Electronic Supporting information

In silico study MMP inhibition

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1. Materials

HF-DFT calculations were performed using the Gaussian03 package. All structures were fully optimized by using the B3LYP hybrid functional. Two basis sets have been used : the LanL2DZ basis set for the Zn atom and the 6-31G** basis set for the other atoms. Thermochemical corrections were obtained from harmonic frequency analysis of the optimized structures for standard conditions.

Gaussian 03, Revision D.02,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

All HF-DFT representations have been made using VMD software developed by the Theoretical and Computational Biophysics Group in the Beckman Institute for Advanced Science and Technology at the University of Illinois at Urbana-Champaign.
http://www.ks.uiuc.edu/Research/vmd/

Humphrey, W.; Dalke, A.; Schulten, K. “VMD -Visual Molecular Dynamics” *J. Molecular Graphics,* **1996**, *14*, 33-38.

Molecular graphics images of docking were produced using the UCSF Chimera package from the Resource for Biocomputing, Visualization, and Informatics at the University of California, San Francisco (supported by NIH P41 RR-01081).

Pettersen, E.F., Goddard, T.D., Huang, C.C., Couch, G.S., Greenblatt, D.M., Meng, E.C., and Ferrin, T.E. "UCSF Chimera - A Visualization System for Exploratory Research and Analysis." *J. Comput. Chem.* **2004**, *25*, 1605-1612.

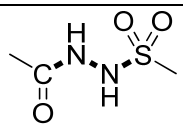
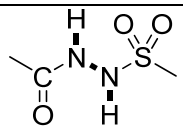
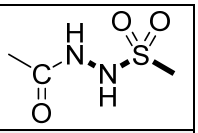
Affinity grid maps were calculated for each atom type constituting the MMPs with AutoGrid program. Grid maps were centered on the MMP catalytic site, with 120 x 120 x 120 grid points and a spacing of 0.214 Å between the grid points. The distance-dependent dielectric permittivity of Mehler and Solmajer[1] was used for the calculations of the electrostatic grid maps. Random starting positions on the entire protein surface, random orientations and torsions were used for all ligands. The AutoDock program, version 4.1 was used for docking computations, with a Lamarckian genetic algorithm.[2] Each docking experiment was performed with two runs constituted of a series of 250 simulations. Each docking simulation was carried out with an initial population of 250 individuals, a maximum number of 5,000,000 energy evaluations and a maximum number of 50,000 generations. The pseudo-Solis and Wets modification methods were used with default parameters. Docked conformations of the ligands were clustered with a root mean square deviation (RMSD) cut-off of 0.5 Å.

Michel F. Sanner, M. F. *J. Mol. Graphics Mod.* **1999**, *17*, 57-61.

[1] Mehler, E. L.; Solmajer, T. *Protein Eng.* **1991**, *4*, 903.

[2] (a) Morris, G. M.; Goodsell, D. S.; Halliday, R. S.; Huey, R.; Hart, W. E.; Belew, R. K.; Olson, A. J. *J. Comput. Chem.* **1998**, *19*, 1639; (b) Huey, R.;Morris, G. M.; Olson, A. J.; Goodsell, D. S. *J. Comput. Chem.* **2007**, *28*, 1145.

2. Calculated torsion angles (degrees) for free (unindexed) and zinc-bound ligands 3-10 in type I (a) and type II (b)

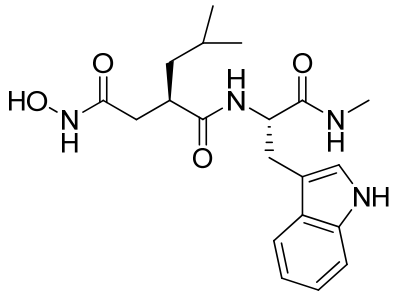
Ligand			
3 ***trans***	-92.9	-136.8	-101.9
3a	-136.5	-62.9	-90.7
3b	-106.9	-39.1	-28.0
4 ***trans***	-96.8	-138.0	-92.2
4 ***cis***	-103.7	-75.9	-61.4
4a	-107.1	-50.1	147.6
4b	-106.4	-40.7	-24.6
5 ***trans***	-97.5	-138.2	-91.0
5 ***cis***	-104.2	-76.1	-60.8
5a	-106.5	-50.1	147.1
5b	-105.9	-40.3	-23.0
6 ***trans***	-97.5	-138.0	-90.8
6 ***cis***	-103.4	-76.2	-61.7
6a	-105.8	-50.9	146.1
6b	-100.2	-35.6	-20.3
7 ***trans***	-97.3	-138.4	-90.6
7 ***cis***	-104.7	-75.6	-60.3
7a	-105.7	-50.3	145.3
7b	-103.2	-38.3	-21.8
8 ***trans***	-97.3	-136.9	-91.35
8 ***cis***	-103.8	-75.7	-61.7
8a	-106.3	-49.5	147.1
8b	-106.2	-39.9	-24.0
9 ***trans***	-95.5	-135.2	-94.2
9a-1	-112.1	-51.4	158.1
9a-2	-106.4	-49.2	147.7
9b	-106.3	-39.8	-24.9
10 ***trans***	-80.1	-163.2	-117.6
10b-1	-118.4	-45.8	-1.0
10b-2	-103.2	-46.7	-166.4

3. Coordinates and Energies for free ligands

Zinc(II)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	0.000000	0.000000	0.000000

SCF Done: E(RB+HF-LYP) = -64.6263106902 A.U. after 10 cycles
Zero-point correction= 0.000000 (Hartree/Particle)
Thermal correction to Energy= 0.001416
Thermal correction to Enthalpy= 0.002360
Thermal correction to Gibbs Free Energy= -0.015877
Sum of electronic and zero-point Energies= -64.626311
Sum of electronic and thermal Energies= -64.624894
Sum of electronic and thermal Enthalpies= -64.623950
Sum of electronic and thermal Free Energies= -64.642188

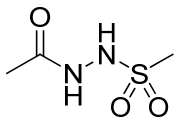


Galardine **1**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	4.777935	-0.583256	-2.200591
2	6	0	5.252730	-0.158721	-0.978183
3	6	0	4.142308	0.360218	-0.255137
4	6	0	2.979934	0.224490	-1.100260
5	6	0	3.418644	-0.351180	-2.268099
6	6	0	6.548370	-0.177905	-0.451790
7	6	0	6.731618	0.337793	0.825271
8	6	0	5.650252	0.866568	1.559445
9	6	0	4.365724	0.882971	1.031514
10	6	0	1.560217	0.588965	-0.770190
11	6	0	0.678039	-0.631566	-0.388377
12	7	0	-0.701517	-0.231010	-0.089682
13	6	0	-1.593371	0.061814	-1.084890
14	6	0	-3.058466	0.245309	-0.659564
15	6	0	-3.665612	-1.158650	-0.425912
16	6	0	-5.182788	-1.115521	-0.392770
17	7	0	-5.786681	-1.988063	0.463961
18	8	0	-7.177718	-1.858437	0.589506
19	6	0	1.224667	-1.448980	0.792861
20	7	0	1.259115	-0.776971	1.991439
21	6	0	1.892625	-1.369537	3.161895
22	8	0	1.546932	-2.621245	0.678656

23	8	0	-1.251746	0.119339	-2.262134
24	6	0	-3.306119	1.193734	0.534705
25	6	0	-3.262714	2.701111	0.207242
26	1	0	-4.302966	0.976290	0.937717
27	8	0	-5.873017	-0.415261	-1.134992
28	1	0	7.382033	-0.580525	-1.020097
29	1	0	7.725019	0.337517	1.263554
30	1	0	5.829556	1.271011	2.551285
31	1	0	3.545560	1.304214	1.606707
32	1	0	5.330883	-1.006097	-2.927645
33	1	0	2.859309	-0.616016	-3.154536
34	1	0	1.536732	1.327985	0.040379
35	1	0	1.069951	1.058562	-1.627427
36	1	0	0.660293	-1.315643	-1.239575
37	1	0	1.201455	0.231100	1.958971
38	1	0	1.421853	-0.989721	4.072393
39	1	0	1.759098	-2.449708	3.104919
40	1	0	2.967446	-1.154881	3.193027
41	1	0	-1.029697	-0.341686	0.858070
42	1	0	-3.556490	0.653893	-1.542865
43	1	0	-2.603951	0.980986	1.355038
44	1	0	-3.380761	-1.815060	-1.257062
45	1	0	-3.272733	-1.619719	0.489058
46	6	0	-3.672697	3.518929	1.440732
47	6	0	-1.905206	3.173876	-0.332767
48	1	0	-4.014452	2.875332	-0.575961
49	1	0	-5.366782	-2.249616	1.345472
50	1	0	-7.355474	-1.186822	-0.106407
51	1	0	-3.708394	4.588389	1.209209
52	1	0	-4.660748	3.223427	1.810026
53	1	0	-2.955441	3.382596	2.259881
54	1	0	-1.926976	4.250353	-0.532881
55	1	0	-1.105717	2.989999	0.395512
56	1	0	-1.635109	2.671452	-1.265286

SCF Done: E(RB+HF-LYP) = -1298.92992702 A.U. after 15 cycles
Zero-point correction= 0.470238 (Hartree/Particle)
Thermal correction to Energy= 0.499935
Thermal correction to Enthalpy= 0.500880
Thermal correction to Gibbs Free Energy= 0.404108
Sum of electronic and zero-point Energies= -1298.459689
Sum of electronic and thermal Energies= -1298.429992
Sum of electronic and thermal Enthalpies= -1298.429047
Sum of electronic and thermal Free Energies= -1298.525819

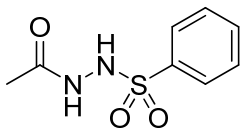


N'-acetylmethanesulfonylhydrazide **3**

***Trans** conformation*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.449498	-1.240662	-0.214277
2	16	0	-1.361018	0.141406	0.170557
3	8	0	-0.834511	-0.066201	1.519327
4	8	0	-2.018138	1.384410	-0.238654
5	7	0	-0.103192	-0.101530	-1.037675
6	7	0	1.053624	-0.685961	-0.530471
7	6	0	2.088305	0.122124	-0.094699
8	6	0	3.337464	-0.611638	0.342466
9	8	0	1.968307	1.335639	-0.076858
10	1	0	0.129377	0.852566	-1.336544
11	1	0	1.218002	-1.639565	-0.817761
12	1	0	3.299356	-1.688314	0.157171
13	1	0	4.200512	-0.182866	-0.171965
14	1	0	3.473655	-0.446339	1.414787
15	1	0	-1.905257	-2.172197	-0.054102
16	1	0	-3.294469	-1.175447	0.473051
17	1	0	-2.780804	-1.147630	-1.247985

SCF Done: E(RB+HF-LYP) = -852.430341158 a.u. after 10 cycles
Zero-point correction= 0.128816 (Hartree/Particle)
Thermal correction to Energy= 0.139536
Thermal correction to Enthalpy= 0.140480
Thermal correction to Gibbs Free Energy= 0.091438
Sum of electronic and zero-point Energies= -852.301526
Sum of electronic and thermal Energies= -852.290805
Sum of electronic and thermal Enthalpies= -852.289861
Sum of electronic and thermal Free Energies= -852.338903



N'-acetylbenzenesulfonylhydrazide **4**

***Trans** conformation*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.539473	-0.012349	-1.072376
2	6	0	-2.329446	0.644041	-0.856793
3	6	0	-1.471549	0.165142	0.135764
4	6	0	-1.800673	-0.940288	0.920008
5	6	0	-3.016289	-1.588021	0.693672
6	6	0	-3.880381	-1.127021	-0.300712
7	16	0	0.087201	1.006045	0.425177
8	8	0	0.632987	0.504042	1.687686
9	1	0	-4.826112	-1.632599	-0.471604
10	8	0	-0.077437	2.435133	0.147423

11	7	0	1.036567	0.446085	-0.943068
12	7	0	1.783252	-0.698301	-0.670198
13	6	0	3.113513	-0.566663	-0.315083
14	8	0	3.612665	0.533946	-0.148722
15	6	0	3.868434	-1.868998	-0.157806
16	1	0	1.693522	1.215051	-1.121718
17	1	0	1.439111	-1.544302	-1.101089
18	1	0	3.280536	-2.749841	-0.428906
19	1	0	4.773578	-1.832197	-0.768605
20	1	0	4.177146	-1.961866	0.887019
21	1	0	-1.119509	-1.266551	1.697815
22	1	0	-3.289380	-2.447080	1.298681
23	1	0	-4.219204	0.349016	-1.837765
24	1	0	-2.054185	1.519152	-1.434939

SCF Done: E(RB+HF-LYP) = -1044.16759387 a.u. after 11 cycles
Zero-point correction= 0.181856 (Hartree/Particle)
Thermal correction to Energy= 0.195695
Thermal correction to Enthalpy= 0.196640
Thermal correction to Gibbs Free Energy= 0.138595
Sum of electronic and zero-point Energies= -1043.985738
Sum of electronic and thermal Energies= -1043.971898
Sum of electronic and thermal Enthalpies= -1043.970954
Sum of electronic and thermal Free Energies= -1044.028999

***Cis** conformation*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.364516	-0.215419	0.159942
2	16	0	-0.057962	-1.301712	0.347342
3	8	0	-3.757120	-0.129380	-0.115236
4	6	0	-2.942278	0.742532	-0.313933
5	6	0	-3.216473	2.221269	-0.091218
6	8	0	-0.657950	-1.006539	1.643874
7	8	0	0.331551	-2.642939	-0.085875
8	7	0	-1.168013	-0.795294	-0.846549
9	7	0	-1.650156	0.492754	-0.783470
10	1	0	-0.908747	-1.122557	-1.773573
11	1	0	-0.986999	1.257387	-0.854857
12	1	0	-2.561927	2.879805	-0.669916
13	1	0	-4.255932	2.423317	-0.352183
14	1	0	-3.085219	2.448465	0.971890
15	6	0	2.386976	-0.573491	-0.723130
16	6	0	3.468861	0.289821	-0.890045
17	6	0	3.521775	1.494307	-0.183513
18	6	0	2.498678	1.837242	0.702432
19	6	0	1.411861	0.980054	0.882745
20	1	0	2.338636	-1.522547	-1.246163
21	1	0	4.274591	0.018586	-1.565117
22	1	0	4.367981	2.161532	-0.316414
23	1	0	2.551181	2.765243	1.263378
24	1	0	0.625662	1.208929	1.593838

```
SCF Done:  E(RB+HF-LYP) =  -1044.15928482     a.u. after   11 cycles
Zero-point correction=                        0.181703 (Hartree/Particle)
Thermal correction to Energy=                     0.195556
Thermal correction to Enthalpy=                   0.196500
Thermal correction to Gibbs Free Energy=          0.139040
Sum of electronic and zero-point Energies=           -1043.977581
Sum of electronic and thermal Energies=              -1043.963729
Sum of electronic and thermal Enthalpies=            -1043.962785
Sum of electronic and thermal Free Energies=         -1044.020245
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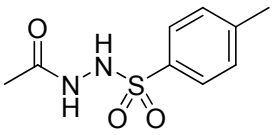

N'-acetyl-4-methylbenzenesulfonylhydrazide **5**

Trans *conformation*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.892607	-0.917803	-0.829995
2	6	0	1.060402	-0.425665	0.178234
3	6	0	1.488240	0.584395	1.038061
4	6	0	2.768576	1.113411	0.875511
5	6	0	3.624584	0.643777	-0.128669
6	6	0	3.165799	-0.377259	-0.976688
7	16	0	-0.578543	-1.116813	0.382809
8	8	0	-0.555496	-2.535842	0.018097
9	7	0	-1.432942	-0.382123	-0.965594
10	7	0	-2.045356	0.827378	-0.641696
11	6	0	-3.390700	0.837485	-0.322095
12	6	0	-3.990813	2.211114	-0.111315
13	8	0	-1.103855	-0.640939	1.664301
14	8	0	-4.022003	-0.202162	-0.227029
15	1	0	-2.172686	-1.057872	-1.191257
16	1	0	-1.594464	1.647277	-1.021699
17	1	0	-3.287836	3.027663	-0.295789
18	1	0	-4.860279	2.324243	-0.763459
19	1	0	-4.341281	2.276566	0.922206
20	1	0	0.829011	0.934429	1.824543
21	1	0	3.108587	1.899576	1.544055
22	6	0	5.020712	1.196832	-0.280486
23	1	0	3.818375	-0.756049	-1.758699
24	1	0	1.546331	-1.715491	-1.477927
25	1	0	5.302298	1.287623	-1.333943
26	1	0	5.115163	2.181640	0.184553
27	1	0	5.755954	0.536451	0.195186

```
SCF Done:  E(RB+HF-LYP) =  -1083.48904493     a.u. after   11 cycles
Zero-point correction=                        0.209249 (Hartree/Particle)
Thermal correction to Energy=                     0.224975
Thermal correction to Enthalpy=                   0.225919
Thermal correction to Gibbs Free Energy=          0.162672
```

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Sum of electronic and zero-point Energies=          -1083.279796
Sum of electronic and thermal Energies=             -1083.264070
Sum of electronic and thermal Enthalpies=           -1083.263126
Sum of electronic and thermal Free Energies=        -1083.326373
```
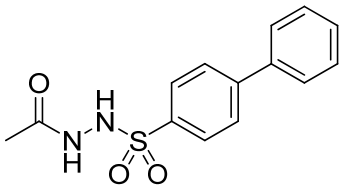

***Cis** conformation*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.202811	0.564905	0.963819
2	6	0	0.944062	-0.568822	0.189694
3	6	0	1.897733	-1.055630	-0.708565
4	6	0	3.114481	-0.391059	-0.832681
5	6	0	3.398542	0.754634	-0.073285
6	6	0	2.426191	1.219182	0.822713
7	16	0	-0.646147	-1.393217	0.325058
8	7	0	-1.632424	-0.671274	-0.868892
9	7	0	-1.872771	0.681957	-0.778719
10	6	0	-3.106760	1.151998	-0.323025
11	6	0	-3.110272	2.649844	-0.061472
12	8	0	-1.211333	-1.033378	1.621187
13	8	0	-0.488903	-2.770207	-0.142200
14	8	0	-4.072162	0.440208	-0.163819
15	1	0	-1.412329	-1.013803	-1.800640
16	1	0	-1.078667	1.312930	-0.810603
17	1	0	-2.338515	3.192119	-0.615888
18	1	0	-4.091795	3.044737	-0.326248
19	1	0	-2.954382	2.822022	1.008611
20	1	0	1.690450	-1.953229	-1.281510
21	1	0	3.860685	-0.771312	-1.525070
22	6	0	4.734921	1.445525	-0.192539
23	1	0	2.632499	2.098424	1.426947
24	1	0	0.465799	0.904063	1.683598
25	1	0	4.667255	2.501052	0.084592
26	1	0	5.474228	0.979843	0.470465
27	1	0	5.128424	1.383393	-1.211202

```
SCF Done:  E(RB+HF-LYP) =  -1083.48084661     a.u. after   11 cycles
Zero-point correction=                        0.209080 (Hartree/Particle)
Thermal correction to Energy=                 0.224819
Thermal correction to Enthalpy=               0.225763
Thermal correction to Gibbs Free Energy=      0.163394
Sum of electronic and zero-point Energies=          -1083.271766
Sum of electronic and thermal Energies=             -1083.256028
Sum of electronic and thermal Enthalpies=           -1083.255084
Sum of electronic and thermal Free Energies=        -1083.317453
```



N'-acetylbiphenyl-4-sulfonylhydrazide **6**

Trans *conformation*

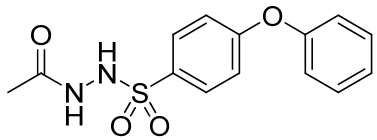
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.271786	-1.331131	-0.815991
2	6	0	-0.502201	-0.775468	0.205020
3	6	0	0.063374	0.068540	1.160201
4	6	0	1.421296	0.368593	1.080759
5	6	0	2.225754	-0.167953	0.061159
6	6	0	1.626313	-1.024564	-0.881400
7	16	0	-2.246058	-1.170988	0.302777
8	8	0	-2.460053	-2.537505	-0.180616
9	7	0	-2.893429	-0.189162	-1.002130
10	7	0	-3.289922	1.083779	-0.594971
11	6	0	-4.624435	1.315878	-0.315243
12	6	0	-4.975508	2.755620	-0.007258
13	8	0	-2.732800	-0.709927	1.604583
14	8	0	-5.436070	0.405154	-0.326050
15	1	0	-3.732868	-0.697509	-1.305221
16	1	0	-2.683111	1.833613	-0.894259
17	1	0	-4.131088	3.442290	-0.109100
18	1	0	-5.786000	3.073891	-0.667395
19	1	0	-5.346232	2.805354	1.020095
20	1	0	-0.556149	0.474176	1.952194
21	1	0	1.859740	1.043740	1.808636
22	6	0	3.672765	0.154618	-0.017658
23	1	0	2.237337	-1.478684	-1.654762
24	1	0	-0.180556	-2.009211	-1.531248
25	6	0	4.302024	0.338846	-1.260293
26	6	0	5.660057	0.642317	-1.335458
27	6	0	6.417704	0.766381	-0.169761
28	6	0	5.806042	0.584924	1.071685
29	6	0	4.447637	0.283029	1.147322
30	1	0	3.716465	0.269724	-2.172109
31	1	0	6.125101	0.789367	-2.305813
32	1	0	7.476106	1.001767	-0.228291
33	1	0	6.389155	0.669684	1.983951
34	1	0	3.988228	0.115742	2.116772

```
SCF Done:  E(RB+HF-LYP) =  -1275.23156972     a.u. after   11 cycles
Zero-point correction=                        0.262866 (Hartree/Particle)
Thermal correction to Energy=                     0.281345
Thermal correction to Enthalpy=                   0.282289
Thermal correction to Gibbs Free Energy=          0.213039
Sum of electronic and zero-point Energies=          -1274.968704
Sum of electronic and thermal Energies=             -1274.950225
Sum of electronic and thermal Enthalpies=           -1274.949280
Sum of electronic and thermal Free Energies=        -1275.018531
```

***Cis** conformation*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.147629	0.106094	1.021634
2	6	0	-0.632687	-0.943732	0.236694
3	6	0	0.219390	-1.652790	-0.614118
4	6	0	1.562250	-1.296325	-0.684439
5	6	0	2.076630	-0.235961	0.084257
6	6	0	1.198750	0.453223	0.939115
7	16	0	-2.378530	-1.362741	0.294383
8	7	0	-3.110504	-0.408587	-0.918642
9	7	0	-3.039778	0.961587	-0.797793
10	6	0	-4.152314	1.690734	-0.369936
11	6	0	-3.825113	3.142621	-0.059083
12	8	0	-2.894396	-0.892368	1.575542
13	8	0	-2.536341	-2.731039	-0.196888
14	8	0	-5.259987	1.214825	-0.268349
15	1	0	-2.933819	-0.774691	-1.850598
16	1	0	-2.121965	1.394080	-0.778687
17	1	0	-2.936794	3.510999	-0.580842
18	1	0	-4.685034	3.756226	-0.329782
19	1	0	-3.662006	3.245729	1.018870
20	1	0	-0.168800	-2.479403	-1.199514
21	1	0	2.220209	-1.835254	-1.358539
22	6	0	3.510813	0.138289	0.003282
23	1	0	1.583481	1.245170	1.573601
24	1	0	-0.811870	0.609369	1.715777
25	6	0	3.906863	1.485194	0.057905
26	6	0	5.253026	1.837157	-0.018254
27	6	0	6.230847	0.849664	-0.148252
28	6	0	5.851913	-0.492601	-0.202481
29	6	0	4.505669	-0.844944	-0.128644
30	1	0	3.152714	2.262854	0.133234
31	1	0	5.537783	2.884571	0.016654
32	1	0	7.279795	1.124033	-0.206307
33	1	0	6.606173	-1.268485	-0.293795
34	1	0	4.223935	-1.893417	-0.143684

SCF Done: E(RB+HF-LYP) = -1275.22329003 a.u. after 12 cycles
Zero-point correction= 0.262656 (Hartree/Particle)
Thermal correction to Energy= 0.281163
Thermal correction to Enthalpy= 0.282107
Thermal correction to Gibbs Free Energy= 0.213249
Sum of electronic and zero-point Energies= -1274.960634
Sum of electronic and thermal Energies= -1274.942127
Sum of electronic and thermal Enthalpies= -1274.941183
Sum of electronic and thermal Free Energies= -1275.010041



N'-acetyl-4-phenoxybenzenesulfonylhydrazide **7**

Trans *conformation*

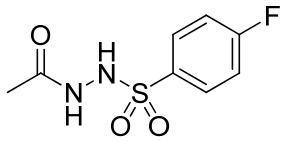
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.209711	-0.832852	-0.572200
2	6	0	-0.774831	-0.528397	0.370270
3	6	0	-0.486504	0.274567	1.476688
4	6	0	0.798288	0.780047	1.636854
5	6	0	1.787802	0.480802	0.692144
6	6	0	1.495726	-0.325579	-0.416655
7	16	0	-2.420827	-1.191736	0.170493
8	8	0	-2.341494	-2.507753	-0.469464
9	7	0	-3.053914	-0.174032	-1.115129
10	7	0	-3.703858	0.967522	-0.649038
11	6	0	-5.081878	0.961464	-0.535398
12	6	0	-5.699513	2.284441	-0.135722
13	8	0	-3.142651	-0.967827	1.425121
14	8	0	-5.725913	-0.052412	-0.749186
15	1	0	-3.752719	-0.764457	-1.581683
16	1	0	-3.195359	1.829966	-0.781173
17	1	0	-4.978638	3.104426	-0.080685
18	1	0	-6.487866	2.538893	-0.847996
19	1	0	-6.165933	2.162026	0.845684
20	1	0	-1.261283	0.478331	2.207169
21	1	0	1.058282	1.400465	2.487456
22	8	0	3.011045	1.057612	0.910309
23	1	0	2.265329	-0.553925	-1.144073
24	1	0	-0.029465	-1.467983	-1.418087
25	6	0	4.147265	0.578406	0.267463
26	6	0	4.866249	1.469043	-0.527057
27	6	0	6.059483	1.046901	-1.115239
28	6	0	6.522650	-0.254310	-0.914154
29	6	0	5.791676	-1.135335	-0.113676
30	6	0	4.602181	-0.723294	0.486924
31	1	0	4.488150	2.476034	-0.667647
32	1	0	6.624989	1.737837	-1.733090
33	1	0	7.449983	-0.579809	-1.374905
34	1	0	6.151322	-2.146181	0.053101
35	1	0	4.033125	-1.394653	1.121510

```
SCF Done:  E(RB+HF-LYP) =  -1350.43914712     a.u. after   12 cycles
Zero-point correction=                        0.266493 (Hartree/Particle)
Thermal correction to Energy=                     0.286090
Thermal correction to Enthalpy=                   0.287034
Thermal correction to Gibbs Free Energy=          0.213500
Sum of electronic and zero-point Energies=          -1350.172654
Sum of electronic and thermal Energies=             -1350.153057
Sum of electronic and thermal Enthalpies=           -1350.152113
Sum of electronic and thermal Free Energies=        -1350.225647
```

***Cis** conformation*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.192597	-0.075354	0.628027
2	6	0	-0.984244	-1.084390	0.073569
3	6	0	-0.441849	-1.992786	-0.843960
4	6	0	0.893300	-1.885028	-1.207104
5	6	0	1.688395	-0.868901	-0.656817
6	6	0	1.147177	0.039322	0.261146
7	16	0	-2.714576	-1.204550	0.523216
8	7	0	-3.557090	-0.281899	-0.643768
9	7	0	-3.254005	1.057728	-0.748230
10	6	0	-4.125134	2.022152	-0.237599
11	6	0	-3.526779	3.420182	-0.232669
12	8	0	-2.876881	-0.523128	1.803417
13	8	0	-3.160515	-2.573701	0.265636
14	8	0	-5.243564	1.770918	0.150061
15	1	0	-3.642897	-0.778264	-1.527129
16	1	0	-2.301450	1.317588	-0.982183
17	1	0	-2.684046	3.540368	-0.919879
18	1	0	-4.310485	4.132786	-0.493270
19	1	0	-3.184810	3.652856	0.781051
20	1	0	-1.059558	-2.790620	-1.242128
21	1	0	1.345991	-2.580731	-1.905071
22	8	0	2.980847	-0.821496	-1.103745
23	1	0	1.767013	0.817066	0.690712
24	1	0	-0.620188	0.597012	1.363825
25	6	0	3.943776	-0.092446	-0.411656
26	6	0	4.316100	-0.451209	0.885023
27	6	0	5.342647	0.253291	1.513782
28	6	0	5.994794	1.295240	0.850169
29	6	0	5.617338	1.634314	-0.450025
30	6	0	4.585972	0.942752	-1.087563
31	1	0	3.811479	-1.271836	1.384231
32	1	0	5.638252	-0.020351	2.522039
33	1	0	6.796207	1.836515	1.343031
34	1	0	6.124127	2.439977	-0.972470
35	1	0	4.278768	1.186044	-2.099117

SCF Done: E(RB+HF-LYP) = -1350.43091834 a.u. after 11 cycles
Zero-point correction= 0.266325 (Hartree/Particle)
Thermal correction to Energy= 0.285952
Thermal correction to Enthalpy= 0.286896
Thermal correction to Gibbs Free Energy= 0.214114
Sum of electronic and zero-point Energies= -1350.164593
Sum of electronic and thermal Energies= -1350.144967
Sum of electronic and thermal Enthalpies= -1350.144023
Sum of electronic and thermal Free Energies= -1350.216805



N'-acetyl-4-fluorobenzenesulfonylhydrazide **8**

***Trans** conformation*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.927934	0.895420	-0.829949
2	6	0	-1.093765	0.397780	0.175358
3	6	0	-1.511030	-0.624344	1.029349
4	6	0	-2.783415	-1.170977	0.870177
5	6	0	-3.600583	-0.673564	-0.139524
6	6	0	-3.198498	0.352174	-0.992338
7	16	0	0.537682	1.104559	0.390581
8	8	0	0.495433	2.525922	0.038930
9	7	0	1.402378	0.392267	-0.960967
10	7	0	2.033599	-0.809711	-0.645171
11	6	0	3.379662	-0.795567	-0.322065
12	6	0	4.007478	-2.158380	-0.125070
13	8	0	1.059785	0.620944	1.669936
14	8	0	3.986855	0.256438	-0.212070
15	1	0	2.130276	1.082125	-1.183206
16	1	0	1.606484	-1.631496	-1.048424
17	1	0	3.324603	-2.987147	-0.329298
18	1	0	4.886238	-2.242459	-0.768994
19	1	0	4.348069	-2.231790	0.911260
20	1	0	-0.848113	-0.969901	1.814389
21	1	0	-3.148510	-1.962163	1.515190
22	9	0	-4.828470	-1.198459	-0.296161
23	1	0	-3.878547	0.711307	-1.756442
24	1	0	-1.587098	1.705112	-1.465351

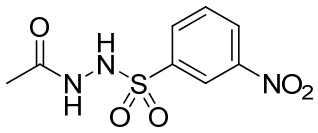
```
SCF Done:  E(RB+HF-LYP) =  -1143.39891987     a.u. after   11 cycles
Zero-point correction=                        0.173702 (Hartree/Particle)
Thermal correction to Energy=                     0.188308
Thermal correction to Enthalpy=                   0.189252
Thermal correction to Gibbs Free Energy=          0.129591
Sum of electronic and zero-point Energies=           -1143.225217
Sum of electronic and thermal Energies=              -1143.210612
Sum of electronic and thermal Enthalpies=            -1143.209668
Sum of electronic and thermal Free Energies=         -1143.269329
```

***Cis** conformation*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.227679	0.613996	0.958534
2	6	0	0.990439	-0.526335	0.184305
3	6	0	1.952341	-1.005824	-0.711082

4	6	0	3.162202	-0.330469	-0.844686
5	6	0	3.378892	0.811299	-0.076950
6	6	0	2.436538	1.295065	0.825369
7	16	0	-0.584041	-1.380848	0.327666
8	7	0	-1.589687	-0.687991	-0.861314
9	7	0	-1.881648	0.653168	-0.775758
10	6	0	-3.131379	1.079909	-0.318088
11	6	0	-3.196650	2.580663	-0.085430
12	8	0	-1.145545	-1.025464	1.626067
13	8	0	-0.396203	-2.755151	-0.135019
14	8	0	-4.061864	0.329140	-0.134114
15	1	0	-1.391402	-1.042967	-1.792941
16	1	0	-1.119573	1.318419	-0.850976
17	1	0	-2.455700	3.144815	-0.659664
18	1	0	-4.197323	2.927435	-0.345777
19	1	0	-3.036409	2.780915	0.979097
20	1	0	1.758899	-1.911615	-1.275409
21	1	0	3.936488	-0.676680	-1.520017
22	9	0	4.545804	1.464809	-0.206306
23	1	0	2.661410	2.177132	1.414347
24	1	0	0.483896	0.938557	1.677639

SCF Done: E(RB+HF-LYP) = -1143.39022750 a.u. after 17 cycles
Zero-point correction= 0.173351 (Hartree/Particle)
Thermal correction to Energy= 0.188089
Thermal correction to Enthalpy= 0.189033
Thermal correction to Gibbs Free Energy= 0.129203
Sum of electronic and zero-point Energies= -1143.216877
Sum of electronic and thermal Energies= -1143.202139
Sum of electronic and thermal Enthalpies= -1143.201194
Sum of electronic and thermal Free Energies= -1143.261025



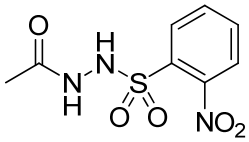
N'-acetyl-3-nitrobenzenesulfonylhydrazide **9**

Trans *conformation*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.814094	0.188261	-0.186141
2	6	0	1.623735	-0.474187	0.090260
3	6	0	0.576704	0.280368	0.615884
4	6	0	0.711823	1.644971	0.874318
5	6	0	1.924678	2.277416	0.589106
6	6	0	2.985514	1.551673	0.053221
7	16	0	-0.979612	-0.538000	1.003309
8	8	0	-1.785869	0.416675	1.764005
9	1	0	3.937488	2.012707	-0.177602
10	8	0	-0.691972	-1.893195	1.473950
11	7	0	-1.628747	-0.796466	-0.601544

12	7	0	-2.470053	0.224772	-1.037433
13	6	0	-3.839928	0.072025	-0.880408
14	8	0	-4.295400	-0.879843	-0.270684
15	6	0	-4.683444	1.158282	-1.510420
16	1	0	-2.182323	-1.657152	-0.512113
17	1	0	-2.097392	0.783772	-1.792176
18	1	0	-4.101065	1.889567	-2.076738
19	1	0	-5.426350	0.696830	-2.165342
20	1	0	-5.222003	1.679198	-0.714135
21	1	0	-0.121321	2.188822	1.305171
22	1	0	2.043041	3.336876	0.790205
23	7	0	3.939339	-0.583100	-0.750612
24	1	0	1.529599	-1.537072	-0.092809
25	8	0	4.982778	0.025188	-0.981090
26	8	0	3.759374	-1.780681	-0.956831

```
SCF Done:  E(RB+HF-LYP) =  -1248.66275812     a.u. after   11 cycles
Zero-point correction=                          0.184353 (Hartree/Particle)
Thermal correction to Energy=                   0.200682
Thermal correction to Enthalpy=                 0.201626
Thermal correction to Gibbs Free Energy=        0.137149
Sum of electronic and zero-point Energies=          -1248.478405
Sum of electronic and thermal Energies=             -1248.462077
Sum of electronic and thermal Enthalpies=           -1248.461132
Sum of electronic and thermal Free Energies=        -1248.525609
```



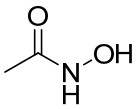
N'-acetyl-2-nitrobenzenesulfonylhydrazide **10**

Trans *conformation*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.462696	0.388293	-0.449225
2	6	0	-2.114688	0.516287	-0.124075
3	6	0	-1.300341	-0.613364	0.047930
4	6	0	-1.871373	-1.875806	-0.113072
5	6	0	-3.216789	-2.009782	-0.461295
6	6	0	-4.013335	-0.879082	-0.626566
7	16	0	0.408907	-0.614189	0.677505
8	8	0	0.793307	-2.021900	0.832705
9	1	0	-5.061124	-0.976357	-0.890663
10	8	0	0.474450	0.295056	1.821596
11	7	0	1.287988	-0.106742	-0.753600
12	7	0	2.600360	-0.578306	-0.728590
13	6	0	3.642179	0.260353	-0.400268
14	8	0	3.444454	1.431961	-0.119291
15	6	0	5.015583	-0.375357	-0.455683
16	1	0	1.324976	0.917708	-0.755985
17	1	0	2.722006	-1.532480	-1.029006

18	1	0	5.000334	-1.424763	-0.760864
19	1	0	5.641027	0.193346	-1.148279
20	1	0	5.468773	-0.301441	0.536356
21	1	0	-1.248290	-2.746442	0.053478
22	1	0	-3.638934	-3.001006	-0.591273
23	1	0	-4.055127	1.287439	-0.563214
24	7	0	-1.599524	1.893022	-0.019465
25	8	0	-2.397660	2.771961	0.286628
26	8	0	-0.413197	2.083667	-0.282327

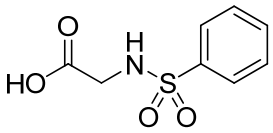
SCF Done: E(RB+HF-LYP) = -1248.65211362 a.u. after 13 cycles
Zero-point correction= 0.184259 (Hartree/Particle)
Thermal correction to Energy= 0.200683
Thermal correction to Enthalpy= 0.201627
Thermal correction to Gibbs Free Energy= 0.137735
Sum of electronic and zero-point Energies= -1248.467854
Sum of electronic and thermal Energies= -1248.451431
Sum of electronic and thermal Enthalpies= -1248.450486
Sum of electronic and thermal Free Energies= -1248.514379



N-acetohydroxamic acid **AHA 11**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.814909	-0.443597	0.023444
2	1	0	1.810773	-1.534957	-0.039332
3	1	0	2.313881	-0.135374	0.946314
4	1	0	2.392202	-0.043124	-0.813847
5	6	0	0.429216	0.155586	-0.010468
6	8	0	0.195235	1.363678	-0.002745
7	7	0	-0.605138	-0.732144	-0.122593
8	1	0	-0.552827	-1.648633	0.302955
9	8	0	-1.886525	-0.183485	0.040264
10	1	0	-1.662487	0.773621	0.084060

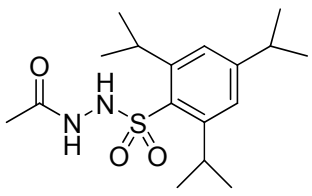
SCF Done: E(RB+HF-LYP) = -284.382279266 a.u. after 9 cycles
Zero-point correction= 0.078065 (Hartree/Particle)
Thermal correction to Energy= 0.083843
Thermal correction to Enthalpy= 0.084787
Thermal correction to Gibbs Free Energy= 0.049332
Sum of electronic and zero-point Energies= -284.304214
Sum of electronic and thermal Energies= -284.298436
Sum of electronic and thermal Enthalpies= -284.297492
Sum of electronic and thermal Free Energies= -284.332948



2-(phenylsulfonamido)acetic acid **12**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.170308	-1.652745	0.063058
2	6	0	-2.969386	-0.843174	-1.058374
3	6	0	-1.984876	0.142872	-1.042044
4	6	0	-1.208564	0.298456	0.109423
5	6	0	-1.404936	-0.493226	1.241782
6	6	0	-2.394507	-1.476355	1.209754
7	1	0	-0.803571	-0.328189	2.128522
8	1	0	-2.559551	-2.100325	2.082216
9	1	0	-3.938843	-2.419305	0.043972
10	1	0	-3.583957	-0.974950	-1.943235
11	1	0	-1.828950	0.794376	-1.894985
12	16	0	0.070342	1.553021	0.131508
13	8	0	-0.314098	2.642141	-0.768843
14	8	0	0.446063	1.783785	1.528782
15	7	0	1.381252	0.790116	-0.683069
16	1	0	1.705988	1.459946	-1.376332
17	6	0	2.450121	0.165559	0.111917
18	1	0	3.415217	0.632277	-0.101861
19	1	0	2.265173	0.309928	1.180479
20	6	0	2.583224	-1.341198	-0.156359
21	8	0	1.678556	-1.852503	-1.007775
22	1	0	1.114813	-1.109043	-1.300406
23	8	0	3.441332	-2.004047	0.370841

SCF Done: E(RB+HF-LYP) = -1064.05945495 A.U. after 15 cycles
Zero-point correction= 0.171338 (Hartree/Particle)
Thermal correction to Energy= 0.184283
Thermal correction to Enthalpy= 0.185227
Thermal correction to Gibbs Free Energy= 0.128846
Sum of electronic and zero-point Energies= -1063.888117
Sum of electronic and thermal Energies= -1063.875172
Sum of electronic and thermal Enthalpies= -1063.874228
Sum of electronic and thermal Free Energies= -1063.930609



N'-acetyl-2,4,6-triisopropylbenzenesulfonylhydrazide **13**

Trans *conformation*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.868936	-0.097561	0.320628
2	6	0	2.273169	1.160661	0.356516
3	6	0	0.930098	1.376522	0.028900
4	6	0	0.165277	0.250293	-0.374326
5	6	0	0.708642	-1.064025	-0.344303
6	6	0	2.062039	-1.186658	-0.008507
7	16	0	-1.502175	0.563323	-1.035553
8	7	0	-2.374150	0.984040	0.433274
9	7	0	-2.797056	-0.142279	1.147339
10	6	0	-4.127127	-0.519773	1.063124
11	6	0	-4.535269	-1.642411	1.992570
12	8	0	-2.055774	-0.648642	-1.643493
13	8	0	-1.515529	1.810182	-1.806692
14	8	0	-4.889628	0.032048	0.287346
15	6	0	4.344820	-0.270593	0.650359
16	1	0	-3.218644	1.470526	0.105280
17	1	0	-2.271524	-0.318996	1.992235
18	1	0	-3.722711	-1.995054	2.632981
19	1	0	-5.369347	-1.306215	2.613766
20	1	0	-4.892334	-2.477911	1.384750
21	6	0	-0.049600	-2.366255	-0.638344
22	1	0	2.498053	-2.179460	-0.005185
23	1	0	2.878651	2.013842	0.646617
24	6	0	0.416194	2.816396	0.154031
25	1	0	-0.663314	2.824342	0.032113
26	6	0	0.698633	3.397741	1.553519
27	6	0	1.000773	3.709562	-0.956150
28	1	0	0.607056	4.727657	-0.866618
29	1	0	2.093439	3.766388	-0.895251
30	1	0	0.726897	3.325870	-1.941511
31	1	0	0.234338	4.385765	1.639248
32	1	0	0.280917	2.760685	2.339516
33	1	0	1.767686	3.522781	1.753274
34	6	0	0.294445	-3.490435	0.358563
35	1	0	-1.114961	-2.175460	-0.536427
36	6	0	0.194703	-2.828030	-2.087993
37	1	0	-0.362439	-3.748689	-2.292068
38	1	0	-0.137366	-2.069715	-2.799989
39	1	0	1.257677	-3.030229	-2.263402
40	1	0	-0.392928	-4.328844	0.205054
41	1	0	1.307992	-3.883765	0.229875
42	1	0	0.193658	-3.157370	1.396872
43	6	0	4.555954	-1.147536	1.898663
44	6	0	5.135139	-0.817201	-0.553309
45	1	0	4.740453	0.727575	0.878379
46	1	0	5.620548	-1.210002	2.147677
47	1	0	4.027060	-0.739334	2.765398
48	1	0	4.193358	-2.168044	1.735455
49	1	0	6.203453	-0.870469	-0.318426
50	1	0	4.803534	-1.825612	-0.823049
51	1	0	5.010524	-0.178639	-1.432939

SCF Done: E(RB+HF-LYP) = -1398.00993909 a.u. after 11 cycles
Zero-point correction= 0.435861 (Hartree/Particle)

Thermal correction to Energy=	0.462708
Thermal correction to Enthalpy=	0.463652
Thermal correction to Gibbs Free Energy=	0.377146
Sum of electronic and zero-point Energies=	-1397.574078
Sum of electronic and thermal Energies=	-1397.547231
Sum of electronic and thermal Enthalpies=	-1397.546287
Sum of electronic and thermal Free Energies=	-1397.632794

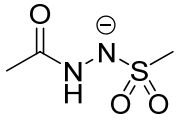
***Cis** conformation*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.640370	-1.617701	-0.125558
2	6	0	0.348580	-1.210859	-0.489232
3	6	0	0.085599	0.187015	-0.493252
4	6	0	1.067986	1.119058	-0.052696
5	6	0	2.327309	0.624689	0.296749
6	6	0	2.646895	-0.732142	0.248596
7	16	0	-1.503504	0.857508	-1.113145
8	8	0	-1.254365	2.107257	-1.833860
9	6	0	4.037124	-1.236548	0.608092
10	7	0	-2.361894	1.334901	0.295153
11	7	0	-2.561665	0.363554	1.254465
12	6	0	-3.824988	-0.199431	1.444457
13	8	0	-4.829864	0.225716	0.921012
14	8	0	-2.283565	-0.204276	-1.738928
15	6	0	-3.804436	-1.395632	2.383548
16	1	0	-2.026515	2.223265	0.659886
17	1	0	-1.746204	-0.078262	1.666555
18	1	0	-2.960840	-1.388500	3.080252
19	1	0	-4.738827	-1.409142	2.945691
20	1	0	-3.753509	-2.313940	1.789161
21	6	0	0.880389	2.637308	0.085015
22	1	0	3.086213	1.333141	0.612399
23	1	0	1.868912	-2.677939	-0.138758
24	6	0	-0.638953	-2.324129	-0.867110
25	1	0	4.022694	-2.327446	0.488217
26	6	0	5.108594	-0.679456	-0.347900
27	6	0	4.392934	-0.937406	2.076561
28	1	0	5.370795	-1.361483	2.327323
29	1	0	4.441531	0.140695	2.263960
30	1	0	3.652156	-1.363052	2.760429
31	1	0	6.090558	-1.101798	-0.110425
32	1	0	4.876175	-0.921056	-1.389341
33	1	0	5.187719	0.410008	-0.267116
34	6	0	1.679687	3.389859	-0.995611
35	1	0	-0.161158	2.896165	-0.089363
36	6	0	1.237661	3.132769	1.500506
37	1	0	1.523410	4.469245	-0.897864
38	1	0	2.754193	3.196021	-0.908631
39	1	0	1.351572	3.088081	-1.992836
40	1	0	0.998861	4.197619	1.589922
41	1	0	0.674670	2.594708	2.270933
42	1	0	2.301666	3.018776	1.729266

43	6	0	-0.533690	-3.559365	0.048765
44	1	0	-1.650317	-1.940640	-0.760118
45	6	0	-0.462028	-2.726386	-2.344731
46	1	0	-1.371964	-4.231356	-0.161306
47	1	0	0.382459	-4.136772	-0.111510
48	1	0	-0.577526	-3.287815	1.109011
49	1	0	-1.178760	-3.510289	-2.611161
50	1	0	-0.635907	-1.874534	-3.005168
51	1	0	0.547069	-3.112447	-2.529408

```
SCF Done:  E(RB+HF-LYP) =  -1398.00020502     A.U. after   15 cycles
Zero-point correction=                        0.435579 (Hartree/Particle)
Thermal correction to Energy=                     0.462486
Thermal correction to Enthalpy=                   0.463430
Thermal correction to Gibbs Free Energy=          0.377246
Sum of electronic and zero-point Energies=           -1397.564626
Sum of electronic and thermal Energies=              -1397.537719
Sum of electronic and thermal Enthalpies=            -1397.536775
Sum of electronic and thermal Free Energies=         -1397.622959
```

4. Coordinates and Energies for free deprotonated ligands

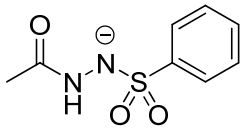


N'-acetylmethanesulfonylhydrazide **3**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.042313	1.530257	-0.047049

2	16	0	1.372690	-0.178658	0.069072
3	7	0	0.144781	-0.257647	-0.996007
4	7	0	-0.983122	0.426136	-0.497644
5	6	0	-2.132950	-0.171165	-0.086509
6	8	0	-2.326324	-1.374513	0.047125
7	8	0	1.014337	-0.297557	1.506735
8	8	0	2.464247	-1.031213	-0.452067
9	6	0	-3.260736	0.828963	0.216022
10	1	0	-1.036038	1.425652	-0.669936
11	1	0	-2.990510	1.880881	0.069407
12	1	0	-4.122930	0.595088	-0.417033
13	1	0	-3.572804	0.691874	1.255618
14	1	0	1.263434	2.245963	0.233172
15	1	0	2.884235	1.626541	0.642631
16	1	0	2.370128	1.711043	-1.072573

SCF Done: E(RB+HF-LYP) = -851.856161378 a.u. after 10 cycles
Zero-point correction= 0.114842 (Hartree/Particle)
Thermal correction to Energy= 0.125228
Thermal correction to Enthalpy= 0.126172
Thermal correction to Gibbs Free Energy= 0.077853
Sum of electronic and zero-point Energies= -851.741320
Sum of electronic and thermal Energies= -851.730933
Sum of electronic and thermal Enthalpies= -851.729989
Sum of electronic and thermal Free Energies= -851.778309



N'-acetylbenzenesulfonylhydrazide **4**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.412544	2.878582	-0.271593
2	6	0	-3.274440	2.211474	-0.161192
3	1	0	-4.022820	2.475333	-0.915693
4	1	0	-3.726362	2.383010	0.820021
5	6	0	-2.944712	0.716316	-0.285715
6	8	0	-3.822193	-0.125716	-0.132455
7	7	0	-1.638384	0.478449	-0.578606
8	1	0	-1.060651	1.286160	-0.791265
9	7	0	-1.113570	-0.785576	-0.921698
10	16	0	-0.118782	-1.312462	0.248828
11	8	0	-0.572982	-1.122912	1.649903
12	8	0	0.369048	-2.647446	-0.159759
13	6	0	1.352598	-0.230313	0.142399
14	6	0	1.419708	0.943859	0.898814
15	6	0	2.502066	1.814546	0.744607
16	6	0	3.523066	1.512683	-0.158420