

Supporting Information:

A DFT study of the mechanism of NHC catalysed annulation reactions involving α,β -unsaturated acyl azoliums and β -naphthol.

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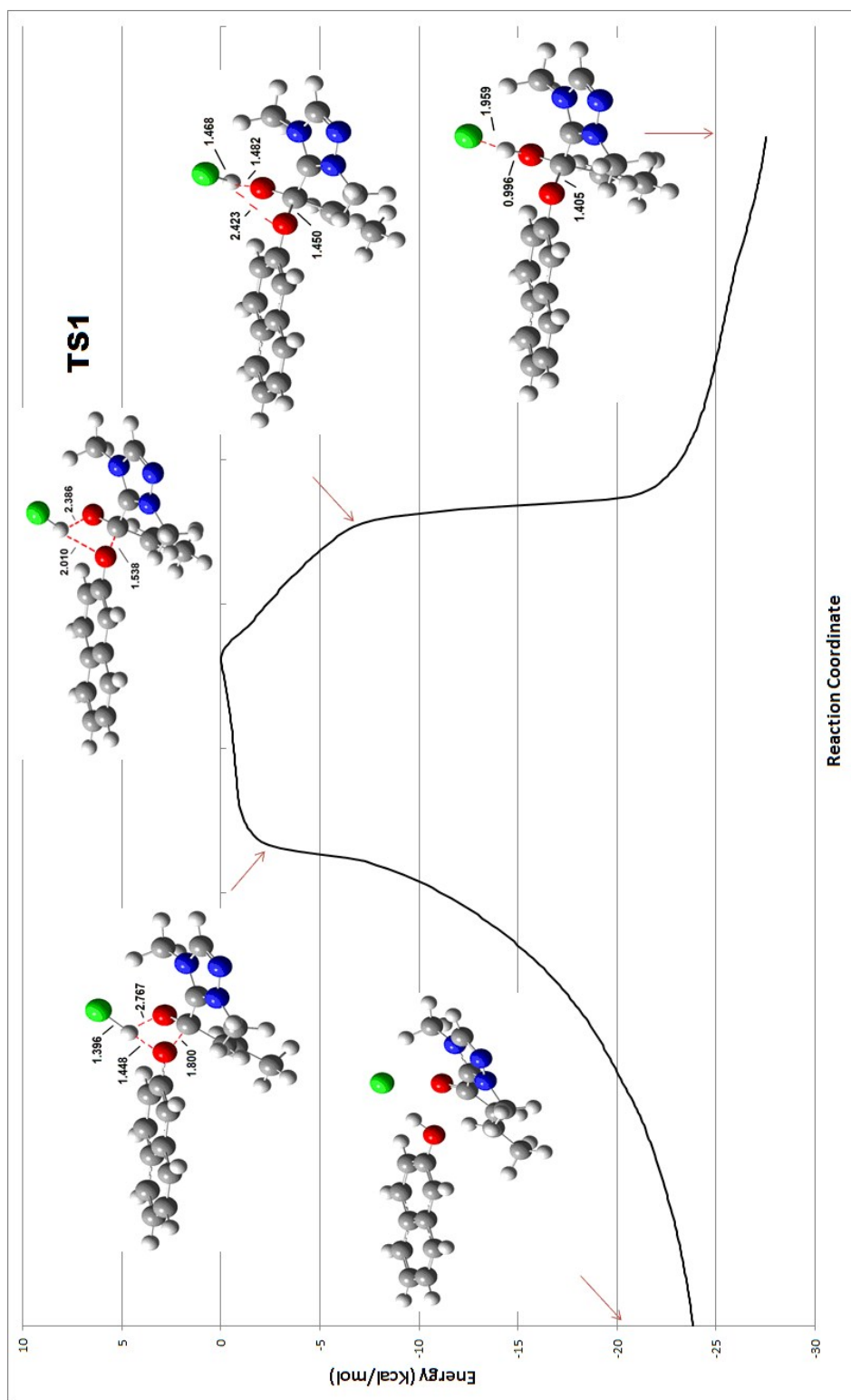


Figure S1. Energy profile (IRC, ΔE) corresponding to the transition state **TS1** in toluene

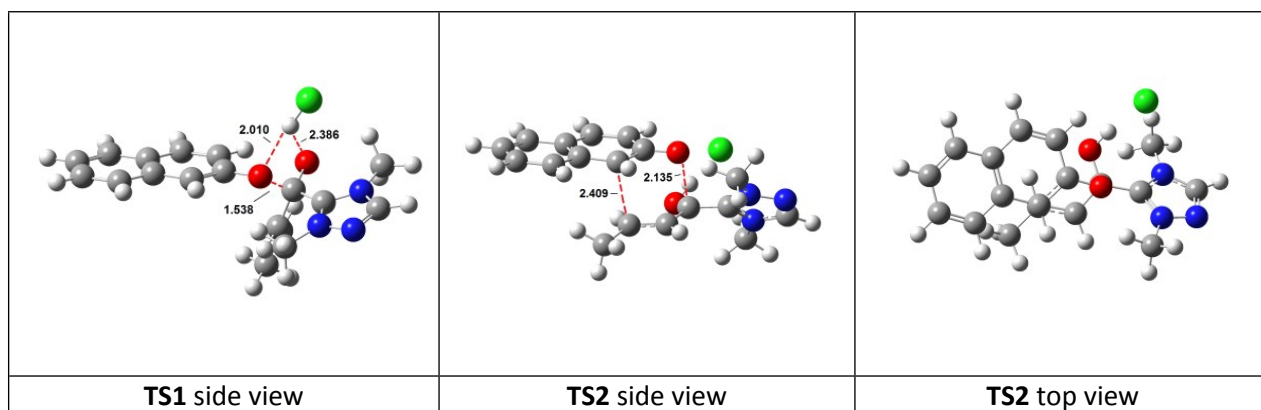


Figure S2. Geometries, in toluene, of the TS involved in the reaction of ion pair **6** with naphthol **7** via 1, 2-addition/Claisen rearrangement . The bond lengths (in black) are given in angstroms.

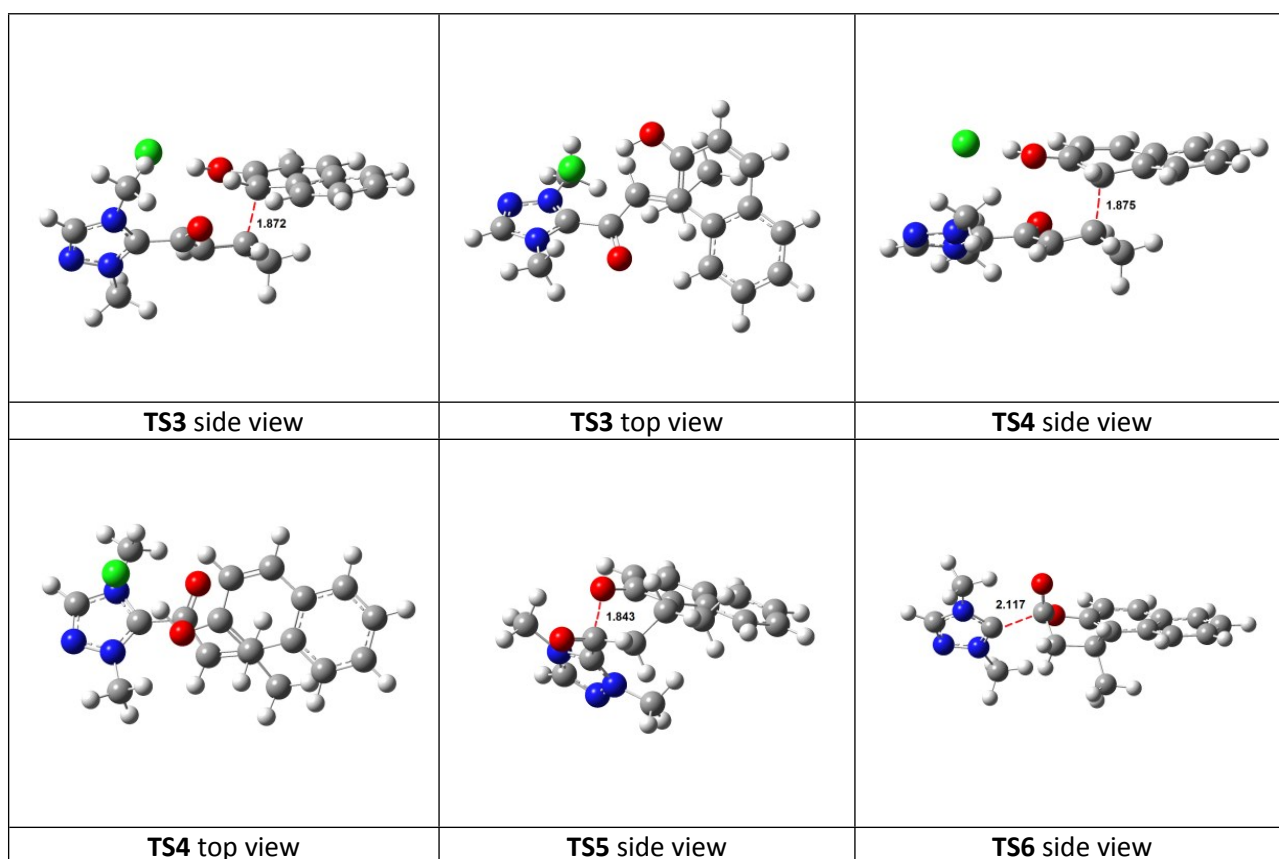


Figure S3. Geometries, in toluene, of the TS involved in the reaction of ion pair **6** with naphthol **7** via 1, 4-addition. The bond lengths (in black) are given in angstroms.

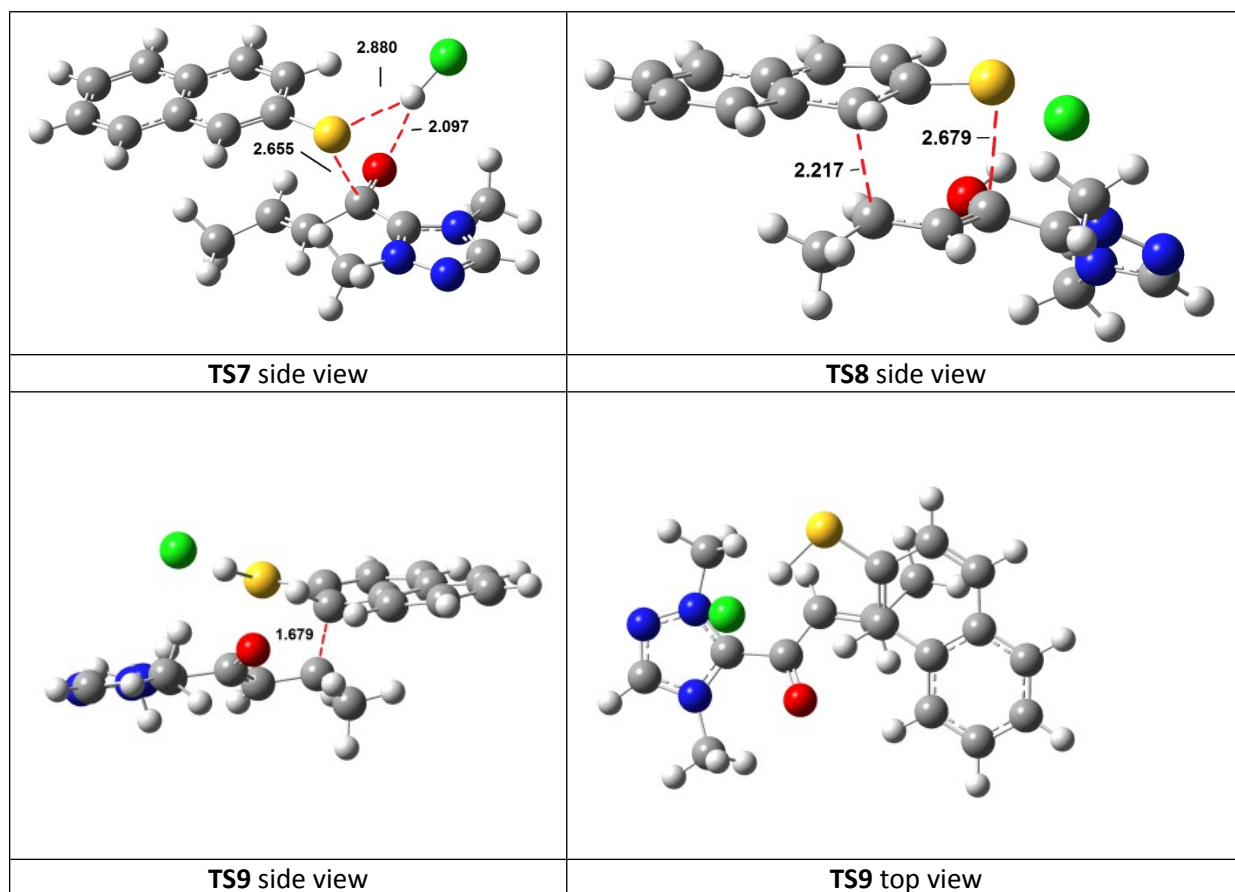


Figure S4. Geometries, in toluene, of the TS involved in the reaction of ion pair **6** with naphthothiol **9** via 1, 2-addition/Claisen rearrangement (**TS7** and **TS8**) and via 1, 4-addition (**TS9**). The bond lengths (in black) are given in angstroms.

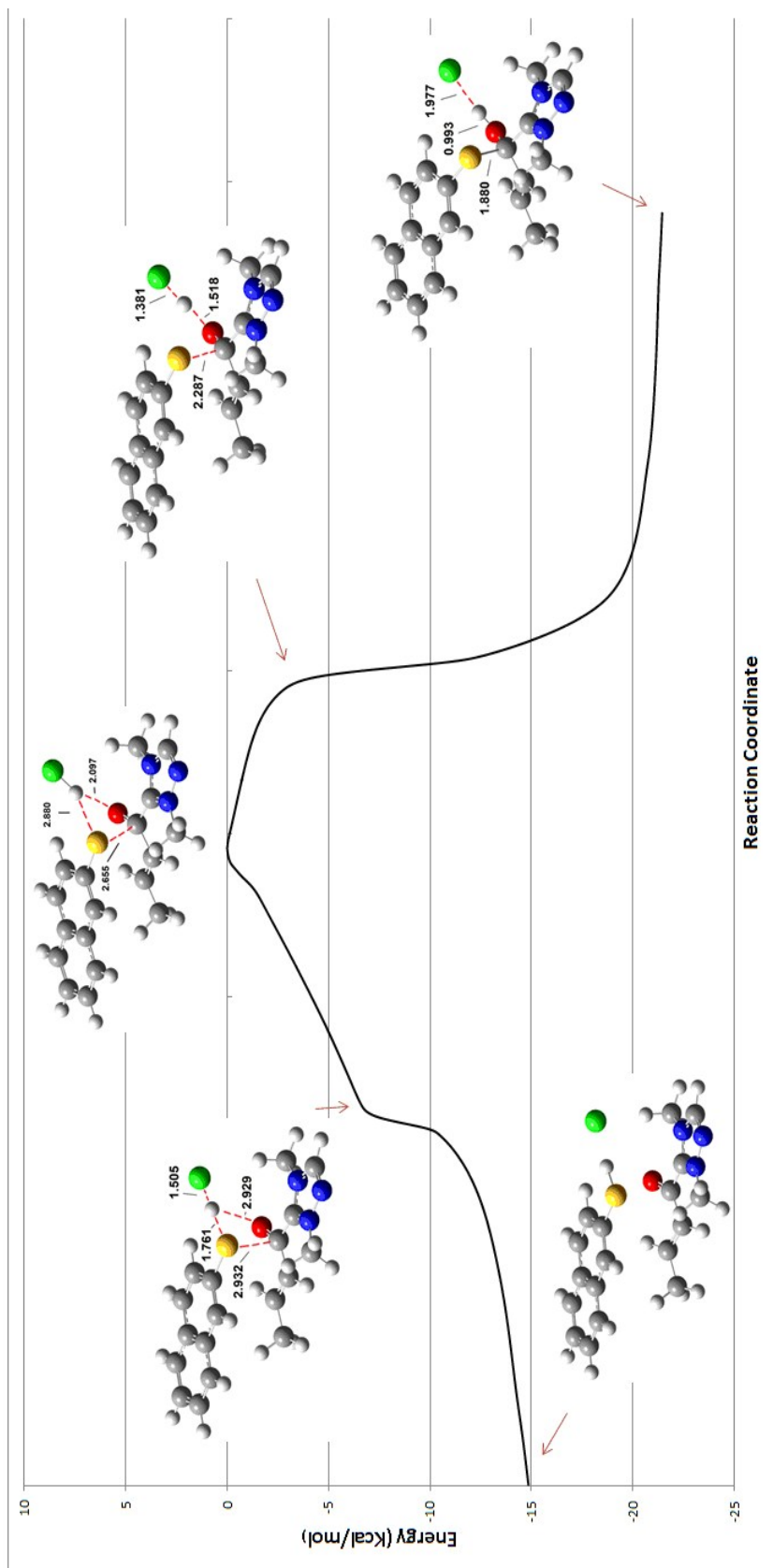


Figure S5. Energy profile (IRC, ΔE) corresponding to the transition state TS7 in toluene

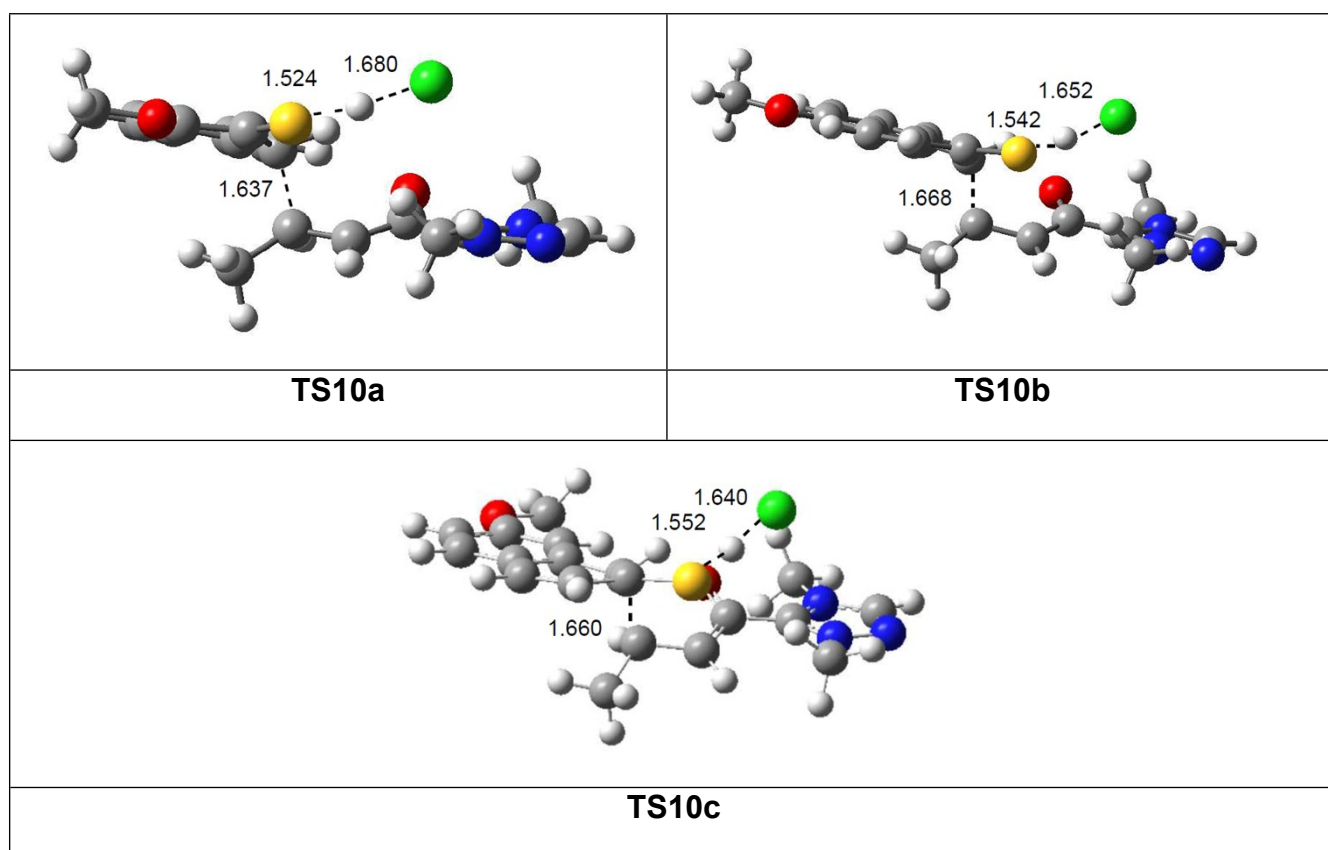
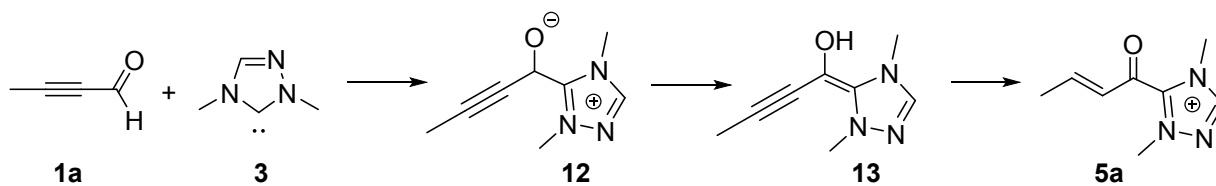


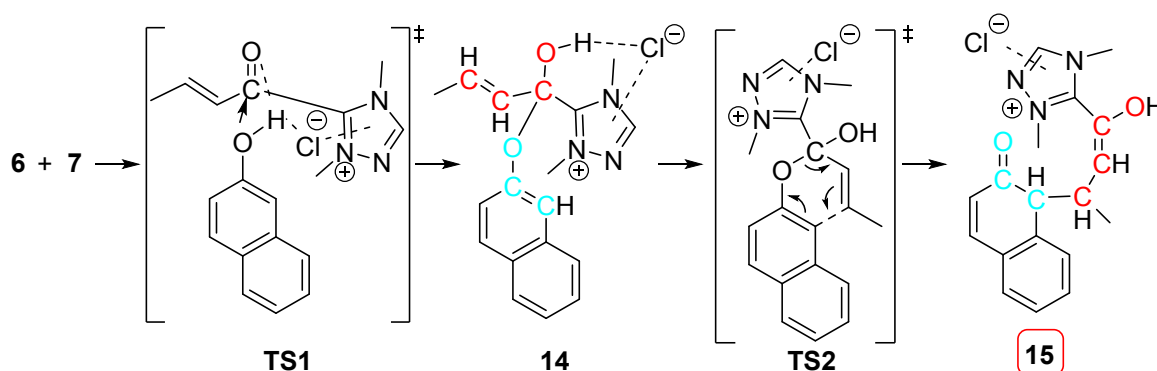
Figure S6. Geometries, in toluene, of **TS10a-c** involved in the 1, 4-addition reaction of methoxy substituted β -naphthalenethiols **26a-c** to IP **6**

Table S1. Absolute energies (E, H, G in hartree and S in Cal/Mol-Kelvin), in toluene, of the stationary points involved Formation of acyl azolium **5a**.



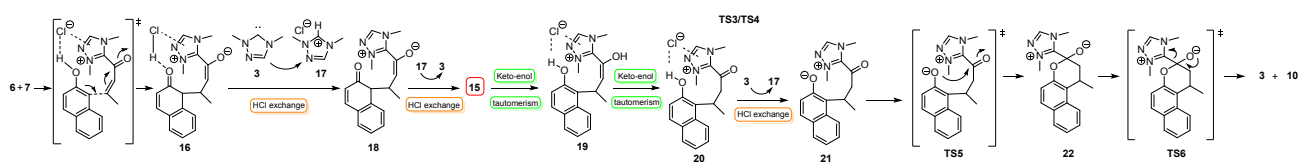
	E	H	S	G
1a	-229.9142511	-229.839381	77.718	-229.878165
3	-320.748475	-320.621656	82.781	-320.662966
12	-550.6702906	-550.465351	115.581	-550.52303
13	-550.692246	-550.486502	118.537	-550.545657
5a	-551.1855937	-550.966342	115.982	-551.024221

Table S2. Absolute energies (E, H, G in hartree and S in Cal/Mol-Kelvin) and relative energies (ΔE , ΔH and ΔG in Kcal/Mol), in toluene, of the stationary points involved in the NHC catalysed reaction of ion pair **6** with naphthol **7** via 1,2-addition/Claisen rearrangement.



	E	ΔE	H	ΔH	S	G	ΔG
6	-1011.656065		-1011.433353		121.315	-1011.493893	
7	-460.995574		-460.830708		88.572	-460.874909	
6+7	-1472.651639	0.0	-1472.264061	0.0	209.887	-1472.368802	0.0
TS1	-1472.623304	17.8	-1472.238769	15.9	170.760	-1472.323984	28.1
14	-1472.670223	-11.7	-1472.281250	-10.8	163.053	-1472.362619	3.9
TS2	-1472.625461	16.4	-1472.238023	16.3	158.056	-1472.327622	25.8
15	-1472.676465	-15.6	-1472.285119	-13.2	163.310	-1472.366617	1.4

Table S3. Absolute energies (E, H, G in hartree and S in Cal/Mol-Kelvin) and relative energies (ΔE , ΔH and ΔG in Kcal/Mol), in toluene, of the stationary points involved in the NHC catalysed reaction of ion pair **6** with naphthol **7** via 1,4-addition.



	E	ΔE	H	ΔH	S	G	ΔG
6	-1011.656065		-1011.433353		121.315	-1011.493893	
7	-460.995574		-460.830708		88.572	-460.874909	
3	-320.748475		-320.621656		82.781	-320.662966	
17	-781.674861		-781.531677		97.950	-781.580558	
6+7	-1472.651639	0.0	-1472.264061	0.0	209.887	-1472.368802	0.0
6+7+3	-1793.400113		-1792.885717		292.668	-1793.031768	
TS3	-1472.644413	4.5 ^a	-1472.255862	5.1 ^a	157.499	-1472.334460	21.5 ^a
TS4	-1472.640764	6.8 ^a	-1472.252864	7.0 ^a	157.823	-1472.331624	23.3 ^a
16	-1472.645736	3.7 ^a	-1472.256485	4.8 ^a	158.323	-1472.335494	20.9 ^a
16+3	-1793.394211	3.7 ^b	-1792.878141	4.8 ^b	241.104	-1792.998460	20.9 ^b
18+17	-1793.421853	-13.6 ^b	-1792.904096	-11.5 ^b	251.942	-1793.029825	1.2 ^b
18	-1011.746992	-13.6 ^c	-1011.372419	-11.5 ^c	153.992	-1011.449267	1.2 ^c
15+3	-1793.424939	-15.6 ^b	-1792.906775	-13.2 ^b	246.091	-1793.029583	1.4 ^b
15	-1472.676465	-15.6 ^a	-1472.285119	-13.2 ^a	163.310	-1472.366617	1.4 ^a
19	-1472.679388	-17.4 ^a	-1472.289076	-15.7 ^a	162.181	-1472.370010	-0.8 ^a
20	-1472.691489	-25.0 ^a	-1472.299739	-22.4 ^a	156.460	-1472.377818	-5.7 ^a
20+3	-1793.439964	-25.0 ^b	-1792.921395	-22.4 ^b	239.241	-1793.040784	-5.7 ^b
21+17	-1793.432800	-20.5 ^b	-1792.914273	-17.9 ^b	243.494	-1793.035786	-2.5 ^b
21	-1011.757940	-20.5 ^d	-1011.382596	-17.9 ^d	145.544	-1011.455228	-2.5 ^d
TS5	-1011.754778	-18.5 ^d	-1011.380921	-16.9 ^d	142.281	-1011.451924	-0.4 ^d
22	-1011.768419	-27.1 ^d	-1011.393115	-24.5 ^d	144.124	-1011.465038	-8.7 ^d
TS6	-1011.752008	-16.8 ^d	-1011.378539	-15.4 ^d	148.798	-1011.452794	-1.0 ^d
10+3	-1011.763826	-24.2 ^d	-1011.391262	-23.4 ^d	193.161	-1011.487656	-22.9 ^d
10	-691.015351	-24.2 ^e	-690.769606	-23.4 ^e	110.380	-690.824690	-22.9 ^e

(a) Relative to **6 + 7**

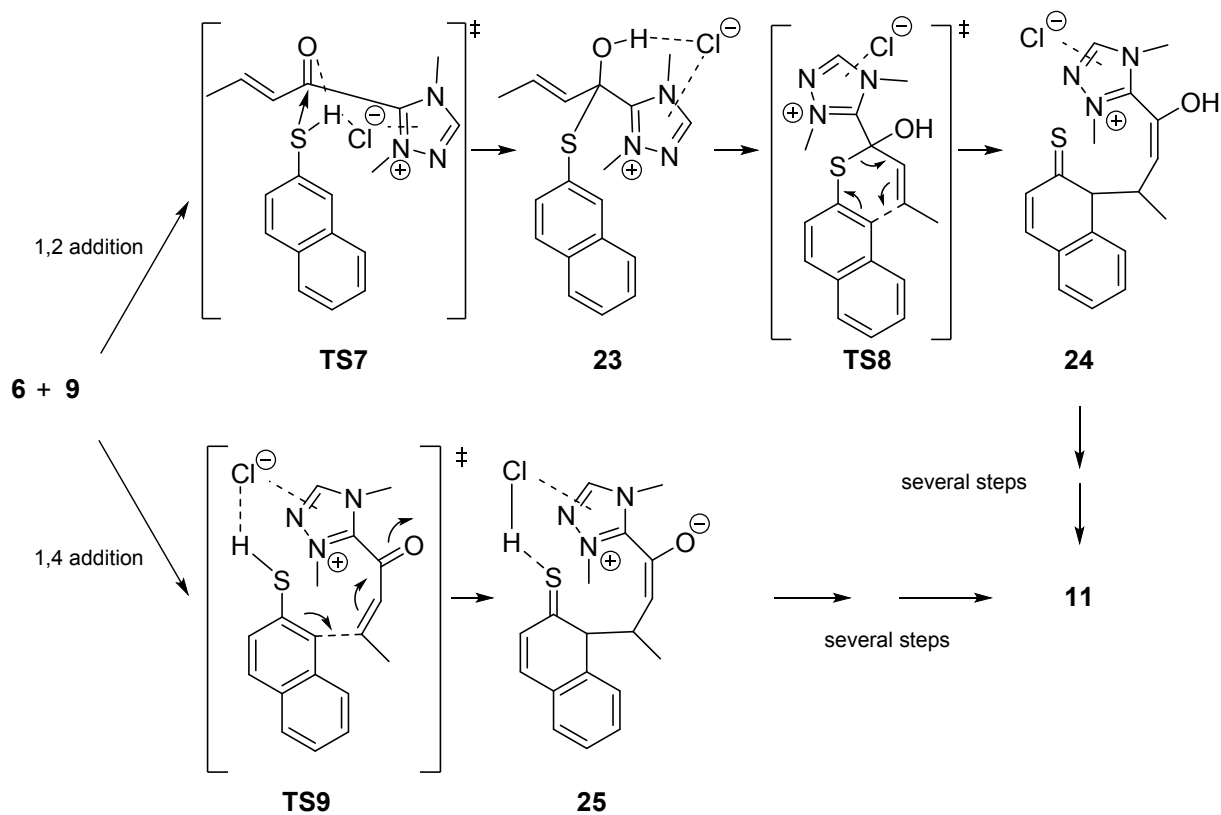
(b) Relative to **6 + 7 + 3**

(c) From **(18 + 17) - (6 + 7 + 3)**

(d) Relative to **18**

(e) Relative to **18 - 3**

Table S4. Absolute energies (E, H, G in hartree and S in Cal/Mol-Kelvin) and relative energies (ΔE , ΔH and ΔG in Kcal/Mol), in toluene, of the stationary points involved in the NHC catalysed reaction of ion pair **6** with naphthothiol **9** via 1,2-addition/Claisen rearrangement and via 1,4-addition.



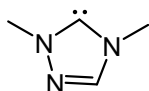
	E	ΔE	H	ΔH	S	G	ΔG
6	-1011.656065		-1011.433353		121.315	-1011.493893	
9	-784.029695		-783.869074		93.364	-783.915666	
6+9	-1795.685761	0.0	-1795.302427	0.0	214.679	-1795.409559	0.0
TS7	-1795.665399	12.8	-1795.284430	11.3	168.075	-1795.368306	25.9
23	-1795.703624	-11.2	-1795.315697	-8.3	165.883	-1795.398479	7.0
TS8	-1795.666118	12.3	-1795.281663	13.0	158.965	-1795.360992	30.5
24	-1795.697422	-7.3	-1795.308265	-3.7	167.305	-1795.391756	11.2
TS9	-1795.661078	15.5	-1795.281317	13.2	155.080	-1795.358708	31.9
25	-1795.665993	12.4	-1795.281420	13.2	164.540	-1795.363532	28.9

Table S5. Absolute energies (E, H, G in hartree and S in Cal/Mol-Kelvin) and relative energies (ΔE , ΔH and ΔG in Kcal/Mol), in toluene, of **TSa-c** involved in the 1,4-additions of methoxy substituted β -naphthalenethiols **26a-c** to IP **6**.

	E	ΔE	H	ΔH	S	G	ΔG
6	-1011,656065		-1011,433353		121,315	-1011,493893	
26a	-898.531563		-898.334970		105.734	-898.387735	
6+26a	-1910.187628		-1909.768323		227.049	-1909.881628	
TS10a	-1910.172689	9.4	-1909.755069	8.3	173.180	-1909.841492	25.2
26b	-898.531396		-898.334423		104.888	-898.386766	
6+26b	-1910.187461		-1909.767776		226.203	-1909.880659	
TS10b	-1910.163612	15.0	-1909.747836	12.5	169.933	-1909.832639	30.1
26c	-898.5312942		-898.335967		103.428	-898.387581	
6+26c	-1910.187359		-1909.769320		224.743	-1909.881474	
TS10c	-1910.166091	13.3	-1909.749942	12.2	168.800	-1909.83418	29.7

Z-Matrix

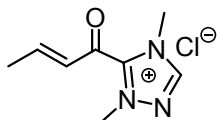
Compound 3



E=-320,748475

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	2.222882
3	1	0	0.376558	0.000000	3.227253
4	7	0	0.778722	0.000505	1.113715
5	7	0	-1.214420	-0.004432	0.554470
6	7	0	-1.245596	-0.002908	1.909130
7	6	0	2.218310	0.007258	1.100100
8	1	0	2.603062	0.887720	1.603735
9	1	0	2.611499	-0.882016	1.581273
10	1	0	2.532931	0.021897	0.066171
11	6	0	-2.460604	-0.020034	-0.158026
12	1	0	-3.022022	-0.914620	0.088158
13	1	0	-3.050246	0.852920	0.099490
14	1	0	-2.231302	-0.009602	-1.214104

Compound 6

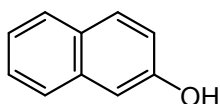


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2	6	0	0.000000	0.000000	1.476971
3	6	0	1.087982	0.000000	2.238613
4	6	0	0.942827	-0.046978	3.687734
5	8	0	-0.073372	-0.324780	4.268870
6	6	0	2.093263	0.360232	4.558260
7	7	0	2.207175	-0.004696	5.836139
8	6	0	3.265389	0.672565	6.324829
9	7	0	3.764245	1.474036	5.448266
10	7	0	3.005770	1.290016	4.358790
11	6	0	1.498763	-1.087055	6.489572
12	6	0	3.368092	1.961170	3.133867
13	1	0	1.004550	0.019321	-0.406640
14	1	0	-0.506613	-0.889847	-0.368337
15	1	0	-0.556248	0.852748	-0.383587
16	1	0	-0.958974	-0.021144	1.976771
17	1	0	2.080294	-0.019271	1.824510
18	1	0	3.632722	0.553635	7.324170

19	1	0	0.476906	-0.797955	6.685268
20	1	0	1.530410	-1.947514	5.831710
21	1	0	2.018909	-1.310170	7.410761
22	1	0	3.977431	2.808441	3.411799
23	1	0	2.478251	2.294020	2.617067
24	1	0	3.936741	1.279107	2.511020
25	17	0	3.296177	-1.896549	3.550363

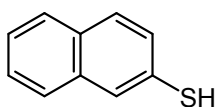
Compound 7



E=-460,995574

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1	6	0	1.401504	0.544323	0.000000
2	6	0	1.983265	-0.687230	0.000000
3	6	0	1.187750	-1.848390	0.000000
4	6	0	-0.165041	-1.745062	0.000000
5	6	0	-0.802588	-0.487688	0.000000
6	6	0	0.000000	0.673981	0.000000
7	6	0	-2.203015	-0.356287	0.000000
8	6	0	-0.633006	1.931792	0.000000
9	6	0	-1.991034	2.027999	0.000000
10	6	0	-2.788214	0.872830	0.000000
11	8	0	3.316230	-0.880714	0.000000
12	1	0	2.011991	1.435219	0.000000
13	1	0	1.682516	-2.805027	0.000000
14	1	0	-0.773423	-2.635835	0.000000
15	1	0	-2.806546	-1.250629	0.000000
16	1	0	-0.022704	2.821369	0.000000
17	1	0	-2.460652	2.998268	0.000000
18	1	0	-3.861854	0.963629	0.000000
19	1	0	3.763107	-0.038882	0.000000

Compound 9

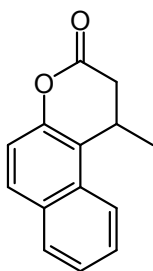


E=-784,029695

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
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2	6	0	0.000000	0.000000	1.362040
3	6	0	1.223414	0.000000	2.062675
4	6	0	2.399936	0.019456	1.384042
5	6	0	2.430071	0.009673	-0.024721
6	6	0	1.206111	-0.008915	-0.724540
7	6	0	3.634164	0.015051	-0.752248
8	6	0	1.223911	-0.018384	-2.132286

9	6	0	2.403660	-0.013188	-2.810292
10	6	0	3.622341	0.003460	-2.113549
11	1	0	-0.932822	0.014115	-0.540979
12	1	0	1.219078	-0.017839	3.139937
13	1	0	3.333269	0.028205	1.924612
14	1	0	4.567886	0.028212	-0.212341
15	1	0	0.285689	-0.030246	-2.664011
16	1	0	2.406941	-0.021721	-3.887895
17	1	0	4.549722	0.007233	-2.662291
18	16	0	-1.541830	-0.088017	2.220718
19	1	0	-1.221226	0.750978	3.209624

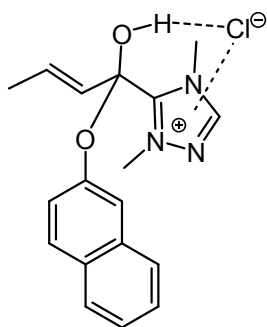
Compound 10



E=-691,015351

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
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1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.485612
3	6	0	1.358670	0.000000	2.175892
4	6	0	1.126906	-0.601589	3.559355
5	6	0	2.358221	-0.767033	1.357870
6	6	0	2.032585	-1.208223	0.108776
7	6	0	3.669435	-1.053902	1.829726
8	6	0	2.855419	-2.071985	-0.629149
9	6	0	4.048813	-2.458619	-0.121369
10	6	0	4.503449	-1.934269	1.104537
11	6	0	4.213494	-0.428841	2.970219
12	6	0	5.788551	-2.235483	1.589837
13	6	0	5.474471	-0.714412	3.400066
14	6	0	6.265757	-1.649214	2.720960
15	1	0	1.703188	1.028996	2.286222
16	8	0	-0.779212	0.567451	-0.692442
17	1	0	0.826628	-1.641392	3.457526
18	1	0	0.321864	-0.066784	4.056608
19	1	0	1.994530	-0.572088	4.203440
20	8	0	0.910358	-0.810435	-0.570688
21	1	0	2.504972	-2.405590	-1.590843
22	1	0	4.681602	-3.138023	-0.669110
23	1	0	3.641614	0.322630	3.485395
24	1	0	6.398309	-2.928564	1.031879
25	1	0	7.255171	-1.879514	3.079584
26	1	0	5.870277	-0.207787	4.265042
27	1	0	-0.514770	-0.924742	1.753241
28	1	0	-0.621196	0.819592	1.822943

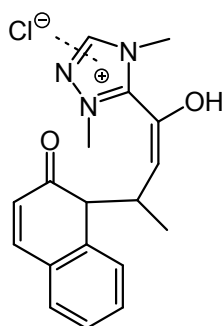
Compound 14



E=-1472,670223

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.320503
3	6	0	1.253228	0.000000	2.145549
4	8	0	1.175722	0.985307	3.150639
5	8	0	2.342419	0.126089	1.349719
6	6	0	1.328871	-1.296031	2.936249
7	6	0	1.084192	2.289233	2.734050
8	7	0	1.577481	-2.484680	2.383760
9	7	0	1.099167	-1.523924	4.212756
10	6	0	-0.128117	2.901265	2.723817
11	6	0	2.254831	2.986672	2.400122
12	6	0	1.534744	-3.383854	3.389242
13	6	0	2.030266	-2.759494	1.035708
14	7	0	1.237802	-2.824060	4.507302
15	6	0	0.909568	-0.603105	5.317829
16	6	0	-1.217673	0.023834	-0.845341
17	1	0	0.957442	0.015550	-0.501256
18	1	0	-0.920796	-0.001098	1.885853
19	1	0	3.136102	-0.091248	1.897229
20	1	0	-1.010831	2.346231	2.997380
21	1	0	1.722041	-4.429868	3.255571
22	1	0	1.410443	-2.226679	0.329433
23	1	0	3.061367	-2.441372	0.944083
24	1	0	1.946583	-3.825052	0.870594
25	1	0	0.075176	0.052392	5.122238
26	1	0	0.723230	-1.222082	6.182750
27	1	0	1.814418	-0.024246	5.446627
28	1	0	-2.124356	0.001023	-0.250254
29	1	0	-1.231033	0.920742	-1.460314
30	1	0	-1.229224	-0.822284	-1.528761
31	17	0	4.288090	-0.905584	3.298852
32	6	0	2.173843	4.298783	2.053406
33	1	0	3.067865	4.845780	1.799617
34	6	0	-0.233963	4.258600	2.369956
35	6	0	0.935593	4.970334	2.025327
36	6	0	0.826989	6.329879	1.674596
37	1	0	1.723087	6.870729	1.413880
38	6	0	-0.383018	6.951899	1.664853
39	1	0	-0.454048	7.992756	1.395113
40	6	0	-1.472265	4.928367	2.351839
41	1	0	-2.363288	4.381416	2.617405
42	6	0	-1.545560	6.242496	2.007315
43	1	0	-2.498562	6.745644	1.997006
44	1	0	3.196061	2.465799	2.439678

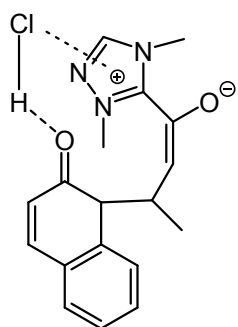
Compound 15



E=-1472,676465

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.489351
3	6	0	1.136180	0.000000	2.176606
4	6	0	1.111629	0.040561	3.636298
5	7	0	0.494165	0.907303	4.411636
6	7	0	1.704569	-0.832532	4.452411
7	7	0	0.686042	0.630387	5.706695
8	6	0	-0.232953	2.099988	4.038268
9	6	0	1.433728	-0.418812	5.707382
10	6	0	2.585470	-1.909282	4.053079
11	6	0	-1.307920	-0.492643	-0.583413
12	6	0	0.398926	1.413263	-0.526012
13	6	0	-0.764209	2.343504	-0.303597
14	8	0	-1.105190	2.645814	0.818827
15	6	0	-1.503082	2.802914	-1.469002
16	1	0	-0.935514	0.032952	2.023595
17	8	0	2.334298	-0.095629	1.596919
18	1	0	-1.248957	2.018110	4.403240
19	1	0	-0.235230	2.198842	2.960903
20	1	0	0.259305	2.946905	4.497714
21	1	0	1.795106	-0.913510	6.586090
22	1	0	2.628026	-2.630709	4.857443
23	1	0	3.568020	-1.497289	3.854494
24	1	0	2.189027	-2.377179	3.161888
25	1	0	3.011563	0.363961	2.162987
26	1	0	-2.147656	0.093545	-0.217146
27	1	0	-1.479767	-1.529003	-0.309385
28	1	0	-1.297274	-0.428083	-1.668237
29	1	0	1.215997	1.751741	0.107424
30	17	0	3.993086	1.292175	3.568539
31	6	0	-1.072227	2.552748	-2.708290
32	1	0	-1.634675	2.921099	-3.553713
33	6	0	0.891143	1.315229	-1.933852
34	6	0	0.150035	1.833042	-2.991189
35	1	0	-2.395725	3.375393	-1.278911
36	6	0	2.090411	0.679421	-2.194189
37	1	0	2.668899	0.295115	-1.366882
38	6	0	0.611586	1.687077	-4.294110
39	1	0	0.029546	2.091282	-5.107445
40	6	0	1.802933	1.043814	-4.544568
41	1	0	2.157304	0.937165	-5.556248
42	6	0	2.547154	0.544982	-3.490000
43	1	0	3.487444	0.053429	-3.677996
44	1	0	0.802591	-0.656573	-0.327270

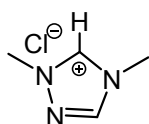
Compound 16



E=-1472,645736

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.457502
3	6	0	1.233325	0.000000	2.052406
4	6	0	1.312900	0.114761	3.530249
5	7	0	0.496869	-0.323116	4.473315
6	7	0	2.340266	0.672373	4.176954
7	7	0	0.949854	-0.035901	5.702291
8	6	0	-0.751786	-1.032053	4.340401
9	6	0	2.065445	0.572268	5.493047
10	6	0	3.491105	1.343871	3.600461
11	6	0	-1.315886	-0.339428	-0.651219
12	6	0	0.630309	1.442422	-0.551797
13	6	0	-0.475941	2.374090	-0.562883
14	8	0	-0.982425	2.828345	0.513490
15	6	0	-1.113768	2.717485	-1.777619
16	1	0	-0.906352	0.173873	2.009999
17	8	0	2.339100	-0.019768	1.465073
18	1	0	-0.869497	-1.635399	5.229108
19	1	0	-0.712730	-1.652934	3.456176
20	1	0	-1.571676	-0.327806	4.261606
21	1	0	2.706062	0.956177	6.260941
22	1	0	4.042781	1.792346	4.416383
23	1	0	3.136639	2.108783	2.923205
24	1	0	4.094806	0.626859	3.065779
25	1	0	-0.373620	2.818444	1.338220
26	1	0	-2.117857	0.297032	-0.284609
27	1	0	-1.574898	-1.367233	-0.415339
28	1	0	-1.266499	-0.245189	-1.732803
29	1	0	1.370581	1.661046	0.215244
30	17	0	0.673364	3.237430	2.792973
31	6	0	-0.567012	2.344021	-2.954906
32	1	0	-1.044858	2.642412	-3.875819
33	6	0	1.264401	1.196692	-1.857490
34	6	0	0.644960	1.593235	-3.041841
35	1	0	-2.001047	3.324285	-1.726568
36	6	0	2.459487	0.496679	-1.910413
37	1	0	2.912885	0.187743	-0.980241
38	6	0	1.232532	1.283791	-4.270276
39	1	0	0.746065	1.595212	-5.180960
40	6	0	2.417721	0.595518	-4.312095
41	1	0	2.873096	0.359035	-5.259033
42	6	0	3.031961	0.204880	-3.127335
43	1	0	3.965815	-0.331905	-3.162706
44	1	0	0.779945	-0.670753	-0.347754

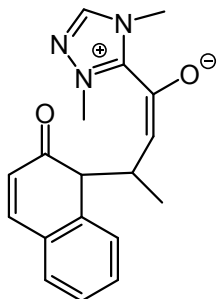
Compound 17



E=-781,674861

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	2.144056
3	1	0	0.361702	0.000000	3.152489
4	7	0	0.804009	-0.012098	1.054423
5	7	0	-1.223559	0.018276	0.466401
6	7	0	-1.244463	0.019150	1.806734
7	6	0	2.256428	-0.037223	1.010760
8	1	0	2.612636	-0.941748	1.486177
9	1	0	2.551646	-0.023730	-0.032167
10	1	0	2.644004	0.834882	1.520860
11	6	0	-2.453423	0.034373	-0.289279
12	1	0	-3.009370	0.928419	-0.039888
13	1	0	-2.204213	0.031397	-1.341155
14	1	0	-3.032100	-0.845288	-0.040441
15	1	0	0.354499	-0.011337	-1.036169
16	17	0	1.824860	-0.068318	-2.590960

Compound 18

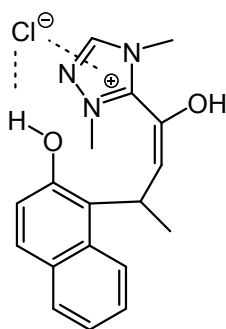


E=-1011,746992

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.482160
3	6	0	1.197870	0.000000	2.121668
4	6	0	1.144143	0.163295	3.596838
5	7	0	0.358718	-0.415028	4.491775
6	7	0	1.976716	0.934837	4.307587
7	7	0	0.644751	-0.024369	5.745463
8	6	0	-0.690107	-1.380918	4.277241
9	6	0	1.627232	0.794446	5.605534
10	6	0	2.998529	1.815013	3.772391
11	6	0	-1.359023	-0.291533	-0.598501
12	6	0	0.633638	1.334541	-0.548811

13	6	0	-0.347641	2.446970	-0.355718
14	8	0	-0.562247	2.918845	0.738458
15	6	0	-1.084897	2.905082	-1.530434
16	1	0	-0.920116	0.139234	2.025486
17	8	0	2.354764	-0.039178	1.619101
18	1	0	-0.664965	-2.079991	5.101747
19	1	0	-0.508100	-1.880223	3.335435
20	1	0	-1.652777	-0.884285	4.243833
21	1	0	2.118738	1.303789	6.410060
22	1	0	3.757717	1.957008	4.529981
23	1	0	2.552753	2.766424	3.507741
24	1	0	3.402955	1.338932	2.889999
25	1	0	-2.108384	0.405022	-0.227638
26	1	0	-1.678495	-1.295039	-0.331694
27	1	0	-1.340312	-0.217739	-1.683177
28	1	0	1.495942	1.498955	0.094240
29	6	0	-0.722939	2.544780	-2.763848
30	1	0	-1.261527	2.930175	-3.617602
31	6	0	1.095329	1.127362	-1.949762
32	6	0	0.403478	1.675890	-3.026415
33	1	0	-1.897438	3.590382	-1.351622
34	6	0	2.202801	0.333329	-2.190730
35	1	0	2.732396	-0.078676	-1.343921
36	6	0	0.821457	1.407802	-4.324807
37	1	0	0.277116	1.836087	-5.152264
38	6	0	1.921116	0.611754	-4.554457
39	1	0	2.241402	0.409619	-5.563223
40	6	0	2.616732	0.078417	-3.482275
41	1	0	3.484248	-0.537476	-3.655667
42	1	0	0.704616	-0.763758	-0.327788

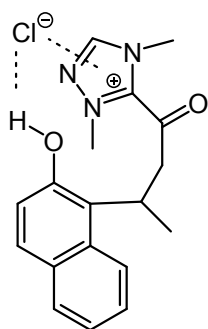
Compound 19



E=-1472,679388

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.503306
3	6	0	1.120341	0.000000	2.221547
4	6	0	1.026127	-0.040476	3.690392
5	7	0	0.644038	0.922981	4.498434
6	7	0	1.262019	-1.102057	4.457243
7	7	0	0.661102	0.527482	5.775789
8	6	0	0.472134	2.322738	4.186569
9	6	0	1.045657	-0.701012	5.729707
10	6	0	1.813239	-2.365434	4.016745
11	6	0	-1.406757	-0.152822	-0.563423
12	6	0	0.706758	1.195644	-0.598666
13	6	0	0.293656	2.461396	-0.275413
14	8	0	-0.674001	2.712951	0.640131
15	6	0	0.839547	3.601250	-0.884044
16	1	0	-0.940803	-0.044169	2.034409
17	8	0	2.328033	-0.075406	1.693061
18	1	0	-0.351932	2.703702	4.772979
19	1	0	0.266849	2.426727	3.130433
20	1	0	1.391011	2.840024	4.435604
21	1	0	1.172457	-1.336595	6.582701
22	1	0	1.170906	-3.175689	4.335910
23	1	0	2.808989	-2.470254	4.428588
24	1	0	1.881674	-2.351543	2.938210
25	1	0	3.013014	0.151703	2.378469
26	1	0	-2.007969	0.735683	-0.387973
27	1	0	-1.913019	-1.002655	-0.113058
28	1	0	-1.362885	-0.310034	-1.635685
29	1	0	-0.853845	1.918394	1.136551
30	17	0	3.930970	0.600604	4.038055
31	6	0	1.809364	3.469862	-1.819595
32	1	0	2.230489	4.341509	-2.294511
33	6	0	1.746585	1.050358	-1.557571
34	6	0	2.294873	2.197529	-2.175104
35	1	0	0.462862	4.564764	-0.584389
36	6	0	2.277247	-0.201115	-1.937255
37	1	0	1.911746	-1.106739	-1.489220
38	6	0	3.312708	2.062472	-3.136475
39	1	0	3.710219	2.957351	-3.589217
40	6	0	3.791737	0.838596	-3.485282
41	1	0	4.573745	0.747047	-4.220638
42	6	0	3.263249	-0.303983	-2.870739
43	1	0	3.646131	-1.276950	-3.132645
44	1	0	0.555667	-0.885094	-0.287318

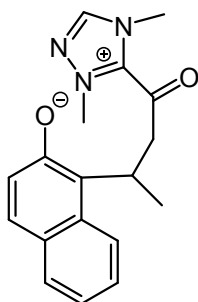
Compound 20



E=-1472,691489

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.486322
3	6	0	1.436726	0.000000	2.052153
4	6	0	1.480495	0.604579	3.449122
5	6	0	2.111083	-1.343605	1.935786
6	6	0	0.737916	-1.097814	-0.721972
7	7	0	0.575157	-2.403295	-0.687642
8	7	0	1.716548	-0.859972	-1.589335
9	7	0	1.439146	-3.020276	-1.497537
10	6	0	-0.422191	-3.188618	0.006150
11	6	0	2.141105	-2.069433	-2.020468
12	6	0	2.225239	0.434586	-2.017206
13	6	0	3.256021	-1.428601	1.170756
14	6	0	1.601906	-2.528492	2.531618
15	6	0	3.903636	-2.662015	0.953047
16	6	0	3.393199	-3.799642	1.478501
17	6	0	2.230820	-3.770933	2.270003
18	6	0	0.455276	-2.555103	3.359052
19	6	0	1.682213	-4.961077	2.781866
20	6	0	-0.056763	-3.724239	3.837948
21	6	0	0.550691	-4.949593	3.538388
22	1	0	2.016069	0.672480	1.425863
23	8	0	-0.464355	0.861070	-0.686305
24	1	0	-1.003747	-3.722145	-0.734409
25	1	0	-1.066943	-2.530933	0.570431
26	1	0	0.069826	-3.884458	0.673644
27	1	0	2.973952	-2.192200	-2.684849
28	1	0	3.241354	0.282820	-2.357848
29	1	0	2.232579	1.108900	-1.173063
30	1	0	1.590117	0.823725	-2.802239
31	1	0	0.895050	0.051146	4.174456
32	1	0	1.111941	1.626585	3.428472
33	1	0	2.507087	0.623112	3.799658
34	8	0	3.743177	-0.318133	0.609397
35	1	0	4.789362	-2.672489	0.339610
36	1	0	3.874080	-4.746423	1.291515
37	1	0	-0.027704	-1.637561	3.639569
38	1	0	2.182181	-5.890542	2.558482
39	1	0	0.136941	-5.867584	3.921169
40	1	0	-0.932823	-3.701725	4.465533
41	1	0	-0.560094	-0.854758	1.853211
42	1	0	-0.528521	0.899842	1.783613
43	1	0	4.392237	-0.540801	-0.093235
44	17	0	5.337571	-1.080093	-1.836412

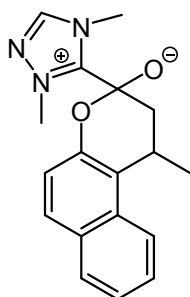
Compound 21



E=-1011,757940

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.496411
3	6	0	1.407988	0.000000	2.131751
4	6	0	1.348687	0.707110	3.473305
5	6	0	2.002333	-1.374088	2.009135
6	6	0	-0.070758	-1.261432	-0.807998
7	7	0	-0.440104	-2.492680	-0.493088
8	7	0	0.147804	-1.273837	-2.129174
9	7	0	-0.426320	-3.301790	-1.569041
10	6	0	-0.816740	-3.081436	0.777862
11	6	0	-0.059388	-2.540842	-2.538132
12	6	0	0.748159	-0.217772	-2.921514
13	6	0	2.352984	-1.657782	0.682167
14	6	0	2.105605	-2.380140	2.999388
15	6	0	2.878670	-2.941603	0.363057
16	6	0	3.011931	-3.898615	1.308660
17	6	0	2.622842	-3.658289	2.641847
18	6	0	1.690700	-2.235369	4.347191
19	6	0	2.732790	-4.677601	3.602376
20	6	0	1.801918	-3.247270	5.253436
21	6	0	2.335069	-4.489775	4.890159
22	1	0	2.010375	0.621324	1.472724
23	8	0	-0.095315	1.025233	-0.625523
24	1	0	-1.077258	-4.105830	0.557039
25	1	0	-1.678829	-2.571295	1.187887
26	1	0	0.017645	-3.054270	1.467688
27	1	0	0.068426	-2.862050	-3.552284
28	1	0	1.046204	-0.653047	-3.866326
29	1	0	1.613109	0.141351	-2.380425
30	1	0	0.043318	0.585063	-3.075236
31	1	0	0.518628	0.378264	4.092162
32	1	0	1.209091	1.770955	3.299962
33	1	0	2.269668	0.578926	4.033265
34	8	0	2.135836	-0.797025	-0.248301
35	1	0	3.160149	-3.119963	-0.663001
36	1	0	3.407125	-4.870906	1.054835
37	1	0	1.274297	-1.306804	4.680207
38	1	0	3.141060	-5.626597	3.288568
39	1	0	2.423436	-5.280246	5.616958
40	1	0	1.472743	-3.083658	6.267502
41	1	0	-0.579347	-0.813898	1.917364
42	1	0	-0.500978	0.929956	1.752348

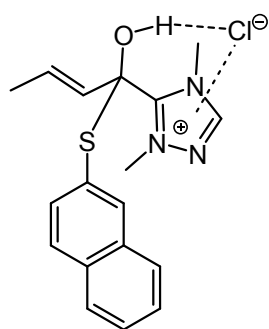
Compound 22



E=-1011,768419

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.520961
3	6	0	1.443397	0.000000	2.009534
4	6	0	1.423895	-0.405651	3.479282
5	6	0	2.298930	-0.917583	1.173101
6	6	0	-1.439167	-0.165740	-0.543610
7	7	0	-2.334874	-1.116668	-0.352763
8	7	0	-2.034759	0.724901	-1.341126
9	7	0	-3.486104	-0.869496	-0.995613
10	6	0	-2.218052	-2.326532	0.429200
11	6	0	-3.277224	0.253036	-1.589413
12	6	0	-1.494116	1.957544	-1.896034
13	6	0	1.760267	-1.596396	0.108407
14	6	0	3.681629	-1.101173	1.445686
15	6	0	2.495394	-2.576383	-0.585907
16	6	0	3.776754	-2.846700	-0.246869
17	6	0	4.416451	-2.095736	0.758489
18	6	0	4.390857	-0.287836	2.356462
19	6	0	5.775654	-2.294657	1.056288
20	6	0	5.715460	-0.487041	2.608895
21	6	0	6.418090	-1.516939	1.970031
22	1	0	1.830778	1.013179	1.910597
23	8	0	0.613815	0.947997	-0.563235
24	1	0	-2.773816	-3.097627	-0.085702
25	1	0	-2.640057	-2.167812	1.414738
26	1	0	-1.173107	-2.589483	0.493380
27	1	0	-3.988764	0.759736	-2.209867
28	1	0	-0.643346	1.727123	-2.517515
29	1	0	-1.154264	2.595302	-1.094930
30	1	0	-2.290503	2.426931	-2.459455
31	1	0	1.019835	-1.410612	3.577730
32	1	0	0.783000	0.268823	4.043141
33	1	0	2.402899	-0.403667	3.941573
34	8	0	0.514153	-1.386337	-0.340212
35	1	0	1.999913	-3.092139	-1.391898
36	1	0	4.334839	-3.609371	-0.767050
37	1	0	3.884153	0.533434	2.833676
38	1	0	6.307136	-3.071627	0.528325
39	1	0	7.462257	-1.673757	2.185387
40	1	0	6.229874	0.162349	3.298934
41	1	0	-0.516222	-0.874231	1.916306
42	1	0	-0.510888	0.887381	1.886786

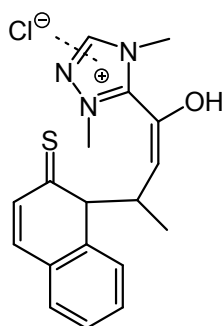
Compound 23



E=-1795,703624

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.322083
3	6	0	1.254212	0.000000	2.133993
4	8	0	2.338480	-0.230226	1.344551
5	6	0	1.154592	-1.105518	3.165540
6	6	0	1.953048	2.564002	1.561078
7	7	0	1.240887	-2.391992	2.810775
8	7	0	0.857140	-1.106150	4.450076
9	6	0	1.078940	3.207714	0.736635
10	6	0	3.340025	2.621431	1.320533
11	6	0	1.045441	-3.111168	3.934515
12	6	0	1.658741	-2.940108	1.535745
13	7	0	0.801271	-2.352268	4.942143
14	6	0	0.771006	-0.013642	5.397050
15	6	0	-1.218669	0.084960	-0.841559
16	1	0	0.955702	-0.034739	-0.502529
17	1	0	-0.919088	0.063893	1.886397
18	1	0	3.106818	-0.389064	1.942398
19	1	0	0.019710	3.159728	0.930918
20	1	0	1.086728	-4.181045	3.966359
21	1	0	1.134634	-2.436418	0.736338
22	1	0	2.726186	-2.795218	1.428313
23	1	0	1.415083	-3.994026	1.539385
24	1	0	0.017910	0.698841	5.088702
25	1	0	0.495433	-0.462873	6.339390
26	1	0	1.740443	0.462606	5.473908
27	1	0	-2.124579	0.075145	-0.244273
28	1	0	-1.206729	0.998027	-1.433555
29	1	0	-1.260433	-0.740975	-1.547789
30	17	0	4.111808	-1.017636	3.564539
31	6	0	3.814388	3.319686	0.257046
32	1	0	4.875128	3.367031	0.068823
33	6	0	1.547952	3.937143	-0.372252
34	6	0	2.937430	3.993309	-0.616634
35	6	0	3.403167	4.724833	-1.725119
36	1	0	4.465010	4.768407	-1.908713
37	6	0	2.531752	5.365192	-2.551282
38	1	0	2.900190	5.921630	-3.397466
39	6	0	0.669896	4.610299	-1.243618
40	1	0	-0.390367	4.564913	-1.049919
41	6	0	1.149679	5.307345	-2.308953
42	1	0	0.470967	5.819820	-2.970717
43	1	0	4.006297	2.106939	1.993204
44	16	0	1.371089	1.677722	2.966396

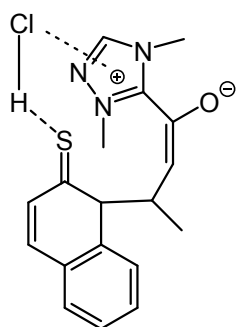
Compound 24



E=-1795,697422

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.488786
3	6	0	1.106437	0.000000	2.226821
4	8	0	2.334126	0.010997	1.718993
5	6	0	1.018093	-0.173302	3.679565
6	6	0	0.688537	2.379355	-0.077462
7	7	0	1.658697	-1.115337	4.376729
8	7	0	0.286509	0.488786	4.552102
9	6	0	-0.319648	1.413560	-0.613842
10	6	0	1.977528	2.357086	-0.711411
11	6	0	1.297000	-0.944662	5.664823
12	6	0	2.646472	-2.044699	3.869066
13	7	0	0.450812	0.017070	5.793964
14	6	0	-0.560511	1.638105	4.341663
15	6	0	-0.980399	-1.052882	-0.487105
16	1	0	1.002072	-0.252287	-0.339735
17	1	0	-0.951111	-0.079852	1.994336
18	1	0	2.944865	0.466020	2.361544
19	1	0	-1.312337	1.706144	-0.284926
20	1	0	1.670321	-1.546197	6.468739
21	1	0	2.294017	-2.466413	2.937425
22	1	0	3.575623	-1.510085	3.712132
23	1	0	2.776391	-2.829021	4.601874
24	1	0	-0.412469	2.002564	3.334839
25	1	0	-1.595185	1.354684	4.491572
26	1	0	-0.274330	2.395831	5.058075
27	1	0	-2.004370	-0.771751	-0.247476
28	1	0	-0.909624	-1.203273	-1.557583
29	1	0	-0.771550	-2.000731	-0.000391
30	17	0	3.775120	1.283297	3.915840
31	6	0	2.107764	1.890198	-1.961289
32	1	0	3.070313	1.922468	-2.448252
33	6	0	-0.262040	1.307056	-2.105881
34	6	0	0.973219	1.449275	-2.738354
35	6	0	1.073540	1.247471	-4.108467
36	1	0	2.033558	1.356547	-4.587827
37	6	0	-0.043797	0.936131	-4.852092
38	1	0	0.038881	0.789309	-5.916071
39	6	0	-1.378115	1.011046	-2.862478
40	1	0	-2.338054	0.920969	-2.378367
41	6	0	-1.273735	0.831917	-4.229406
42	1	0	-2.155092	0.611213	-4.808786
43	1	0	2.807116	2.794723	-0.183448
44	16	0	0.372259	3.350873	1.189959

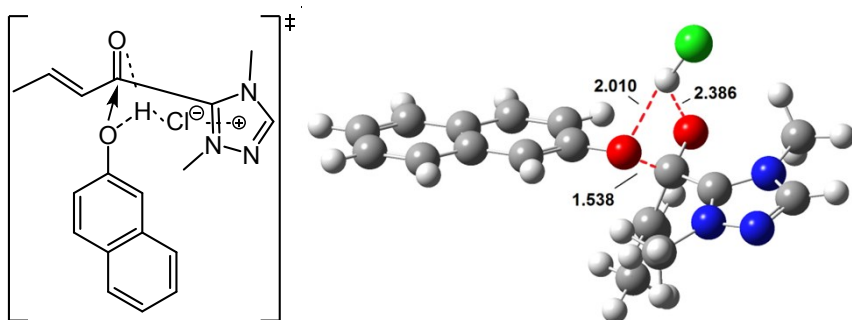
Compound 25



E=-1795,665993

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.471572
3	6	0	1.222237	0.000000	2.077885
4	6	0	1.272890	-0.057420	3.560959
5	7	0	0.468466	0.442249	4.485145
6	7	0	2.273805	-0.633346	4.239681
7	7	0	0.911476	0.195606	5.727565
8	6	0	-0.728811	1.228679	4.314898
9	6	0	2.006882	-0.455769	5.551312
10	6	0	3.430455	-1.318734	3.693940
11	6	0	-1.319517	-0.401760	-0.614246
12	6	0	0.567928	1.396941	-0.578581
13	6	0	-0.506540	2.400902	-0.515498
14	16	0	-0.924209	3.144536	0.901049
15	6	0	-1.244727	2.675040	-1.705138
16	1	0	-0.921352	-0.045890	2.024248
17	8	0	2.345622	0.024519	1.516209
18	1	0	-0.738317	1.976845	5.094959
19	1	0	-1.604034	0.594332	4.397759
20	1	0	-0.700297	1.692383	3.338399
21	1	0	2.639096	-0.816445	6.337630
22	1	0	3.980800	-1.737891	4.526309
23	1	0	4.029076	-0.616498	3.134998
24	1	0	3.105475	-2.106116	3.028495
25	1	0	0.854062	3.172379	2.041307
26	1	0	-2.127541	0.241561	-0.273380
27	1	0	-1.560057	-1.420821	-0.324865
28	1	0	-1.285647	-0.359669	-1.699526
29	1	0	1.379350	1.624789	0.109242
30	17	0	1.905604	3.352394	2.832033
31	6	0	-0.801854	2.266972	-2.909051
32	1	0	-1.355353	2.533946	-3.796900
33	6	0	1.117251	1.142060	-1.934297
34	6	0	0.416581	1.528059	-3.074275
35	1	0	-2.128404	3.284755	-1.619010
36	6	0	2.311721	0.454523	-2.068870
37	1	0	2.836159	0.157871	-1.172285
38	6	0	0.920006	1.217741	-4.336024
39	1	0	0.369112	1.520726	-5.212688
40	6	0	2.108260	0.539173	-4.459543
41	1	0	2.498475	0.304397	-5.435923
42	6	0	2.806213	0.160341	-3.321593
43	1	0	3.741997	-0.365918	-3.417525
44	1	0	0.779189	-0.687694	-0.325838

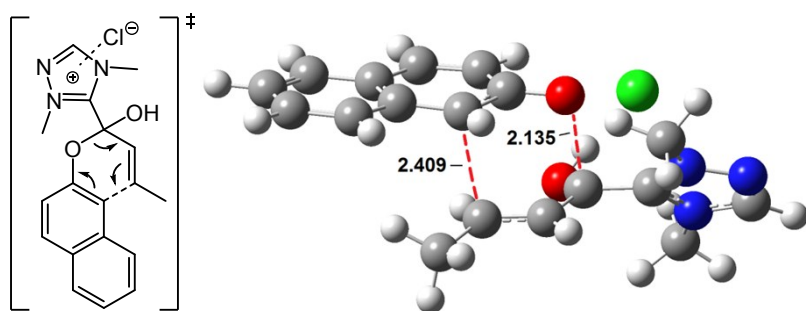
Compound TS1



E=-1472,623304; 1 imaginary frequencies= -261.3459

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.319110
3	6	0	1.307019	0.000000	2.079629
4	8	0	1.183077	1.110930	3.135777
5	8	0	2.385265	0.053309	1.421959
6	6	0	1.299127	-1.204283	3.056188
7	6	0	0.847632	2.348880	2.703379
8	7	0	2.187031	-2.201373	3.010366
9	7	0	0.474010	-1.513787	4.038716
10	6	0	0.090225	3.137279	3.519653
11	6	0	1.293953	2.843369	1.459208
12	6	0	1.842531	-3.068802	3.988029
13	6	0	3.324921	-2.379701	2.120030
14	7	0	0.798370	-2.673347	4.628356
15	6	0	-0.693746	-0.801090	4.501659
16	6	0	-1.203758	0.036670	-0.864742
17	1	0	0.972863	-0.012397	-0.474044
18	1	0	-0.925382	0.029177	1.879584
19	1	0	3.141549	0.882748	3.527059
20	1	0	-0.229776	2.756205	4.476772
21	1	0	2.385001	-3.969027	4.196208
22	1	0	2.988320	-2.358735	1.095267
23	1	0	4.031541	-1.578746	2.270264
24	1	0	3.763729	-3.339276	2.362305
25	1	0	-0.597666	0.235370	4.218242
26	1	0	-1.583476	-1.242121	4.067582
27	1	0	-0.726393	-0.894639	5.578226
28	1	0	-2.120092	0.038172	-0.283342
29	1	0	-1.195083	0.927303	-1.489821
30	1	0	-1.223291	-0.816450	-1.539960
31	17	0	4.152553	0.605700	4.290234
32	6	0	0.950460	4.098166	1.069127
33	1	0	1.291475	4.475140	0.117311
34	6	0	-0.264590	4.443651	3.136574
35	6	0	0.163729	4.934516	1.884565
36	6	0	-0.200157	6.236753	1.495803
37	1	0	0.134286	6.603102	0.537535
38	6	0	-0.958985	7.021636	2.308880
39	1	0	-1.232849	8.017558	2.001470
40	6	0	-1.046281	5.279918	3.958281
41	1	0	-1.373016	4.907757	4.916813
42	6	0	-1.385839	6.534939	3.554522
43	1	0	-1.984882	7.162559	4.194336
44	1	0	1.908470	2.205166	0.849625

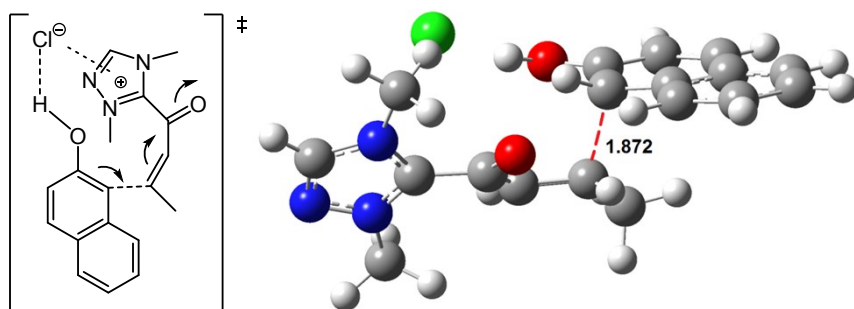
Compound TS2



E=-1472,625461; 1 imaginary frequencies= -293.9134

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.368498
3	6	0	1.210378	0.000000	2.049094
4	8	0	1.538363	2.093649	1.786777
5	8	0	2.291699	-0.422358	1.456002
6	6	0	1.217346	0.008218	3.518626
7	6	0	1.644653	2.176500	0.529798
8	7	0	1.812521	-0.916401	4.281055
9	7	0	0.594680	0.821216	4.350838
10	6	0	0.509247	2.337213	-0.286918
11	6	0	2.911460	1.994458	-0.122573
12	6	0	1.536527	-0.584218	5.558107
13	6	0	2.572873	-2.081293	3.858845
14	7	0	0.790880	0.463995	5.623144
15	6	0	-0.255529	1.958749	4.072307
16	6	0	-1.240504	-0.092052	-0.802288
17	1	0	0.930442	-0.232669	-0.495680
18	1	0	-0.909496	0.160911	1.924088
19	1	0	3.129142	-0.099455	1.927328
20	1	0	-0.427840	2.573753	0.191328
21	1	0	1.898371	-1.134898	6.402888
22	1	0	2.074143	-2.547153	3.020486
23	1	0	3.572169	-1.769668	3.580764
24	1	0	2.601935	-2.767990	4.693403
25	1	0	-0.048199	2.293583	3.067031
26	1	0	-1.290318	1.663643	4.202729
27	1	0	-0.000717	2.730859	4.784573
28	1	0	-2.105749	0.269991	-0.255697
29	1	0	-1.151487	0.452124	-1.737110
30	1	0	-1.417075	-1.135438	-1.061638
31	17	0	4.601360	0.462891	2.952266
32	6	0	3.018362	2.070280	-1.464026
33	1	0	3.979949	1.948070	-1.938492
34	6	0	0.627943	2.500233	-1.687730
35	6	0	1.889864	2.331863	-2.291846
36	6	0	2.001952	2.457383	-3.680612
37	1	0	2.970535	2.326835	-4.137405
38	6	0	0.908629	2.746840	-4.450498
39	1	0	1.010171	2.842969	-5.518944
40	6	0	-0.476548	2.808538	-2.496920
41	1	0	-1.437652	2.959342	-2.029860
42	6	0	-0.340237	2.929127	-3.851896
43	1	0	-1.195991	3.170976	-4.460810
44	1	0	3.766757	1.824081	0.510817

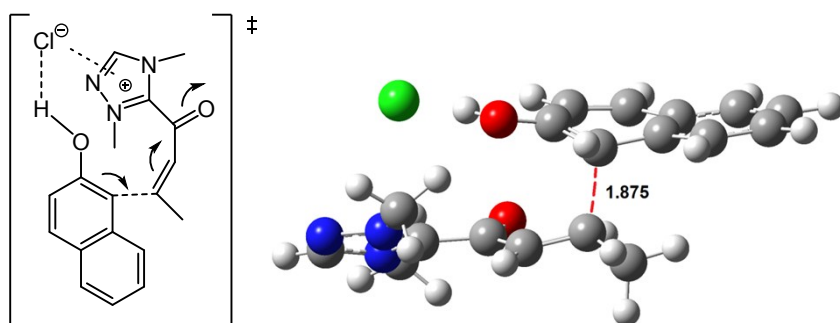
Compound TS3



E=-1472,644413; 1 imaginary frequencies= -350.2907

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.420007
3	6	0	1.237842	0.000000	2.040688
4	6	0	1.291788	0.053514	3.528432
5	7	0	0.453357	-0.420652	4.432255
6	7	0	2.312929	0.567486	4.218275
7	7	0	0.885735	-0.197984	5.680138
8	6	0	-0.801722	-1.109285	4.246185
9	6	0	2.011521	0.408220	5.522009
10	6	0	3.478125	1.261122	3.698987
11	6	0	-1.279921	-0.295313	-0.715206
12	6	0	0.668192	1.658546	-0.552738
13	6	0	-0.499483	2.460219	-0.532296
14	8	0	-1.059077	2.835003	0.568522
15	6	0	-1.165229	2.777592	-1.737755
16	1	0	-0.904855	0.187875	1.970332
17	8	0	2.340560	0.002158	1.475413
18	1	0	-0.948381	-1.735074	5.114654
19	1	0	-0.749499	-1.706892	3.346874
20	1	0	-1.609168	-0.391006	4.168254
21	1	0	2.640902	0.747573	6.319586
22	1	0	4.020144	1.656118	4.548005
23	1	0	3.137229	2.069039	3.065698
24	1	0	4.086676	0.571945	3.134225
25	1	0	-0.445731	2.825355	1.364793
26	1	0	-2.098229	0.306544	-0.329970
27	1	0	-1.529646	-1.341841	-0.558631
28	1	0	-1.192211	-0.131174	-1.784608
29	1	0	1.354737	1.778182	0.276660
30	17	0	0.691028	3.155214	2.860657
31	6	0	-0.611358	2.448014	-2.926694
32	1	0	-1.116394	2.718753	-3.841302
33	6	0	1.295764	1.423234	-1.837328
34	6	0	0.635550	1.767235	-3.021760
35	1	0	-2.091990	3.321404	-1.673056
36	6	0	2.529625	0.781564	-1.903416
37	1	0	3.014884	0.505457	-0.979638
38	6	0	1.226084	1.468515	-4.254353
39	1	0	0.711349	1.739971	-5.162497
40	6	0	2.442305	0.842718	-4.304150
41	1	0	2.895812	0.615337	-5.254411
42	6	0	3.095496	0.500048	-3.121279
43	1	0	4.053931	0.008949	-3.164871
44	1	0	0.852119	-0.533460	-0.401742

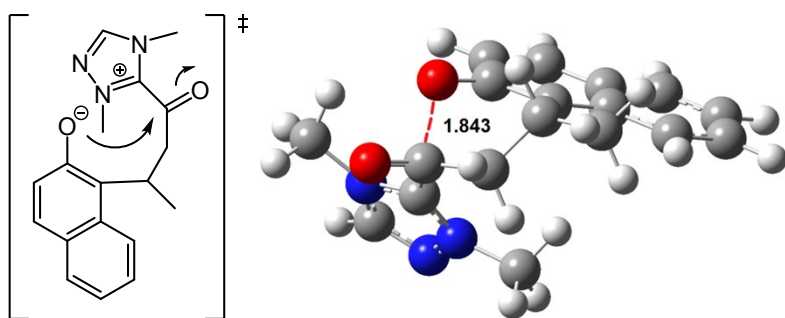
Compound TS4



E=-1472.640764; 1 imaginary frequencies= -362.7169

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.421001
3	6	0	1.230018	0.000000	2.055712
4	6	0	1.295326	-0.233611	3.526040
5	7	0	0.504045	-0.942324	4.311960
6	7	0	2.292378	0.190752	4.304034
7	7	0	0.964367	-0.989174	5.567358
8	6	0	-0.657442	-1.731943	3.970998
9	6	0	2.054056	-0.304142	5.534845
10	6	0	3.505635	0.870378	3.893812
11	6	0	-1.278738	0.433116	-0.656210
12	6	0	0.296619	-1.732490	-0.652424
13	6	0	1.427493	-2.122562	0.121856
14	8	0	1.181214	-2.585942	1.294943
15	6	0	2.735919	-1.907038	-0.367854
16	1	0	0.894560	0.446493	-0.419930
17	1	0	-0.923297	-0.093079	1.964699
18	8	0	2.325452	0.123658	1.493297
19	1	0	-0.737806	-2.497486	4.728738
20	1	0	-0.500620	-2.177723	2.997883
21	1	0	-1.549098	-1.116095	3.972490
22	1	0	2.700524	-0.141352	6.373122
23	1	0	4.129143	0.158718	3.369094
24	1	0	3.993636	1.232990	4.789017
25	1	0	3.261857	1.692211	3.237803
26	1	0	1.997781	-2.677962	1.895902
27	1	0	-2.120936	-0.165263	-0.317421
28	1	0	-1.227376	0.389257	-1.736266
29	1	0	-1.472700	1.464953	-0.375608
30	1	0	-0.629299	-2.194937	-0.342125
31	17	0	3.326891	-2.781777	3.202766
32	6	0	2.899166	-1.546240	-1.658181
33	1	0	3.894405	-1.385479	-2.041975
34	6	0	0.501983	-1.615848	-2.084859
35	6	0	1.804290	-1.435621	-2.567887
36	1	0	3.564241	-2.050342	0.304462
37	6	0	-0.555491	-1.654261	-2.989764
38	1	0	-1.554702	-1.831646	-2.624381
39	6	0	2.009918	-1.238564	-3.936220
40	1	0	3.015481	-1.089935	-4.296820
41	6	0	0.954826	-1.257095	-4.809340
42	1	0	1.122012	-1.113979	-5.863882
43	6	0	-0.333265	-1.483263	-4.333519
44	1	0	-1.160119	-1.527436	-5.023109

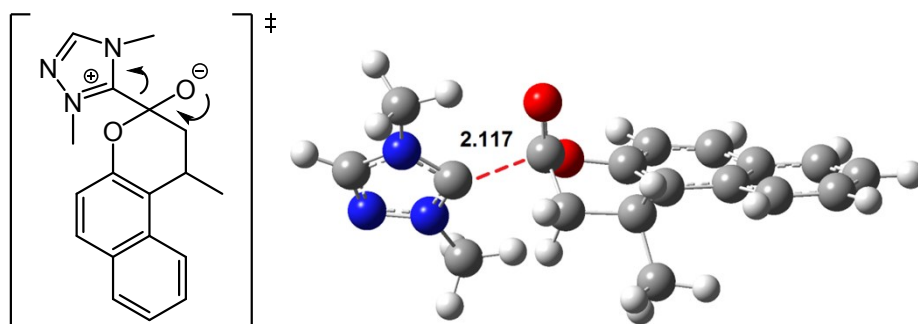
Compound TS5



E=-1011,754778; 1 imaginary frequencies= -100.2999

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.510984
3	6	0	1.364874	0.000000	2.201742
4	6	0	1.158538	0.039114	3.701121
5	6	0	2.299621	-1.004263	1.571521
6	6	0	0.066288	-1.329447	-0.744577
7	7	0	-0.086688	-2.590459	-0.380657
8	7	0	0.218186	-1.357299	-2.071380
9	7	0	-0.031206	-3.425664	-1.433203
10	6	0	-0.307235	-3.172597	0.926949
11	6	0	0.157722	-2.651753	-2.443542
12	6	0	0.432244	-0.222108	-2.951256
13	6	0	2.501107	-0.697123	0.231977
14	6	0	2.989087	-2.107209	2.141178
15	6	0	3.410012	-1.439896	-0.554711
16	6	0	4.101444	-2.468874	-0.011741
17	6	0	3.902879	-2.838316	1.332340
18	6	0	2.816660	-2.572116	3.467870
19	6	0	4.603368	-3.934434	1.866408
20	6	0	3.504358	-3.644541	3.952504
21	6	0	4.418781	-4.338677	3.151582
22	1	0	1.800659	0.959100	1.920084
23	8	0	-0.643710	0.838929	-0.618565
24	1	0	-0.255013	-4.242151	0.787450
25	1	0	-1.287418	-2.900235	1.297707
26	1	0	0.469525	-2.854617	1.608527
27	1	0	0.259594	-2.982774	-3.457460
28	1	0	0.880456	-0.596172	-3.862939
29	1	0	1.093350	0.466697	-2.446282
30	1	0	-0.511880	0.263204	-3.153159
31	1	0	0.575189	-0.802936	4.065601
32	1	0	0.604186	0.940291	3.951075
33	1	0	2.099143	0.071468	4.241180
34	8	0	1.799823	0.262243	-0.315765
35	1	0	3.541640	-1.146868	-1.584432
36	1	0	4.806020	-3.033459	-0.603050
37	1	0	2.124976	-2.078327	4.120328
38	1	0	5.295100	-4.456060	1.222587
39	1	0	4.960602	-5.181269	3.548186
40	1	0	3.338713	-3.960395	4.970223
41	1	0	-0.608178	-0.821624	1.882622
42	1	0	-0.526222	0.913776	1.770732

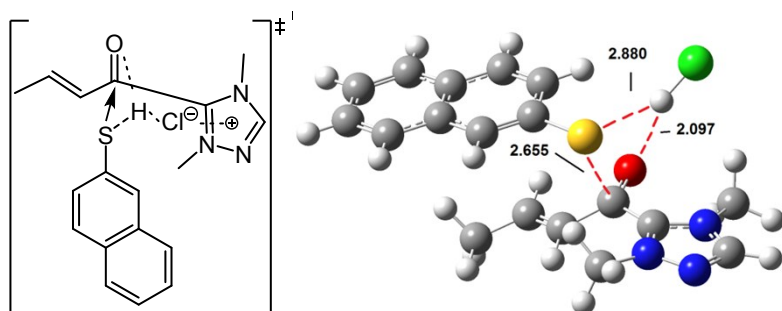
Compound TS6



E=-1011,752008; 1 imaginary frequencies= -166.1919

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.493236
3	6	0	1.443694	0.000000	1.998123
4	6	0	1.423928	-0.532544	3.426564
5	6	0	2.327775	-0.818461	1.093585
6	6	0	-1.973445	-0.681508	-0.352379
7	7	0	-2.521125	-1.889378	-0.331672
8	7	0	-2.921511	0.057378	-0.959863
9	7	0	-3.750776	-1.955206	-0.886874
10	6	0	-1.943321	-3.088651	0.213218
11	6	0	-3.970436	-0.746390	-1.263713
12	6	0	-2.840802	1.476822	-1.224467
13	6	0	1.813810	-1.436322	-0.015858
14	6	0	3.717552	-0.968341	1.352134
15	6	0	2.576340	-2.332580	-0.786014
16	6	0	3.871642	-2.568529	-0.473062
17	6	0	4.488249	-1.870548	0.584434
18	6	0	4.390705	-0.201900	2.326437
19	6	0	5.857484	-2.029887	0.859856
20	6	0	5.724584	-0.359472	2.557039
21	6	0	6.468649	-1.298752	1.831823
22	1	0	1.808188	1.027544	2.002439
23	8	0	0.158864	0.977588	-0.685497
24	1	0	-1.944732	-3.862929	-0.544103
25	1	0	-2.519854	-3.420380	1.069180
26	1	0	-0.926618	-2.866605	0.501412
27	1	0	-4.861683	-0.411779	-1.756940
28	1	0	-3.089189	1.668970	-2.261438
29	1	0	-1.825420	1.792463	-1.033362
30	1	0	-3.527529	2.015303	-0.581055
31	1	0	1.051153	-1.553806	3.430212
32	1	0	0.756787	0.070367	4.037924
33	1	0	2.399791	-0.538905	3.895672
34	8	0	0.546229	-1.235600	-0.453876
35	1	0	2.096372	-2.807181	-1.625344
36	1	0	4.457113	-3.263441	-1.053941
37	1	0	3.850104	0.549370	2.875719
38	1	0	6.420760	-2.736048	0.269685
39	1	0	7.520454	-1.423282	2.029693
40	1	0	6.213447	0.251783	3.298274
41	1	0	-0.500762	-0.897725	1.844442
42	1	0	-0.539624	0.863634	1.864493

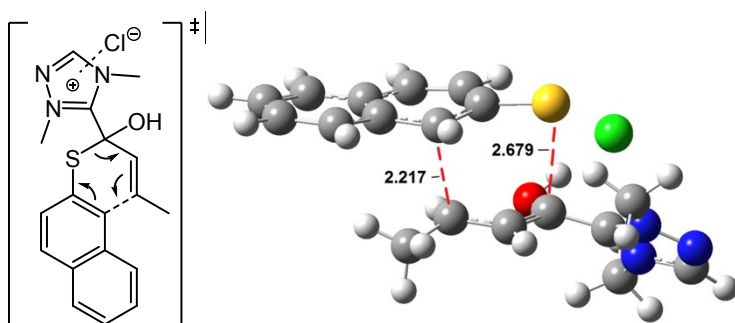
Compound TS7



E=-1795,665399; 1 imaginary frequencies= -321.6409

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.330535
3	6	0	1.258535	0.000000	2.055986
4	16	0	1.264978	2.607060	2.559145
5	8	0	2.353734	-0.136031	1.527090
6	6	0	1.195514	-0.245417	3.532082
7	6	0	1.099941	2.866356	0.851023
8	7	0	2.145815	-0.925823	4.190405
9	7	0	0.259572	0.013777	4.435125
10	6	0	-0.098467	3.243764	0.291029
11	6	0	2.194590	2.640913	-0.019775
12	6	0	1.735453	-1.013962	5.474178
13	6	0	3.363852	-1.536758	3.680855
14	7	0	0.592244	-0.450745	5.645189
15	6	0	-0.983678	0.736663	4.292887
16	6	0	-1.204782	-0.027954	-0.854039
17	1	0	0.962610	0.019320	-0.491928
18	1	0	-0.926394	-0.006296	1.878934
19	1	0	3.779280	1.253228	2.186384
20	1	0	-0.945334	3.424215	0.934535
21	1	0	2.302228	-1.498901	6.243197
22	1	0	3.146181	-2.082688	2.775756
23	1	0	4.104607	-0.779545	3.472371
24	1	0	3.723801	-2.209882	4.447611
25	1	0	-0.830809	1.530882	3.571853
26	1	0	-1.772861	0.060799	3.984186
27	1	0	-1.214331	1.149726	5.264140
28	1	0	-2.119915	-0.024990	-0.271045
29	1	0	-1.210696	0.833194	-1.519608
30	1	0	-1.197760	-0.911927	-1.489348
31	17	0	5.014544	1.534897	2.449681
32	6	0	2.068287	2.773575	-1.366623
33	1	0	2.916597	2.594310	-2.009257
34	6	0	-0.253977	3.404032	-1.094647
35	6	0	0.843772	3.152252	-1.948599
36	6	0	0.678155	3.291105	-3.338836
37	1	0	1.523343	3.101274	-3.982356
38	6	0	-0.522469	3.657540	-3.866029
39	1	0	-0.638119	3.760411	-4.932619
40	6	0	-1.484818	3.784113	-1.670879
41	1	0	-2.322772	3.978856	-1.019497
42	6	0	-1.616437	3.906203	-3.019959
43	1	0	-2.562761	4.198491	-3.445655
44	1	0	3.144033	2.365152	0.403156

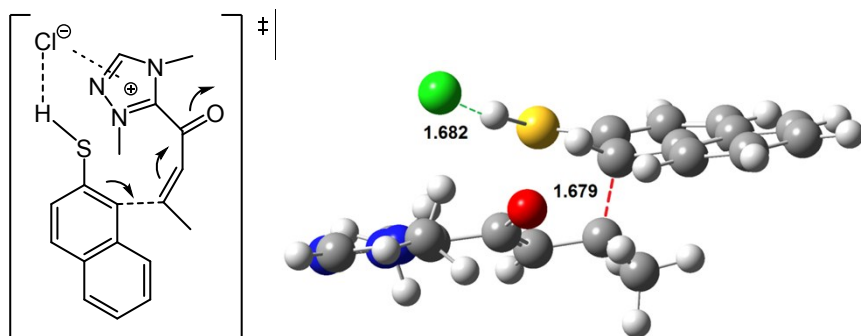
Compound TS8



E=-1795,666118; 1 imaginary frequencies= -346.2935

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.386745
3	6	0	1.186007	0.000000	2.087493
4	8	0	2.308354	-0.274816	1.467554
5	6	0	1.180501	-0.184374	3.542904
6	6	0	1.466226	2.314484	0.246185
7	7	0	1.924032	-1.089095	4.194191
8	7	0	0.428815	0.393842	4.465381
9	6	0	0.308846	2.128774	-0.537553
10	6	0	2.732342	2.069587	-0.365974
11	6	0	1.593931	-0.980751	5.497847
12	6	0	2.848333	-2.073436	3.651369
13	7	0	0.683048	-0.091130	5.684820
14	6	0	-0.599255	1.399035	4.323910
15	6	0	-1.251037	-0.324669	-0.735144
16	1	0	0.935185	-0.252172	-0.478598
17	1	0	-0.929019	0.059180	1.929824
18	1	0	3.121695	0.100599	1.942082
19	1	0	-0.634470	2.432703	-0.112714
20	1	0	2.042145	-1.573500	6.269550
21	1	0	2.419556	-2.512426	2.762008
22	1	0	3.789251	-1.589638	3.419190
23	1	0	2.983747	-2.834770	4.407232
24	1	0	-0.485830	1.884238	3.364006
25	1	0	-1.571146	0.926650	4.409081
26	1	0	-0.467047	2.116260	5.121921
27	1	0	-2.121829	0.127432	-0.268762
28	1	0	-1.203595	-0.019968	-1.773116
29	1	0	-1.392737	-1.404535	-0.725774
30	17	0	4.603122	0.709655	2.906914
31	6	0	2.825337	1.827961	-1.689129
32	1	0	3.789894	1.650985	-2.138754
33	6	0	0.414419	2.055585	-1.961700
34	6	0	1.679974	1.855665	-2.537192
35	6	0	1.785866	1.739705	-3.926546
36	1	0	2.758996	1.580325	-4.363537
37	6	0	0.677840	1.844634	-4.723659
38	1	0	0.773313	1.761883	-5.793759
39	6	0	-0.702662	2.175981	-2.795068
40	1	0	-1.668363	2.361368	-2.350973
41	6	0	-0.574444	2.075302	-4.154764
42	1	0	-1.440705	2.178687	-4.787217
43	1	0	3.606528	2.100131	0.263315
44	16	0	1.347509	2.665731	1.878634

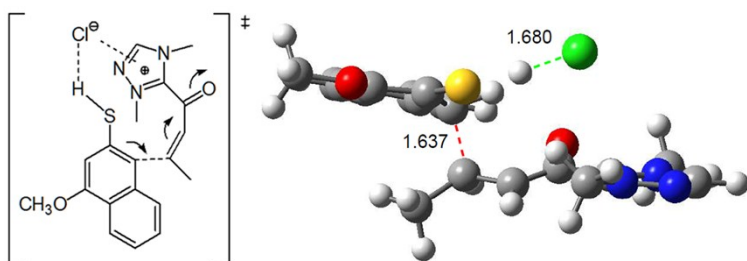
Compound TS9



E=-1795,661078; 1 imaginary frequencies= -265.0697

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.453338
3	6	0	1.240283	0.000000	2.044449
4	6	0	1.348139	-0.005718	3.526877
5	7	0	0.484592	0.332410	4.470516
6	7	0	2.460825	-0.366733	4.178123
7	7	0	1.004441	0.201311	5.698060
8	6	0	-0.842766	0.881322	4.339239
9	6	0	2.201935	-0.221785	5.494787
10	6	0	3.734454	-0.795663	3.627474
11	6	0	-1.301516	-0.388787	-0.648728
12	6	0	0.590246	1.467281	-0.563571
13	6	0	-0.515682	2.400505	-0.500981
14	16	0	-1.058861	3.023527	0.958895
15	6	0	-1.237994	2.706383	-1.676637
16	1	0	-0.920000	-0.035306	2.003616
17	8	0	2.331633	0.006747	1.438505
18	1	0	-1.052457	1.406658	5.259195
19	1	0	-1.566306	0.088032	4.190224
20	1	0	-0.852450	1.566835	3.503062
21	1	0	2.915796	-0.435234	6.264455
22	1	0	4.337085	-1.146940	4.455280
23	1	0	4.207703	0.035841	3.127596
24	1	0	3.574553	-1.586913	2.911099
25	1	0	0.198939	2.975751	1.813270
26	1	0	-2.126582	0.215896	-0.280198
27	1	0	-1.520090	-1.427032	-0.415605
28	1	0	-1.258632	-0.290466	-1.729795
29	1	0	1.374978	1.656094	0.166271
30	17	0	1.509914	3.158005	2.850814
31	6	0	-0.774399	2.325408	-2.888655
32	1	0	-1.324382	2.599388	-3.776116
33	6	0	1.152972	1.232372	-1.904763
34	6	0	0.449373	1.610273	-3.048921
35	1	0	-2.131820	3.301678	-1.593764
36	6	0	2.362022	0.565482	-2.036146
37	1	0	2.887574	0.273163	-1.139373
38	6	0	0.966524	1.313264	-4.312133
39	1	0	0.414450	1.609510	-5.190115
40	6	0	2.164711	0.658052	-4.429611
41	1	0	2.565745	0.432822	-5.403687
42	6	0	2.864432	0.286720	-3.286394
43	1	0	3.809638	-0.222458	-3.381125
44	1	0	0.811801	-0.633970	-0.346893

Compound TS10a

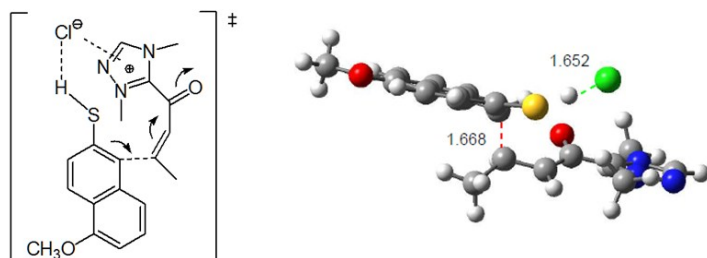


E=-1910.17269066; 1 imaginary frequencies= -599.0150

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.465037
3	6	0	1.233395	0.000000	2.054481
4	6	0	1.329931	0.026435	3.534904
5	7	0	0.465524	0.399655	4.465401
6	7	0	2.432737	-0.335576	4.203976
7	7	0	0.974086	0.286383	5.700601
8	6	0	-0.854562	0.959241	4.312156
9	6	0	2.166281	-0.158461	5.515294
10	6	0	3.701921	-0.797552	3.671152
11	6	0	-1.309031	-0.390307	-0.637685
12	6	0	0.584997	1.421991	-0.561459
13	6	0	-0.514442	2.381308	-0.588778
14	16	0	-1.109543	3.053861	0.837139
15	6	0	-1.168289	2.668989	-1.788097
16	1	0	-0.921709	-0.030897	2.013276
17	8	0	2.335127	-0.004868	1.455384
18	1	0	-1.054873	1.531632	5.205920
19	1	0	-1.588670	0.168716	4.203614
20	1	0	-0.858306	1.601961	3.442691
21	1	0	2.871506	-0.365523	6.294639
22	1	0	4.292815	-1.143399	4.509918
23	1	0	4.193104	0.015010	3.157807
24	1	0	3.532603	-1.598694	2.968106
25	1	0	0.128099	3.015032	1.726164
26	1	0	-2.125490	0.238267	-0.289557
27	1	0	-1.544325	-1.417763	-0.375756
28	1	0	-1.263424	-0.324167	-1.721897
29	1	0	1.343530	1.669719	0.178873
30	17	0	1.432865	3.217708	2.765117
31	6	0	-0.655951	2.240681	-2.985176
32	6	0	1.215187	1.168296	-1.873189
33	6	0	0.584448	1.512303	-3.063146
34	1	0	-2.042013	3.294531	-1.756798
35	6	0	2.432595	0.504672	-1.918258
36	1	0	2.898007	0.235348	-0.981805
37	6	0	1.167530	1.192144	-4.288800
38	1	0	0.663446	1.468414	-5.198550
39	6	0	2.373670	0.540446	-4.318566
40	1	0	2.830300	0.295532	-5.262932
41	6	0	3.008262	0.200531	-3.129448
42	1	0	3.959747	-0.305116	-3.157214

43	1	0	0.788410	-0.672255	-0.332419
44	8	0	-1.213733	2.491708	-4.148447
45	6	0	-2.423007	3.218834	-4.200456
46	1	0	-2.282849	4.222535	-3.810796
47	1	0	-2.692200	3.267014	-5.245344
48	1	0	-3.201437	2.707360	-3.642218

Compound TS10b

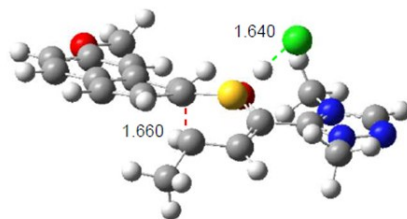
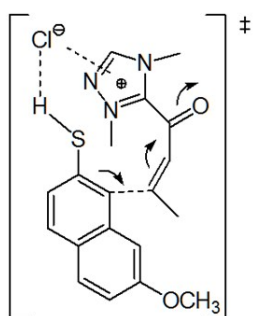


E=- 1910.16358346; 1 imaginary frequencies= - 533.9477

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.454305
3	6	0	1.237711	0.000000	2.048886
4	6	0	1.338616	-0.001034	3.531430
5	7	0	0.471227	0.339504	4.470745
6	7	0	2.448791	-0.359772	4.188267
7	7	0	0.985864	0.210773	5.700955
8	6	0	-0.857689	0.883003	4.332742
9	6	0	2.184776	-0.211038	5.503514
10	6	0	3.723704	-0.791243	3.642909
11	6	0	-1.301741	-0.391491	-0.647158
12	6	0	0.587090	1.468823	-0.562850
13	6	0	-0.524754	2.398030	-0.513647
14	16	0	-1.078334	3.027177	0.942397
15	6	0	-1.235874	2.690301	-1.694441
16	1	0	-0.921243	-0.032350	2.002727
17	8	0	2.333215	0.004793	1.449242
18	1	0	-1.076212	1.402649	5.253876
19	1	0	-1.576357	0.086955	4.174988
20	1	0	-0.865001	1.572215	3.499504
21	1	0	2.895868	-0.421350	6.276618
22	1	0	4.322997	-1.141786	4.473465
23	1	0	4.199510	0.038692	3.142907
24	1	0	3.565342	-1.583409	2.927143
25	1	0	0.175670	2.984509	1.802602
26	1	0	-2.127129	0.213768	-0.280407
27	1	0	-1.519303	-1.429115	-0.410055
28	1	0	-1.259337	-0.296443	-1.728518
29	1	0	1.366129	1.665759	0.170570
30	17	0	1.484757	3.171253	2.841305
31	6	0	-0.763579	2.295096	-2.902105
32	1	0	-1.303835	2.554110	-3.797331
33	6	0	1.164914	1.224645	-1.895909
34	6	0	0.459189	1.585051	-3.042538
35	1	0	-2.130357	3.286406	-1.627495
36	6	0	2.379792	0.564761	-2.001264

37	1	0	2.901315	0.288529	-1.098307
38	6	0	0.986835	1.272124	-4.311059
39	6	0	2.196148	0.621682	-4.406487
40	1	0	2.618062	0.379044	-5.365064
41	6	0	2.881756	0.277442	-3.247242
42	1	0	3.830838	-0.225607	-3.337869
43	1	0	0.811759	-0.633824	-0.347917
44	8	0	0.245988	1.644908	-5.360285
45	6	0	0.726795	1.359136	-6.647554
46	1	0	-0.014431	1.738427	-7.336998
47	1	0	1.677635	1.855006	-6.829723
48	1	0	0.842528	0.287362	-6.793505

Compound TS10c



E= -1910.16599479; 1 imaginary frequencies= -529.3366

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.458854
3	6	0	1.234703	0.000000	2.051733
4	6	0	1.330349	0.020894	3.532958
5	7	0	0.464896	0.391490	4.463222
6	7	0	2.433081	-0.341680	4.201532
7	7	0	0.972732	0.275608	5.698002
8	6	0	-0.857907	0.946696	4.312101
9	6	0	2.165457	-0.168226	5.513079
10	6	0	3.701973	-0.804483	3.668899
11	6	0	-1.302142	-0.399947	-0.643439
12	6	0	0.580345	1.452489	-0.554624
13	6	0	-0.541516	2.380488	-0.567021
14	16	0	-1.140889	3.031605	0.861076
15	6	0	-1.202040	2.649798	-1.779497
16	1	0	-0.921294	-0.032299	2.007609
17	8	0	2.335260	-0.001067	1.453694
18	1	0	-1.061148	1.512166	5.209525
19	1	0	-1.588155	0.153528	4.198283
20	1	0	-0.864814	1.595070	3.446941
21	1	0	2.869896	-0.377071	6.292664
22	1	0	4.291659	-1.153254	4.507132
23	1	0	4.195229	0.008546	3.158124
24	1	0	3.531758	-1.604539	2.964727
25	1	0	0.129677	3.023030	1.753147
26	1	0	-2.128199	0.209210	-0.284753
27	1	0	-1.519390	-1.434927	-0.395035
28	1	0	-1.258069	-0.316638	-1.725866
29	1	0	1.329052	1.688618	0.198236

30	17	0	1.424358	3.210361	2.742528
31	6	0	-0.670739	2.237731	-2.960464
32	1	0	-1.179262	2.485869	-3.880115
33	6	0	1.215449	1.200720	-1.860907
34	6	0	0.558377	1.535757	-3.044628
35	1	0	-2.100332	3.243432	-1.761800
36	6	0	2.438696	0.554370	-1.891913
37	1	0	2.900127	0.306035	-0.949241
38	6	0	1.155055	1.205034	-4.269210
39	1	0	0.652102	1.461205	-5.188231
40	6	0	2.360439	0.571598	-4.304581
41	1	0	2.838456	0.312411	-5.233692
42	6	0	3.014479	0.246117	-3.109475
43	1	0	0.804529	-0.647745	-0.340224
44	8	0	4.193143	-0.361330	-3.245962
45	6	0	4.898782	-0.706890	-2.079523
46	1	0	4.328676	-1.402078	-1.468055
47	1	0	5.812035	-1.180335	-2.411906
48	1	0	5.138053	0.176141	-1.492250
