Supporting Information for:

The Influence of Intramolecular Sulfur–Lone Pair Interactions on Small-Molecule Drug Design and Receptor Binding

Brandi M. Hudson, Elizabeth Nguyen, Dean J. Tantillo*

Department of Chemistry, University of California, Davis CA 95618

I. FRED Receptor specifications

Table S1: FRED Receptor specifications for each active site.

PDB ID	Box Volume (A^3)	Inner Contour (A^3)	Outer Contour (A^3)	Constraints
3H0E	5714	62	1809	ARG207, HIS121B
1HSK	11937	83	3900	None
4MLH	9612	62	2060	ARG63
3UW4	5040	60	1859	None

II. Calculated coordinates and energies

i. Implicit solvation and MP2 calculations of 1

Table S1. Electronic energy differences[a] of conformations of **1** using various model chemistries, basis sets, and solvation models.

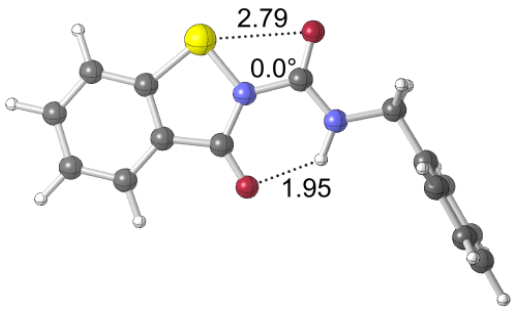
M06-2X/6-31+G(d,p)[b]	SMD(H_2O) M06-2X/6-31+G(d,p)	CPCM(H_2O) M06-2X/6-31+G(d,p)	MP2/6-31+G(d,p)	MP2/cc-PVTZ
11.4	7.1	7.7	11.9	11.5

[a] Energies reported are relative to the lowest energy conformation of **1** exhibiting a sulfur–lone pair interaction.
[b] Fully optimizatized conformations of **1** at M06-2X/6-31+G(d,p) were used for single point calculations implementing solvation models and testing functionals and basis sets.

II. Calculated coordinates and energies

ii. M06-2X/6-31+G(d,p) calculations of ligands

1 (w/ S–lone pair interaction):



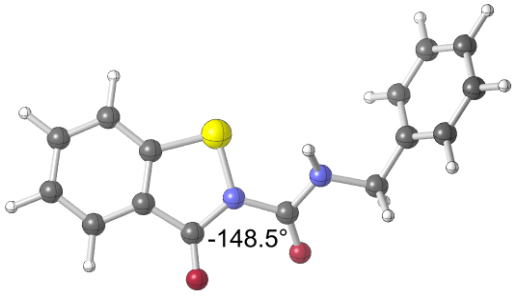
Charge = 0 Multiplicity = 1
Link 0: opt freq=noraman m062x/6-31+g(d,p)
HF = -1236.6640728 hartrees (-776019.072322728 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.246234 (Hartree/Particle)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Sum of electronic and thermal Free Energies =
-1236.464956 hartrees (-775894.12453956 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.484503	0.283430	-0.000109
2	6	2.714955	-0.879989	0.000039
3	6	3.310561	-2.141448	0.000173
4	6	4.695033	-2.219671	0.000147
5	6	5.467553	-1.046527	-0.000006
6	6	4.880142	0.212253	-0.000138
7	6	1.270034	-0.615856	0.000051
8	1	2.679951	-3.025053	0.000278
9	1	5.186954	-3.186281	0.000251
10	1	6.550483	-1.122298	-0.000017
11	1	5.488997	1.110338	-0.000251
12	16	2.513683	1.739995	-0.000245
13	7	1.080950	0.765533	-0.000160
14	8	0.365926	-1.438843	0.000187
15	6	-0.143359	1.493098	0.000100
16	8	-0.102086	2.712057	-0.000141
17	7	-1.262740	0.750590	0.000688
18	1	-1.190641	-0.262928	0.000469
19	6	-2.557894	1.425164	0.000533
20	1	-2.623440	2.072235	-0.880757
21	1	-2.623851	2.071927	0.882020
22	6	-3.665023	0.401846	0.000158
23	6	-4.171337	-0.092129	-1.204496
24	6	-4.171950	-0.092273	1.204492
25	6	-5.170135	-1.063335	-1.206742
26	1	-3.779723	0.289700	-2.144179
27	6	-5.170750	-1.063479	1.206130
28	1	-3.780803	0.289453	2.144411
29	6	-5.671570	-1.550123	-0.000463
30	1	-5.558293	-1.438113	-2.148680
31	1	-5.559376	-1.438367	2.147830
32	1	-6.451964	-2.304870	-0.000717

1 (lacking S–lone pair interaction):

Charge = 0 Multiplicity = 1
Link 0: opt freq=noraman m062x/6-31+g(d,p)
HF = -1236.6458306 hartrees (-776007.625159806 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.245911 (Hartree/Particle)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Sum of electronic and thermal Free Energies =
-1236.447102 hartrees (-775882.92097602 kcal/mol)



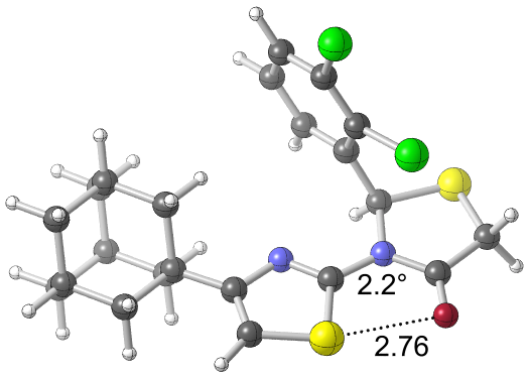
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	6	2.790810	-1.040226	-0.038514
2	6	3.313669	0.236614	0.140443
3	6	4.675666	0.423737	0.369368
4	6	5.503710	-0.690068	0.408885
5	6	4.969046	-1.974009	0.224741
6	6	3.610882	-2.168793	-0.000697
7	6	2.304497	1.316201	0.081109
8	1	5.052662	1.432260	0.509823
9	1	6.567597	-0.571249	0.583312
10	1	5.626657	-2.836952	0.257996
11	1	3.205942	-3.165611	-0.141115
12	16	1.058636	-1.016246	-0.312317
13	7	1.051437	0.715070	-0.168103
14	8	2.490550	2.496771	0.250528
15	6	-0.156115	1.446460	-0.355829
16	8	-0.173527	2.564595	-0.809569
17	7	-1.270629	0.728137	-0.018491
18	1	-1.182566	-0.005235	0.674352
19	6	-2.576665	1.365517	-0.145429
20	1	-2.606812	1.842111	-1.130009
21	1	-2.694959	2.161542	0.599644
22	6	-3.675900	0.340901	-0.001634
23	6	-3.723470	-0.768006	-0.853804
24	6	-4.658885	0.486854	0.977190
25	6	-4.740045	-1.710162	-0.729173
26	1	-2.957322	-0.886408	-1.616282
27	6	-5.681075	-0.454615	1.102415
28	1	-4.626517	1.344120	1.644615
29	6	-5.722644	-1.554583	0.250275
30	1	-4.769270	-2.565320	-1.397279
31	1	-6.440811	-0.328094	1.867255
32	1	-6.515506	-2.289529	0.347165

---

2 (with S–lone pair interaction):



Charge = 0 Multiplicity = 1
HF = -2752.6357786 hartrees (-1727306.47742929 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.407670 (Hartree/Particle)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Sum of electronic and thermal Free Energies =
-2752.284462 hartrees (-1727086.02274962 kcal/mol)

Coordinates (from last standard orientation):

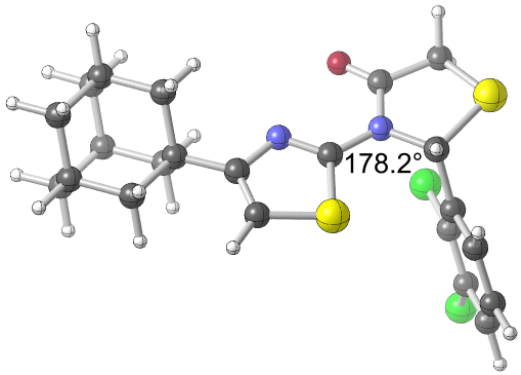
Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.191478	-2.362715	-1.474083
2	6	1.426404	-1.446192	-0.494400
3	6	-0.730414	-1.772421	-0.151223
4	16	-0.470296	-2.853769	-1.489151

5	1	1.887715	-2.774004	-2.190507
6	7	0.315995	-1.128008	0.263200
7	7	-1.971243	-1.562420	0.449522
8	6	-2.065882	-0.522238	1.464224
9	6	-3.111740	-2.232213	0.062128
10	6	-4.334097	-1.791347	0.841361
11	1	-5.040056	-1.336779	0.142481
12	8	-3.133253	-3.075051	-0.809002
13	16	-3.792918	-0.616295	2.110724
14	1	-4.791022	-2.672888	1.293833
15	6	-1.676773	0.871497	1.006244
16	6	-0.783239	1.574713	1.814654
17	6	-2.170869	1.495058	-0.145517
18	6	-0.380576	2.866476	1.498048
19	1	-0.378381	1.081201	2.693754
20	6	-1.749626	2.787964	-0.475668
21	6	-0.859419	3.474837	0.344854
22	1	0.318727	3.394083	2.138156
23	1	-0.553204	4.476732	0.065488
24	17	-3.304601	0.686085	-1.184030
25	17	-2.321421	3.576783	-1.912010
26	6	2.707833	-0.718302	-0.188056
27	6	3.115982	-0.963687	1.281654
28	6	3.859187	-1.161127	-1.105408
29	6	2.470700	0.797390	-0.387885
30	1	3.278500	-2.038905	1.437430
31	1	2.290136	-0.659336	1.936555
32	6	4.390257	-0.176135	1.617461
33	1	3.580858	-0.992182	-2.154938
34	1	4.040603	-2.237931	-0.980841
35	6	5.136311	-0.373042	-0.771386
36	1	1.635633	1.115655	0.248463
37	1	2.172683	0.980515	-1.429487
38	6	3.743303	1.585678	-0.051029
39	1	4.666810	-0.364158	2.662050
40	6	5.529151	-0.630426	0.691597
41	6	4.131215	1.324730	1.412864
42	1	5.945641	-0.703062	-1.433651
43	6	4.883506	1.129335	-0.973832
44	1	3.554550	2.656374	-0.197992
45	1	5.732799	-1.698398	0.844489
46	1	6.451112	-0.085597	0.933200
47	1	3.323344	1.658713	2.078391
48	1	5.028874	1.900286	1.673929
49	1	5.797902	1.695381	-0.753239
50	1	4.621090	1.329585	-2.020850
51	1	-1.393903	-0.786624	2.284145

---

2 (lacking S–lone pair interaction):

Charge = 0 Multiplicity = 1
HF = -2752.6198458 hartrees (-1727296.47943796 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.407529 (Hartree/Particle)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.



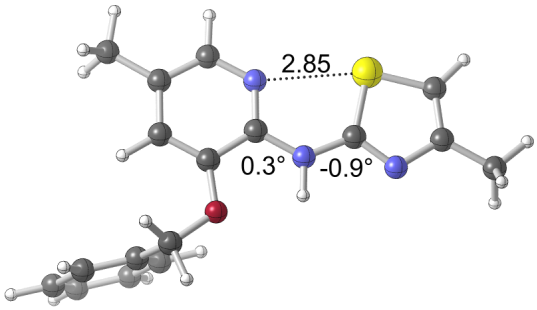
Sum of electronic and thermal Free Energies =
-2752.268709 hartrees (-1727076.13758459 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.367481	-1.111095	-1.696373
2	6	1.937813	-0.301134	-0.761376
3	6	-0.097351	0.554194	-0.708304
4	16	-0.303389	-0.718483	-1.904752
5	1	1.812689	-1.918836	-2.257887
6	7	1.090440	0.642779	-0.214002
7	7	-1.159532	1.407929	-0.389666
8	6	-2.425572	1.272243	-1.092034
9	6	-1.049270	2.409075	0.584003
10	6	-2.290176	3.289478	0.632232
11	1	-2.737500	3.194994	1.623513
12	8	-0.108134	2.585918	1.310640
13	16	-3.427530	2.762247	-0.669706
14	1	-1.972607	4.321676	0.475887
15	6	-3.192223	-0.017337	-0.847954
16	6	-3.693624	-0.672869	-1.973360
17	6	-3.466005	-0.553642	0.417737
18	6	-4.434847	-1.843417	-1.862244
19	1	-3.480896	-0.259658	-2.955971
20	6	-4.196319	-1.741665	0.527874
21	6	-4.680456	-2.385525	-0.608160
22	1	-4.812184	-2.338428	-2.750367
23	1	-5.244626	-3.304099	-0.491254
24	17	-2.927807	0.243527	1.860420
25	17	-4.529350	-2.444453	2.077530
26	6	3.361726	-0.333354	-0.272605
27	6	3.372112	-0.650721	1.240573
28	6	4.196705	-1.393635	-1.008859
29	6	4.006914	1.054092	-0.488770
30	1	2.905692	-1.631556	1.406162
31	1	2.764259	0.096255	1.764779
32	6	4.813467	-0.649816	1.770163
33	1	4.193010	-1.184295	-2.087965
34	1	3.747987	-2.386371	-0.862807
35	6	5.639747	-1.392551	-0.480323
36	1	3.402670	1.811086	0.024432
37	1	3.994904	1.293984	-1.561022
38	6	5.448156	1.055978	0.040332
39	1	4.803003	-0.878341	2.842677
40	6	5.633400	-1.712309	1.022662
41	6	5.440519	0.734537	1.543248
42	1	6.219558	-2.153116	-1.017203
43	6	6.267201	-0.008052	-0.706350
44	1	5.891513	2.045615	-0.122938
45	1	5.202786	-2.707969	1.193366
46	1	6.662300	-1.733112	1.405070
47	1	4.869594	1.497945	2.086592
48	1	6.466089	0.750156	1.935081

49	1	7.304907	-0.005693	-0.348096
50	1	6.292401	0.222148	-1.779734
51	1	-2.226858	1.326003	-2.168234

VO2 (w/ S–lone pair close contact):



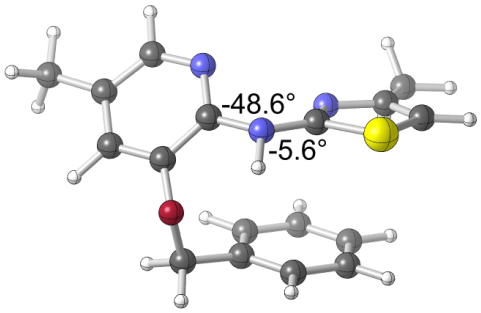
Charge = 0 Multiplicity = 1
HF = -1295.3587971 hartrees (-812850.598768221 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.313615 (Hartree/Particle)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Sum of electronic and thermal Free Energies =
-1295.097900 hartrees (-812686.883229 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	5.619280	-1.106562	0.194899
2	6	4.650343	-0.980860	-0.798812
3	6	3.304877	-1.211425	-0.507256
4	6	2.933513	-1.557210	0.792523
5	6	3.901196	-1.675642	1.788224
6	6	5.245328	-1.454325	1.491850
7	1	6.663117	-0.925380	-0.041883
8	1	4.943167	-0.698501	-1.808006
9	1	1.884765	-1.722878	1.022124
10	1	3.604027	-1.940221	2.798189
11	1	5.997312	-1.548122	2.268847
12	6	2.272393	-1.114396	-1.609495
13	1	2.173720	-2.075266	-2.121965
14	1	2.568954	-0.361656	-2.352704
15	8	0.966390	-0.832951	-1.133497
16	6	0.708846	0.424856	-0.671131
17	6	-0.637919	0.654679	-0.284400
18	6	1.610002	1.460355	-0.553093
19	6	1.172845	2.708960	-0.066042
20	1	2.655167	1.319180	-0.811725
21	6	-0.162540	2.822036	0.277463
22	1	-0.555411	3.760938	0.660469
23	7	-1.051718	1.819479	0.173580
24	6	2.133589	3.858474	0.078092
25	1	2.583909	4.121722	-0.884378
26	1	1.623760	4.744512	0.464019
27	1	2.946632	3.609510	0.767510
28	7	-1.529992	-0.391200	-0.399498
29	6	-2.871578	-0.397262	-0.092133
30	16	-3.746367	0.967131	0.551964
31	6	-4.888546	-1.276706	0.094783
32	6	-5.167898	-0.030202	0.562219
33	1	-6.115923	0.355592	0.908773
34	7	-3.575298	-1.478228	-0.276478
35	1	-1.181287	-1.264455	-0.773578
36	6	-5.855609	-2.410933	-0.045707

37	1	-5.907855	-2.738282	-1.088145
38	1	-5.528344	-3.265745	0.553283
39	1	-6.854627	-2.114811	0.280609

VO2 (lacking S–lone pair close contact):



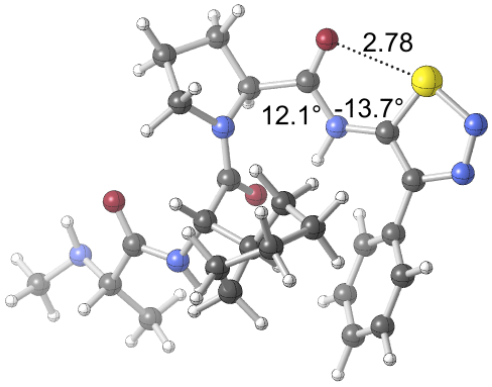
Charge = 0 Multiplicity = 1
HF = -1295.3484576 hartrees (-812844.110628576 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.312971 (Hartree/Particle)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Sum of electronic and thermal Free Energies =
-1295.084581 hartrees (-812678.52542331 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.265539	2.196527	0.299853
2	6	1.068271	2.545419	-0.319568
3	6	-0.156349	2.286124	0.303734
4	6	-0.164161	1.672585	1.558112
5	6	1.032982	1.330341	2.184563
6	6	2.248353	1.593392	1.557644
7	1	3.210662	2.391517	-0.197502
8	1	1.081098	3.020466	-1.298941
9	1	-1.113329	1.453329	2.041826
10	1	1.012814	0.843430	3.154650
11	1	3.181798	1.317222	2.039242
12	6	-1.446639	2.611974	-0.403748
13	1	-1.352031	3.522993	-0.998807
14	1	-2.262451	2.742914	0.317898
15	8	-1.820425	1.595998	-1.355268
16	6	-2.184358	0.398589	-0.782751
17	6	-1.274230	-0.675245	-0.800337
18	6	-3.431011	0.207646	-0.215546
19	6	-3.750267	-1.033246	0.346168
20	1	-4.144920	1.028962	-0.213422
21	6	-2.764770	-2.017794	0.282257
22	1	-2.957504	-3.002831	0.703786
23	7	-1.567810	-1.859327	-0.287083
24	6	-5.094352	-1.296332	0.971341
25	1	-5.897919	-1.196145	0.235068
26	1	-5.140702	-2.307209	1.383406
27	1	-5.298622	-0.591228	1.783000
28	7	-0.043271	-0.486064	-1.440533
29	6	1.157833	-0.879378	-0.874683
30	16	2.623188	-0.719739	-1.825916
31	6	2.659144	-1.606814	0.561519
32	6	3.510513	-1.306281	-0.456843
33	1	4.586394	-1.400338	-0.482270
34	7	1.322421	-1.359873	0.313520
35	1	-0.002406	0.377821	-1.967458
36	6	3.043447	-2.141717	1.904898

37	1	2.561849	-3.108204	2.078740
38	1	4.125534	-2.264442	1.986612
39	1	2.703072	-1.458295	2.689965

PRD (w/ S–lone pair close contact):



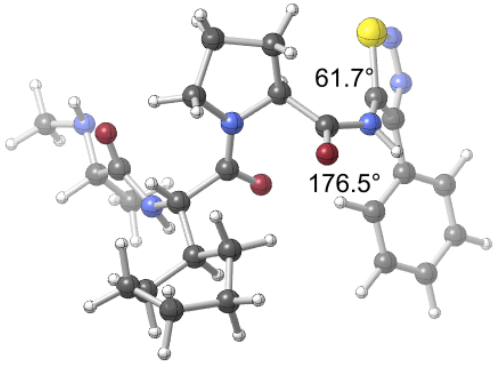
Charge = 0 Multiplicity = 1
HF = -1924.9475356 hartrees (-1207923.82806436 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.586226 (Hartree/Particle)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Sum of electronic and thermal Free Energies =
-1924.428839 hartrees (-1207598.34076089 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.184402	-0.758393	0.913753
2	6	3.456549	0.591262	1.053343
3	16	4.637571	-1.566145	0.502918
4	7	5.511645	-0.107463	0.536512
5	7	4.774720	0.889557	0.819268
6	6	2.489921	1.671799	1.328405
7	6	2.595571	2.883697	0.629880
8	6	1.456312	1.513385	2.256729
9	6	1.671533	3.901488	0.841925
10	1	3.410067	3.011915	-0.076698
11	6	0.525055	2.530333	2.460996
12	1	1.381336	0.600851	2.841796
13	6	0.627498	3.725081	1.753302
14	1	1.764200	4.835032	0.294846
15	1	-0.274666	2.383629	3.180146
16	1	-0.094259	4.519773	1.916017
17	7	1.941757	-1.351845	1.012587
18	1	1.141210	-0.769238	1.271591
19	6	1.666185	-2.608254	0.532870
20	8	2.544493	-3.372911	0.179617
21	6	0.165419	-2.940485	0.459128
22	6	-0.094256	-4.320565	-0.158998
23	1	-0.264896	-2.832249	1.461982
24	6	-1.088000	-2.691633	-1.610282
25	6	-1.308808	-4.102761	-1.066502
26	1	-0.258250	-5.078647	0.608514
27	1	0.781601	-4.617931	-0.741719
28	1	-2.019992	-2.217256	-1.916783
29	1	-0.366559	-2.687028	-2.437002
30	1	-2.238128	-4.114901	-0.487919
31	1	-1.382861	-4.848846	-1.860465
32	7	-0.527341	-1.994475	-0.441471
33	6	-0.895791	-0.781461	0.018250
34	8	-0.654803	-0.423463	1.178046
35	6	-1.506363	0.245915	-0.937987

36	1	-1.831879	-0.216657	-1.873415
37	7	-2.672876	0.826376	-0.299945
38	1	-2.505011	1.592644	0.338455
39	6	-3.747747	0.021827	-0.082897
40	8	-3.801733	-1.107636	-0.560146
41	6	-4.916560	0.613620	0.707221
42	1	-5.513377	1.168690	-0.045909
43	6	-4.478007	1.595424	1.795677
44	1	-4.068453	2.520554	1.376973
45	1	-5.341107	1.877813	2.402760
46	1	-3.740519	1.126940	2.454035
47	7	-5.675189	-0.484187	1.275401
48	6	-0.441702	1.316832	-1.242722
49	6	0.832217	0.652791	-1.812294
50	6	-0.985397	2.387053	-2.215811
51	1	-0.177078	1.793258	-0.286690
52	6	1.623477	1.645184	-2.663170
53	1	0.558361	-0.211389	-2.437073
54	1	1.449246	0.262040	-0.996494
55	6	-0.687441	2.008337	-3.668364
56	1	-2.060388	2.526469	-2.060403
57	1	-0.508161	3.349310	-1.991444
58	6	0.831937	2.017189	-3.931340
59	1	1.816498	2.541873	-2.062154
60	1	2.601827	1.231754	-2.926829
61	1	-1.097502	1.009161	-3.867379
62	1	-1.199147	2.687916	-4.356618
63	1	1.143976	3.007682	-4.280256
64	1	1.068184	1.313222	-4.737234
65	1	-5.574037	-1.291942	0.667315
66	6	-7.077436	-0.174318	1.498802
67	1	-7.592536	-1.072116	1.847142
68	1	-7.180669	0.583493	2.281492
69	1	-7.592252	0.198747	0.596629

PRD (lacking S–lone pair close contact):



Charge = 0 Multiplicity = 1
HF = -1924.9305549 hartrees (-1207913.1725053 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.585636 (Hartree/Particle)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Sum of electronic and thermal Free Energies =
-1924.415341 hartrees (-1207589.87063091 kcal/mol)

Coordinates (from last standard orientation):

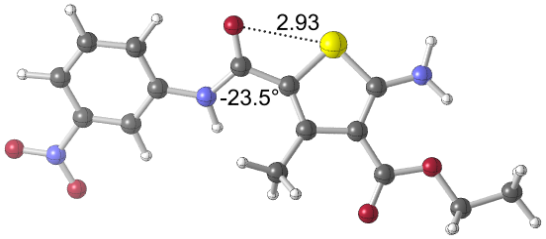
Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.385542	0.314764	1.020924
2	6	4.049389	0.601743	-0.152332
3	16	3.731293	1.556634	2.153627
4	7	4.688854	2.399186	1.016149
5	7	4.765387	1.773546	-0.083403

6	6	4.074979	-0.216432	-1.378284
7	6	5.251309	-0.284351	-2.134703
8	6	2.935297	-0.915351	-1.797800
9	6	5.293695	-1.058500	-3.289954
10	1	6.122746	0.276888	-1.811695
11	6	2.989137	-1.691489	-2.953479
12	1	2.002233	-0.822937	-1.247202
13	6	4.164745	-1.769146	-3.698116
14	1	6.208761	-1.107312	-3.871763
15	1	2.101903	-2.227082	-3.276634
16	1	4.199290	-2.374474	-4.598639
17	7	2.711583	-0.866459	1.316750
18	1	3.126416	-1.722704	0.959789
19	6	1.423890	-1.041688	1.778502
20	8	0.972531	-2.159374	1.924564
21	6	0.606988	0.202186	2.128832
22	6	0.466722	0.389834	3.649651
23	1	1.020217	1.088016	1.635418
24	6	-1.749891	0.167276	2.759153
25	6	-0.952701	0.948583	3.804805
26	1	1.240016	1.046157	4.055417
27	1	0.541452	-0.587362	4.138609
28	1	-2.622676	0.714894	2.398881
29	1	-2.050075	-0.816215	3.144388
30	1	-0.971494	2.014440	3.555624
31	1	-1.351147	0.821345	4.813341
32	7	-0.767730	0.008861	1.679989
33	6	-0.976258	-0.250103	0.375843
34	8	-0.039696	-0.291106	-0.425955
35	6	-2.403178	-0.498817	-0.116075
36	1	-3.123960	-0.429939	0.702615
37	7	-2.740855	0.550940	-1.064435
38	1	-2.278806	0.511878	-1.962868
39	6	-3.215986	1.745207	-0.623995
40	8	-3.507089	1.935309	0.552809
41	6	-3.459981	2.830010	-1.678656
42	1	-4.497747	2.649396	-2.029210
43	6	-2.524877	2.747438	-2.885588
44	1	-2.716797	1.857869	-3.494042
45	1	-2.684905	3.611674	-3.534319
46	1	-1.479495	2.758783	-2.563545
47	7	-3.345267	4.117025	-1.018715
48	6	-2.487078	-1.890339	-0.756244
49	6	-1.945513	-2.948427	0.228917
50	6	-3.932480	-2.215209	-1.193539
51	1	-1.830426	-1.879506	-1.637177
52	6	-2.515813	-4.326910	-0.102490
53	1	-2.234108	-2.683715	1.257939
54	1	-0.851489	-2.949938	0.217889
55	6	-4.677850	-2.974260	-0.094216
56	1	-4.457451	-1.291137	-1.459494
57	1	-3.912209	-2.833292	-2.099590
58	6	-4.039421	-4.357768	0.135448
59	1	-2.292852	-4.555794	-1.152702
60	1	-2.020854	-5.100160	0.492313
61	1	-4.644290	-2.385986	0.832487

62	1	-5.737167	-3.080166	-0.347989
63	1	-4.501132	-5.093391	-0.532883
64	1	-4.248549	-4.690570	1.158330
65	1	-3.654308	4.007678	-0.056884
66	6	-4.077896	5.184429	-1.678873
67	1	-4.040917	6.082033	-1.057978
68	1	-3.611456	5.433590	-2.636857
69	1	-5.135795	4.934501	-1.871664

---

3 (w/ S–lone pair interaction):



Charge = 0 Multiplicity = 1
HF = -1518.7025841 hartrees (-953001.058548591 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.297083 (Hartree/Particle)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Sum of electronic and thermal Free Energies =
-1518.460551 hartrees (-952849.18035801 kcal/mol)

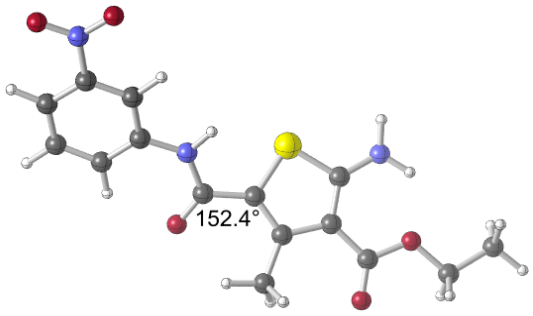
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.801776	1.044282	0.064978
2	6	1.454757	-0.131831	0.327019
3	6	2.869514	-0.034019	0.058959
4	6	3.244068	1.241526	-0.365948
5	16	1.891242	2.314957	-0.445113
6	6	0.817663	-1.366814	0.909065
7	6	-0.611231	1.463655	0.167488
8	7	4.466089	1.690686	-0.742539
9	1	4.615085	2.678143	-0.871625
10	1	5.263138	1.103262	-0.548639
11	8	-0.913751	2.636475	0.333342
12	7	-1.537690	0.456728	0.010084
13	6	3.785072	-1.170096	0.201310
14	8	3.463040	-2.311802	0.453086
15	8	5.084761	-0.825697	0.011475
16	6	6.035631	-1.900703	0.108161
17	6	7.406430	-1.307069	-0.132745
18	6	-2.934270	0.547642	0.102425
19	6	-3.617731	1.713417	0.481625
20	6	-3.661147	-0.610499	-0.193133
21	6	-5.008922	1.701791	0.560255
22	1	-3.059824	2.611953	0.702849
23	6	-5.042568	-0.574539	-0.103408
24	1	-3.171801	-1.532405	-0.489250
25	6	-5.749176	0.560539	0.269064
26	1	-5.523816	2.610278	0.854176
27	1	-6.830013	0.536389	0.323448
28	7	-5.788417	-1.807090	-0.420809
29	8	-5.144461	-2.792118	-0.737902
30	8	-7.002687	-1.765364	-0.346572
31	1	-1.176661	-0.438204	-0.287894

32	1	1.481665	-1.813183	1.649228
33	1	-0.131904	-1.132344	1.392286
34	1	0.664747	-2.135604	0.143503
35	1	5.949562	-2.353870	1.099387
36	1	5.777622	-2.661793	-0.633528
37	1	7.466880	-0.857428	-1.127727
38	1	7.634818	-0.542837	0.615202
39	1	8.166347	-2.089572	-0.064883

---

3 (lacking S–lone pair interaction):



Charge = 0 Multiplicity = 1
HF = -1518.7019945 hartrees (-953000.688568695 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.296978 (Hartree/Particle)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Sum of electronic and thermal Free Energies =
-1518.460186 hartrees (-952848.95131686 kcal/mol)

Coordinates (from last standard orientation):

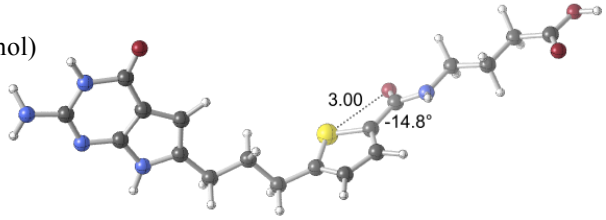
Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.756111	0.518680	-0.261953
2	6	-1.947946	1.077677	0.115183
3	6	-3.050642	0.153044	-0.015885
4	6	-2.657805	-1.093751	-0.494121
5	16	-0.955091	-1.139532	-0.810167
6	6	-2.098972	2.472169	0.649460
7	1	-2.713544	3.067402	-0.031483
8	1	-2.630368	2.451136	1.603186
9	1	-1.128061	2.949260	0.759201
10	6	0.585272	1.140739	-0.243881
11	7	-3.408104	-2.182686	-0.792028
12	1	-2.960655	-3.072106	-0.942020
13	1	-4.377767	-2.169864	-0.511775
14	8	0.765471	2.341782	-0.357857
15	7	1.625719	0.238510	-0.093891
16	6	-4.432138	0.513197	0.327451
17	8	-4.806186	1.598408	0.711653
18	8	-5.298094	-0.522798	0.170379
19	6	-6.672641	-0.237884	0.484720
20	1	-6.732990	0.076579	1.530290
21	1	-7.005604	0.597262	-0.137323
22	6	-7.462350	-1.500992	0.219851
23	1	-7.108649	-2.320971	0.851040
24	1	-8.518721	-1.330941	0.442218
25	1	-7.377582	-1.799471	-0.828698
26	6	3.003174	0.501901	-0.127934
27	6	3.553545	1.736993	-0.503415
28	6	3.855463	-0.553265	0.214066
29	6	4.937632	1.895492	-0.533012
30	1	2.900222	2.558360	-0.759750
31	6	5.224643	-0.350124	0.170686

32	1	3.472530	-1.523641	0.511520
33	6	5.800748	0.857863	-0.196486
34	1	5.347314	2.856056	-0.826927
35	1	6.877601	0.966122	-0.213351
36	7	6.103433	-1.477639	0.534359
37	8	5.574164	-2.534149	0.834075
38	8	7.305014	-1.284342	0.512656
39	1	1.376197	-0.701621	0.181859

---

4 (w/ S–lone pair interaction):

Charge = 0 Multiplicity = 1
HF = -1671.0060974 hartrees (-1048573.03617947 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.392668 (Hartree/Particle)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Sum of electronic and thermal Free Energies =
-1670.677344 hartrees (-1048366.74013344 kcal/mol)



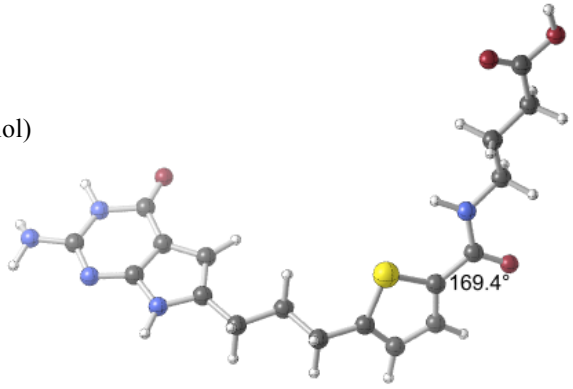
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-5.568016	-0.995057	-0.070608
2	6	-6.474371	0.061520	-0.043925
3	6	-8.296884	-1.206615	0.090422
4	6	-6.085830	-2.333160	-0.024991
5	6	-4.254382	-0.436315	-0.159133
6	6	-4.400649	0.926487	-0.181568
7	1	-7.928498	-3.243736	0.013274
8	1	-3.326134	-0.986808	-0.198874
9	1	-6.171968	2.136614	-0.104158
10	6	-3.393868	2.029895	-0.277322
11	1	-3.575260	2.612487	-1.192147
12	1	-3.527001	2.724900	0.564067
13	6	-1.955327	1.518805	-0.283657
14	1	-1.756427	0.968799	0.643705
15	1	-1.815119	0.811476	-1.109265
16	6	-0.946916	2.665856	-0.430145
17	1	-1.091021	3.387234	0.383866
18	1	-1.139341	3.203501	-1.366211
19	6	0.477632	2.194532	-0.454005
20	6	1.292949	2.052680	-1.547478
21	16	1.279667	1.699332	0.993197
22	6	2.575975	1.533943	-1.217701
23	1	0.983610	2.321882	-2.551378
24	6	2.713576	1.285876	0.123643
25	1	3.368201	1.386159	-1.943719
26	6	3.874528	0.772410	0.893939
27	8	3.941506	0.884433	2.110641
28	7	4.861636	0.185513	0.160280
29	6	6.016762	-0.392354	0.825306
30	1	5.720079	-1.281100	1.400069
31	1	6.384429	0.341715	1.548897

32	6	7.093107	-0.744609	-0.191569
33	1	6.705482	-1.463882	-0.922929
34	1	7.381646	0.150165	-0.753327
35	6	8.318760	-1.339630	0.487884
36	1	8.063032	-2.236369	1.065603
37	1	8.763899	-0.637875	1.202694
38	6	9.386633	-1.729652	-0.501610
39	8	9.294916	-1.655342	-1.702403
40	8	10.493851	-2.190495	0.113180
41	1	11.132780	-2.426963	-0.576816
42	7	-5.758955	1.216059	-0.110241
43	7	-7.833403	0.008984	0.050652
44	7	-7.505718	-2.324370	0.056771
45	7	-9.657096	-1.423650	0.115489
46	1	-9.985591	-2.226141	0.633760
47	1	-10.181420	-0.578028	0.293201
48	1	4.663081	-0.091625	-0.789998
49	8	-5.496582	-3.399489	-0.054797

---

4 (lacking S–lone pair interaction):



Charge = 0 Multiplicity = 1
HF = -1671.0062305 hartrees (-1048573.11970105 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.392774 (Hartree/Particle)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Sum of electronic and thermal Free Energies =
-1670.677084 hartrees (-1048366.57698084 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	4.952170	0.934623	0.370601
2	6	5.886729	0.295414	-0.439416
3	6	7.557490	1.698238	-0.005673
4	6	5.361502	2.115025	1.077539
5	6	3.724836	0.207382	0.273078
6	6	3.948258	-0.840268	-0.582069
7	1	7.044401	3.287639	1.220052
8	1	2.800647	0.442393	0.779780
9	1	5.723566	-1.414134	-1.644509
10	6	3.044306	-1.927426	-1.073012
11	1	2.952043	-1.863969	-2.166841
12	1	3.494485	-2.906680	-0.856127
13	6	1.653536	-1.863467	-0.446847
14	1	1.731465	-1.950120	0.643127
15	1	1.204444	-0.884941	-0.655817
16	6	0.738314	-2.972785	-0.978358
17	1	1.195785	-3.951408	-0.790619
18	1	0.639293	-2.874366	-2.067154
19	6	-0.618105	-2.978840	-0.338442
20	6	-1.172530	-3.939770	0.463877
21	16	-1.714418	-1.654966	-0.557653

22	6	-2.484005	-3.612641	0.912409
23	1	-0.650423	-4.854707	0.720586
24	6	-2.914847	-2.402010	0.448326
25	1	-3.104914	-4.226748	1.553528
26	6	-4.238175	-1.808009	0.776625
27	8	-5.103626	-2.471871	1.329929
28	7	-4.432825	-0.506229	0.421378
29	6	-5.675707	0.168951	0.750705
30	1	-5.686705	0.453009	1.812790
31	1	-6.483165	-0.554987	0.608177
32	6	-5.874792	1.393954	-0.131641
33	1	-5.042694	2.097056	-0.005670
34	1	-5.876387	1.095267	-1.185033
35	6	-7.179596	2.102602	0.205117
36	1	-7.210366	2.409777	1.257822
37	1	-8.044675	1.445422	0.057967
38	6	-7.393332	3.338520	-0.630559
39	8	-6.617485	3.785861	-1.438957
40	8	-8.582657	3.917351	-0.370399
41	1	-8.652788	4.703678	-0.933529
42	7	5.270452	-0.775090	-1.008520
43	7	7.193092	0.625608	-0.646602
44	7	6.724602	2.418865	0.809039
45	7	8.829850	2.199160	-0.171431
46	1	9.256064	2.647833	0.626928
47	1	9.440657	1.555303	-0.655007
48	1	-3.642599	0.057109	0.139106
49	8	4.722525	2.840393	1.819710

III. Full Gaussian Reference

S1. Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2009.**