       -2.85999
N          1.28155       -1.09417       -3.05528
```

C	0.76899	-0.63604	-4.24056
C	-0.25050	0.25220	-4.20010
C	1.40047	-1.17404	-5.48271
H	4.01538	-3.51147	1.78155
H	3.64224	-4.33787	0.25065
H	2.32747	-2.03643	1.36648
H	0.94056	-0.82212	0.15762
H	2.05894	-1.77258	-2.95428
H	-0.69044	0.64427	-5.10511
H	2.46607	-0.93161	-5.50713
H	0.92267	-0.75128	-6.36398
H	1.30977	-2.26276	-5.51864
C	3.61335	1.98037	-3.20313
H	4.44868	1.29804	-3.30790
C	3.00489	2.51480	-4.33546
H	3.36658	2.24848	-5.32165
C	1.93179	3.39136	-4.20087
H	1.45815	3.80738	-5.08229
C	1.46716	3.73349	-2.93396
H	0.63184	4.41583	-2.82920
C	2.07562	3.19907	-1.80163
H	1.71394	3.46540	-0.81544
C	3.14872	2.32251	-1.93622
H	3.62237	1.90650	-1.05478

Molecule DDAA08-R with the benzene probe

37
Energy = -1003.4262857193

C	-2.37955	6.18735	0.00000
C	-3.63506	5.55276	0.00000
C	-3.67311	4.16063	0.00000
N	-1.21435	5.54068	0.00000
C	-1.27095	4.20510	0.00000
C	-2.46244	3.45563	0.00000
N	-0.08028	3.51362	0.00000
C	-2.38732	1.98100	0.00000
C	-0.05268	2.15553	0.00000
N	-1.14244	1.39519	0.00000
N	1.16775	1.54895	0.00000
C	2.40878	2.23467	0.00000
N	3.47811	1.42868	0.00000
O	2.48098	3.47027	0.00000
O	-3.42548	1.30542	0.00000
C	4.81215	1.99749	0.00000
H	4.97880	2.62580	-0.89296
H	5.53265	1.16577	0.00000
H	4.97880	2.62580	0.89296
H	-4.55151	6.14832	0.00000
H	-4.60890	3.59574	0.00000
H	-2.31618	7.28233	0.00000
H	1.15000	0.50057	0.00000
H	3.37968	0.39181	0.00000
H	0.84878	3.98549	0.00000
C	-1.42420	3.97432	3.79999
H	-0.57278	3.30515	3.80001
C	-1.22846	5.35231	3.79999
H	-0.22468	5.75579	3.80001
C	-2.32223	6.21197	3.79999
H	-2.16988	7.28463	3.80001
C	-3.61173	5.69364	3.79999
H	-4.46314	6.36281	3.80001
C	-3.80748	4.31565	3.79999
H	-4.81125	3.91217	3.80001

```
C         -2.71370        3.45600        3.79999
H         -2.86607        2.38333        3.80001
```

Molecule DDAA08-L with the benzene probe

```
37
Energy = -1003.4276332243
C         -2.37955        6.18735        0.00000
C         -3.63506        5.55276        0.00000
C         -3.67311        4.16063        0.00000
N         -1.21435        5.54068        0.00000
C         -1.27095        4.20510        0.00000
C         -2.46244        3.45563        0.00000
N         -0.08028        3.51362        0.00000
C         -2.38732        1.98100        0.00000
C         -0.05268        2.15553        0.00000
N         -1.14244        1.39519        0.00000
N          1.16775        1.54895        0.00000
C          2.40878        2.23467        0.00000
N          3.47811        1.42868        0.00000
O          2.48098        3.47027        0.00000
O         -3.42548        1.30542        0.00000
C          4.81215        1.99749        0.00000
H          4.97880        2.62580       -0.89296
H          5.53265        1.16577        0.00000
H          4.97880        2.62580        0.89296
H         -4.55151        6.14832        0.00000
H         -4.60890        3.59574        0.00000
H         -2.31618        7.28233        0.00000
H          1.15000        0.50057        0.00000
H          3.37968        0.39181        0.00000
H          0.84878        3.98549        0.00000
C         -0.08438        2.11478        3.79999
H          0.90042        1.67946        3.80001
C         -0.23928        3.49825        3.79999
H          0.62494        4.13986        3.80001
C         -1.50441        4.05749        3.79999
H         -1.62500        5.13441        3.80001
C         -2.61463        3.23325        3.79999
H         -3.59943        3.66857        3.80001
C         -2.45974        1.84978        3.79999
H         -3.32396        1.20817        3.80001
C         -1.19461        1.29055        3.79999
H         -1.07403        0.21361        3.80001
```

S1.5 Monomers

Molecule DADA01

```
19
Energy = -676.1319023917
C          0.97944        4.27963        0.00000
N         -0.15844        3.57207        0.00000
C          2.22299        3.69493        0.00000
C         -0.03201        2.24043        0.00000
C          2.24927        2.28843        0.00000
N          1.11633        1.55968        0.00000
N          3.40640        1.55569        0.00000
C          4.70278        2.02843        0.00000
O          5.04750        3.19027        0.00000
N         -1.18990        1.49275        0.00000
C         -2.50226        1.96404        0.00000
O         -3.43426        1.17386        0.00000
```

```
H          5.41605        1.19113        0.00000
H          0.86737        5.35742        0.00000
H          3.13761        4.26312        0.00000
H         -1.09949        0.47056        0.00000
H          3.30899        0.52445        0.00000
O         -2.68114        3.26556        0.00000
H         -1.76794        3.70601        0.00000
```

Molecule DADA02

```
17
Energy = -559.1080382260
C          4.02811        1.51915        0.00000
N          3.31953        2.62903        0.00000
N          3.55464        0.26633        0.00000
C          1.96898        2.43917        0.00000
C          2.20862        0.17300        0.00000
N          1.37322        1.22028        0.00000
N          1.20311        3.52702        0.00000
N          1.62439       -1.06904        0.00000
C          2.22691       -2.33689        0.00000
O          1.51666       -3.34741        0.00000
N          3.57025       -2.38291        0.00000
H          5.11973        1.62295        0.00000
H          1.67928        4.42096        0.00000
H          0.16575        3.46724        0.00000
H          4.09060       -1.49607        0.00000
H          3.99934       -3.29944        0.00000
H          0.58463       -1.08849        0.00000
```

Molecule DADA03

```
18
Energy = -543.0534150514
C          4.15495        1.49042        0.00000
C          3.39911        2.62877        0.00000
N          3.62757        0.25377        0.00000
C          1.99093        2.46276        0.00000
C          2.29171        0.19409        0.00000
N          1.44228        1.22970        0.00000
N          1.16807        3.51606        0.00000
N          1.68719       -1.04962        0.00000
C          2.26860       -2.31461        0.00000
O          1.54839       -3.31986        0.00000
N          3.60887       -2.38435        0.00000
H          5.23885        1.53999        0.00000
H          1.56043        4.44064        0.00000
H          0.14299        3.40400        0.00000
H          4.13877       -1.51248        0.00000
H          4.01887       -3.30126        0.00000
H          0.66224       -1.05572        0.00000
H          3.84733        3.61305        0.00000
```

Molecule DADA04

```
18
Energy = -600.9422394890
C          1.02833        4.23793        0.00000
N         -0.12201        3.55566        0.00000
C          2.27449        3.64333        0.00000
C          0.00878        2.23241        0.00000
C          2.28893        2.24211        0.00000
N          1.14483        1.53060        0.00000
H          0.93653        5.31882        0.00000
H          3.19254        4.20622        0.00000
```

```
N         -1.15730        1.47302        0.00000
C         -2.41111        1.99823        0.00000
O         -3.42118        1.30420        0.00000
H         -2.43865        3.09121        0.00000
N          3.43897        1.48731        0.00000
C          4.73975        1.94018        0.00000
H          5.44199        1.09273        0.00000
O          5.10243        3.09706        0.00000
H         -1.07665        0.44559        0.00000
H          3.32801        0.46096        0.00000
```

Molecule DADA05

```
21
Energy = -690.4972150351
C          1.17978        4.23058        0.00000
N         -0.03815        3.67666        0.00000
C          2.39058        3.55939        0.00000
C          0.01768        2.33751        0.00000
C          2.33018        2.14663        0.00000
N          1.11401        1.55598        0.00000
N          3.43383        1.40542        0.00000
N         -1.17698        1.63361        0.00000
C         -2.48322        2.10722        0.00000
O         -3.43008        1.31231        0.00000
N         -2.66799        3.43865        0.00000
N          1.51484        5.56179        0.00000
N          3.45622        4.44152        0.00000
C          2.89628        5.62240        0.00000
H          3.41883        6.56597        0.00000
H         -1.85232        4.04596        0.00000
H         -3.61782        3.76484        0.00000
H         -1.09569        0.61329        0.00000
H          0.87409        6.33854        0.00000
H          4.31784        1.88602        0.00000
H          3.40133        0.37529        0.00000
```

Molecule DADA06

```
38
Energy = -1136.4447119367
C         -5.51368        1.74136       -2.73635
C         -6.83727        1.92793       -3.11575
C         -5.09548        0.50265       -2.24342
C         -7.75003        0.88350       -3.00058
C         -6.01223       -0.54533       -2.14030
C         -7.33535       -0.35302       -2.51238
C         -3.68937        0.23038       -1.84170
N         -2.99912        1.30135       -1.39601
N         -1.68682        1.21300       -1.00233
C         -1.13444        2.36964       -0.58707
C          0.27355        2.20022       -0.04964
N          0.68459        3.29555        0.58847
N          1.91370        3.39174        1.18644
C          2.24325        4.64487        1.63133
C          3.51740        4.80077        2.38024
C          4.00976        6.10204        2.51429
C          4.20555        3.73658        2.96753
C          5.18597        6.33482        3.21258
C          5.37975        3.97672        3.67220
C          5.87400        5.27184        3.79310
O         -3.18391       -0.89348       -1.89404
O         -1.71808        3.45207       -0.63989
O          0.92831        1.16336       -0.17808
O          1.49236        5.58751        1.38826
```

```
H          -7.15368         2.88577        -3.50947
H          -8.78148         1.03198        -3.29612
H          -4.80524         2.55244        -2.86008
H          -5.67387        -1.50064        -1.76207
H          -8.04336        -1.16763        -2.42135
H           3.45104         6.91234         2.06494
H           5.56548         7.34484         3.30828
H           6.78927         5.45393         4.34359
H           3.83159         2.72420         2.89091
H           5.90385         3.14794         4.13287
H          -3.37835         2.23380        -1.27765
H          -1.33600         0.28123        -0.73106
H           0.15919         4.16779         0.58479
H           2.39549         2.50905         1.36820
```

Molecule DADA07

```
36
Energy = -1155.4264169128
C          -2.79126         4.87350        -0.46473
C          -3.97296         4.05446        -0.31267
C          -1.52798         4.13181        -0.30023
C          -3.89298         2.71186        -0.05798
C          -1.52029         2.75161        -0.03743
N          -2.71188         2.06653         0.07957
C          -0.31627         4.81822        -0.39901
C           0.88682         4.16134        -0.23903
C           0.90561         2.75928         0.02161
C          -0.29866         2.08333         0.11184
C           2.13473         1.92859         0.21975
N           3.29027         2.60054         0.27938
N           4.49711         1.98675         0.47781
C           5.59595         2.79390         0.45679
C           6.91196         2.10137         0.69010
H           6.80419         1.02399         0.80212
H           7.36947         2.52070         1.58763
H           7.57204         2.32100        -0.15005
O           2.07937         0.69320         0.34677
O           5.47717         4.00005         0.26325
O          -2.82637         6.08339        -0.70053
C          -5.09841         1.85761         0.13799
O          -6.26562         2.33445        -0.31666
O          -5.05623         0.78023         0.68696
H          -4.92655         4.56629        -0.35905
H          -0.37459         5.87836        -0.60155
H          -0.28880         1.02174         0.31191
O           2.08370         4.80327        -0.32260
C           2.09488         6.21171        -0.56446
H           1.63227         6.43715        -1.52758
H           3.14552         6.48795        -0.57526
H           1.57104         6.74078         0.23441
H          -2.69419         1.05362         0.24718
H           3.35935         3.60774         0.14123
H           4.49800         0.98030         0.62124
H          -6.11808         3.16787        -0.78873
```

Molecule DADA08

```
20
Energy = -656.2590967401
C           1.01528         4.32551         0.00000
N          -0.14063         3.65017         0.00000
C           2.24888         3.71916         0.00000
C          -0.04012         2.31718         0.00000
C           2.24291         2.31428         0.00000
```

```
N          1.09748        1.60941        0.00000
N          3.38933        1.55965        0.00000
C          4.69025        2.00633        0.00000
O          5.06584        3.16058        0.00000
N         -1.19973        1.56622        0.00000
C         -2.52756        1.98734        0.00000
O         -3.42998        1.14174        0.00000
H          5.38640        1.15397        0.00000
H          0.92995        5.40673        0.00000
H          3.17520        4.26804        0.00000
H         -1.08965        0.54962        0.00000
H          3.27532        0.52858        0.00000
N         -2.76679        3.30551        0.00000
H         -1.97374        3.94500        0.00000
H         -3.72813        3.59786        0.00000
```

Molecule DADA09

```
70
Energy = -1679.2313716053
C         -4.95355        4.49483        0.89834
C         -6.13282        3.79583        0.67287
C         -3.72120        3.84860        0.92819
C         -3.66067        2.45504        0.71226
C         -6.09159        2.41403        0.47490
C         -4.85441        1.77317        0.49351
O         -2.55003        4.51684        1.15415
N         -7.22933        1.62299        0.25767
C         -8.49291        2.04342       -0.04687
C         -9.48884        0.91010       -0.23228
C        -10.41328        1.14433       -1.42543
C        -11.46472        0.04549       -1.55483
O         -8.82215        3.21791       -0.16284
C         -2.41327        1.63042        0.65821
N         -1.25340        2.23116        0.96110
C          0.01160        1.55286        0.89664
C          1.10719        2.56109        1.22666
N          2.35477        2.10256        0.95726
C          3.56319        2.79624        1.13045
C          3.69296        3.94140        1.91768
C          4.92976        4.56451        2.02933
C          6.05088        4.07273        1.36803
C          5.93789        2.91245        0.57583
C          4.68977        2.30283        0.47813
C          7.02797        2.26424       -0.22341
N          8.20687        2.91307       -0.31421
C          9.29035        2.47653       -1.17574
C          9.53419        3.41826       -2.36127
C          9.88184        4.83409       -1.90089
O          6.82541        1.18409       -0.79440
O         -2.45074        0.42825        0.34042
O          0.83941        3.66475        1.69042
O          7.27864        4.68152        1.45946
C         -2.59303        5.91822        1.39314
C          7.39254        5.85235        2.26183
C         10.64128        2.83676       -3.24064
H         -5.00814        5.56339        1.05199
H         -7.07998        4.31094        0.64269
H         -4.79875        0.70617        0.33087
H         -7.08762        0.61722        0.35106
H         -8.96589       -0.04270       -0.33143
H        -10.08781        0.85312        0.68420
H        -10.88738        2.12072       -1.31180
H         -9.81369        1.19455       -2.33939
```

```
H        -12.08217       -0.01329       -0.65386
H        -10.99776       -0.93301       -1.70155
H        -12.12779        0.22789       -2.40314
H         -1.23544        3.20798        1.23646
H          0.05756        0.72491        1.61267
H          0.18608        1.12303       -0.09110
H          2.42085        1.18678        0.50511
H          2.83260        4.34645        2.42595
H          5.00496        5.44950        2.64500
H          4.61139        1.42634       -0.15048
H          8.29033        3.77698        0.20263
H         10.20692        2.39029       -0.58192
H          9.02529        1.48487       -1.53604
H          8.60670        3.45725       -2.94265
H         10.06049        5.48822       -2.75688
H         10.78986        4.82940       -1.28905
H          9.07474        5.27790       -1.31266
H         -3.19106        6.14376        2.28008
H         -2.99988        6.44842        0.52793
H         -1.55927        6.21170        1.55713
H          7.14563        5.63468        3.30379
H          6.74465        6.64766        1.88489
H          8.43349        6.15753        2.18629
H         11.58080        2.76569       -2.68392
H         10.81875        3.46733       -4.11429
H         10.38251        1.83539       -3.59232
```

Molecule DADA10

```
19
Energy = -547.7888108698
N          1.54069       -1.04796        0.00000
C          2.27442       -2.17683        0.00000
C          3.69846       -2.15050        0.00000
C          4.33838       -0.94303        0.00000
C          3.36219        2.66712        0.00000
C          1.92519        2.54946        0.00000
N          1.42648        1.25629        0.00000
C          2.18957        0.12228        0.00000
C          3.59615        0.25371        0.00000
C          4.15108        1.56056        0.00000
N          1.61285       -3.34475        0.00000
H          4.24885       -3.08267        0.00000
H          5.42166       -0.89427        0.00000
H          0.58217       -3.38582        0.00000
H          5.23176        1.66174        0.00000
H          3.76610        3.66928        0.00000
O          1.14883        3.51803        0.00000
H          2.13424       -4.20299        0.00000
H          0.39611        1.15276        0.00000
```

Molecule DDAA01

```
67
Energy = -1639.9932891682
C         -4.43726        3.53041       -3.61104
C         -5.63659        2.85467       -3.40316
C         -3.27197        3.13395       -2.95399
C         -5.69955        1.77283       -2.50399
C         -3.29538        2.03866       -2.06515
C         -4.51783        1.41134       -1.86622
O         -2.09894        3.77951       -3.14073
O         -6.77949        3.21964       -4.04896
C         -6.90555        0.95829       -2.16066
N         -7.97749        1.05642       -2.97626
```

```
O         -6.88805        0.20224       -1.18251
C         -2.12468        1.45166       -1.33988
N         -0.90427        1.90270       -1.66000
O         -2.28976        0.55370       -0.49939
C          0.30833        1.32550       -1.14448
C          1.45700        1.80682       -2.03168
N          2.65203        1.26120       -1.71353
O          1.24863        2.61641       -2.93237
C          3.89502        1.46704       -2.34648
C          4.03845        2.18576       -3.53704
C          5.30556        2.29792       -4.09545
C          6.42963        1.72705       -3.51399
C          6.27929        1.01745       -2.31769
C          5.01252        0.89137       -1.74291
N          7.35049        0.41828       -1.63738
C          8.62932        0.22593       -2.08240
O          9.03942        0.55208       -3.18807
C         -2.01299        4.85670       -4.08960
C         -0.58522        5.35336       -4.07339
C         -6.75717        4.34136       -4.94408
C         -8.16049        4.51185       -5.48173
C         -9.21460        0.32342       -2.76591
C          9.54237       -0.43593       -1.05892
C        -10.39780        1.25824       -2.53670
C         10.47171       -1.45502       -1.71134
H         -4.40420        4.36778       -4.28794
H         -4.54831        0.57326       -1.18587
H         -7.92474        1.73382       -3.72251
H         -0.77901        2.59947       -2.38678
H          0.49492        1.62417       -0.10843
H          0.25705        0.23638       -1.15005
H          2.64707        0.60827       -0.92932
H          3.17771        2.63574       -4.00270
H          5.42071        2.85093       -5.02048
H          7.40459        1.81409       -3.96460
H          4.89952        0.33574       -0.81990
H          7.15037        0.10631       -0.68980
H         -2.29815        4.47776       -5.07608
H         -2.71614        5.64257       -3.79610
H          0.10777        4.54787       -4.31329
H         -0.32560        5.74412       -3.08897
H         -0.47190        6.15437       -4.80638
H         -6.43105        5.22843       -4.39301
H         -6.04214        4.14384       -5.74847
H         -8.86528        4.69413       -4.66937
H         -8.47671        3.62247       -6.02917
H         -8.19164        5.36288       -6.16394
H         -9.40040       -0.31575       -3.63460
H         -9.04944       -0.32331       -1.90669
H          8.95021       -0.88676       -0.26150
H         10.13470        0.36547       -0.60350
H        -10.55852        1.91111       -3.39874
H        -10.23064        1.88524       -1.65991
H        -11.31088        0.68094       -2.37846
H         11.00771       -0.99511       -2.54113
H          9.90539       -2.30160       -2.10523
H         11.19705       -1.83529       -0.98914
```

Molecule DDAA02

```
17
Energy = -562.9050222862
C          1.10895        4.18756       -0.04205
N         -0.05934        3.47850       -0.03552
```

```
C          2.29956        3.53740       -0.02080
C         -0.03121        2.11687       -0.00600
C          2.31317        2.07865        0.00930
N          1.08947        1.41992        0.01408
N         -1.23268        1.46534        0.00505
C         -2.48553        2.10749        0.00557
N         -3.52951        1.27303        0.04496
O          3.37660        1.44083        0.03300
H         -1.18086        0.41585        0.01627
H         -3.44913        0.23061        0.01671
H         -4.44355        1.70976        0.02164
O         -2.58965        3.34557       -0.01915
H         -1.03264        3.86943       -0.04222
H          1.00578        5.27332       -0.06404
H          3.24977        4.06871       -0.02448
```

Molecule DDAA03

```
22
Energy = -641.1212441084
C         -3.83268        3.70308        0.91688
C         -4.84046        2.78097        1.08491
C         -2.56977        3.27149        0.48268
C         -4.56207        1.43750        0.79194
C         -2.37175        1.88232        0.24129
N         -3.38534        0.99300        0.38609
C         -1.46623        4.13147        0.25819
C         -0.27488        3.62114       -0.15256
C         -0.16034        2.20544       -0.32903
N         -1.18170        1.37226       -0.15241
N          1.03301        1.61557       -0.64819
C          2.18028        2.27162       -1.12396
N          3.25482        1.44681       -1.17814
O          2.19240        3.44009       -1.48567
H          4.11539        1.89257       -1.44771
H          3.29504        0.59027       -0.61207
H          1.07091        0.59262       -0.53064
H         -3.99672        4.75723        1.11216
H         -5.82696        3.07068        1.42054
H         -5.34283        0.68898        0.89061
H         -1.57973        5.19732        0.42214
H          0.58722        4.23782       -0.34706
```

Molecule DDAA04

```
20
Energy = -619.1099861599
C         -4.00770        3.22906        0.00000
C         -3.50532        4.54190        0.00000
N         -3.22898        2.15429        0.00000
C         -2.14692        4.73903        0.00000
C         -1.91200        2.35536        0.00000
N         -1.33917        3.64993        0.00000
N         -0.95942        1.43872        0.00000
C          0.02816        3.49371        0.00000
C          0.22882        2.11917        0.00000
N          1.38063        1.39175        0.00000
C          2.65170        1.94671        0.00000
N          3.64432        1.01574        0.00000
O          2.84840        3.15587        0.00000
H         -5.07666        3.05042        0.00000
H         -4.17289        5.39112        0.00000
H          0.72388        4.31043        0.00000
H         -1.66847        5.70808        0.00000
H          1.25822        0.36503        0.00000
```

```
H          3.49064        0.01186        0.00000
H          4.58542        1.36598        0.00000
```

Molecule DDAA05

```
19

S    -2.3906043    2.2719308    0.6013863
O    -3.2901753    1.3733313    1.3007449
O    -2.3165679    3.6401578    1.0829363
N    -0.9531313    1.5241564    0.5439539
C     0.1509392    2.2280299    0.2906138
N     0.2195346    3.5407439    0.0889844
H    -0.5863392    4.0925016    0.3575179
H     1.1568008    3.9207482   -0.0501658
N     1.3076496    1.4964852    0.2213638
C     2.5874961    2.0393220    0.0253852
H     1.1973362    0.4889715    0.3899489
N     3.5848274    1.1334311    0.0999505
H     3.4744514    0.2398709    0.5853896
H     4.5100144    1.5290883    0.0588417
O     2.7752060    3.2270190   -0.2325869
C    -2.9215116    2.3382055   -1.0994095
H    -3.8957798    2.8252151   -1.1113118
H    -2.9925652    1.3228068   -1.4849029
H    -2.1979973    2.9219116   -1.6670245
```

Molecule DDAA06

```
19
Energy = -547.7459157973
N          1.50635       -1.11038        0.00000
C          2.17221       -2.29114        0.00000
C          3.58674       -2.27342        0.00000
C          4.24175       -1.06801        0.00000
C          3.36262        2.54721        0.00000
C          1.91807        2.43546        0.00000
N          1.34046        1.18734        0.00000
C          2.12772        0.11695        0.00000
C          3.54421        0.15003        0.00000
C          4.14321        1.43791        0.00000
N          1.45315       -3.41143        0.00000
H          4.12003       -3.21381        0.00000
H          5.32643       -1.04724        0.00000
H          0.39771       -3.40978        0.00000
H          5.22561        1.51393        0.00000
H          3.77696        3.54614        0.00000
O          1.20087        3.46465        0.00000
H          1.94554       -4.28757        0.00000
H          0.45233       -1.12164        0.00000
```

Molecule DDAA07

```
23
Energy = -641.3891667121
H          4.80022       -3.00135        0.26849
C          3.87499       -3.37573        0.71130
N          2.78852       -2.43233        0.52643
C          2.40301       -2.08960       -0.70201
O          2.92504       -2.53748       -1.73782
N          1.34380       -1.16799       -0.73470
C          0.78010       -0.66729       -1.87010
N         -0.20894        0.19385       -1.76876
C         -0.77644        0.69860       -2.92699
O         -1.71211        1.51304       -2.85999
N          1.28155       -1.09417       -3.05528
```

```
C          0.76899       -0.63604       -4.24056
C         -0.25050        0.25220       -4.20010
C          1.40047       -1.17404       -5.48271
H          4.01538       -3.51147        1.78155
H          3.64224       -4.33787        0.25065
H          2.32747       -2.03643        1.36648
H          0.94056       -0.82212        0.15762
H          2.05894       -1.77258       -2.95428
H         -0.69044        0.64427       -5.10511
H          2.46607       -0.93161       -5.50713
H          0.92267       -0.75128       -6.36398
H          1.30977       -2.26276       -5.51864
```

Molecule DDAA08

```
25
Energy = -771.5802013068
C         -2.37955        6.18735        0.00000
C         -3.63506        5.55276        0.00000
C         -3.67311        4.16063        0.00000
N         -1.21435        5.54068        0.00000
C         -1.27095        4.20510        0.00000
C         -2.46244        3.45563        0.00000
N         -0.08028        3.51362        0.00000
C         -2.38732        1.98100        0.00000
C         -0.05268        2.15553        0.00000
N         -1.14244        1.39519        0.00000
N          1.16775        1.54895        0.00000
C          2.40878        2.23467        0.00000
N          3.47811        1.42868        0.00000
O          2.48098        3.47027        0.00000
O         -3.42548        1.30542        0.00000
C          4.81215        1.99749        0.00000
H          4.97880        2.62580       -0.89296
H          5.53265        1.16577        0.00000
H          4.97880        2.62580        0.89296
H         -4.55151        6.14832        0.00000
H         -4.60890        3.59574        0.00000
H         -2.31618        7.28233        0.00000
H          1.15000        0.50057        0.00000
H          3.37968        0.39181        0.00000
H          0.84878        3.98549        0.00000
```

S2 Molecular Geometries

S2.1 Benzene probe

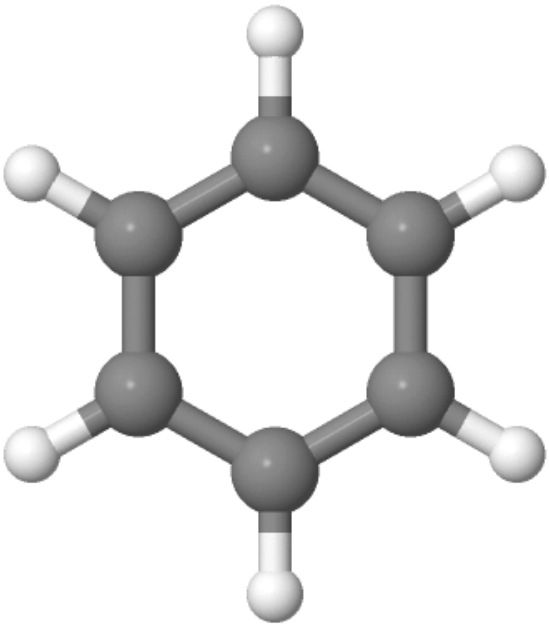


Figure S1 Benzene

S2.2 Dimers with benzene probe

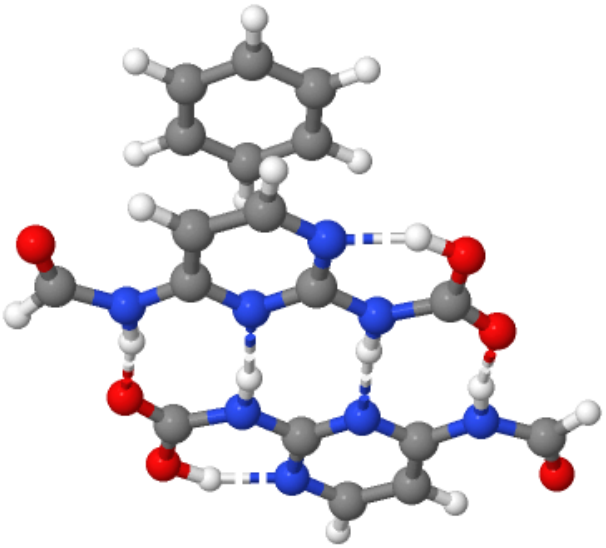


Figure S2 DADA01 + benzene

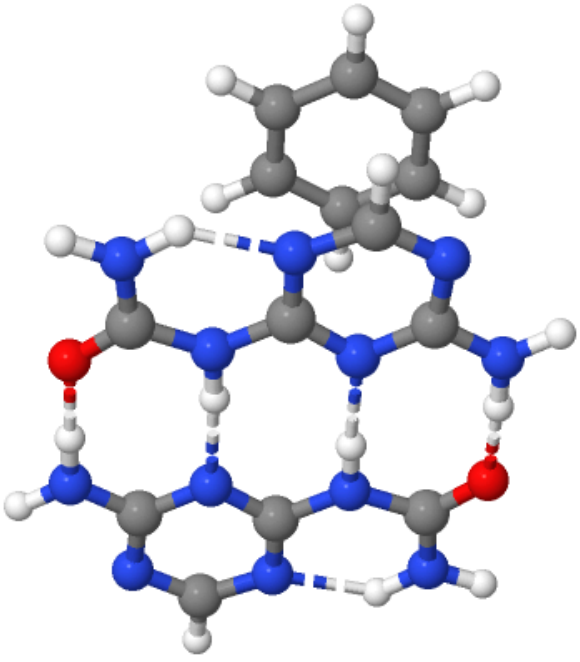


Figure S3 DADA02 + benzene

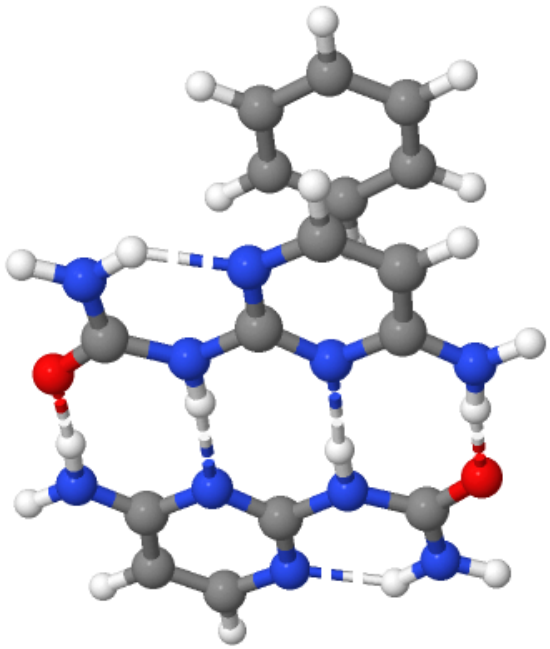


Figure S4 DADA03 + benzene

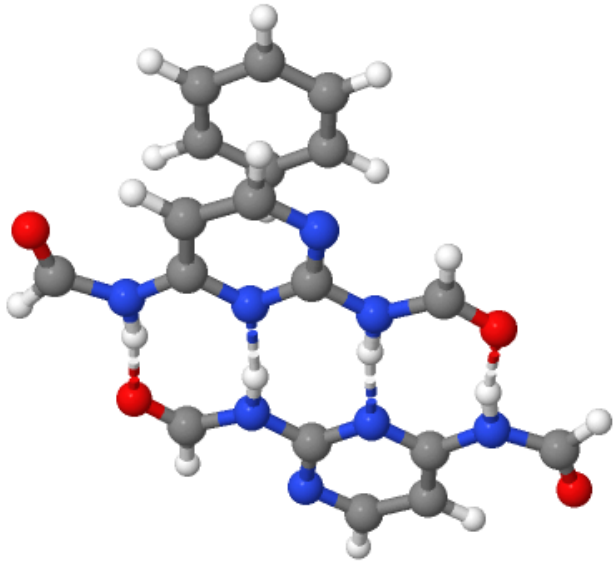


Figure S5 DADA04 + benzene

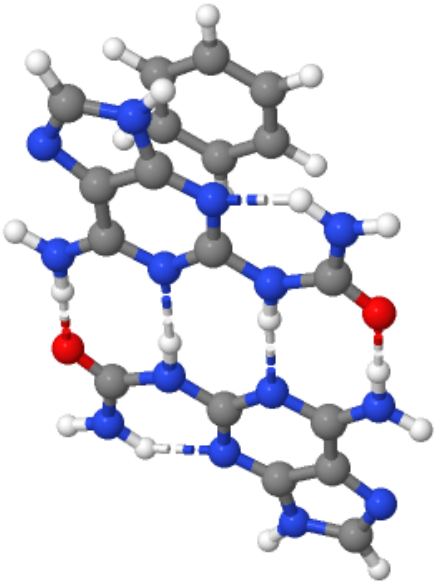


Figure S6 DADA05-R + benzene

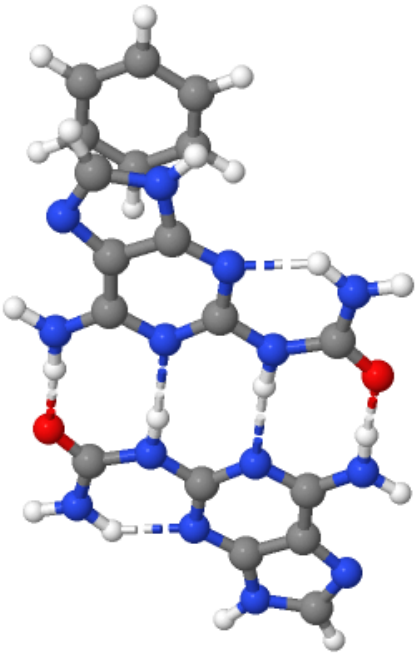


Figure S7 DADA05-L + benzene

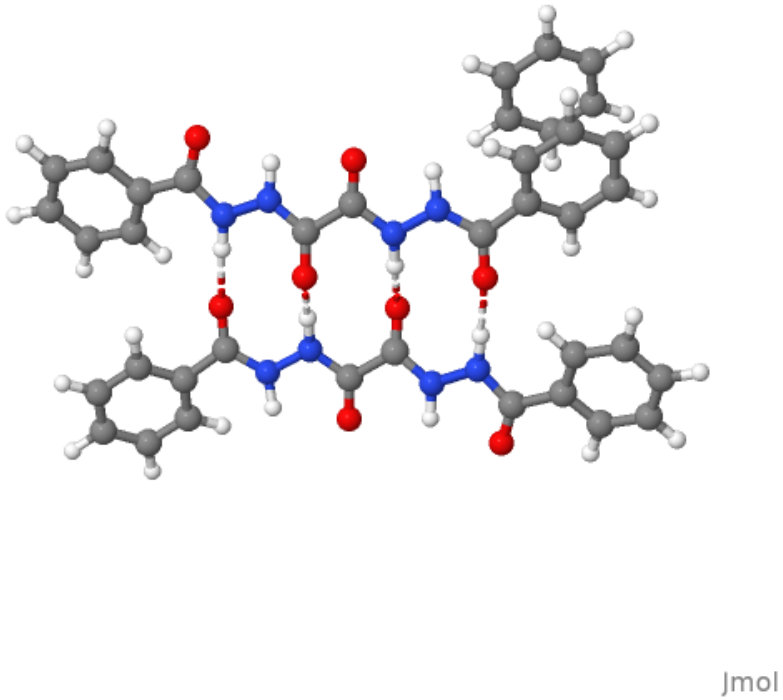


Figure S8 DADA06-R + benzene

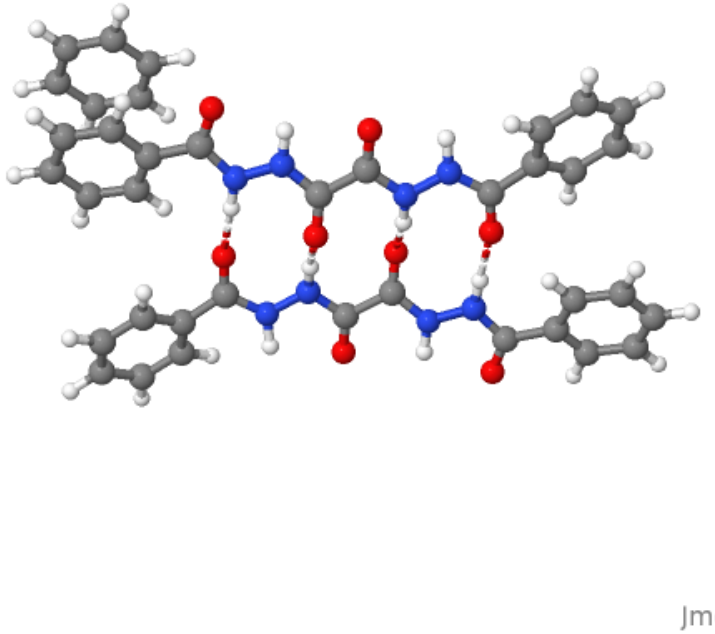


Figure S9 DADA06-L + benzene

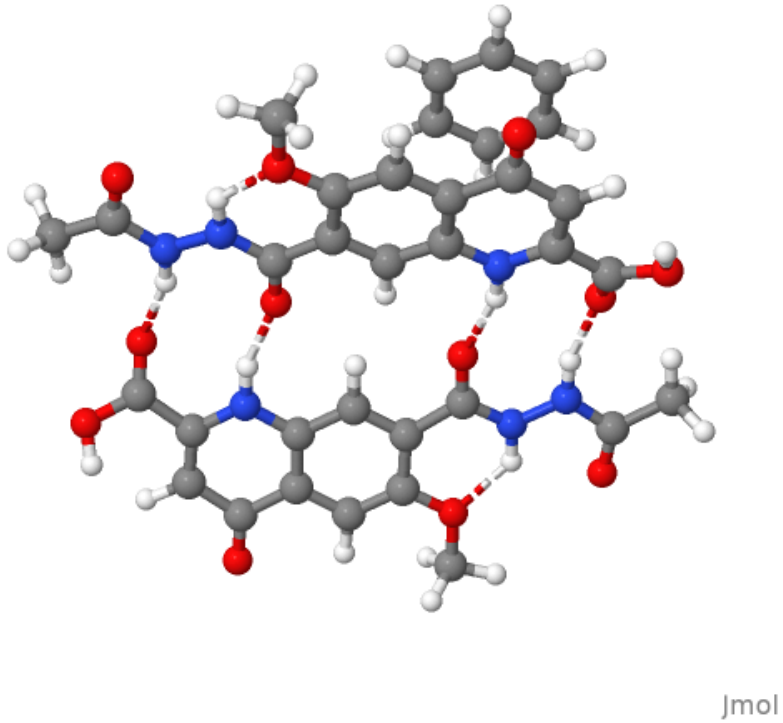


Figure S10 DADA07-R + benzene

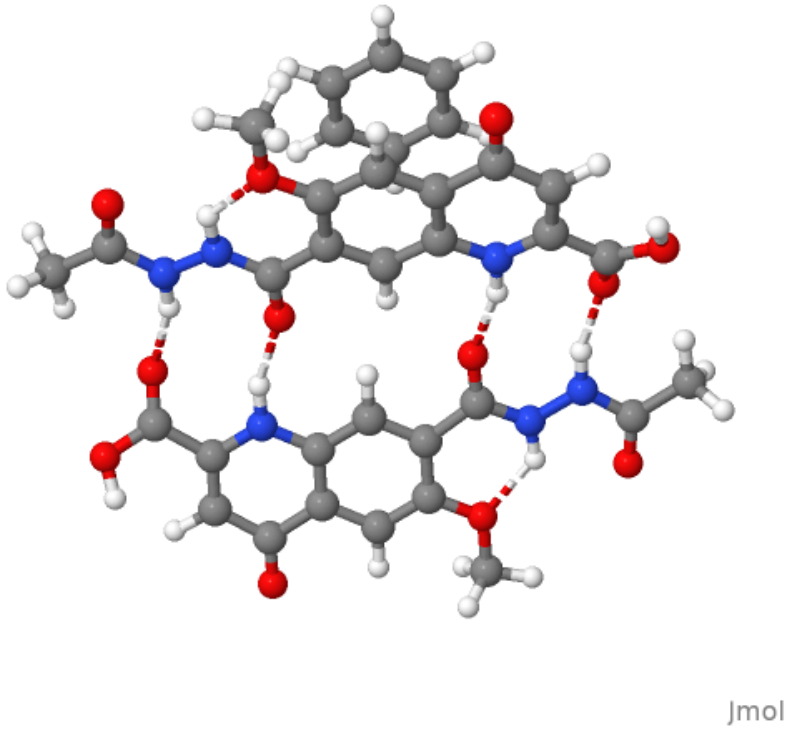


Figure S11 DADA07-L + benzene

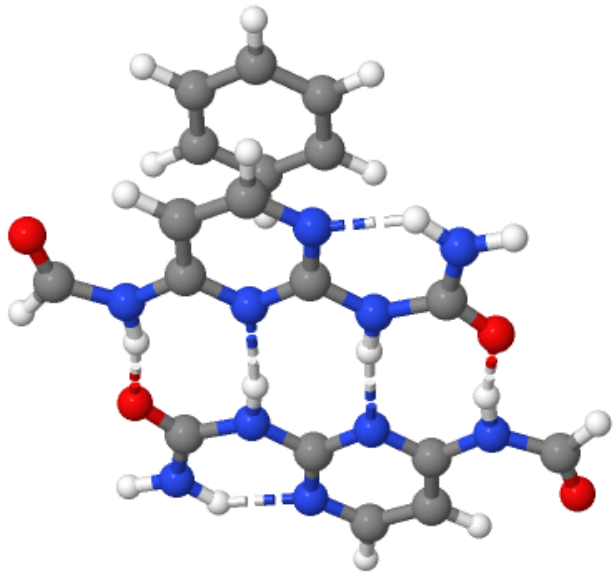


Figure S12 DADA08 + benzene

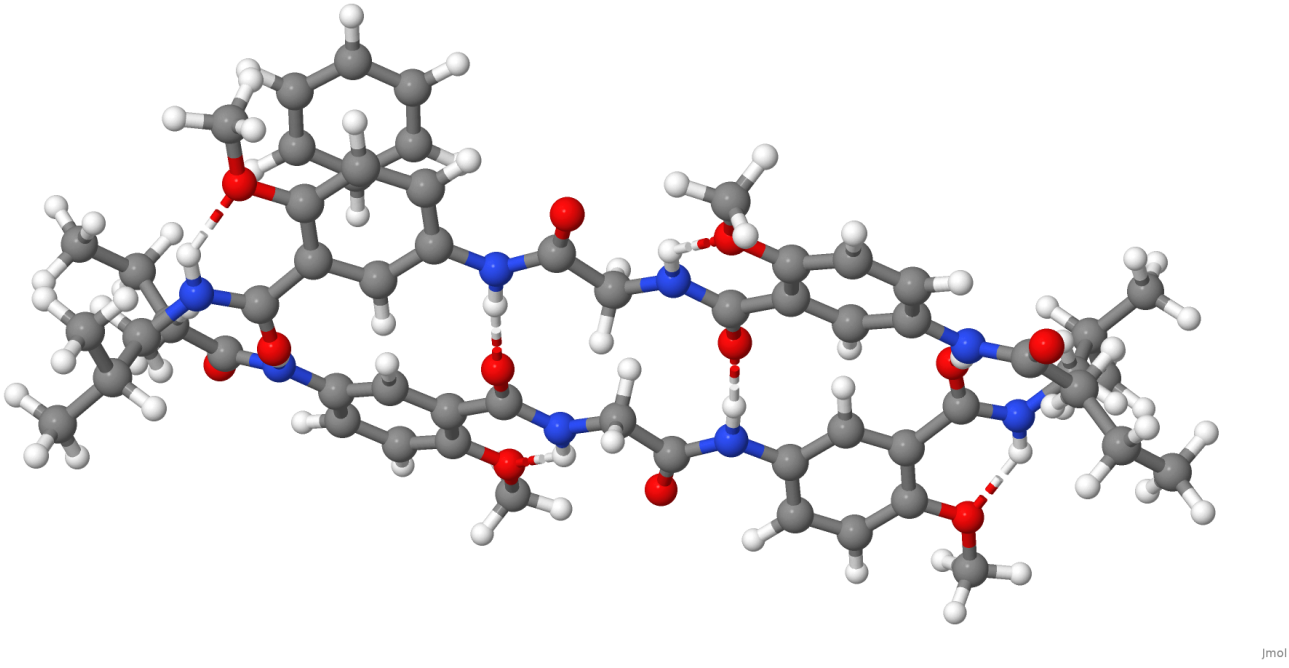


Figure S13 DADA09-R + benzene

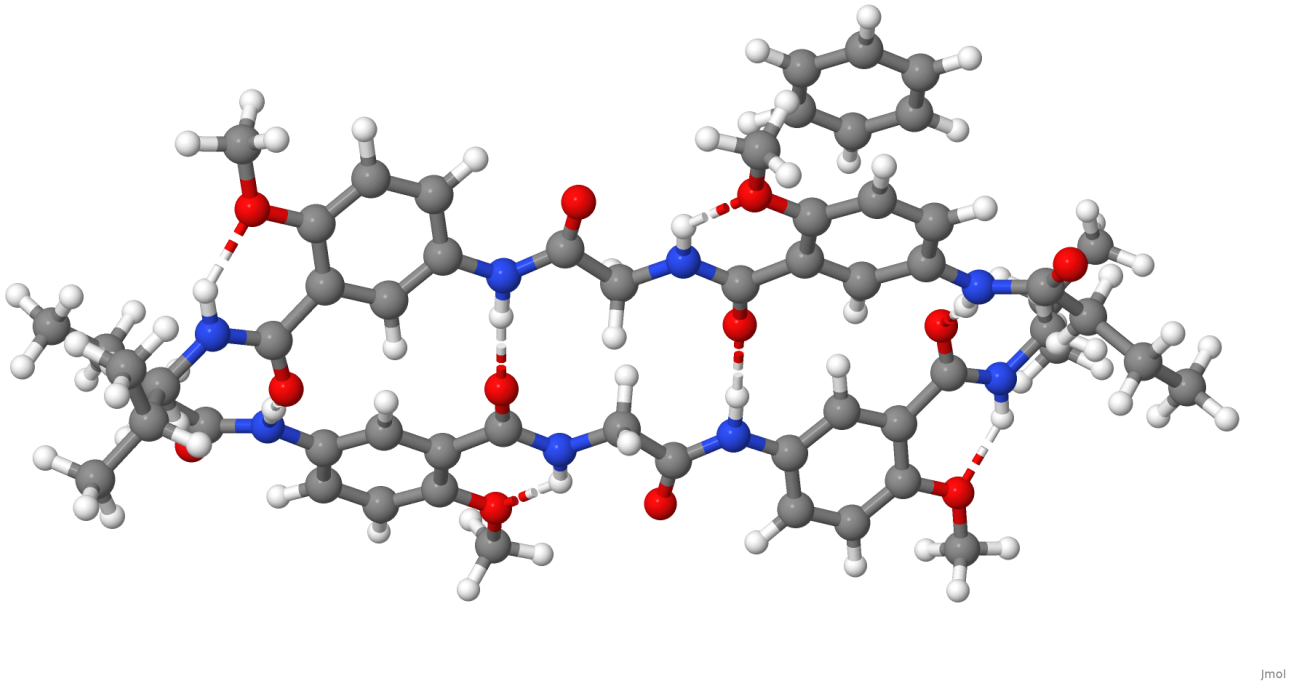


Figure S14 DADA09-L + benzene

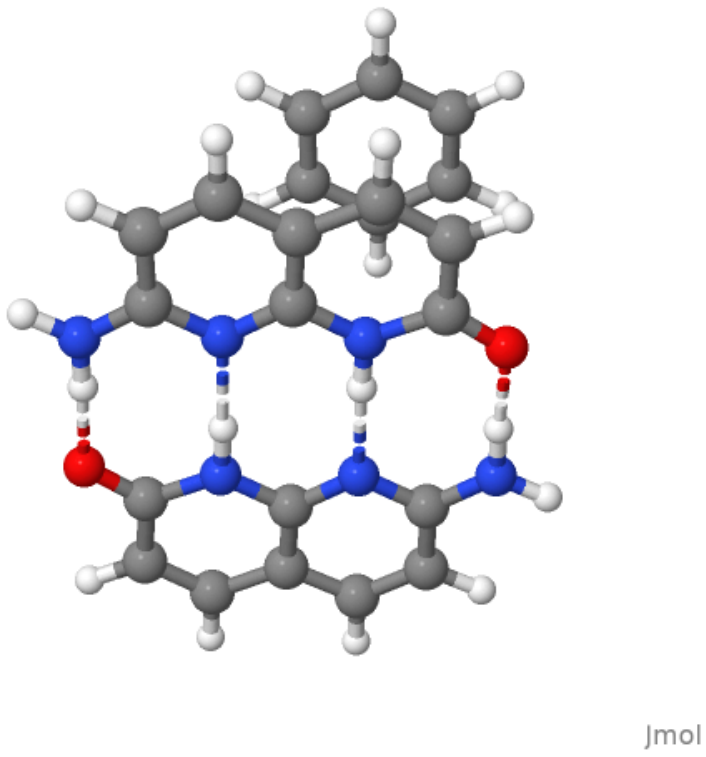


Figure S15 DADA10-R + benzene

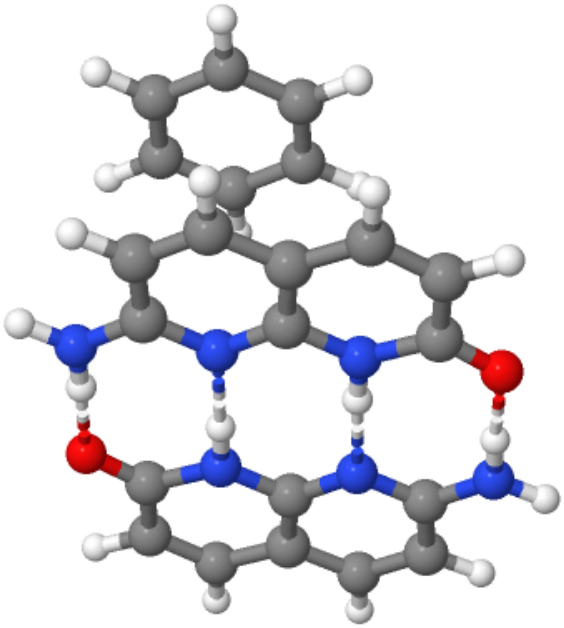


Figure S16 DADA10-L + benzene

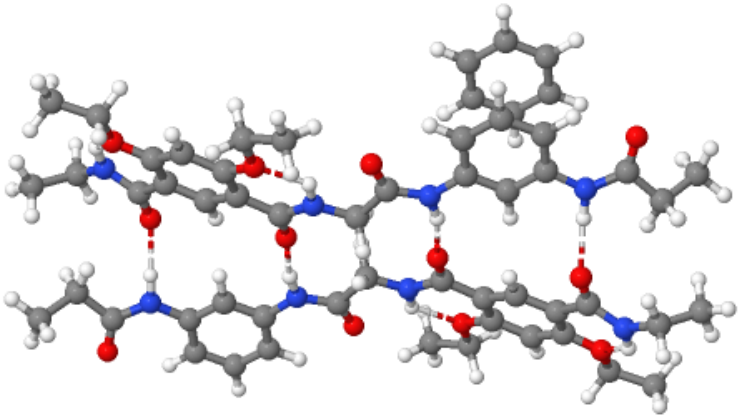


Figure S17 DDAA01-R + benzene

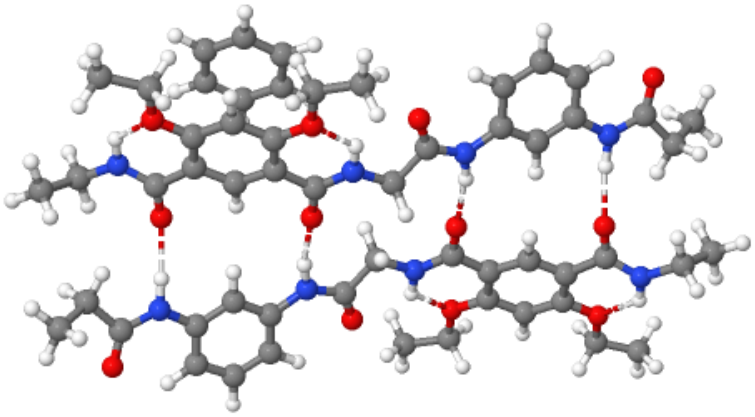


Figure S18 DDAA01-L + benzene

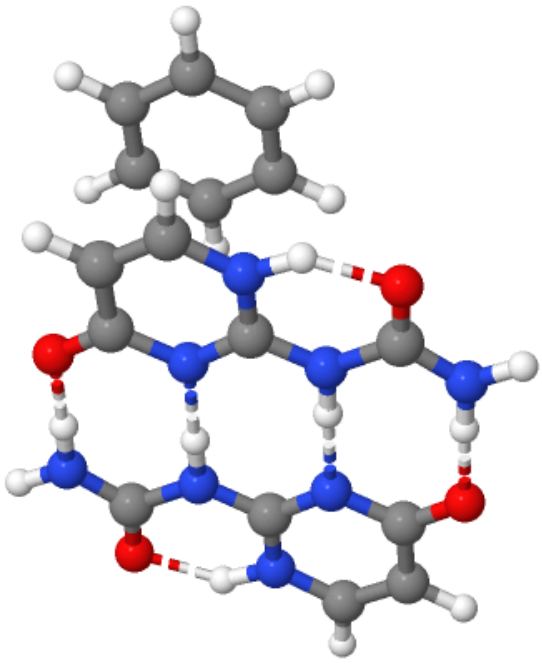


Figure S19 DDAA02 + benzene

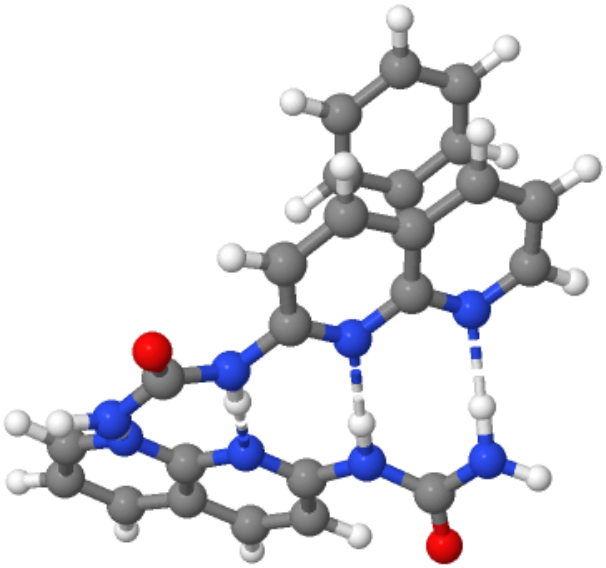


Figure S20 DDAA03-R + benzene

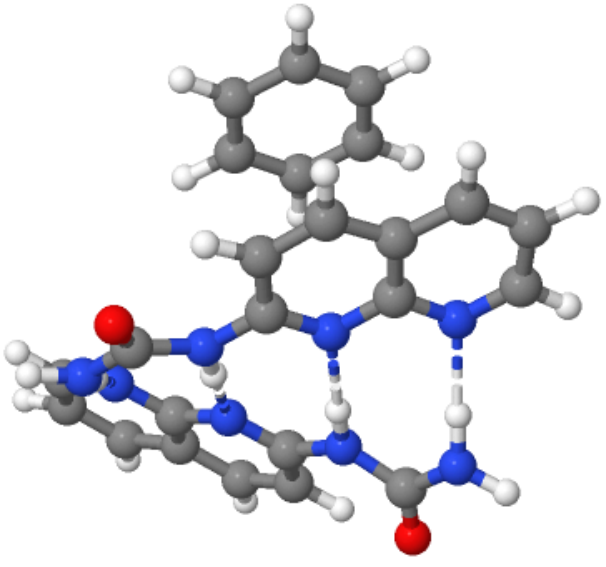


Figure S21 DDAA03-L + benzene

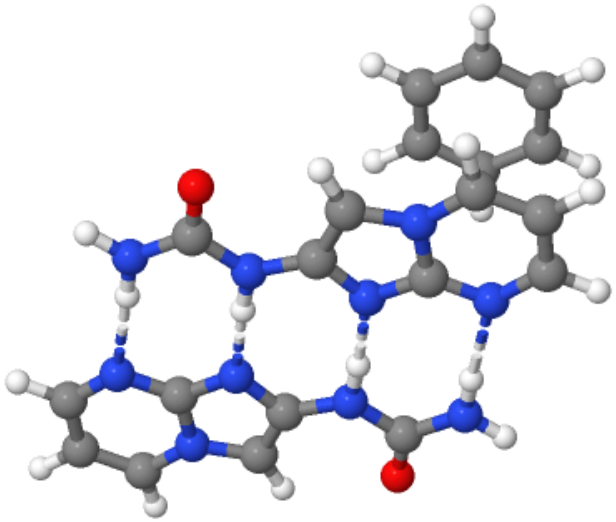


Figure S22 DDAA04-R + benzene

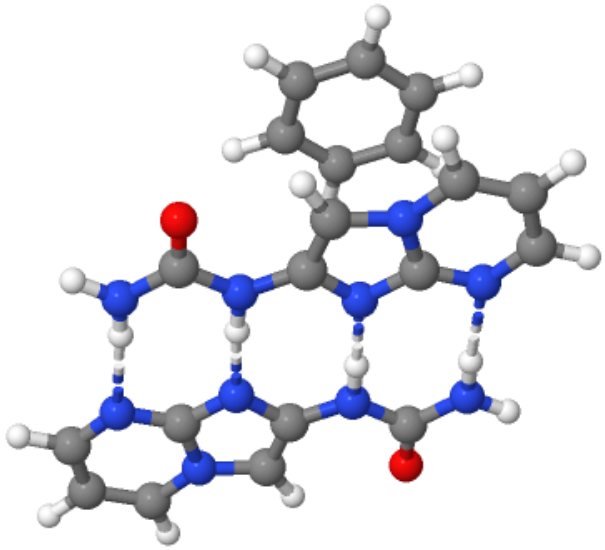


Figure S23 DDAA04-L + benzene

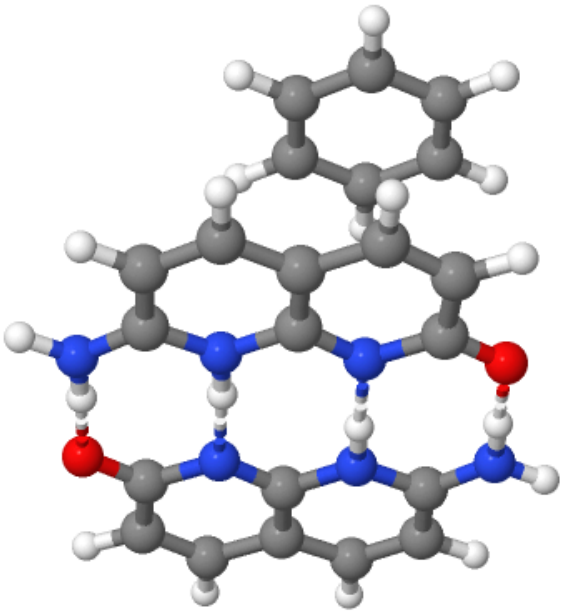


Figure S24 DDAA06-R + benzene

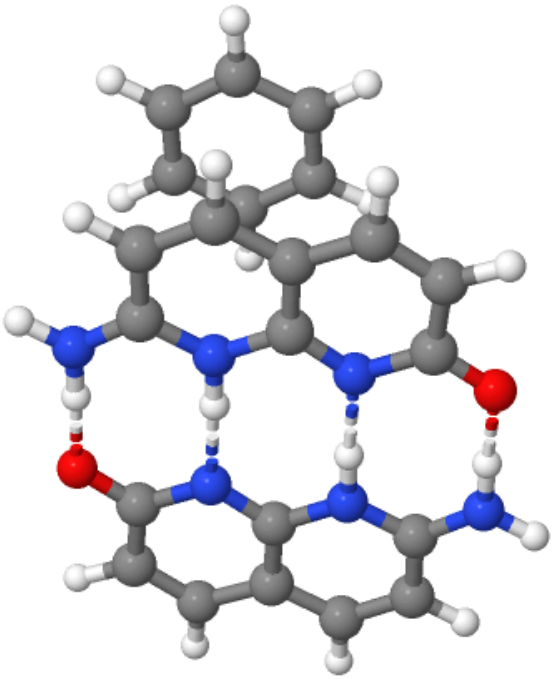


Figure S25 DDAA06-L + benzene

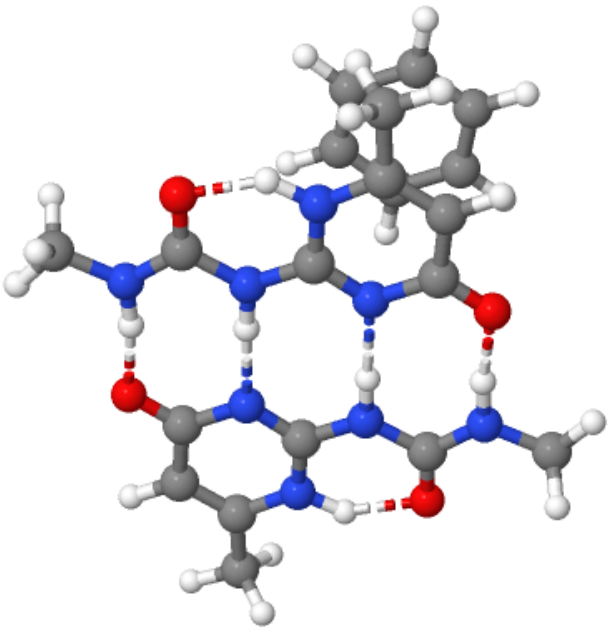


Figure S26 DDAA07 + benzene

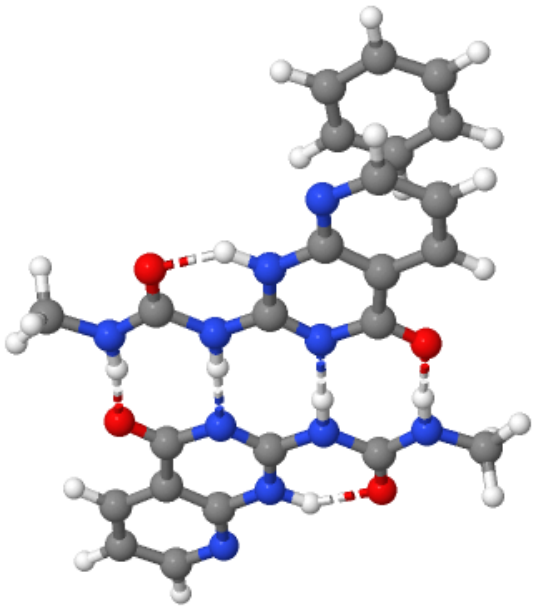


Figure S27 DDAA08-R + benzene

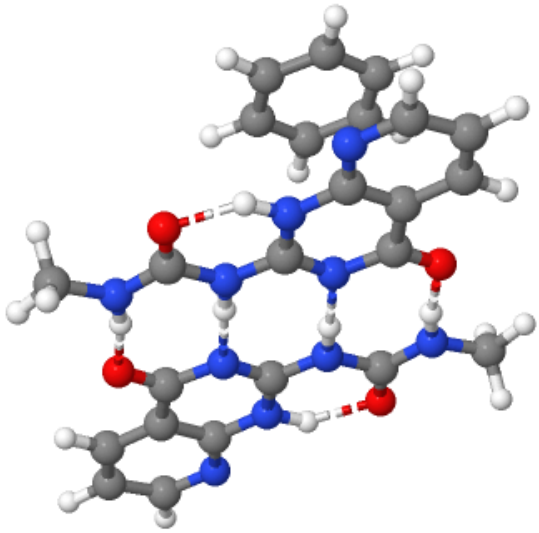


Figure S28 DDAA08-L + benzene

S2.3 Dimers

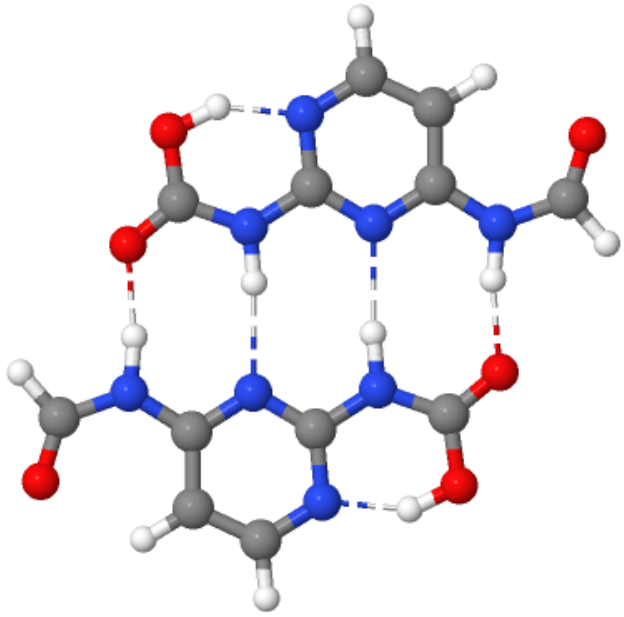


Figure S29 DADA01

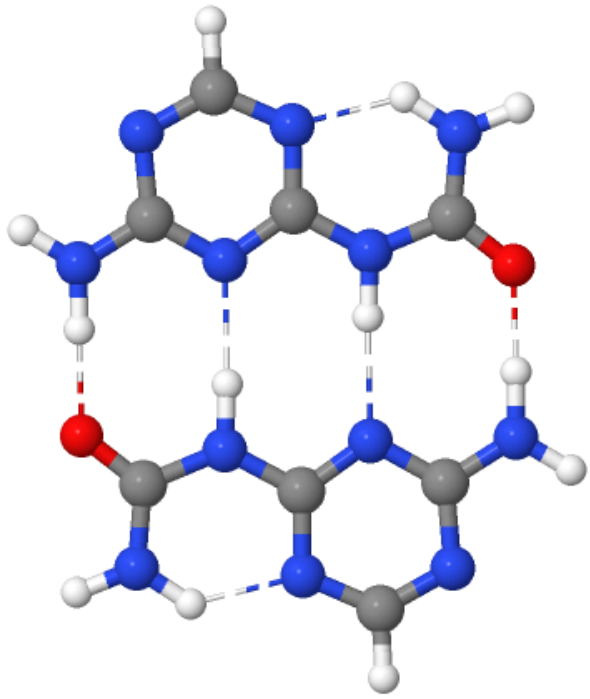


Figure S30 DADA02

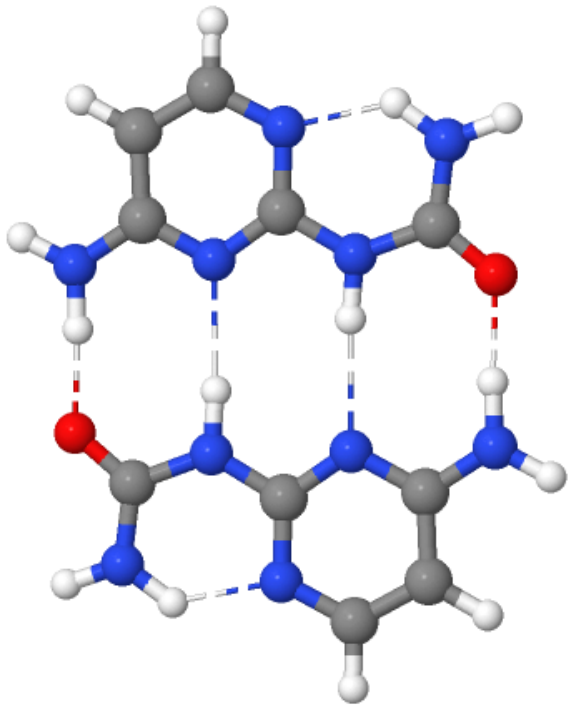


Figure S31 DADA03

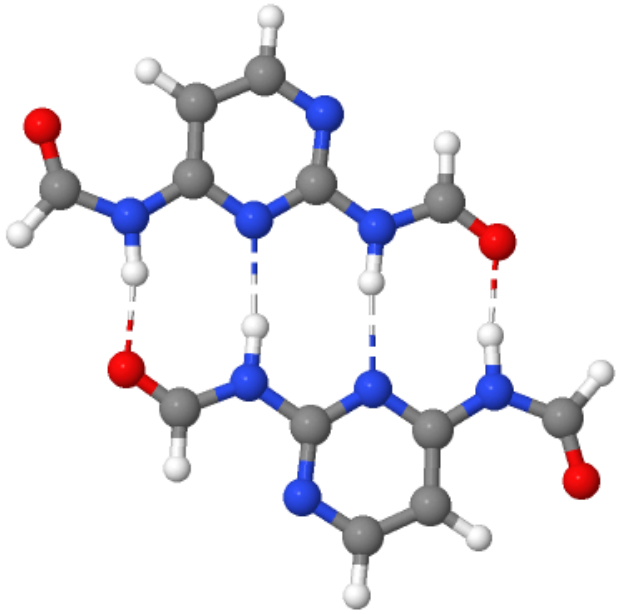


Figure S32 DADA04

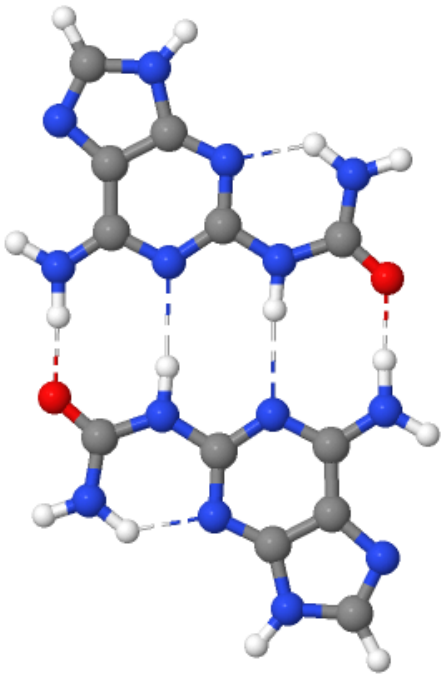


Figure S33 DADA05

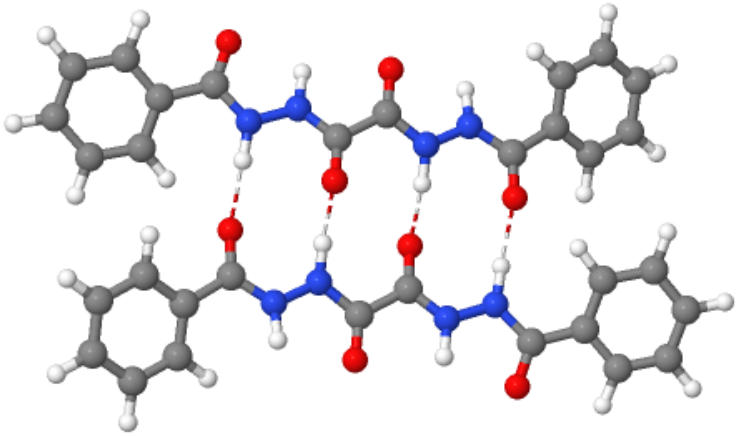


Figure S34 DADA06

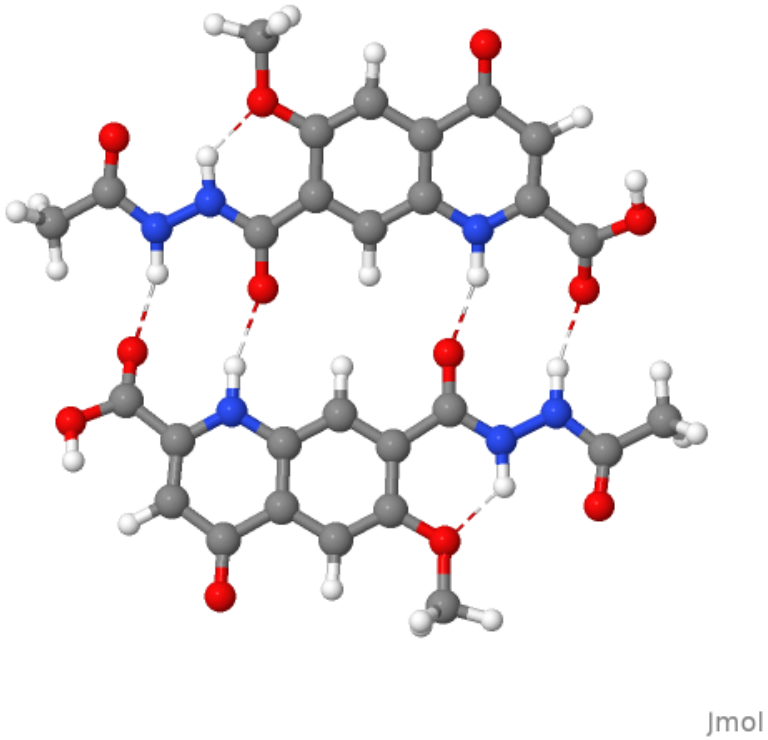


Figure S35 DADA07

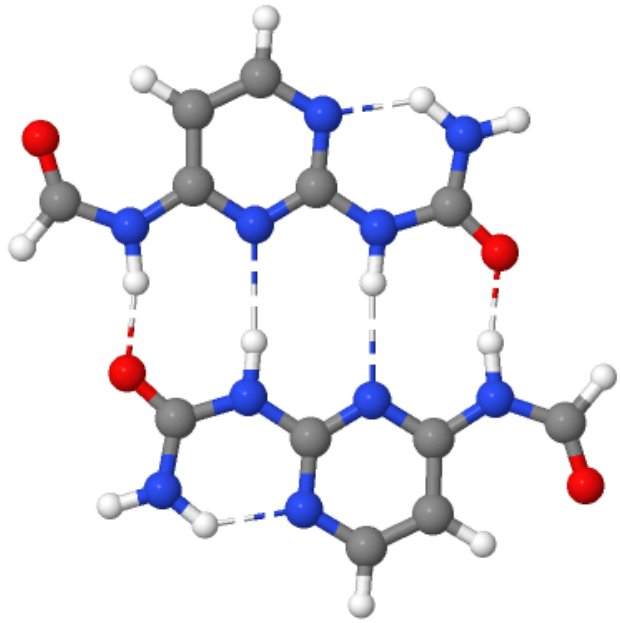


Figure S36 DADA08

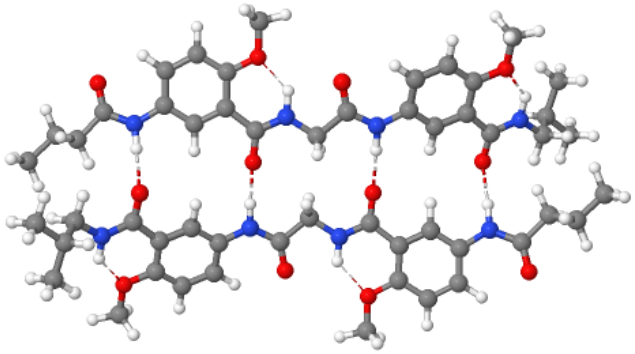


Figure S37 DADA09

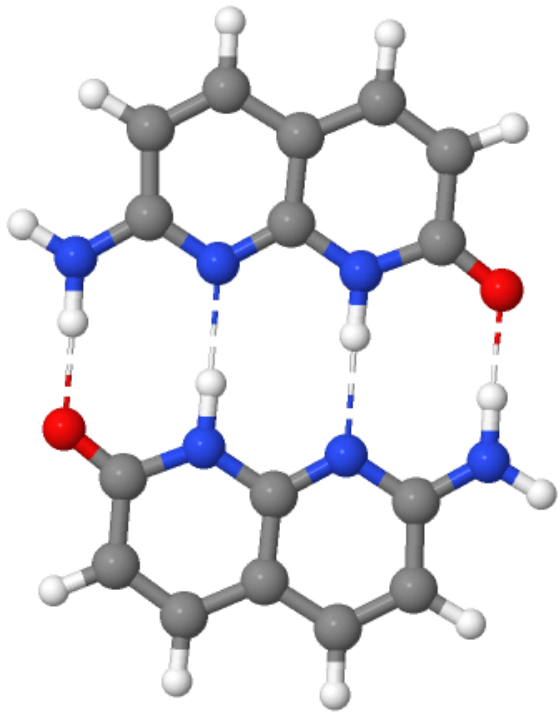


Figure S38 DADA10

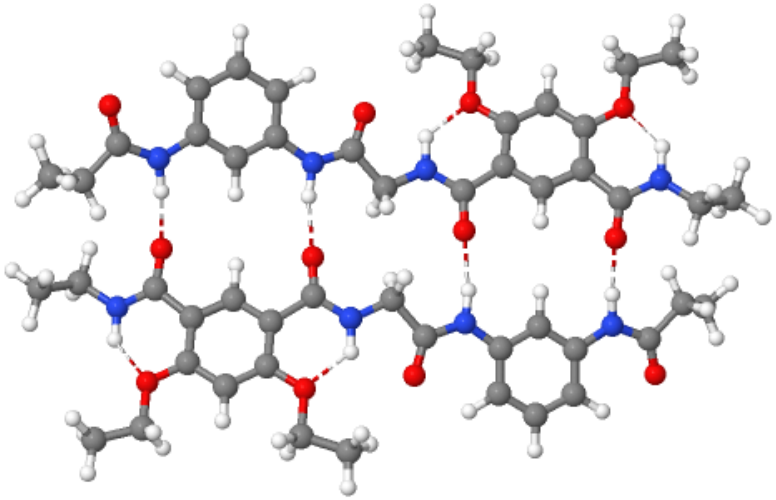


Figure S39 DDAA01

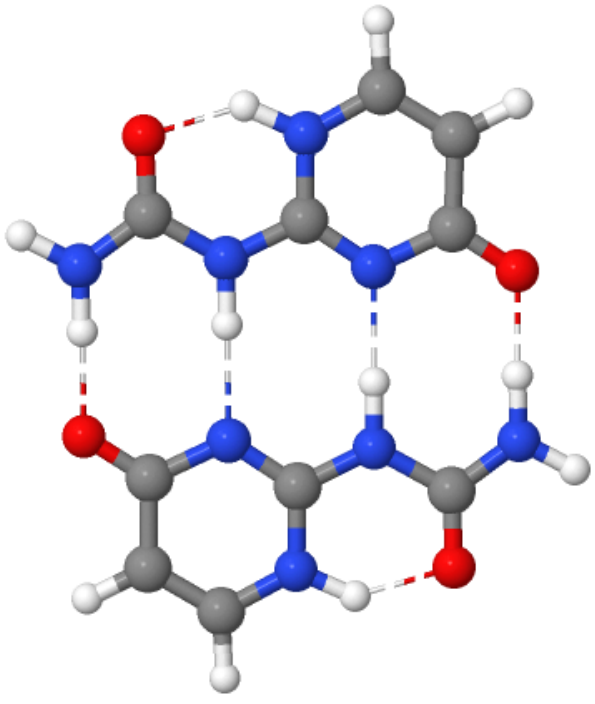


Figure S40 DDAA02

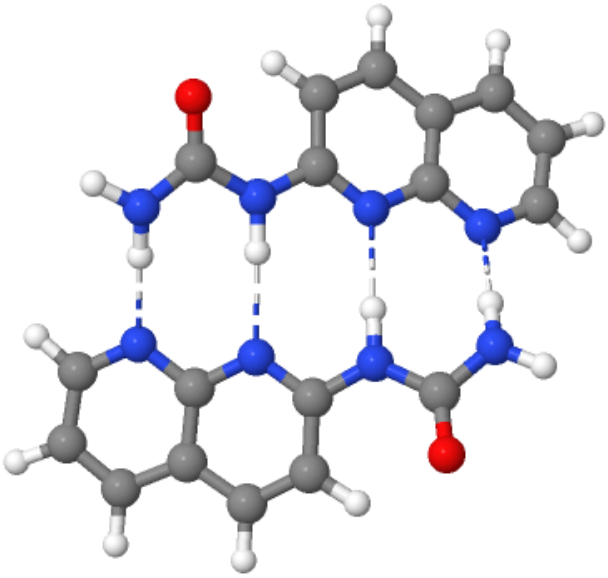


Figure S41 DDAA03

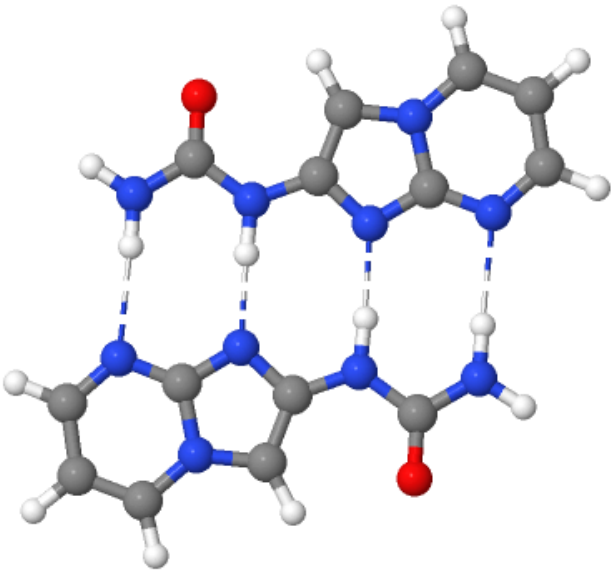


Figure S42 DDAA04

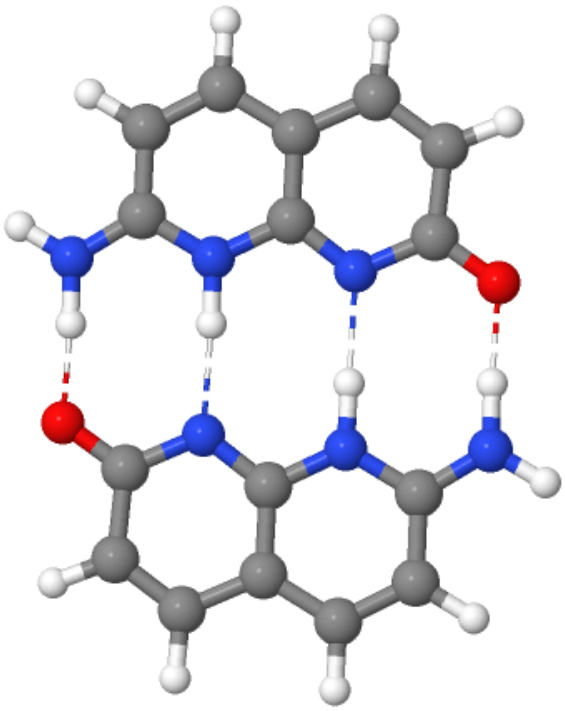


Figure S43 DDAA06

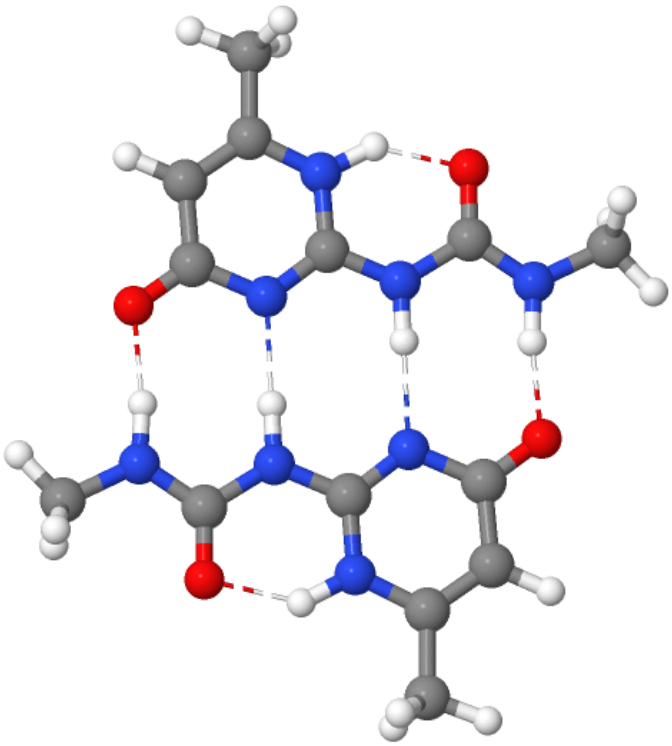


Figure S44 DDAA07

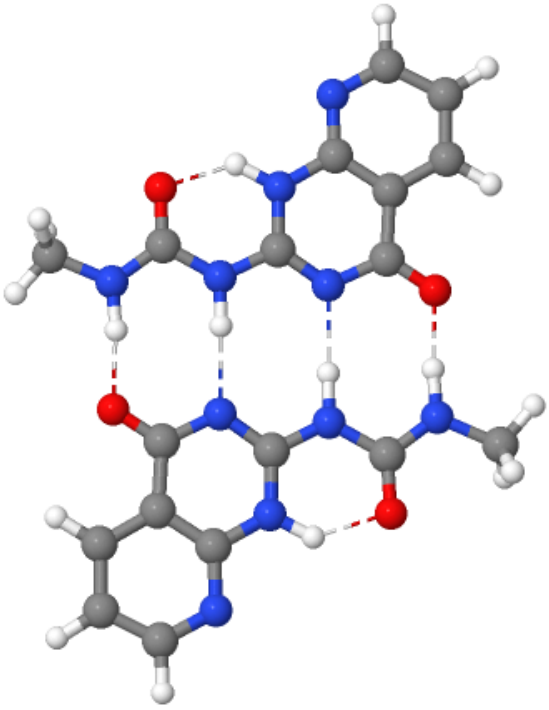


Figure S45 DDAA08

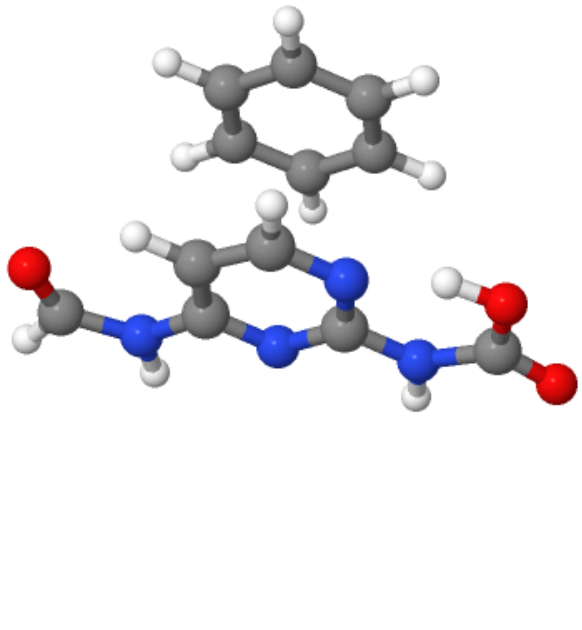


Figure S46 DADA01 + benzene

S2.4 Monomers with benzene probe

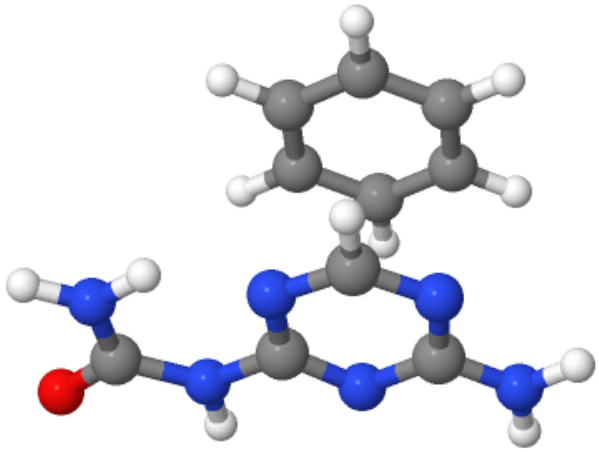


Figure S47 DADA02 + benzene

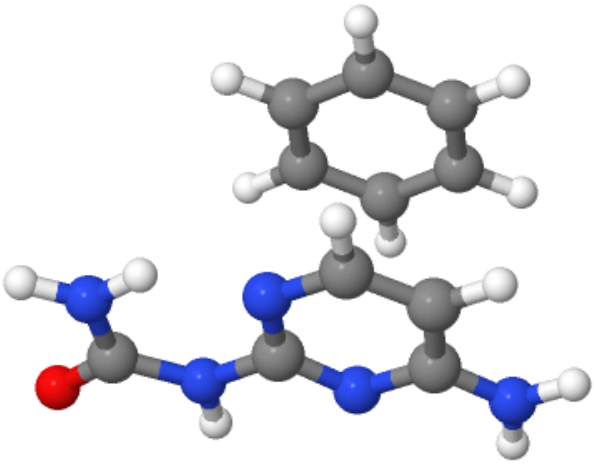


Figure S48 DADA03 + benzene

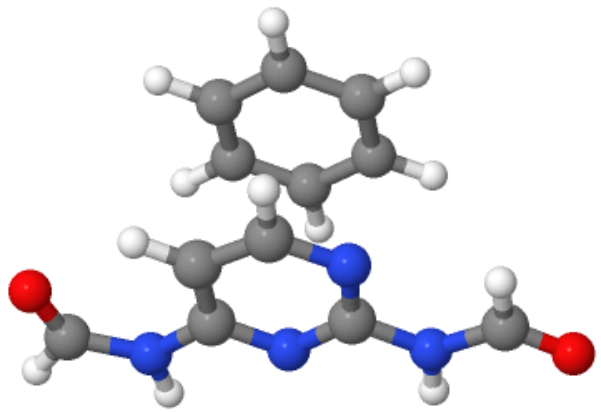


Figure S49 DADA04 + benzene

S2.5 Monomers

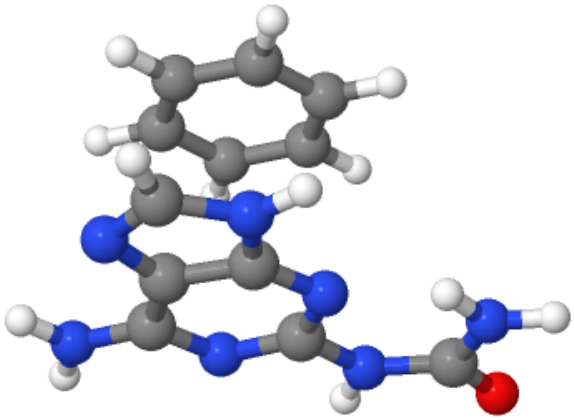


Figure S50 DADA05-R + benzene

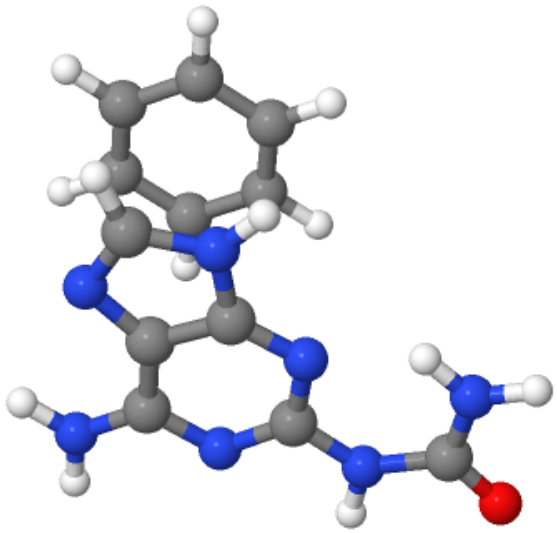


Figure S51 DADA05-L + benzene

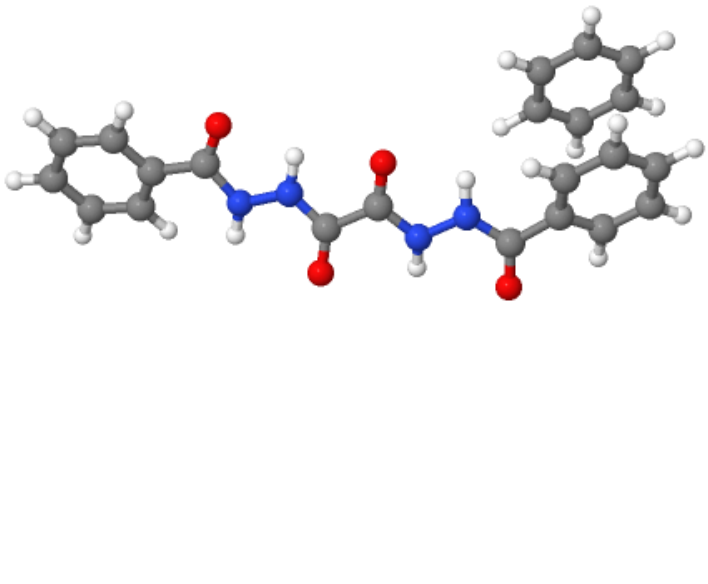


Figure S52 DADA06-R + benzene

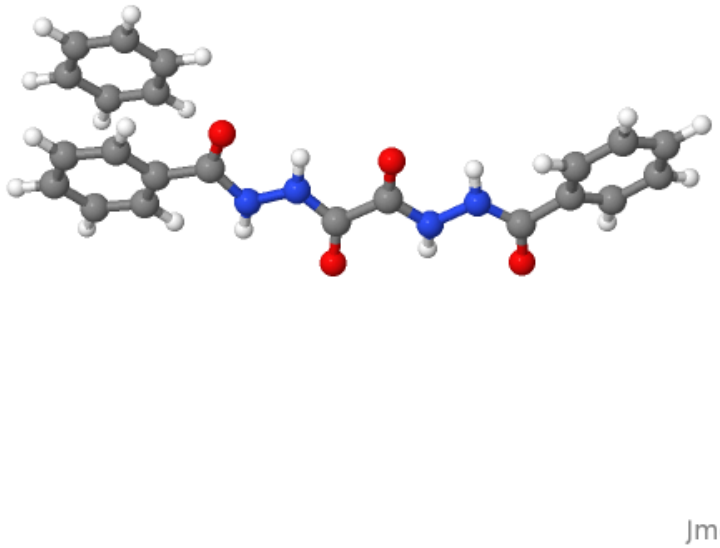


Figure S53 DADA06-L + benzene

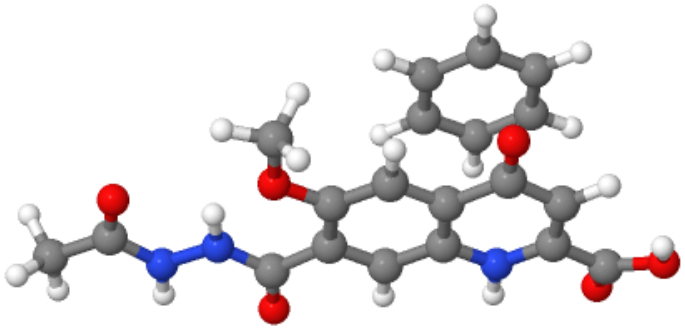


Figure S54 DADA07-R + benzene

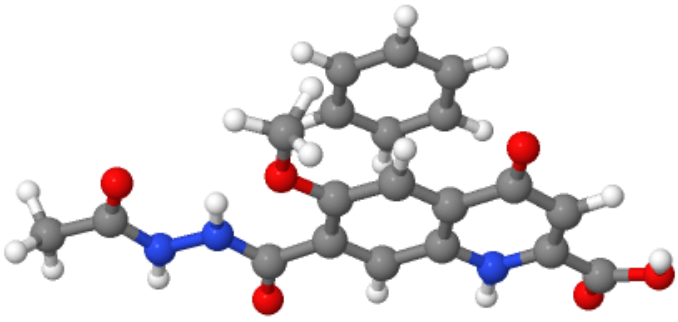


Figure S55 DADA07-L + benzene

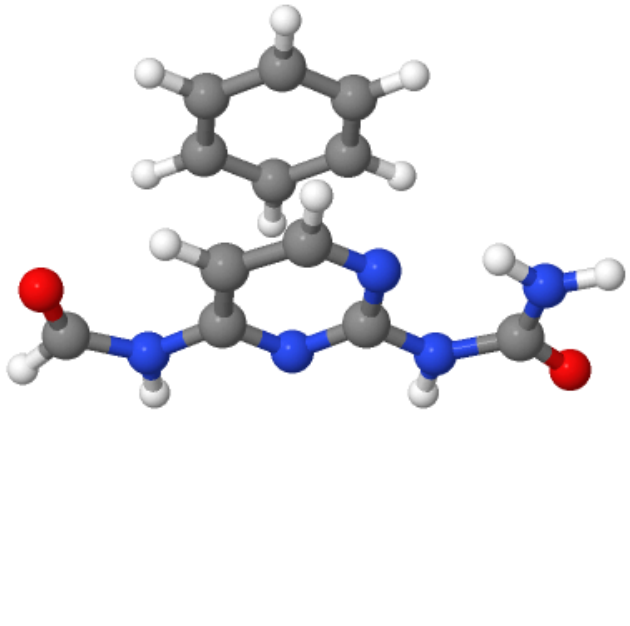


Figure S56 DADA08 + benzene

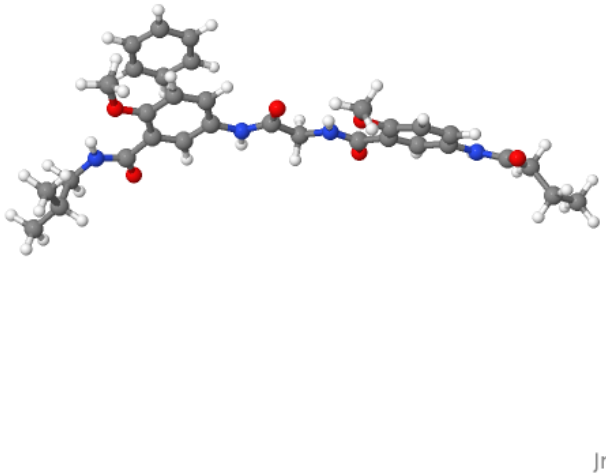
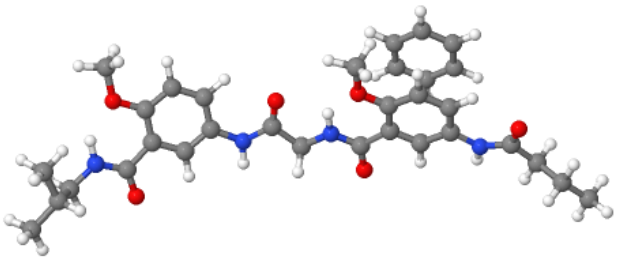
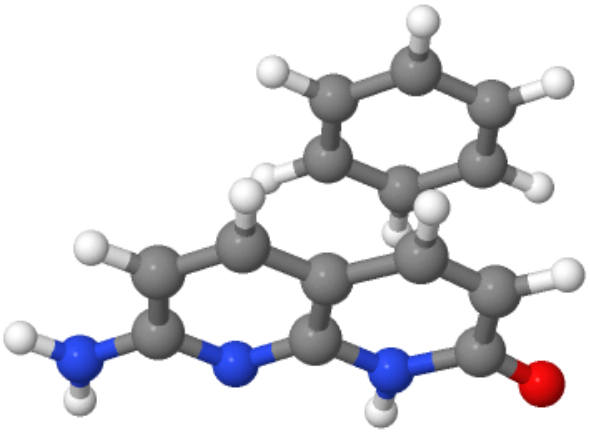


Figure S57 DADA09-R + benzene



Jmol

Figure S58 DADA09-L + benzene



Jmol

Figure S59 DADA10-R + benzene

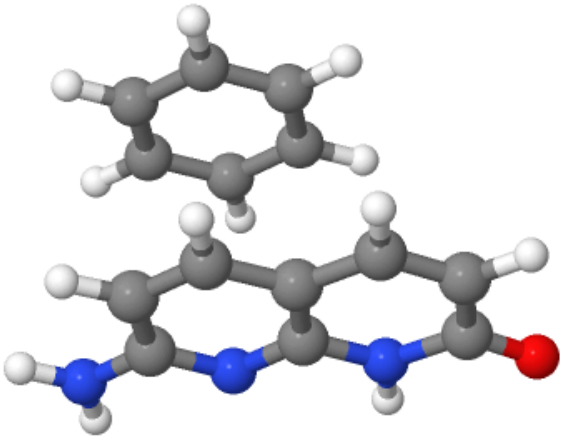


Figure S60 DADA10-L + benzene

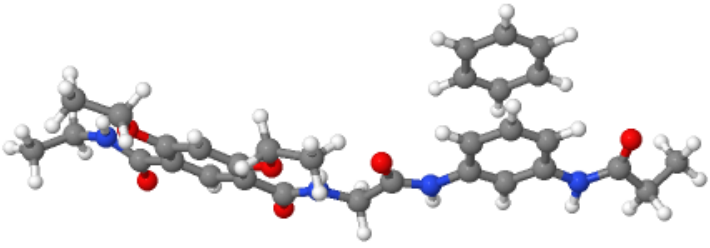
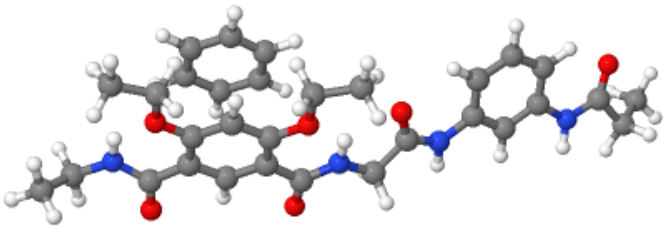
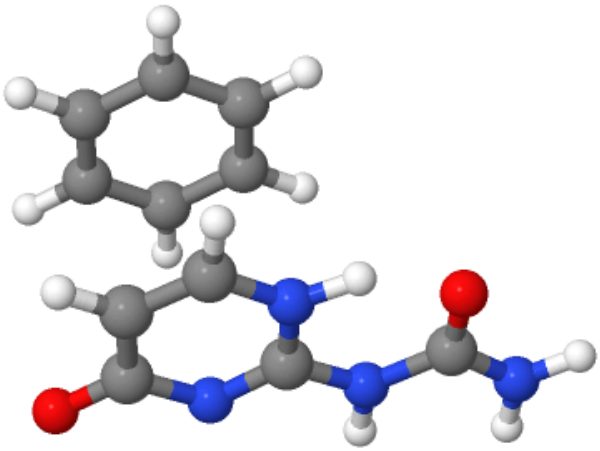


Figure S61 DDAA01-R + benzene



Jmol

Figure S62 DDAA01-L + benzene



Jmol

Figure S63 DDAA02 + benzene

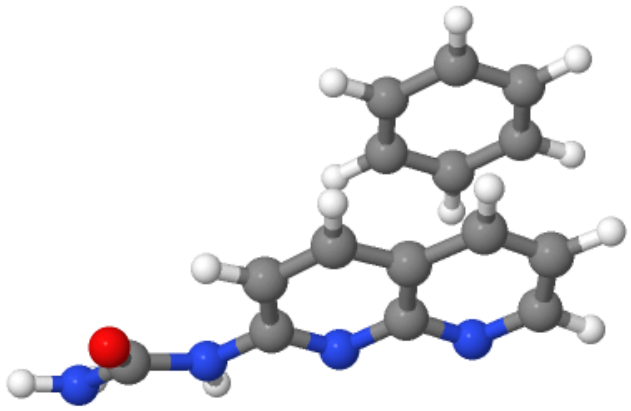


Figure S64 DDAA03-R + benzene

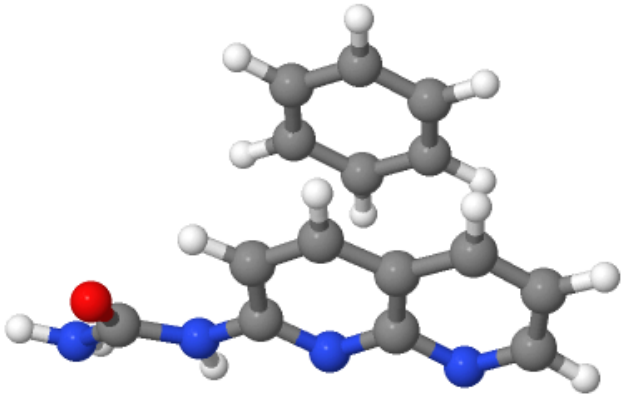


Figure S65 DDAA03-L + benzene

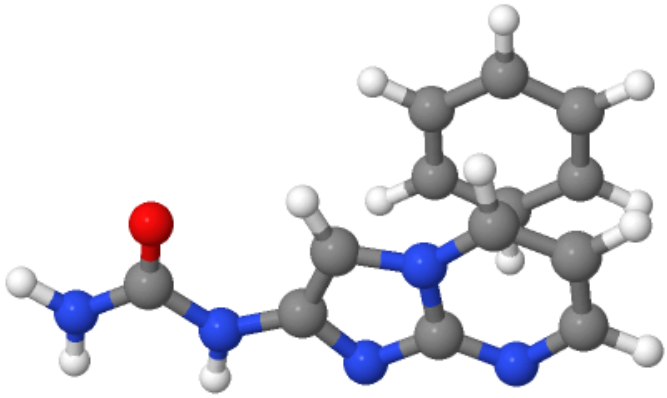


Figure S66 DDAA04-R + benzene

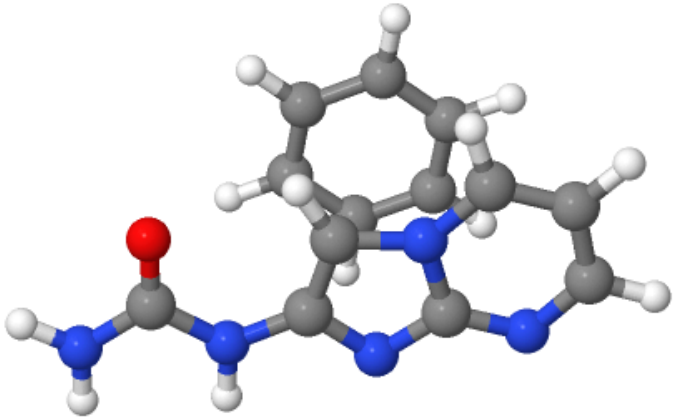


Figure S67 DDAA04-L + benzene

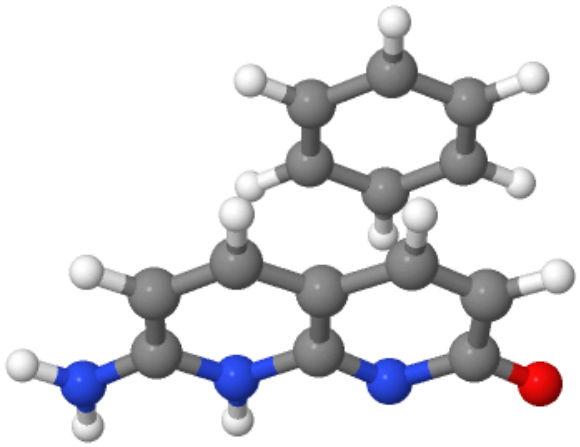


Figure S68 DDAA06-R + benzene

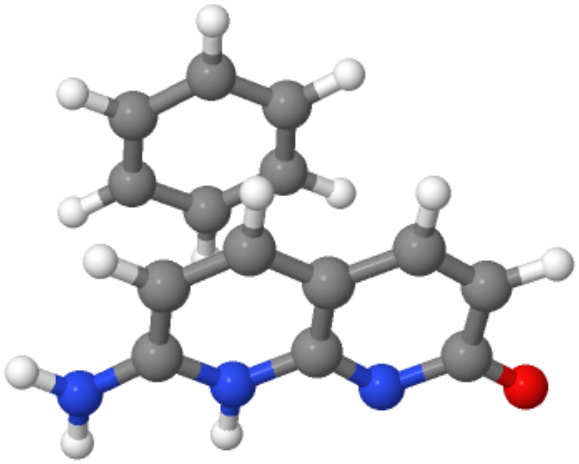


Figure S69 DDAA06-L + benzene

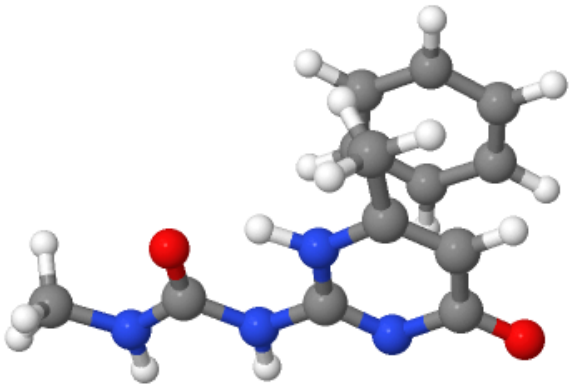


Figure S70 DDAA07 + benzene

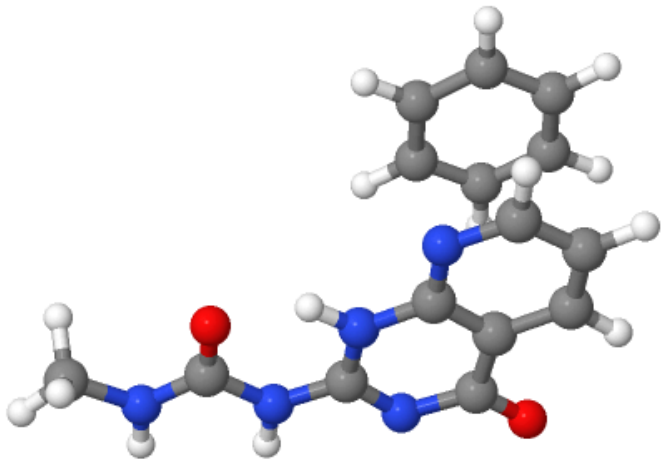


Figure S71 DDAA08-L + benzene

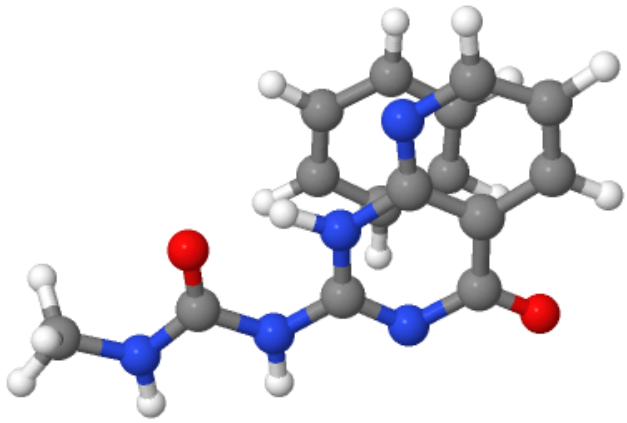


Figure S72 DDAA08-L + benzene

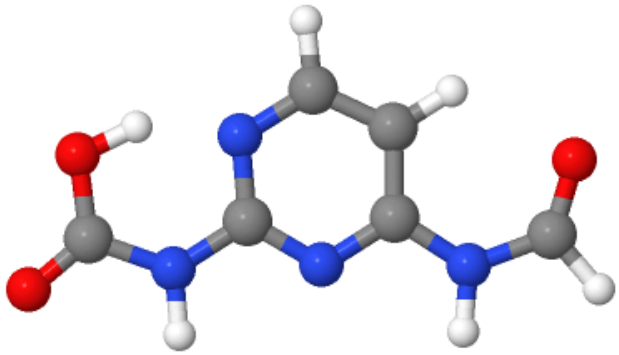


Figure S73 DADA01

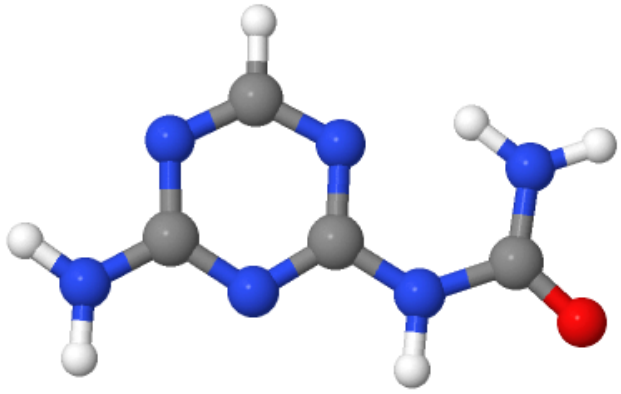


Figure S74 DADA02

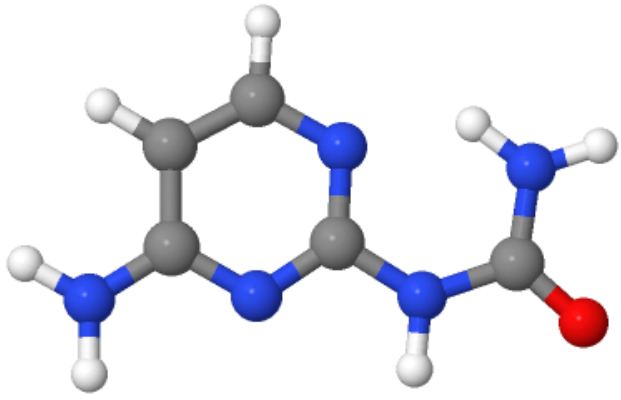


Figure S75 DADA03

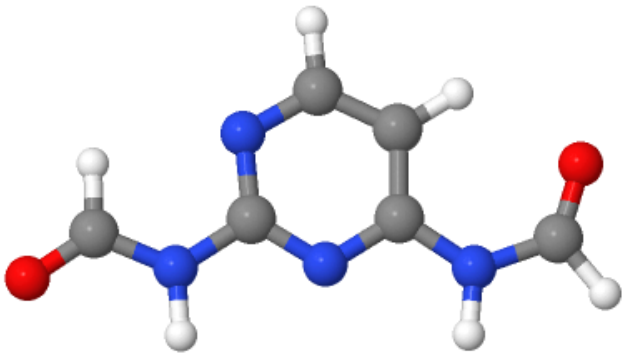


Figure S76 DADA04

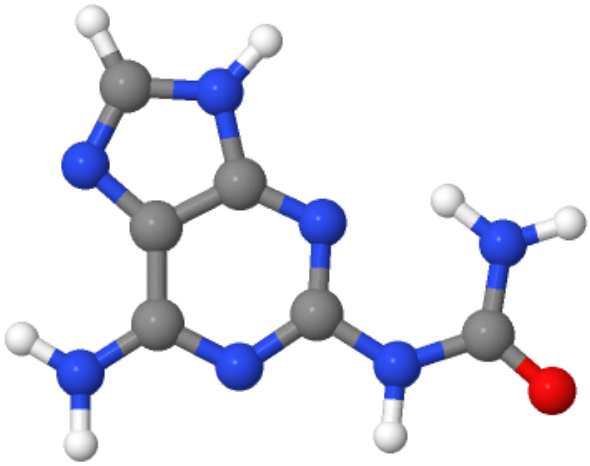


Figure S77 DADA05

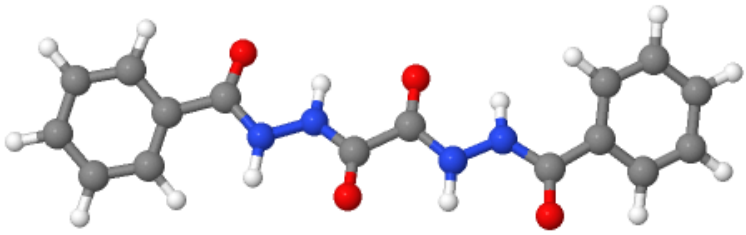


Figure S78 DADA06

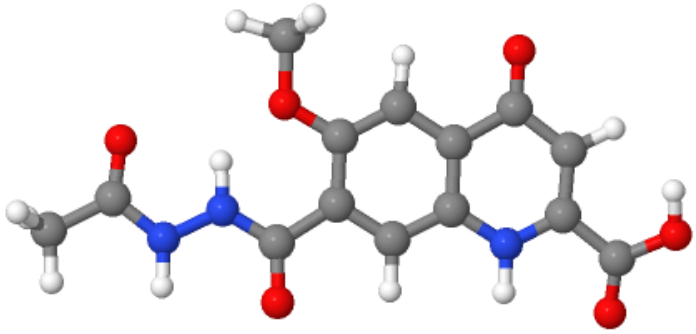
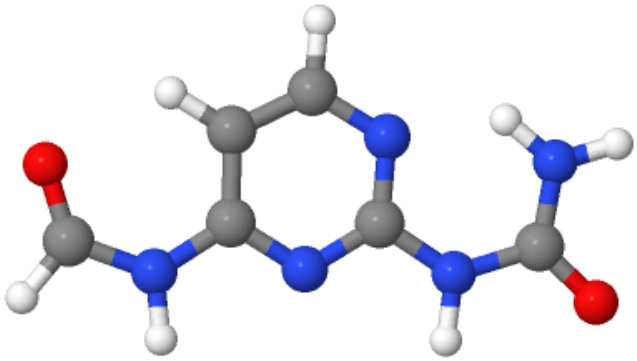
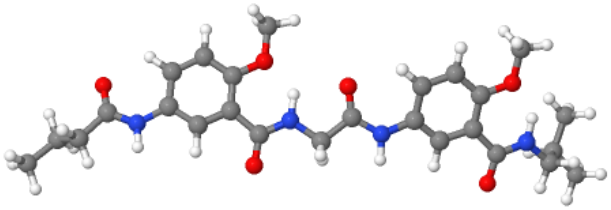


Figure S79 DADA07



Jmol

Figure S80 DADA08



Jmol

Figure S81 DADA09

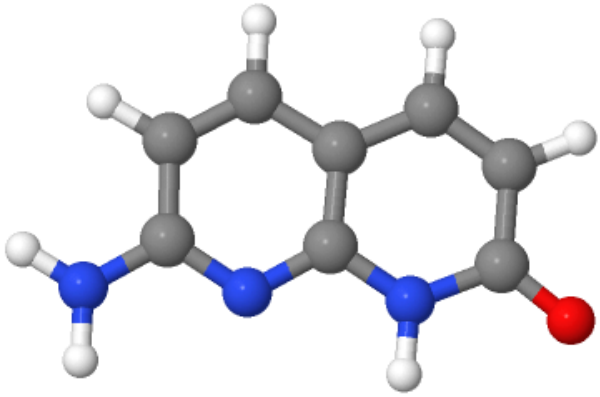


Figure S82 DADA10

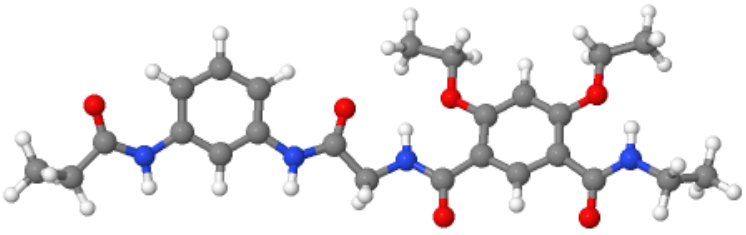


Figure S83 DDAA01

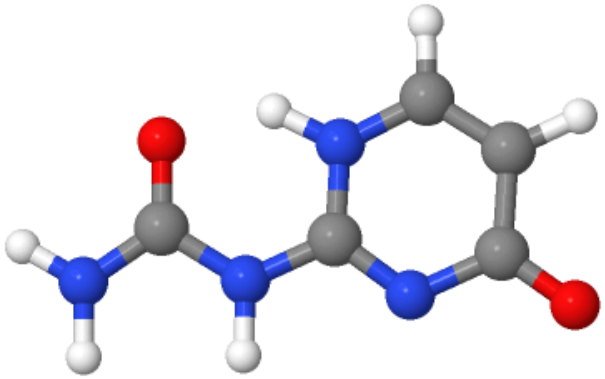


Figure S84 DDAA02

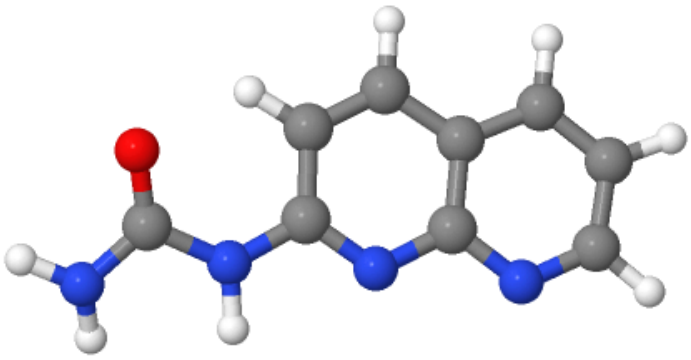


Figure S85 DDAA03

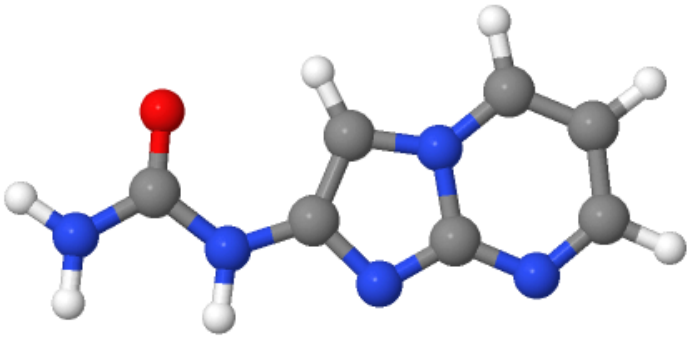


Figure S86 DDAA04

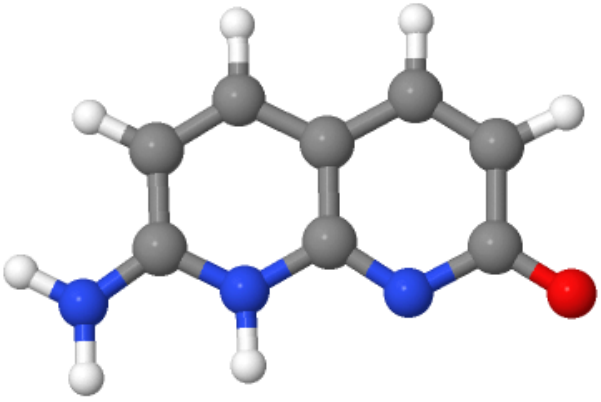


Figure S87 DDAA06

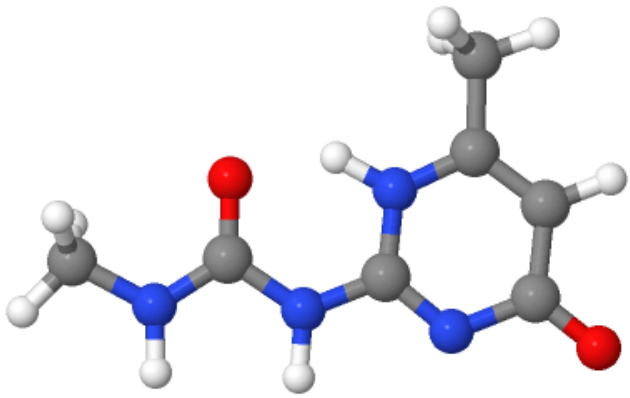


Figure S88 DDAA07

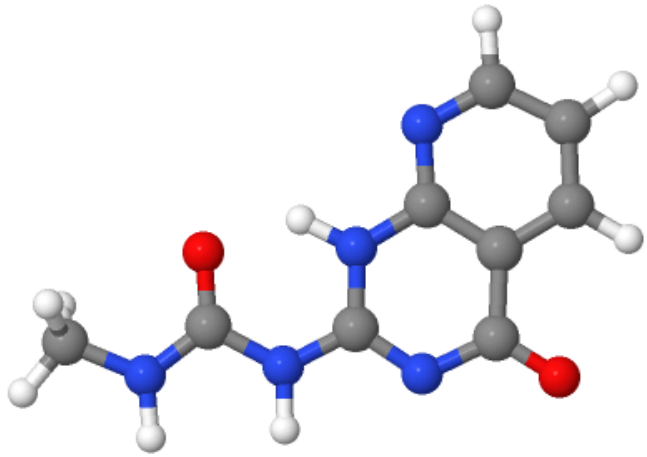


Figure S89 DDAA08