Supporting Information to accompany:

Constrained Bithiazoles: Small Molecule Correctors of Defective ΔF508–CFTR Protein Trafficking

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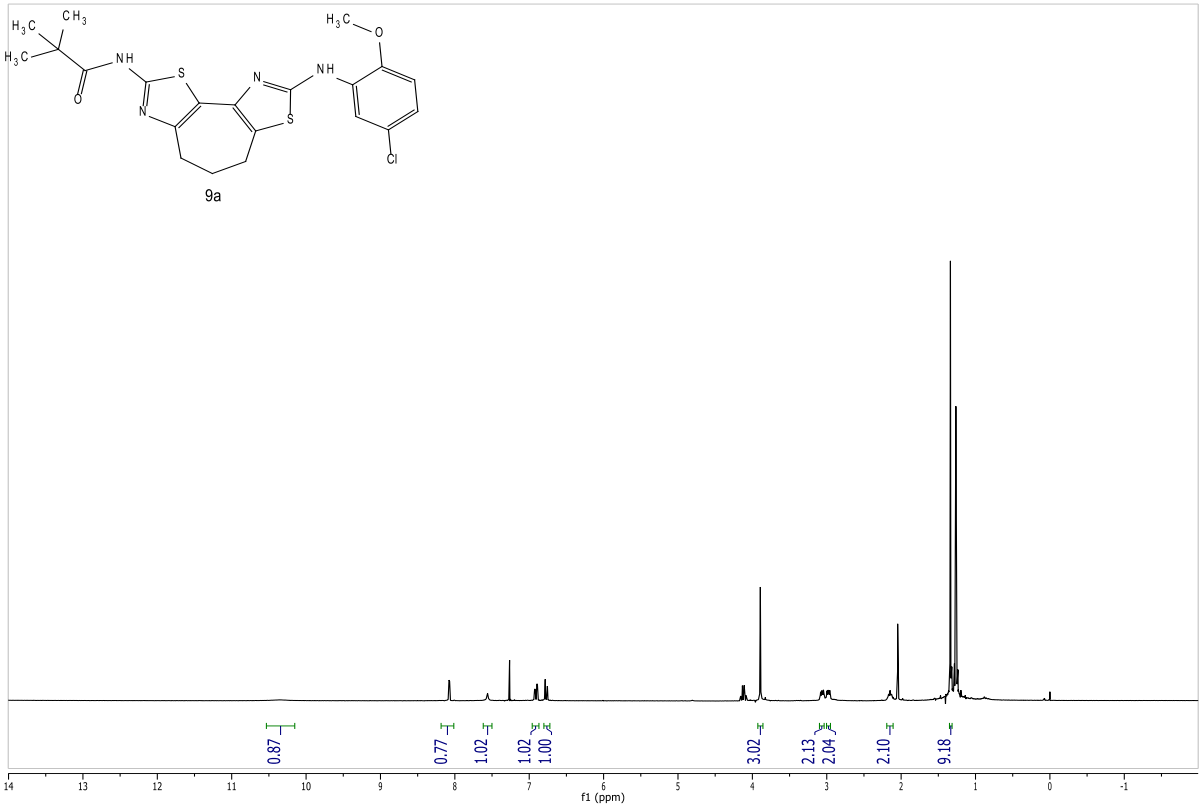
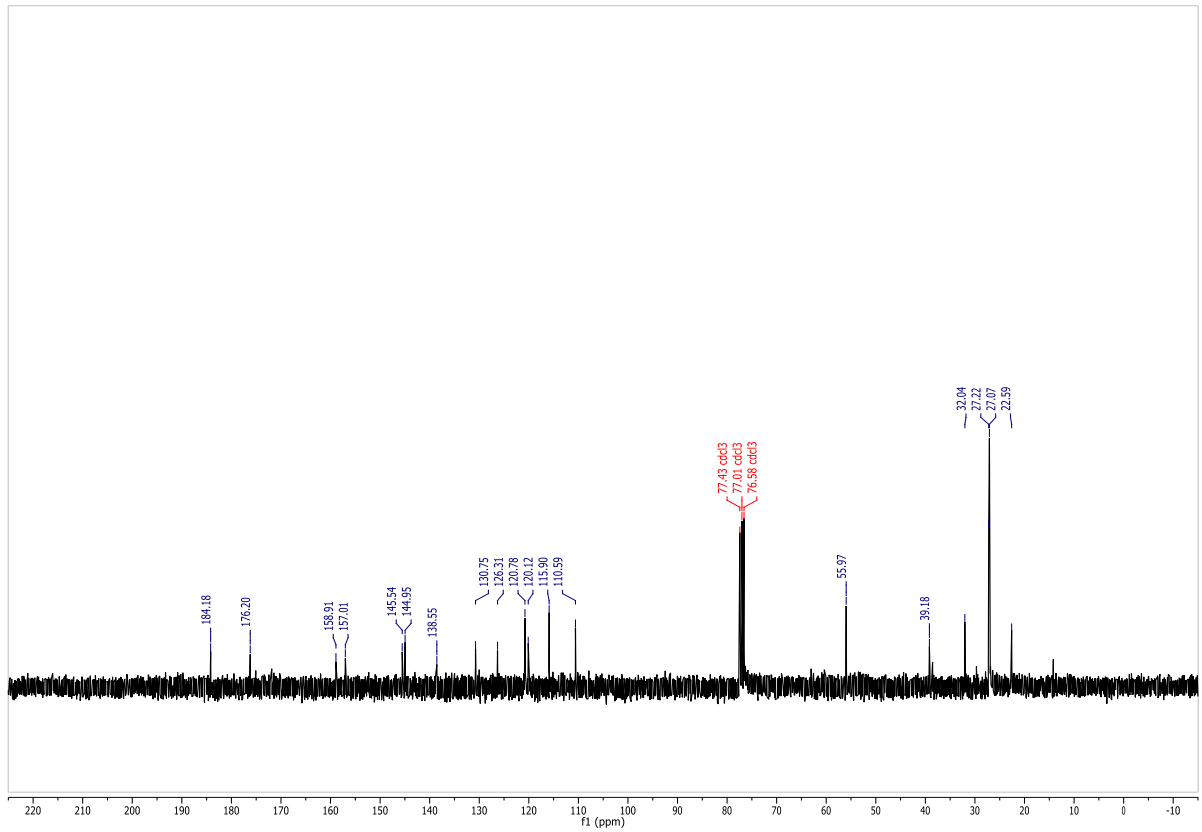
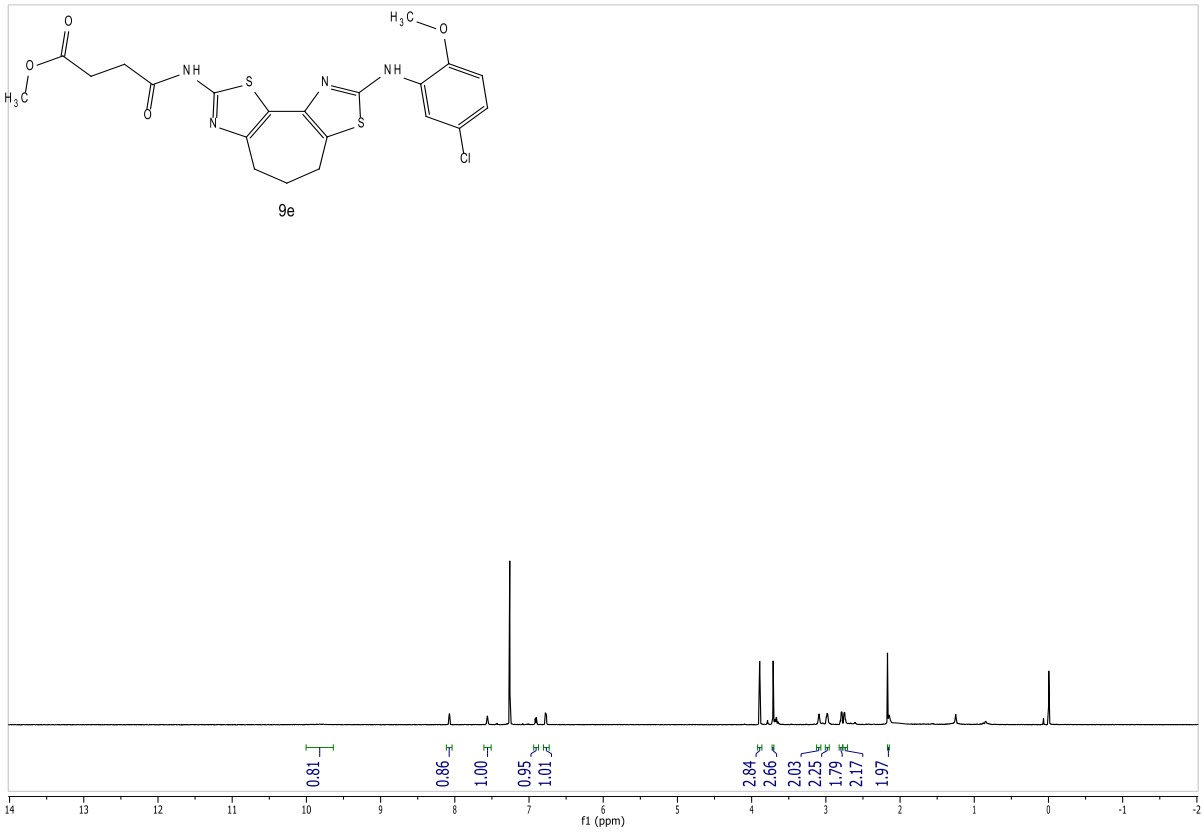
^{1}H and ^{13}C NMR for **9a**, **9e**, **10a**, and **10c**



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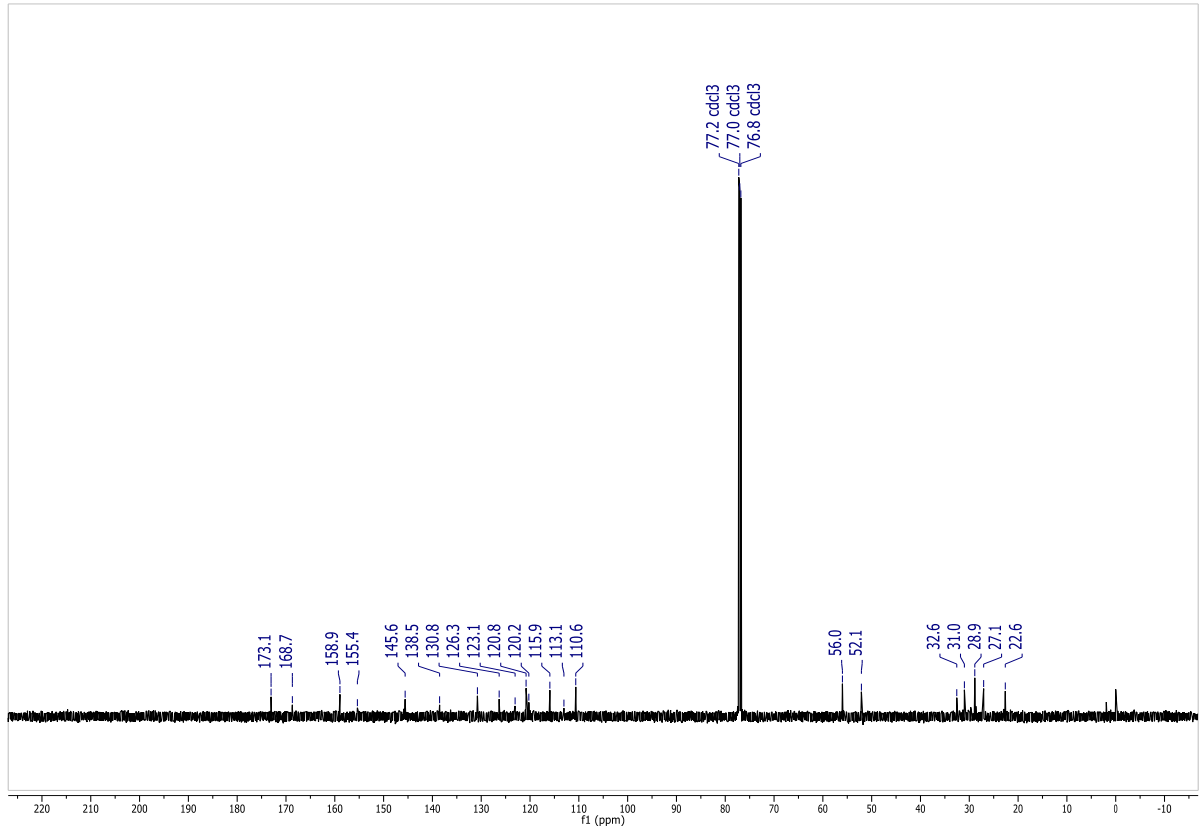
1.97
f1 (ppm)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126.3
123.1
120.8
120.2
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110.6
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31.0
28.9
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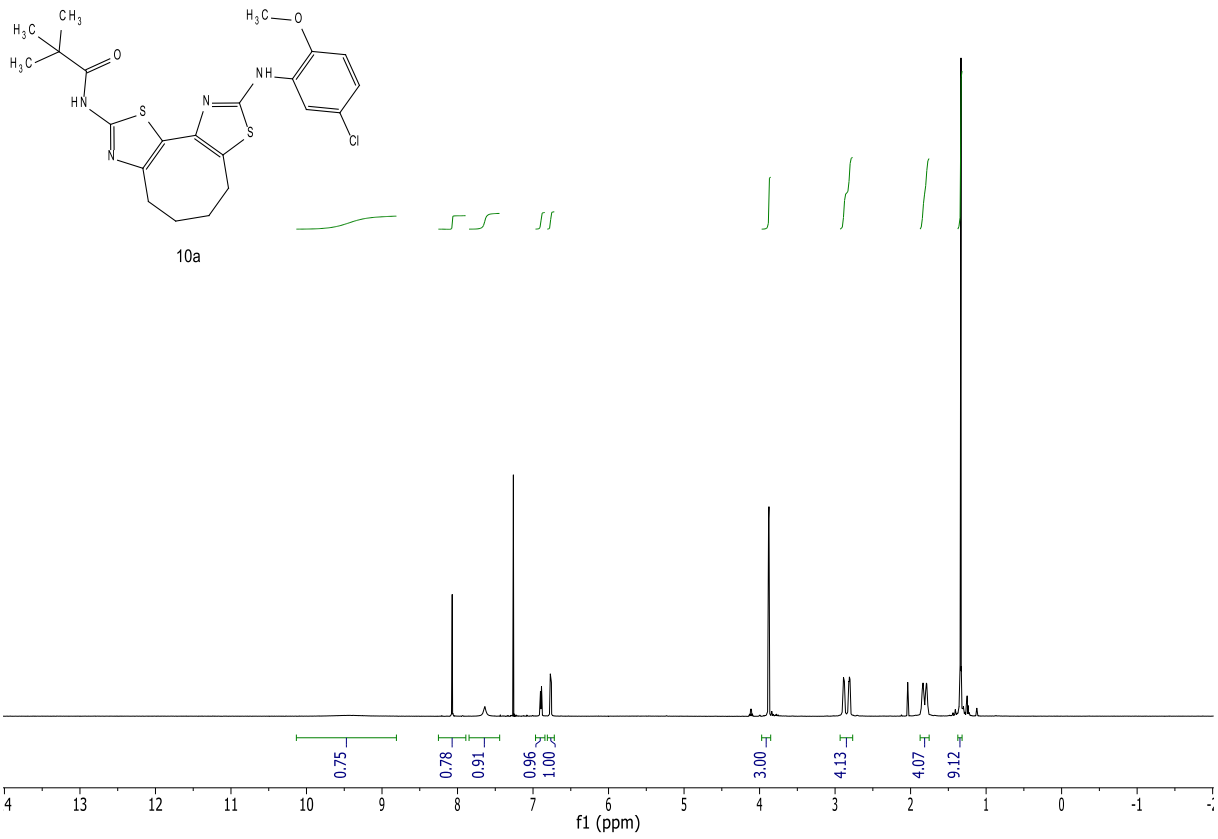
22.6
f1 (ppm)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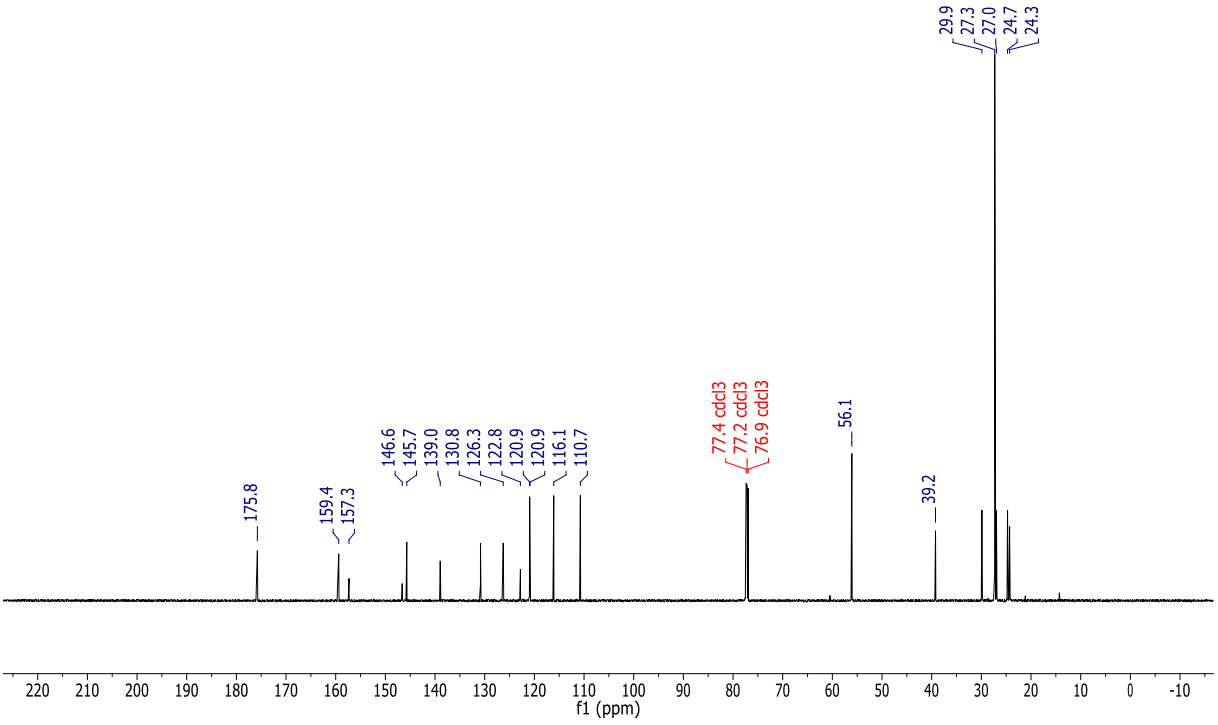
4.13
4.07
9.12
f1 (ppm)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122.8
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76.9 cdcl3
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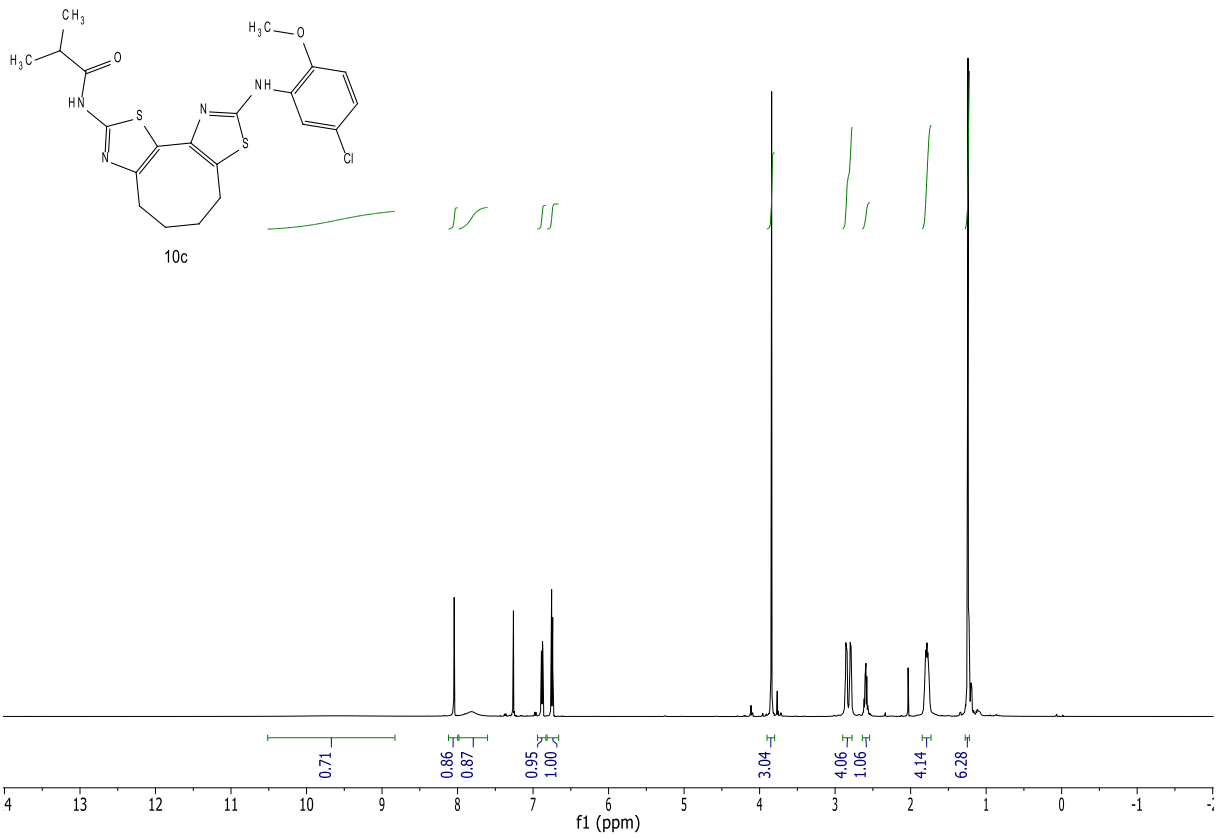
f1 (ppm)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0.95
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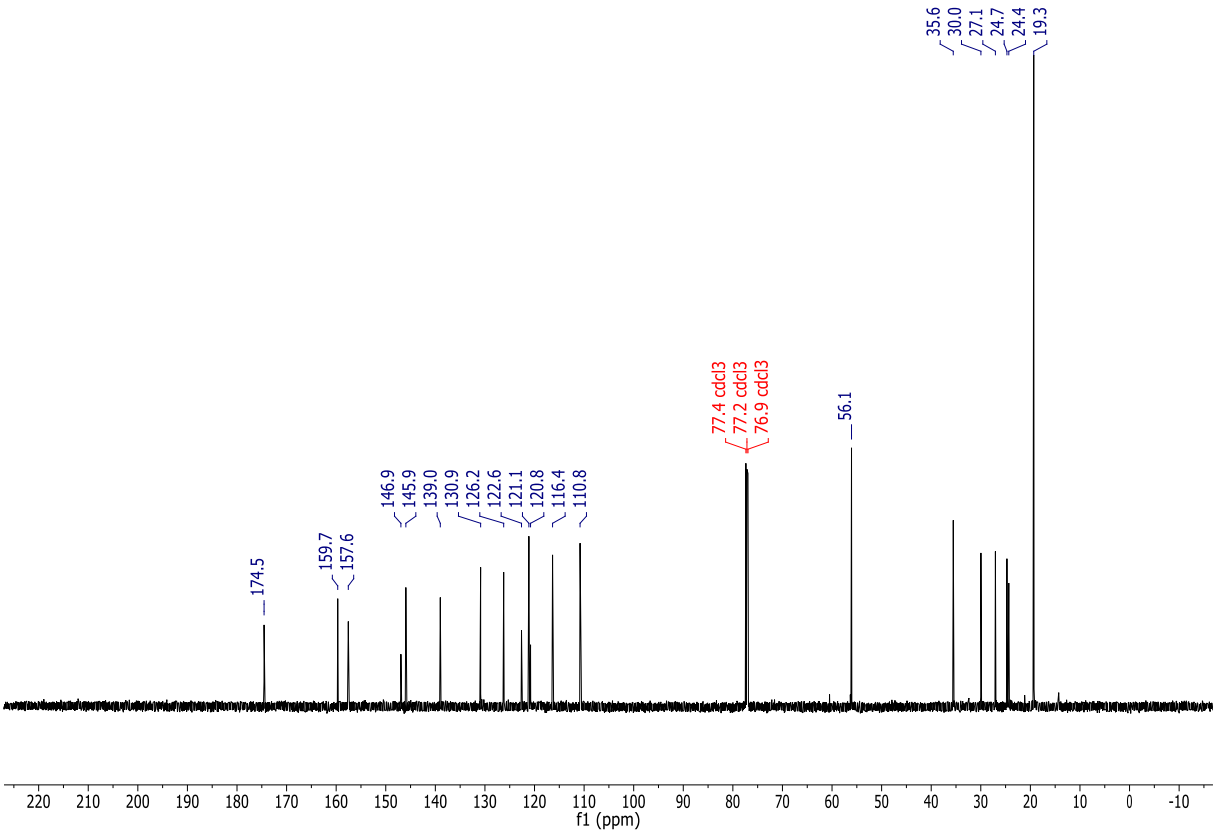
1.06
4.14
6.28
f1 (ppm)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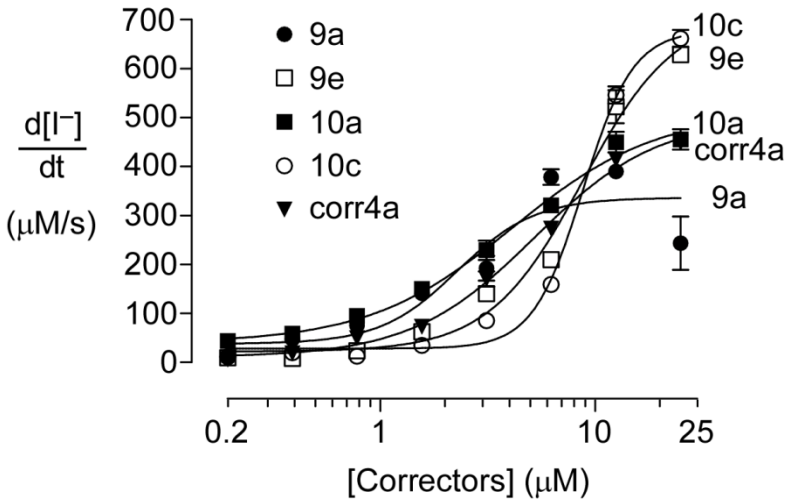
145.9
139.0
130.9
126.2
122.6
121.1
120.8
116.4
110.8
159.7
157.6
174.5
f1 (ppm)

Corrector Activity Figure For **corr4a**, **9a**, **9e**, **10a**, and **10c**



HRMS Data Summary

Number	Formula	[M+H] calc.	[M+H] found	purity
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8a	C17H18ClN4OS2+	393.0605	393.0593	≥95%
9a	C21H24ClN4O2S2+	463.1024	463.1021	≥95%
9b	C20H20ClN4O2S2+	447.0711	447.0708	≥95%
9c	C20H22ClN4O2S2+	449.0867	449.0870	≥95%
9d	C21H24ClN4O2S2+	463.1024	463.1024	≥95%
9e	C21H22ClN4O4S2+	493.0766	493.0758	≥95%
9f	C20H17ClN5O3S2+	474.0456	474.0462	≥95%
9g	C22H27ClN5OS2+	476.1340	476.1338	≥95%
9h	C20H24N5OS2+	414.1417	414.1404	≥95%
9i	C22H28N5OS2+	442.1730	442.1725	≥95%
9j	C21H24N5O4S2+	474.1264	474.1253	≥95%
10a	C22H26ClN4O2S2+	477.1180	477.1176	≥95%
10b	C21H22ClN4O2S2+	461.0867	461.0865	≥95%
10c	C21H24ClN4O2S2+	463.1024	463.1021	≥95%
10d	C22H26ClN4O2S2+	477.1180	477.1176	≥95%
10e	C22H24ClN4O4S2+	507.0922	507.0918	≥95%
10f	C21H19ClN5O3S2+	488.0612	488.0609	≥95%
10g	C23H29ClN5OS2+	490.1497	490.1491	≥95%
10h	C21H26N5OS2+	428.1573	428.1570	≥95%
10i	C23H30N5OS2+	456.1886	456.1884	≥95%
10j	C22H26N5O4S2+	488.1421	488.1415	≥95%

Computational Supporting Information

Gaussian09 Full Reference:

Gaussian 09, Revision B.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.**

Spartan10 Full Reference:

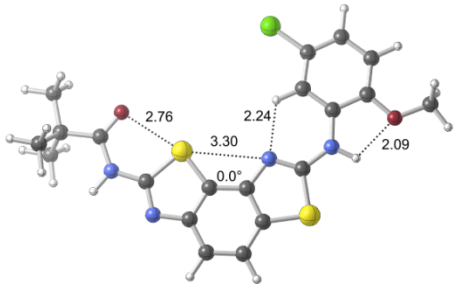
Shao, Y.; Molnar, L.F.; Jung, Y.; Kussmann, J.; Ochsenfeld, C.; Brown, S.T.; Gilbert, A.T.B.; Slipchenko, L.V.; Levchenko, S.V.; O'Neill, D.P.; DiStasio Jr., R.A.; Lochan, R.C.; Wang, T.; Beran, G.J.O.; Besley, N.A.; Herbert, J.M.; Lin, C.Y.; Van Voorhis, T.; Chien, S.H.; Sodt, S.H.; Steele, R.P.; Rassolov, V.A.; Maslen, P.E.; Korambath, P.P.; Adamson, R.D.; Austin, B.; Baker, J.; Byrd, E.F.C.; Dachsel, H.; Doerksen, R.J..; Dreuw, A.; Dunietz, B.D.; Dutoi, A.D.; Furlani, T.R.; Gwaltney, S.R.; Heyden, A.; Hirata, S.; Hsu, C-P.; Kedziora, G.; Khalliulin, R.Z.; Klunzinger, P.; Lee, A.M.; Lee, M.S.; Liang, W.Z.; Lotan, I.; Nair, N.; Peters, B.; Proynov, E.I.; Pieniazek, P.A.; Rhee, Y.M.; Ritchie, J.; Rosta, E.; Sherrill, C.D.; Simmonett, A.C.; Subotnik, J.E.; Woodcock III H.L.; Zhang, W.; Bell, A.T.; Chakraborty, A.K.; Chipman, D.M.; Keil, F.J.; Warshel, A.; Hehre, W.J.; Schaefer, H.F.; Kong, J.; A.I. Krylov, A.I.; Gill, P.M.W.; and Head-Gordon, M. *Phys. Chem. Chem. Phys.,* **2006***, 8*, 3172.

Spartan conformational searching:

The conformational searches of bithiazoles **3**, **1**, and **9** were done using Spartan10. Conformer distribution at the ground state using Molecular Mechanics (MMFF) and keywords "searchmethod=systematic" and "maxenergy=50" were used.

Calculated coordinates and energies for **3**, **9a**, and **10a:**

3: lowest energy conformation



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RMS Force	0.004758	0.000300	NO
Maximum Displacement	0.315191	0.001800	NO
RMS Displacement	0.048115	0.001200	NO

Predicted change in Energy=-9.842131D-03

Imaginary Frequencies: none found

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.069457	-2.083773	-0.218888
2	6	-1.047407	-1.215082	-0.009210
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12	6	5.265213	2.959341	-0.080713
13	6	-5.707774	0.292752	-0.060039
14	6	-6.644878	1.503503	0.092754
15	6	-8.083529	1.003829	-0.060332
16	6	-6.343782	2.542251	-1.003148
17	6	-6.465815	2.132057	1.486917
18	6	7.755093	-0.392524	0.154419
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20	6	-1.797280	-3.533410	-0.524001
21	6	-0.503720	-4.021939	0.165584
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24	1	2.270247	1.315509	-0.087317
25	1	7.192183	2.009641	0.008528
26	1	5.661970	3.966789	-0.112785
27	1	-8.228062	0.536047	-1.036774
28	1	-8.316419	0.256610	0.701789
29	1	-8.775686	1.845276	0.039971

30	1	-7.056199	3.368921	-0.920277
31	1	-5.337840	2.965571	-0.919369
32	1	-6.446005	2.097744	-1.997340
33	1	-6.635559	1.389858	2.272337
34	1	-5.469483	2.561646	1.631997
35	1	-7.192919	2.940111	1.613328
36	1	8.170662	-1.396036	0.223723
37	1	8.108940	0.102939	-0.755020
38	1	8.029651	0.193390	1.036891
39	1	-1.695551	-3.643632	-1.611905
40	1	-2.647728	-4.139994	-0.205011
41	1	-0.194421	-4.973624	-0.273732
42	1	-0.701995	-4.197832	1.232204
43	8	-6.099325	-0.830725	-0.271343
44	8	6.345701	-0.568947	0.100996
45	7	-3.341950	-1.549311	-0.223613
46	7	1.418763	-0.790414	0.005318
47	7	3.783558	-0.978625	0.050332
48	7	-4.349925	0.598631	0.066393
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3: second lowest energy conformation

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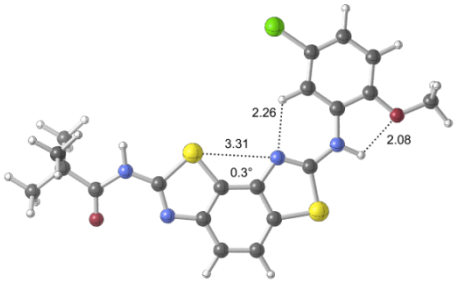

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HF = -2400.3285782 hartrees (-1506230.18610628 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.391473 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies =

-2399.998467 hartrees (-1506023.03802717 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
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5	6	0.709698	3.177964	-0.052424
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7	6	3.964185	-0.505150	-0.012212
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9	6	2.996085	-1.503148	0.069309
10	6	5.710289	-2.195398	0.021290

11	6	3.404014	-2.836453	0.125921
12	6	4.738488	-3.199061	0.103443
13	6	-4.821188	-1.116683	-0.112744
14	6	-6.282945	-1.576474	-0.086518
15	6	-6.308838	-3.089469	-0.308125
16	6	-7.060873	-0.873261	-1.211487
17	6	-6.906876	-1.241262	1.278304
18	6	7.581286	-0.091116	-0.157952
19	17	2.179132	-4.076681	0.221480
20	6	-1.584473	3.980426	0.529137
21	6	-0.263508	4.316549	-0.190084
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23	1	-5.400160	0.852791	0.241549
24	1	1.947523	-1.242261	0.086897
25	1	6.757201	-2.473322	0.003191
26	1	5.026417	-4.242812	0.147470
27	1	-5.856823	-3.352436	-1.267500
28	1	-5.749705	-3.609038	0.473747
29	1	-7.345137	-3.440918	-0.296165
30	1	-8.086678	-1.254647	-1.236112
31	1	-7.115348	0.210856	-1.068284
32	1	-6.601421	-1.065566	-2.185829
33	1	-6.336029	-1.695944	2.093666
34	1	-6.962935	-0.163169	1.461093
35	1	-7.927871	-1.634372	1.316118

36	1	8.085151	0.872102	-0.227807
37	1	7.898386	-0.606859	0.755468
38	1	7.831656	-0.701243	-1.033022
39	1	-1.451713	4.103583	1.613212
40	1	-2.371729	4.671674	0.217586
41	1	0.148303	5.245910	0.212780
42	1	-0.458496	4.486566	-1.258985
43	8	-3.879718	-1.867120	-0.297741
44	8	6.196076	0.192408	-0.121089
45	7	-3.321439	2.154948	0.293754
46	7	1.321991	0.915177	0.005714
47	7	3.698570	0.863683	-0.078079
48	7	-4.618201	0.230372	0.085710
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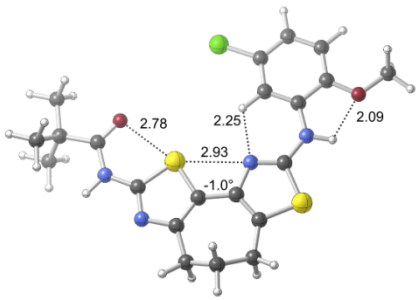
50	16	2.444139	3.253900	-0.139816

9a: lowest energy conformation



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mem = 10GB

HF = -2439.6284424 hartrees (-1530891.24389042 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.420038 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies =

-2439.272639 hartrees (-1530667.97369889 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.045761	2.745385	0.094328
2	6	-0.976214	1.892657	0.025215
3	6	-3.145668	0.836675	0.051985
4	6	0.458597	2.155980	0.023921
5	6	1.078251	3.372586	0.055845
6	6	2.537864	1.395156	0.027597
7	6	3.624066	-0.840308	0.003681
8	6	4.902993	-1.444622	0.005255
9	6	2.487044	-1.644632	-0.014433
10	6	5.028203	-2.824016	-0.010523
11	6	2.640714	-3.031823	-0.030080
12	6	3.886385	-3.633083	-0.028484
13	6	-4.269415	-1.347785	-0.002232
14	6	-5.650852	-2.012124	0.008150
15	6	-6.410347	-1.611290	1.283572
16	6	-5.449585	-3.527783	-0.017579

17	6	-6.437182	-1.571444	-1.237994
18	6	7.257890	-1.098874	0.025573
19	17	1.207479	-4.024362	-0.053444
20	6	-2.012142	4.245518	0.160945
21	6	0.516880	4.764456	0.084201
22	6	-0.852812	4.906528	-0.587940
23	1	4.536882	0.975113	0.036070
24	1	-5.141628	0.541911	0.102623
25	1	1.503509	-1.196554	-0.016490
26	1	6.006402	-3.289414	-0.009128
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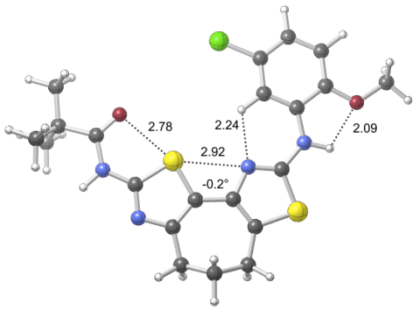
34	1	-6.641928	-0.495894	-1.244690
35	1	-5.891255	-1.820087	-2.153133
36	1	-7.400158	-2.091621	-1.262263
37	1	7.933932	-0.244977	0.040835
38	1	7.425642	-1.716838	0.914991
39	1	7.437559	-1.694029	-0.876949
40	1	-1.999520	4.561951	1.213003
41	1	-2.961908	4.598272	-0.252361

42	1	0.452315	5.118565	1.122238
43	1	1.221698	5.434079	-0.422119
44	1	-1.068819	5.976827	-0.670815
45	1	-0.799905	4.509963	-1.608489
46	8	-3.222383	-1.966885	-0.058369
47	8	5.948833	-0.563751	0.023599
48	7	-3.278015	2.130584	0.106301
49	7	1.292402	1.044351	0.003968
50	7	3.617447	0.555811	0.021724
51	7	-4.271861	0.027969	0.052248
52	16	-1.522666	0.234548	-0.023618
53	16	2.808879	3.128552	0.070477

9a: second lowest energy conformation



Charge = 0 Multiplicity = 1

mem = 6400MB

HF = -2439.6159893 hartrees (-1530883.42944564 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.419806 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies =

-2439.261591 hartrees (-1530661.04096841 kcal/mol)

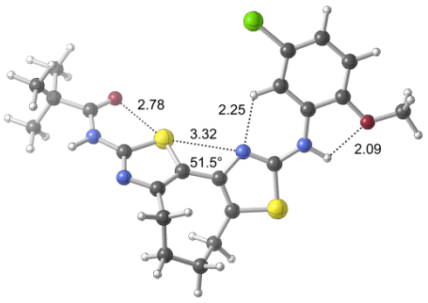
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.097099	2.280332	-0.273660
2	6	0.944365	1.547906	-0.140643
3	6	3.002154	0.274791	-0.329923
4	6	-0.453215	1.960878	-0.069059
5	6	-0.937610	3.237336	-0.045747
6	6	-2.599634	1.426425	0.007458
7	6	-3.918555	-0.680013	0.030993
8	6	-5.255596	-1.142450	0.059320
9	6	-2.876314	-1.603489	-0.004269
10	6	-5.530077	-2.500274	0.051837
11	6	-3.181798	-2.965322	-0.011131
12	6	-4.484109	-3.428987	0.016193
13	6	5.126528	-0.739103	0.370309
14	6	6.105090	-1.877135	0.038084
15	6	5.396455	-3.240221	0.091883
16	6	7.233078	-1.847688	1.070357
17	6	6.681306	-1.635294	-1.367192
18	6	-7.558418	-0.543681	0.126946
19	17	-1.864628	-4.113350	-0.054065

20	6	2.213852	3.777387	-0.319538
21	6	-0.233526	4.563045	-0.063480
22	6	1.183087	4.535740	0.519325
23	1	-4.630435	1.221984	0.075091
24	1	3.787045	-1.510196	-1.012804
25	1	-1.850363	-1.264589	-0.025215
26	1	-6.552812	-2.856610	0.073153
27	1	-4.690821	-4.492589	0.010529
28	1	4.901409	-3.391754	1.056021
29	1	4.650699	-3.366214	-0.700701
30	1	6.135962	-4.036432	-0.039701
31	1	7.959878	-2.633327	0.840644
32	1	7.740462	-0.880538	1.064671
33	1	6.845128	-2.010611	2.079392
34	1	5.908494	-1.674575	-2.141442
35	1	7.169358	-0.657660	-1.424787
36	1	7.425922	-2.405589	-1.594044
37	1	-8.136887	0.378777	0.152244
38	1	-7.822497	-1.118559	-0.767662
39	1	-7.771384	-1.136120	1.023812
40	1	2.164347	4.116212	-1.363484
41	1	3.221163	4.017198	0.033113
42	1	-0.198767	4.949897	-1.090993
43	1	-0.830653	5.279925	0.511798
44	1	1.518697	5.573698	0.612390

45	1	1.153198	4.117137	1.531895
46	8	5.336903	0.093002	1.223888
47	8	-6.199045	-0.154166	0.091994
48	7	3.253058	1.542877	-0.392541
49	7	-1.399470	0.943643	-0.034068
50	7	-3.761704	0.706617	0.042255
51	7	3.973538	-0.725142	-0.406610
52	16	1.327926	-0.146939	-0.112891
53	16	-2.683192	3.179424	0.017673

10a: lowest energy conformation



Charge = 0 Multiplicity = 1

mem = 10GB

HF = -2478.9219167 hartrees (-1555548.29194842 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.449556 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies =

-2478.536709 hartrees (-1555306.57026459 kcal/mol)

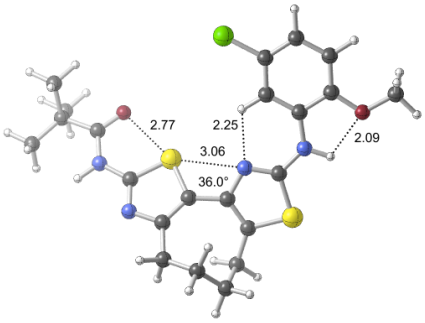
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.885460	1.932353	0.994103
2	6	1.036596	1.270592	0.149466
3	6	3.257426	0.349097	0.312015
4	6	-0.337957	1.637725	-0.167491
5	6	-0.696546	2.902332	-0.535268
6	6	-2.495522	1.236672	-0.372359
7	6	-3.998423	-0.721028	-0.072656
8	6	-5.358960	-1.093403	-0.181757
9	6	-3.058474	-1.670177	0.322316
10	6	-5.757851	-2.389538	0.101050
11	6	-3.488291	-2.967618	0.603951
12	6	-4.815051	-3.343536	0.499425
13	6	4.694021	-1.467341	-0.513867
14	6	6.102431	-2.059431	-0.392596
15	6	6.169989	-3.310384	-1.269866
16	6	6.384659	-2.436584	1.071133
17	6	7.131108	-1.025622	-0.880904
18	6	-7.570115	-0.387455	-0.712576
19	17	-2.300439	-4.148938	1.098721
20	6	1.540158	3.106525	1.866907
21	6	0.171138	4.090242	-0.831675
22	6	1.717775	4.488734	1.210403

23	6	0.530524	4.975698	0.378064
24	1	-4.516847	1.155660	-0.653458
25	1	5.171665	0.025479	0.859120
26	1	-2.015003	-1.400095	0.404430
27	1	-6.798822	-2.677550	0.017837
28	1	-5.118314	-4.359585	0.722680
29	1	5.436228	-4.053713	-0.948187
30	1	5.959311	-3.068779	-2.314270
31	1	7.170422	-3.748749	-1.201419
32	1	7.361071	-2.927170	1.136601
33	1	6.411673	-1.564305	1.732424
34	1	5.628456	-3.129579	1.452110
35	1	6.921655	-0.721564	-1.911030
36	1	7.148087	-0.126518	-0.256388
37	1	8.132051	-1.468076	-0.851622
38	1	-8.051846	0.536182	-1.031113
39	1	-7.726062	-1.163579	-1.470164
40	1	-7.995382	-0.713254	0.243348
41	1	2.193156	3.041559	2.741894
42	1	0.506432	3.003473	2.218272
43	1	1.095273	3.720907	-1.294651
44	1	-0.332135	4.704105	-1.586198
45	1	2.623989	4.476673	0.591186
46	1	1.892719	5.225044	2.002751
47	1	0.767241	5.979263	0.006514

48	1	-0.353140	5.079107	1.021372
49	8	3.828597	-1.923918	-1.238879
50	8	-6.195038	-0.086022	-0.576079
51	7	3.155712	1.400544	1.071109
52	7	-1.352589	0.694578	-0.092514
53	7	-3.711298	0.609080	-0.381818
54	7	4.451093	-0.354086	0.259153
55	16	1.832854	-0.100854	-0.572727
56	16	-2.428970	2.952642	-0.755339

10a: second lowest energy conformation



Charge = 0 Multiplicity = 1

mem = 55GB

HF = -2478.9223142 hartrees (-1555548.54138364 kcal/mol)

Imaginary Frequencies: 1 (-6.7633 1/cm)

Zero-point correction = 0.449389 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies =

-2478.534383 hartrees (-1555305.11067633 kcal/mol)

Coordinates (from last standard orientation):

Center Atomic Coordinates (Angstroms)

Number	Number	X	Y	Z
1	6	1.996593	2.403433	0.649472
2	6	1.014316	1.626061	0.088651
3	6	3.207626	0.616709	0.166556
4	6	-0.398878	1.879791	-0.192690
5	6	-0.918508	3.070326	-0.605236
6	6	-2.492464	1.202616	-0.383052
7	6	-3.721236	-0.932589	-0.056188
8	6	-5.025632	-1.476668	-0.124575
9	6	-2.657185	-1.750913	0.316526
10	6	-5.247906	-2.809977	0.178028
11	6	-2.909303	-3.090625	0.615873
12	6	-4.180242	-3.632636	0.554290
13	6	4.455391	-1.414388	-0.407392
14	6	5.822646	-2.105671	-0.361835
15	6	5.627551	-3.417642	0.413727
16	6	6.923387	-1.270760	0.298803
17	6	6.207276	-2.416894	-1.816721
18	6	-7.321334	-1.063343	-0.602536
19	17	-1.567101	-4.105433	1.079376
20	6	1.934038	3.767464	1.298096
21	6	-0.200111	4.367127	-0.798517
22	6	0.559013	4.352750	1.642269
23	6	-0.080584	5.161113	0.510313

24	1	-4.489934	0.856847	-0.637455
25	1	5.170201	0.302739	0.528793
26	1	-1.655074	-1.349376	0.372101
27	1	-6.245657	-3.228504	0.125810
28	1	-4.346178	-4.676856	0.791596
29	1	5.357505	-3.222815	1.456983
30	1	4.833972	-4.013073	-0.043041
31	1	6.557737	-3.994725	0.401969
32	1	7.857670	-1.839854	0.289657
33	1	7.111391	-0.335118	-0.240352
34	1	6.695079	-1.043815	1.346462
35	1	5.422063	-3.003565	-2.298801
36	1	6.354757	-1.496592	-2.391920
37	1	7.141491	-2.987328	-1.836802
38	1	-7.394118	-1.860669	-1.350842
39	1	-7.678910	-1.431764	0.365526
40	1	-7.924873	-0.212109	-0.914871
41	1	2.496170	4.473445	0.669467
42	1	2.523141	3.669184	2.215912
43	1	0.801547	4.133256	-1.181259
44	1	-0.697887	4.971833	-1.563609
45	1	0.675630	5.015478	2.506221
46	1	-0.115573	3.550202	1.960987
47	1	0.516225	6.062203	0.320759
48	1	-1.076379	5.497902	0.822997

49	8	3.481480	-1.959379	-0.898851
50	8	-5.993373	-0.587355	-0.501792
51	7	3.244192	1.810500	0.677811
52	7	-1.290444	0.820245	-0.088987
53	7	-3.614975	0.420832	-0.381199
54	7	4.362428	-0.152794	0.126952
55	16	1.664434	0.077037	-0.400314
56	16	-2.641264	2.900847	-0.818795