Supporting information

Synthesis of aryl(dihydro)naphthothiophene frames: a comprehensive and structural study

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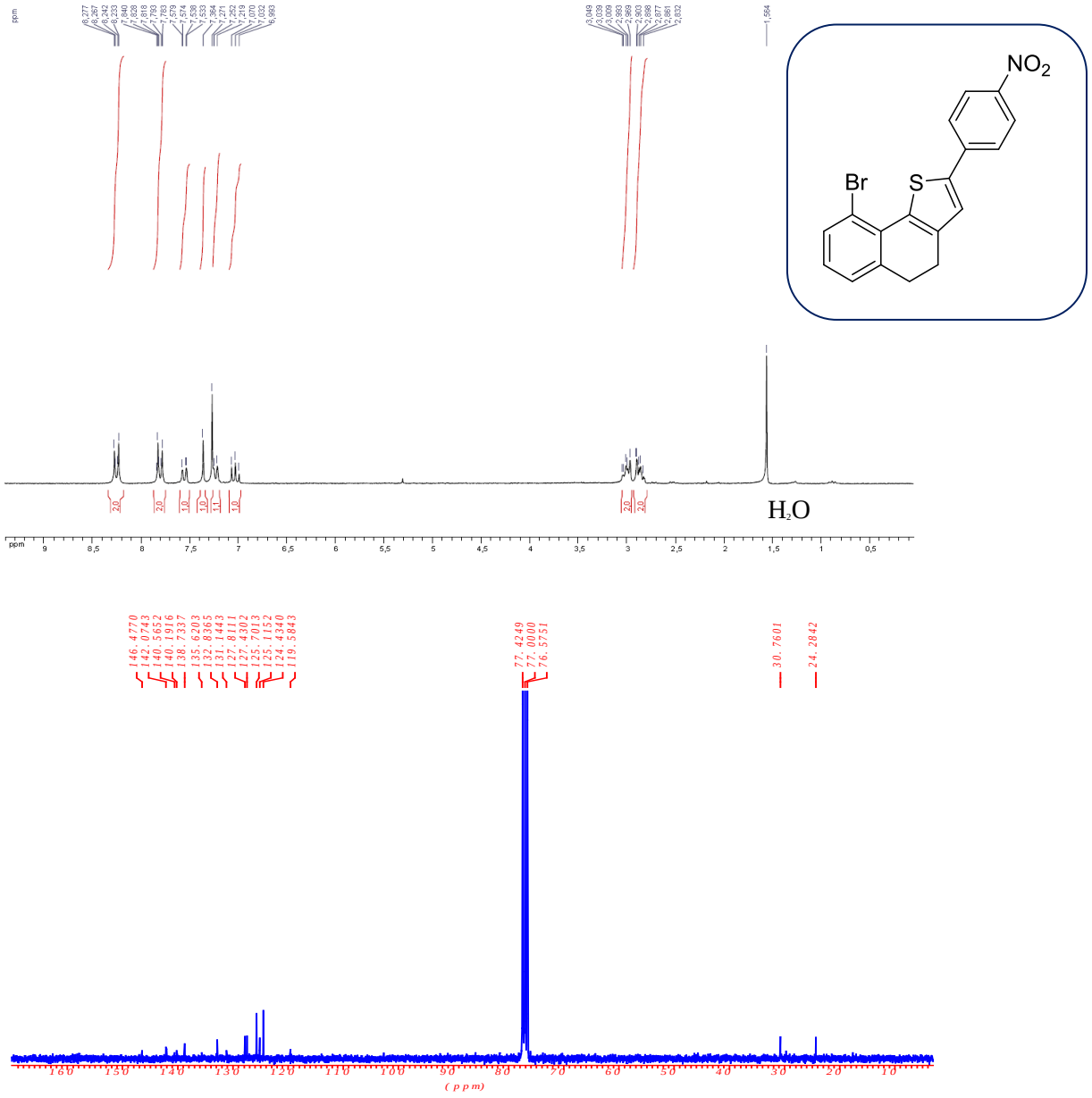
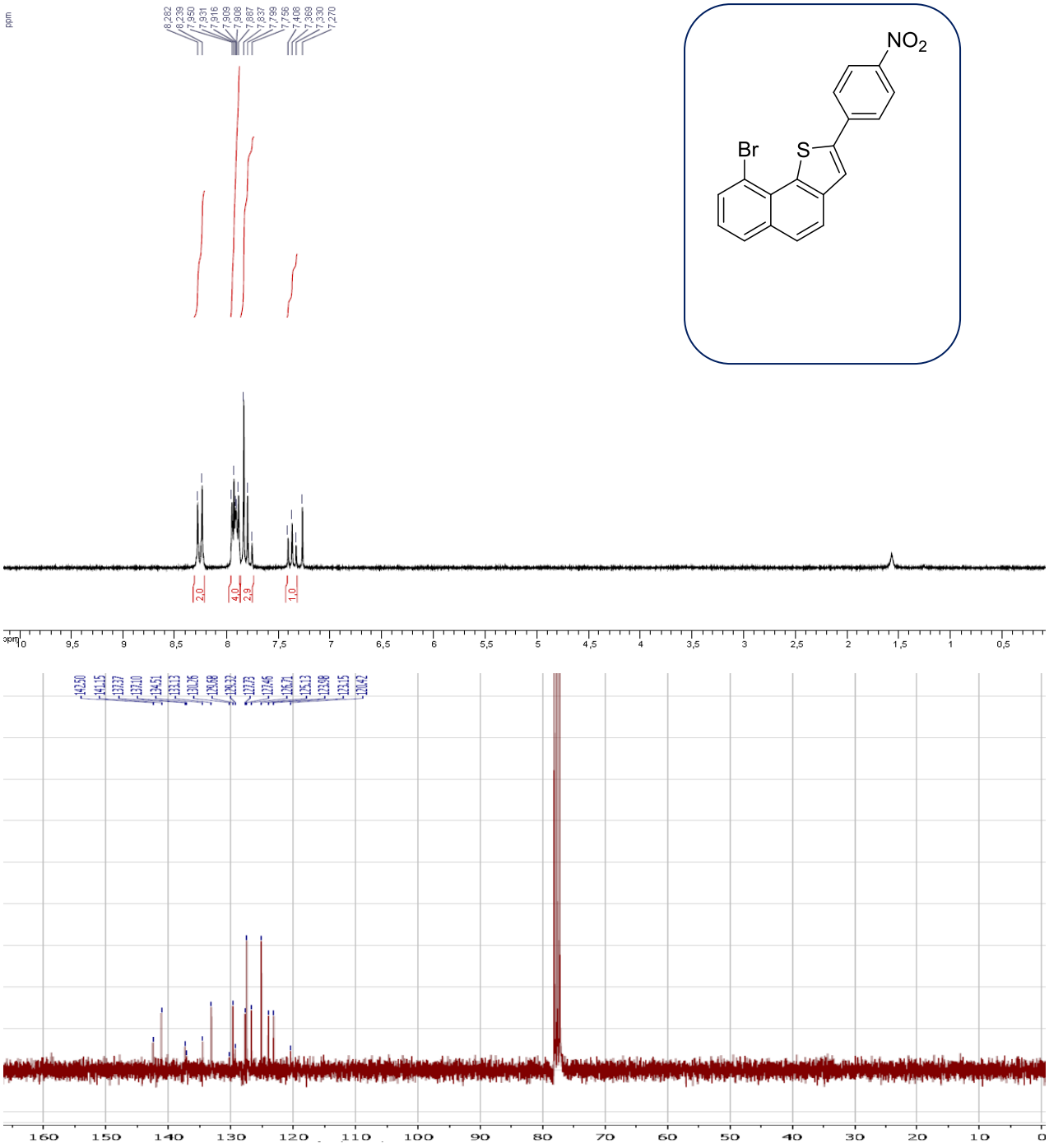
Compound 2b



Compound 3b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7,330
7,270
NO2
Br
S
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4,0
2,9
1,0
ppm
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137,110
134,451
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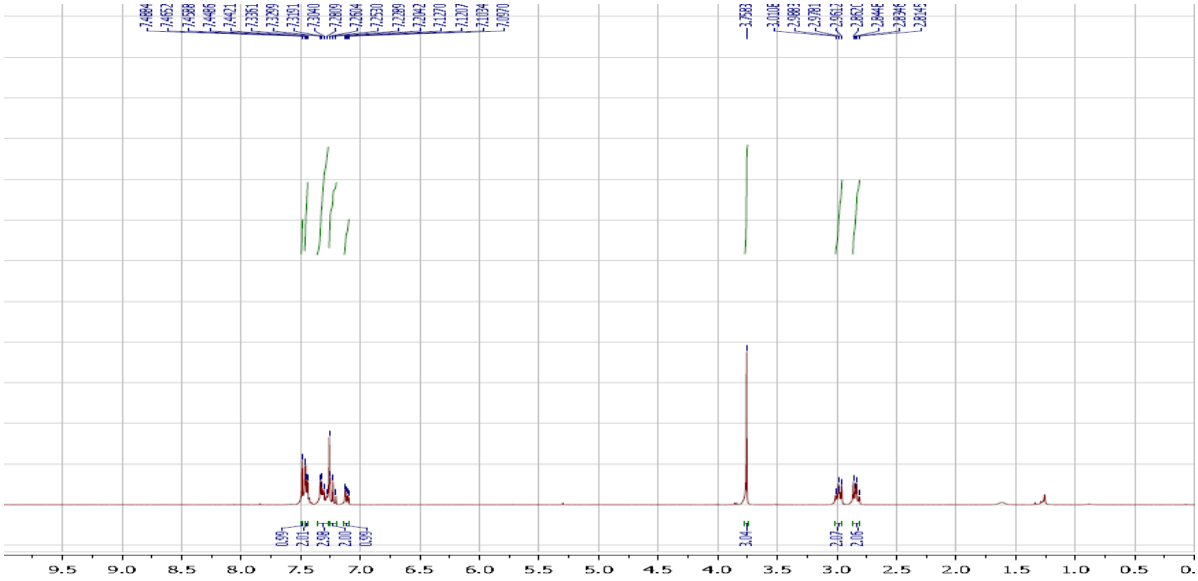
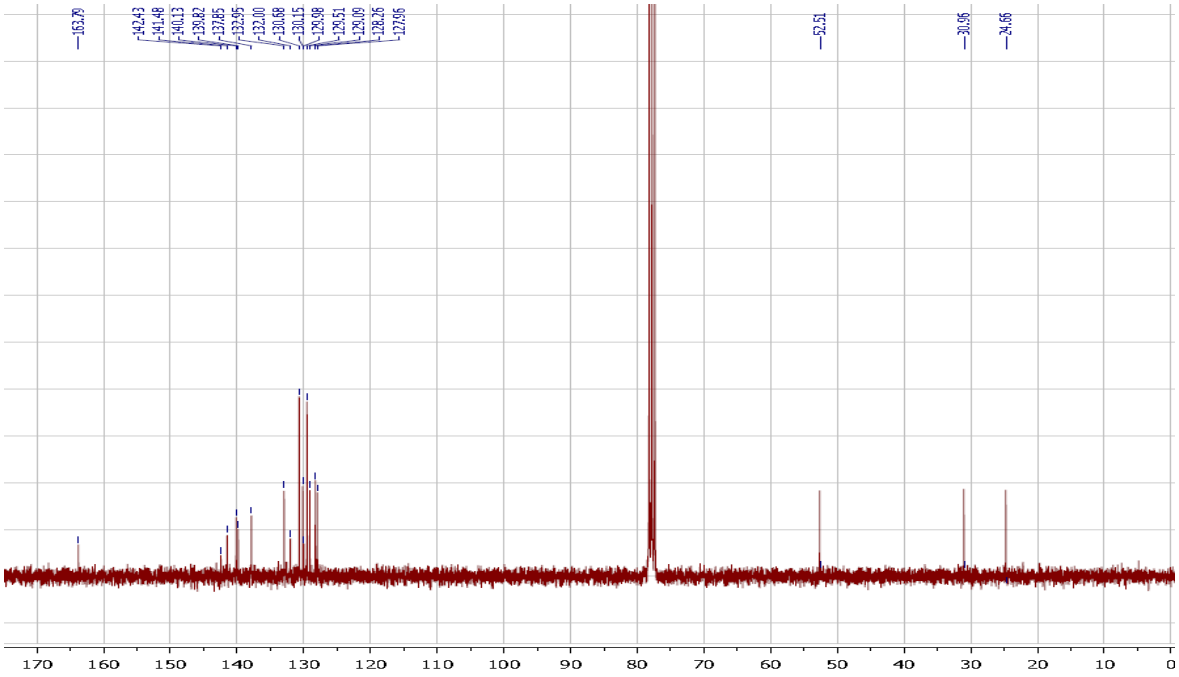
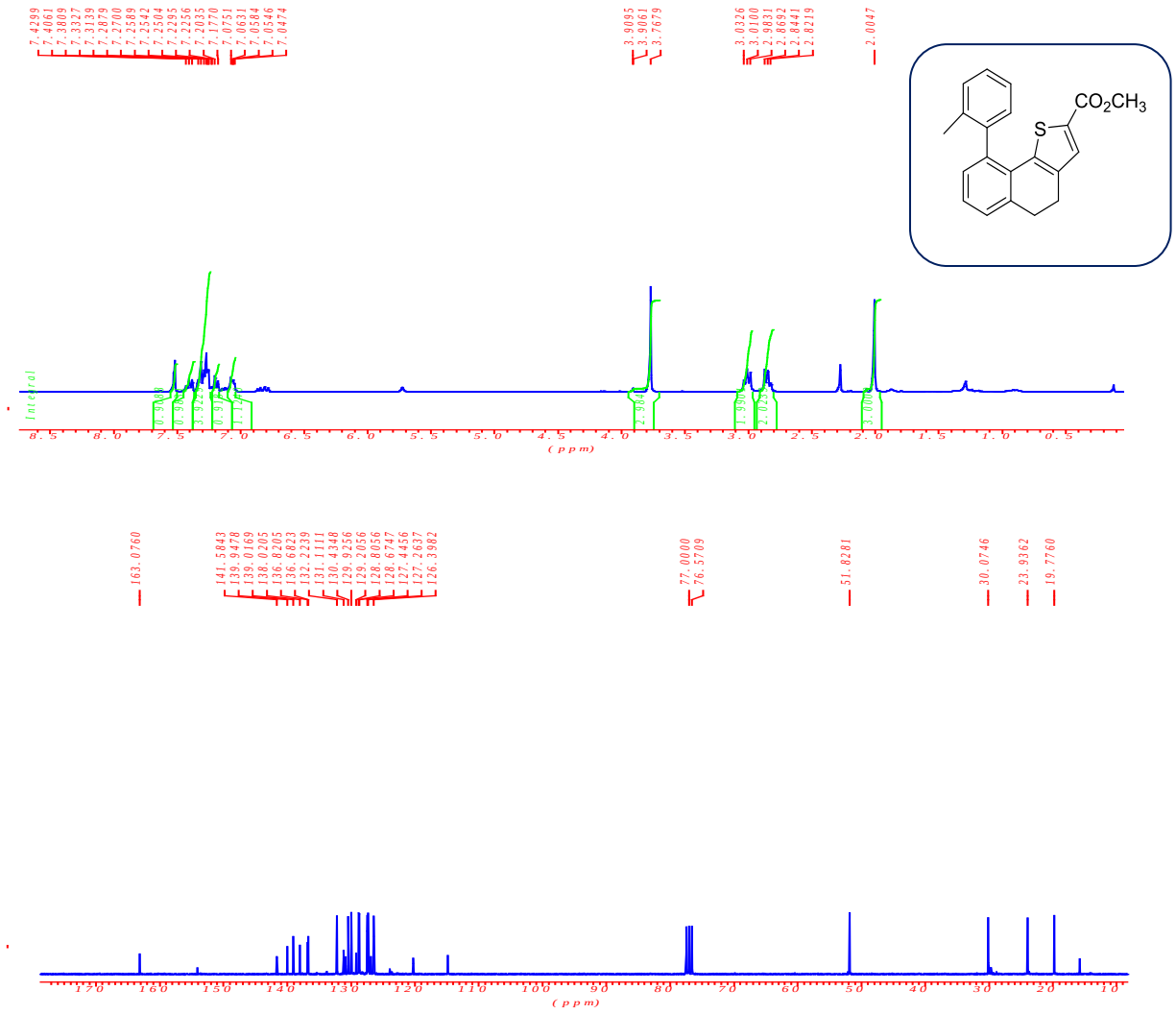
123,598
123,315
120,642

Compound 4a

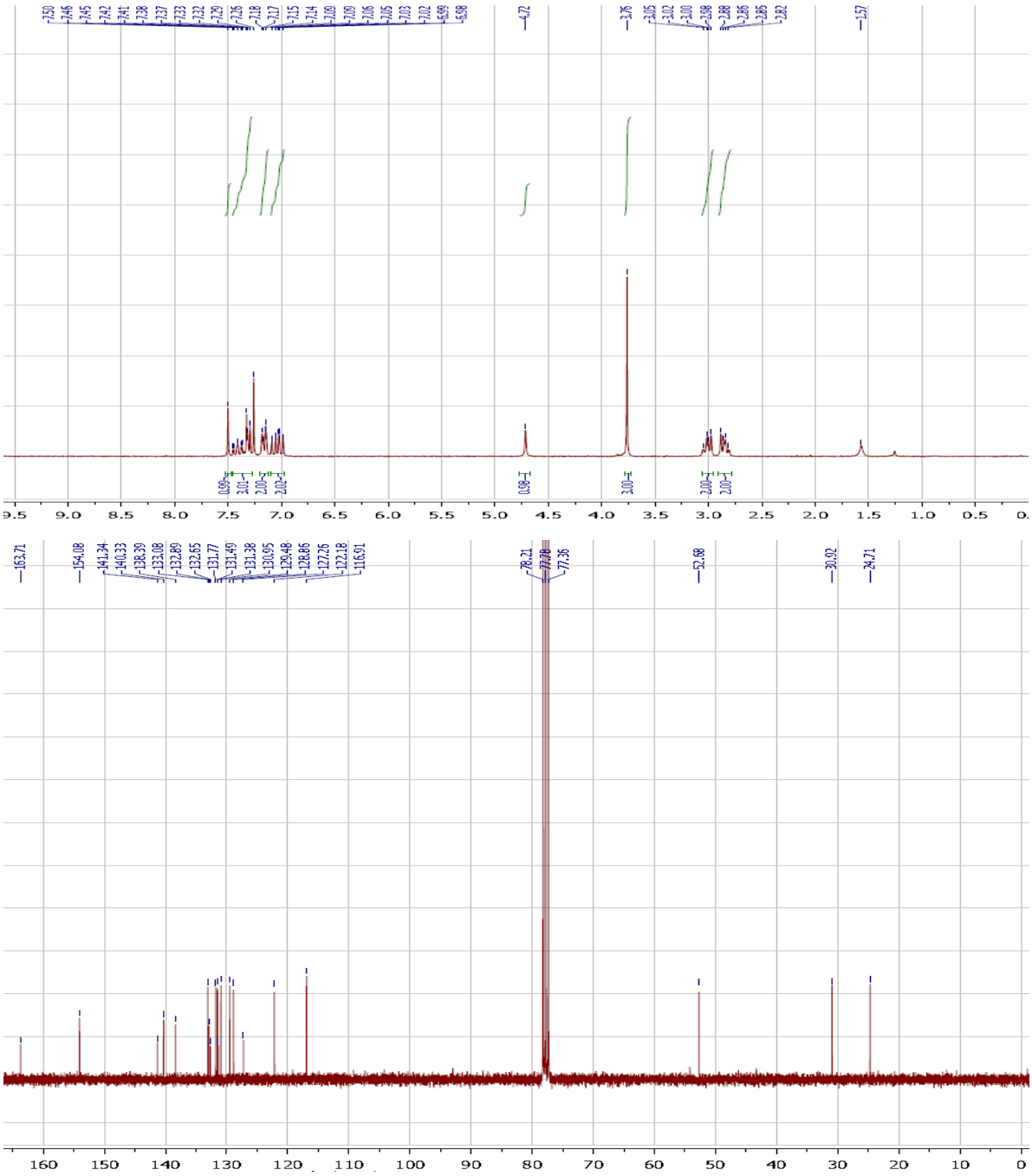




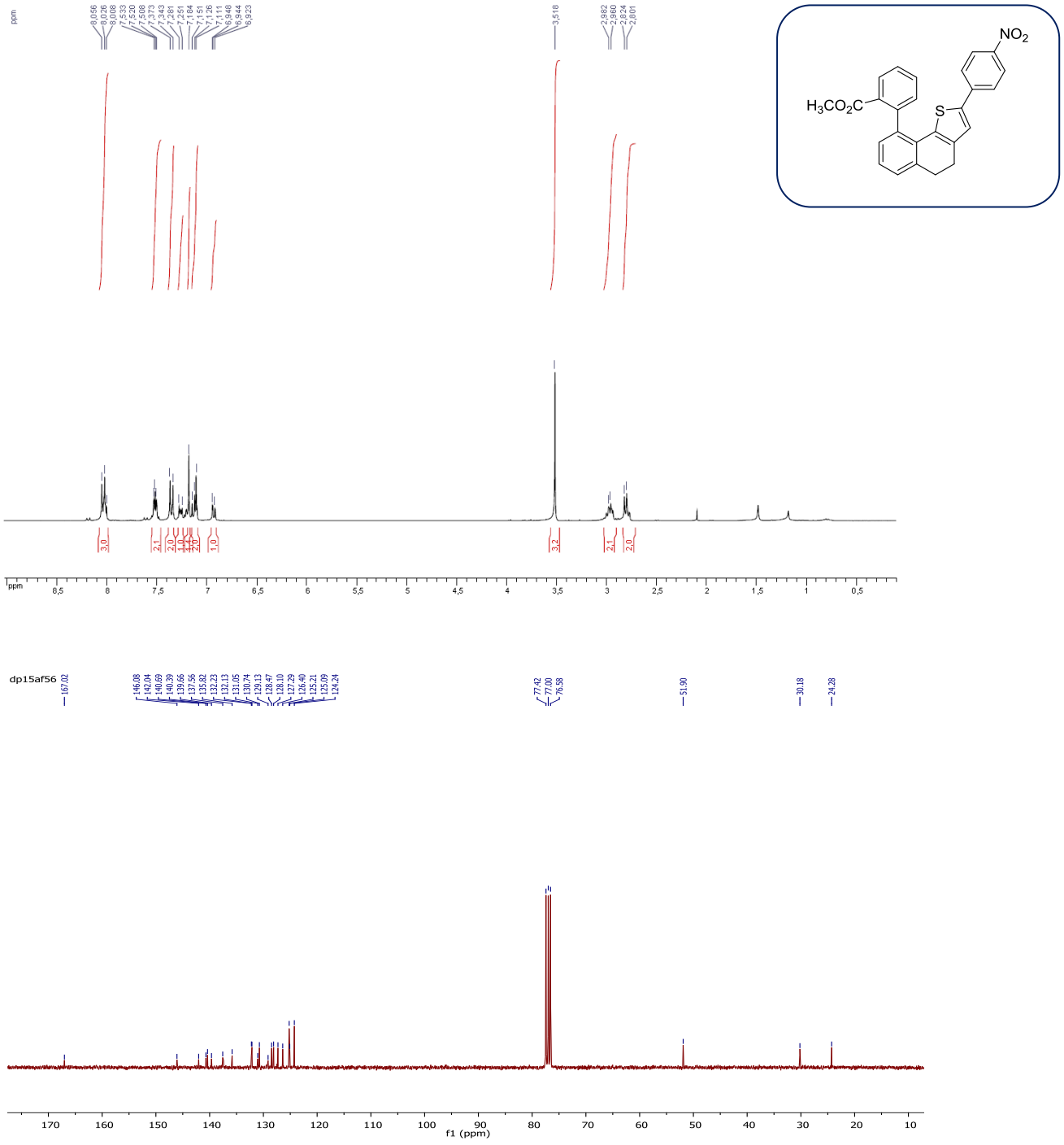
Compound 4b



Compound 4c



Compound 4e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7,111
6,948
6,923
3,516
2,982
2,960
2,824
2,801
NO2
H3CO2C
S
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2,1
2,0
1,0
3,2
2,1
2,0
dp15af56
167,02
146,08
142,04
140,69
140,39
139,66
137,56
135,82
132,23
132,13
131,05
130,74
129,13
128,47
128,10
127,29
126,40
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124,24
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77,00
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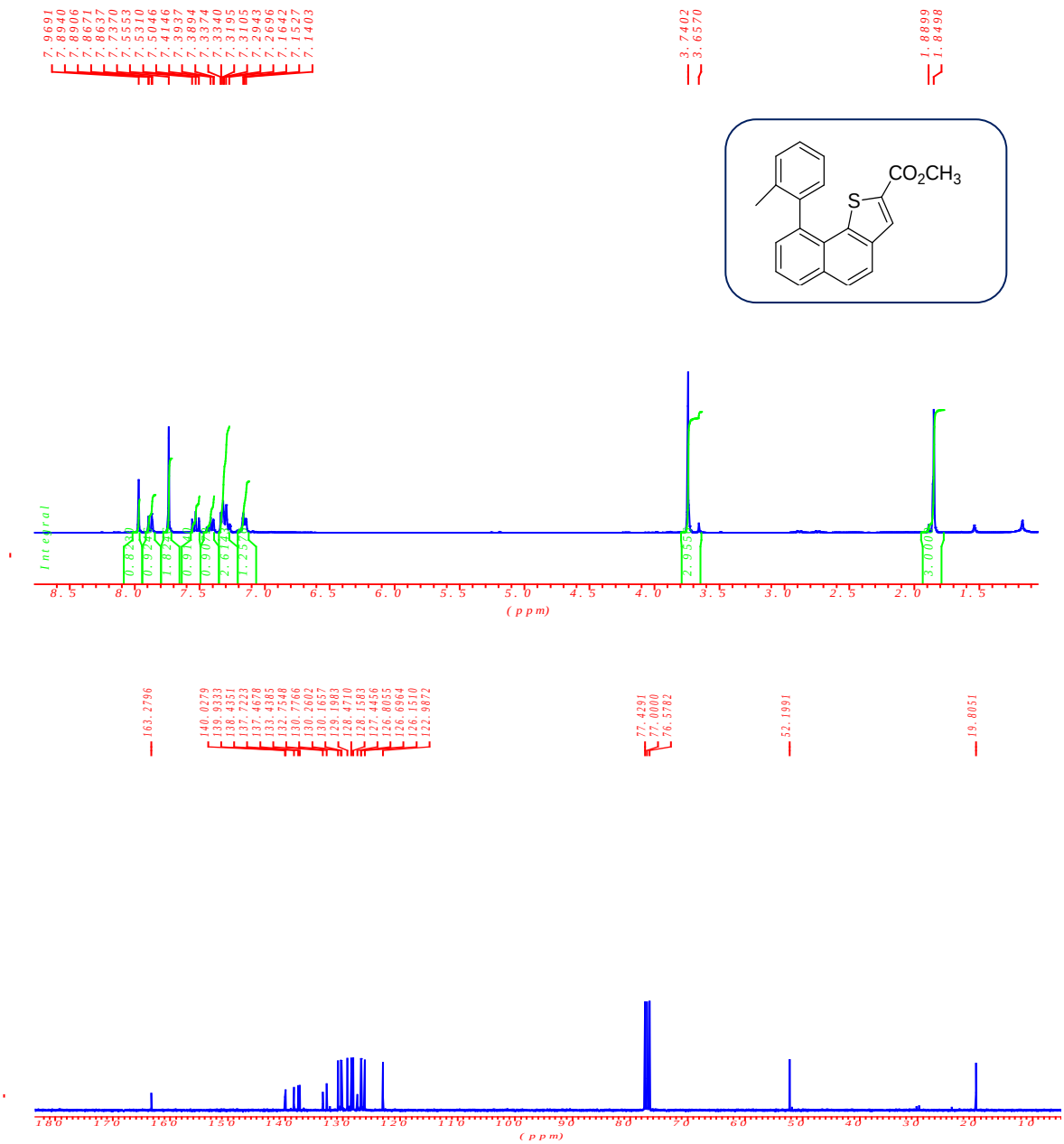
51,90
30,18
24,28
f1 (ppm)

Compound 5a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7.8906
7.8671
7.8637
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7.3937
7.3894
7.3374
7.3340
7.3195
7.3105
7.2943
7.2696
7.1642
7.1527
7.1403
3.7402
3.6570
1.8899
1.8498
CO2CH3
S
Integral
0.83
0.92
1.82
0.91
0.90
2.61
1.25
2.95
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
(ppm)
163.2796
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139.9333
138.4351
137.7223
137.4678
133.4385
132.7548
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128.4710
128.1583
127.4456
126.8055
126.6964
126.1510
122.9872
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77.0000
76.5782
52.1991
19.8051
180
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160
150
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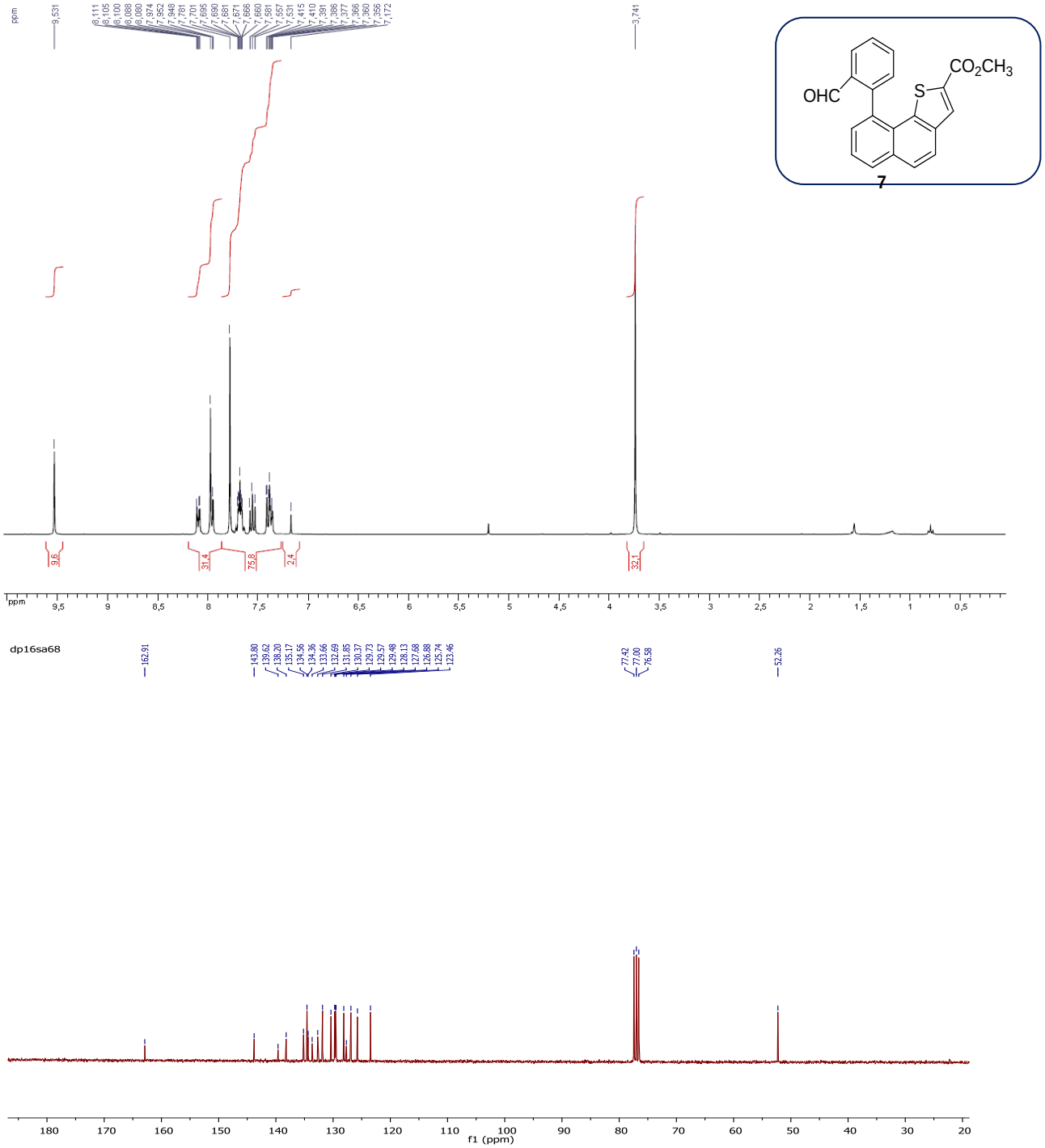
130
120
110
100
90
80
70
60
50
40
30
20
10
(ppm)

Compound 5b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7,690
7,681
7,671
7,666
7,660
7,581
7,557
7,531
7,415
7,410
7,391
7,386
7,377
7,368
7,360
7,396
7,172
3,741
9,6
31,4
75,8
2,4
32,1
OHC
S
CO2CH3
7
dp16sa68
162,91
143,80
139,62
138,20
135,17
134,56
134,36
133,66
132,69
131,85
130,37
129,73
129,57
129,48
128,13
127,68
126,88
125,74
123,46
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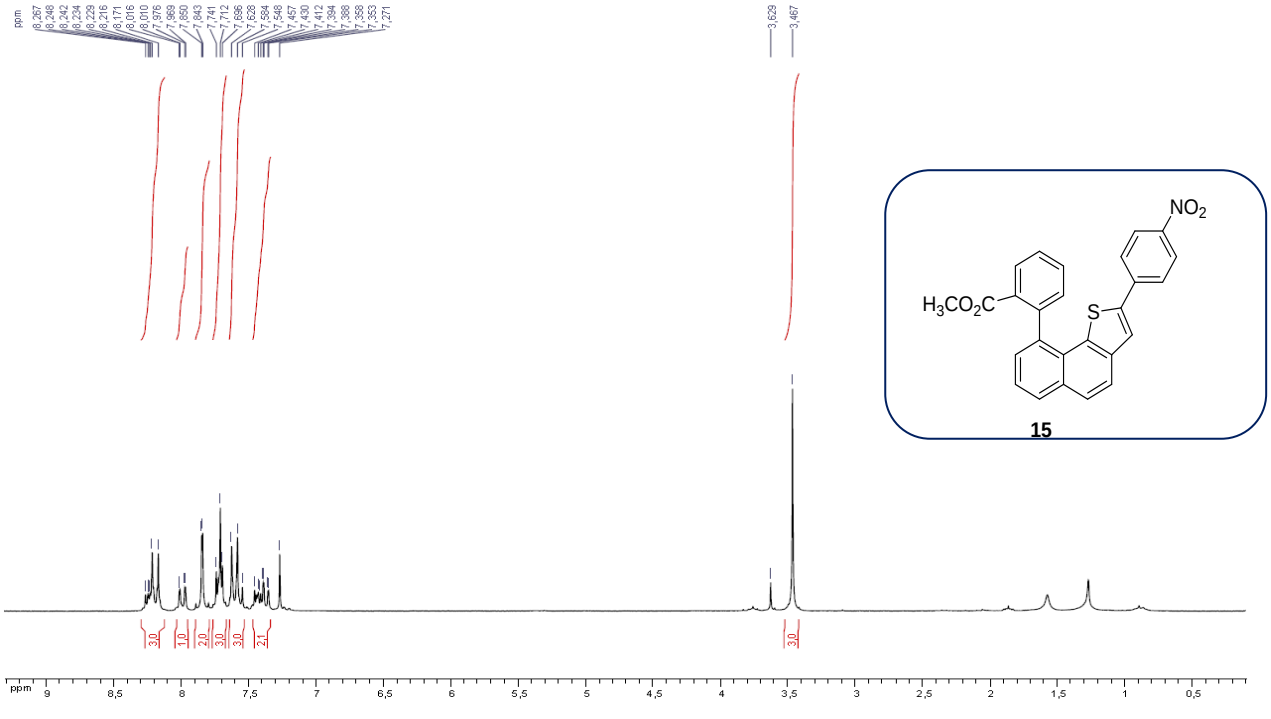
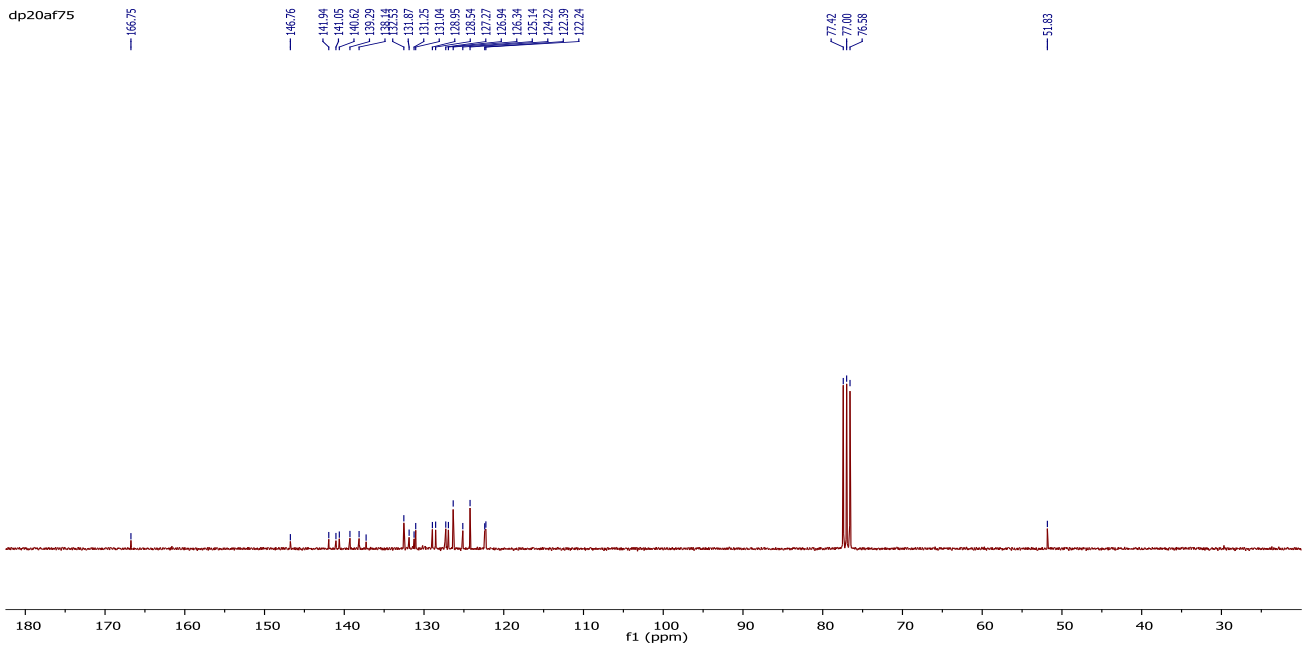
77,00
76,58
52,26
f1 (ppm)

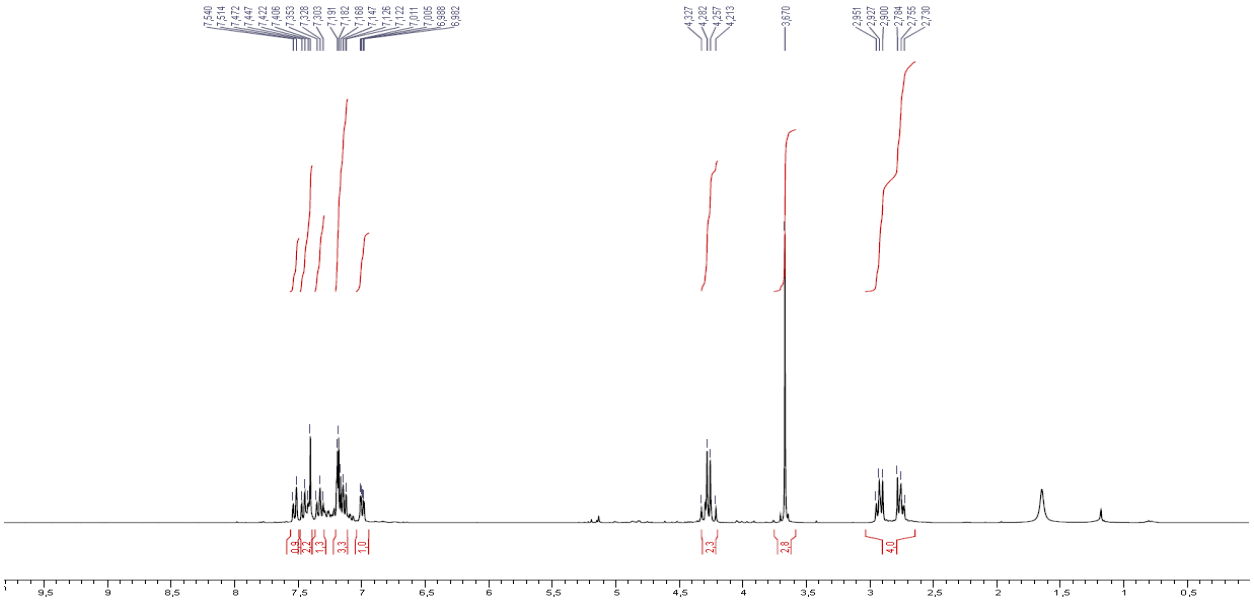
Compound 5d

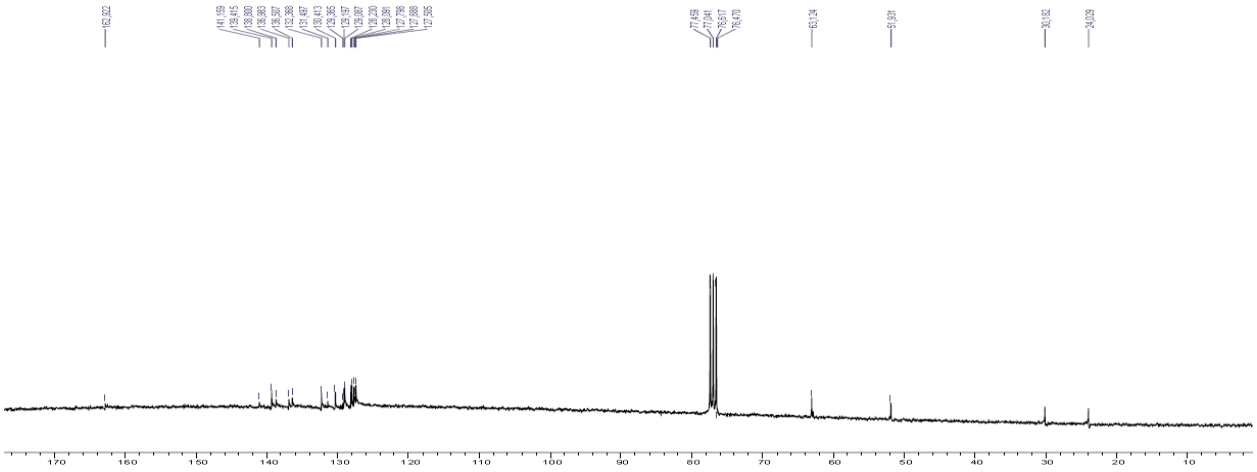


15

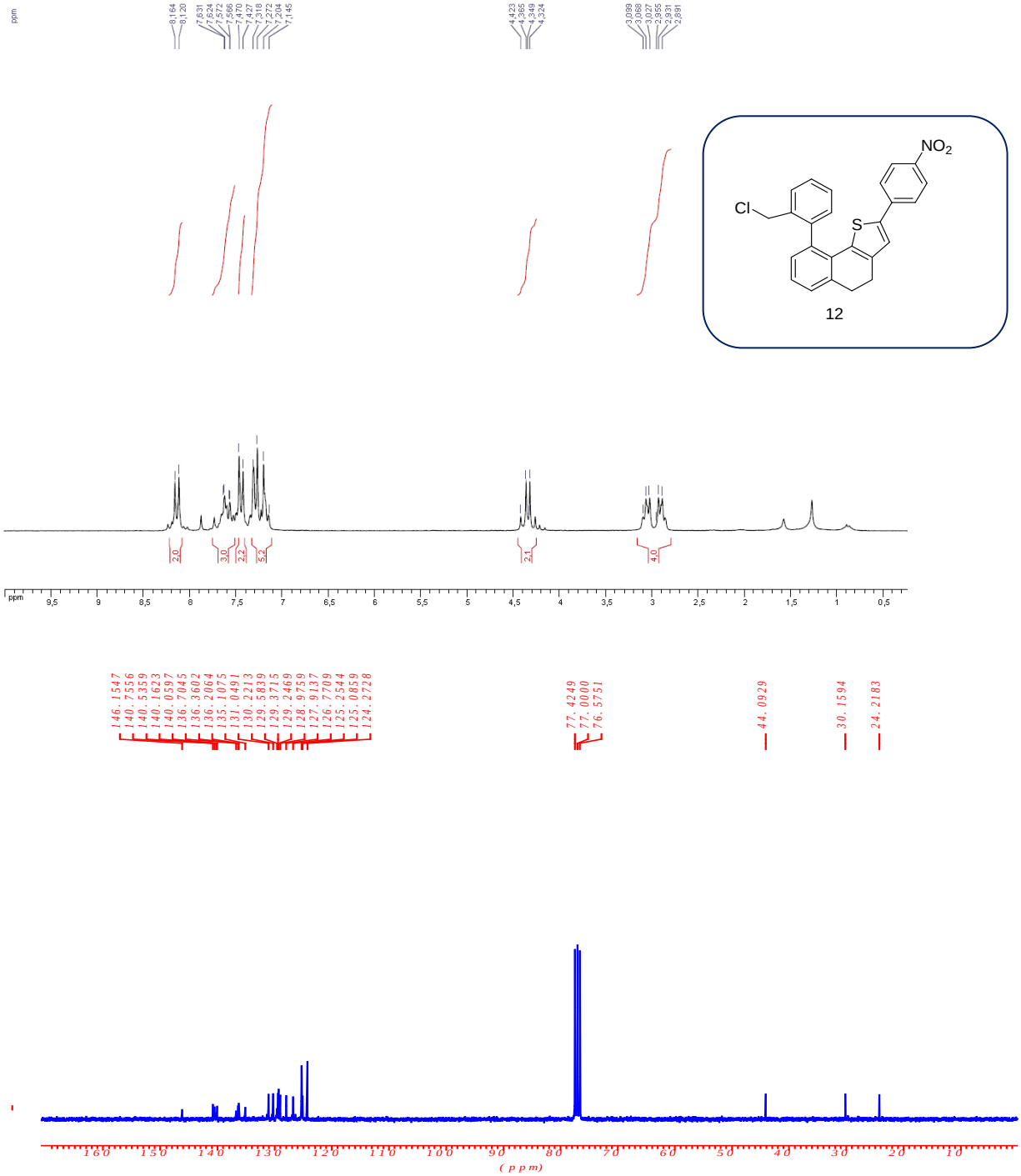


Compound 7





Compound 8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4,365
4,349
4,324
3,099
3,068
3,027
2,965
2,931
2,891
NO2
Cl
S
12
2,0
3,0
2,2
5,0
2,1
4,0
146.1547
140.7556
140.5359
140.1623
140.0597
136.7045
136.3602
136.2064
135.1075
131.0491
130.2213
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129.3715
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127.9137
126.7709
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77.0000
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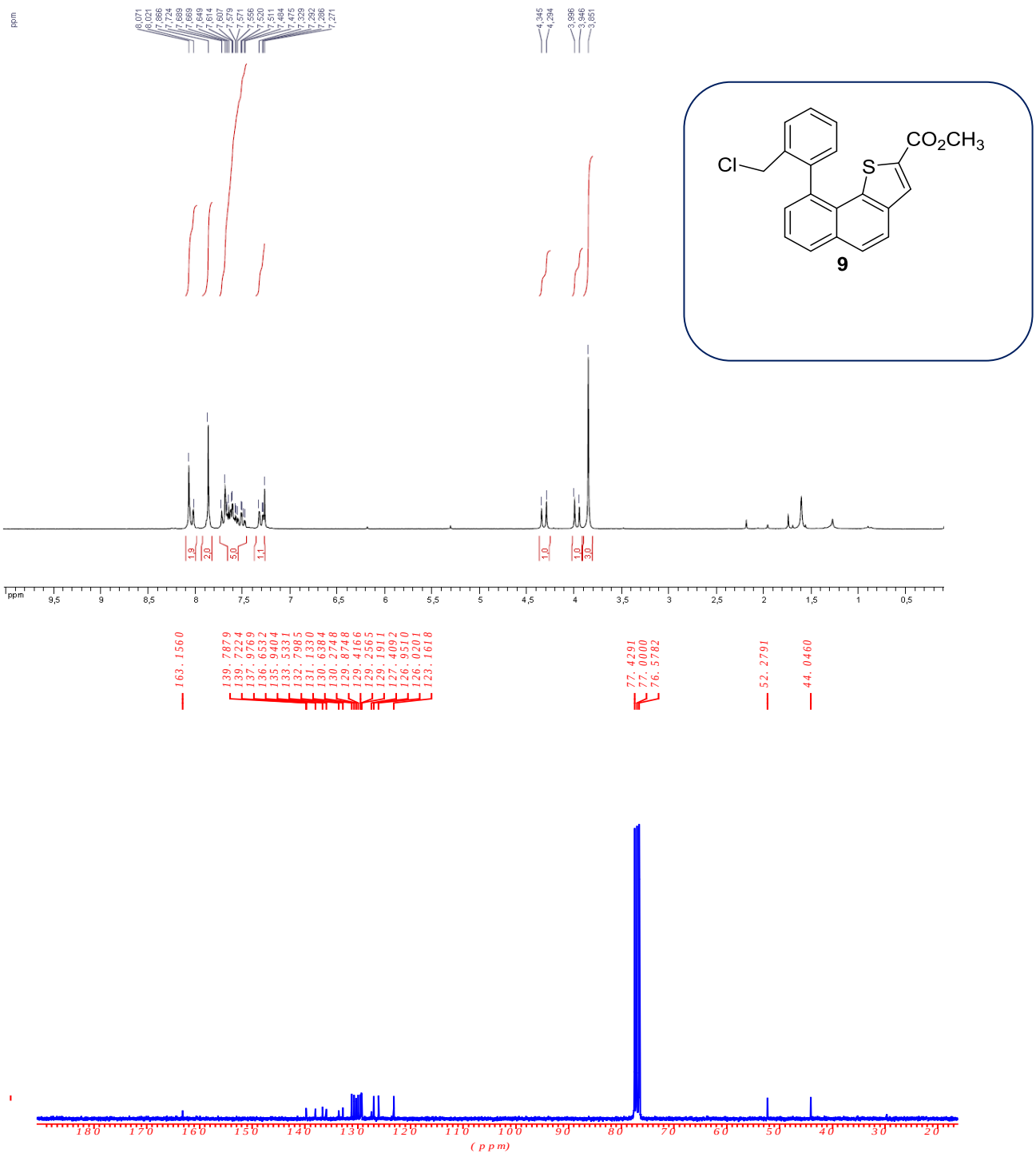
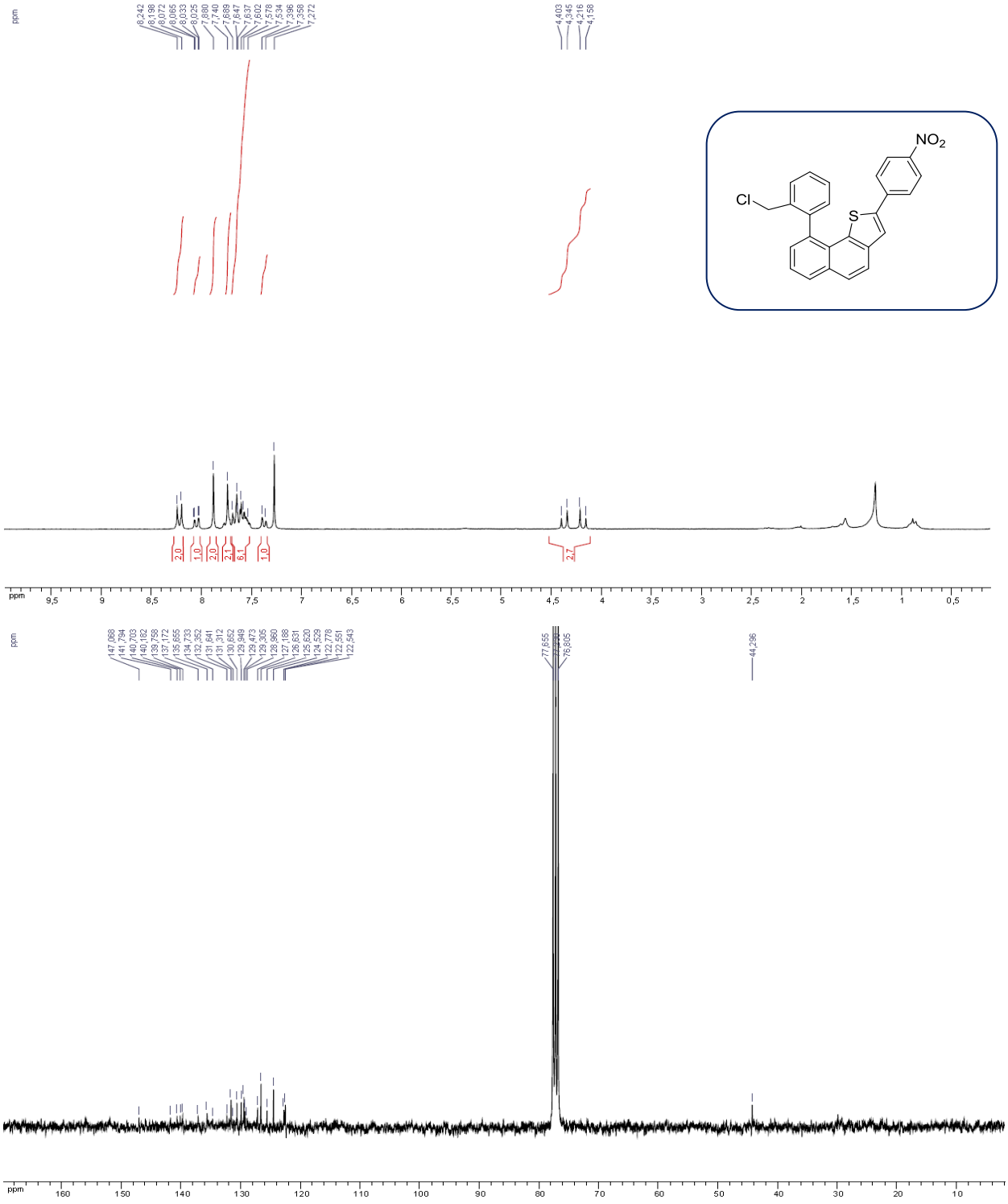
30.1594
24.2183
(ppm)

Compound 9



Compound 10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7,534
7,396
7,358
7,272
4,403
4,345
4,216
4,158
NO2
Cl
S
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1,0
2,0
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1,0
2,7
9,5
9
8,5
8
7,5
7
6,5
6
5,5
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4,5
4
3,5
3
2,5
2
1,5
1
0,5
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140,162
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135,695
134,733
132,892
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131,312
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122,543
77,655
76,805
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60
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40
30
20
10

X-ray structures

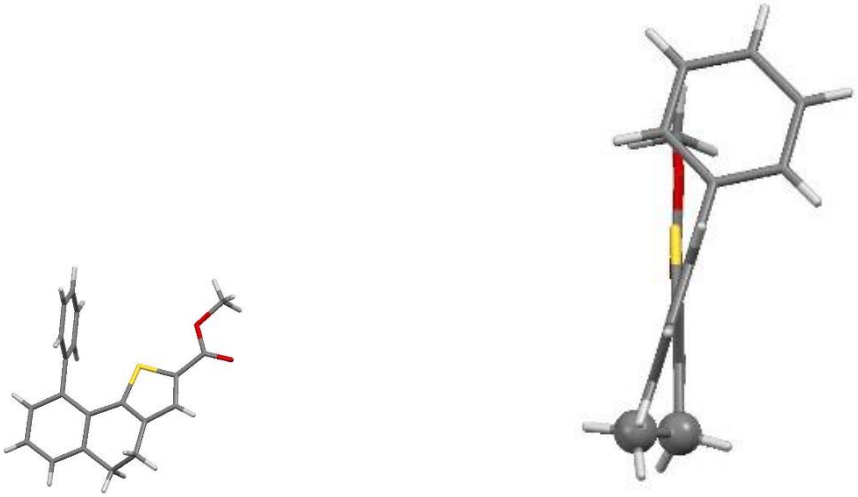


Figure S 1: X-ray structure of compounds **4a**.

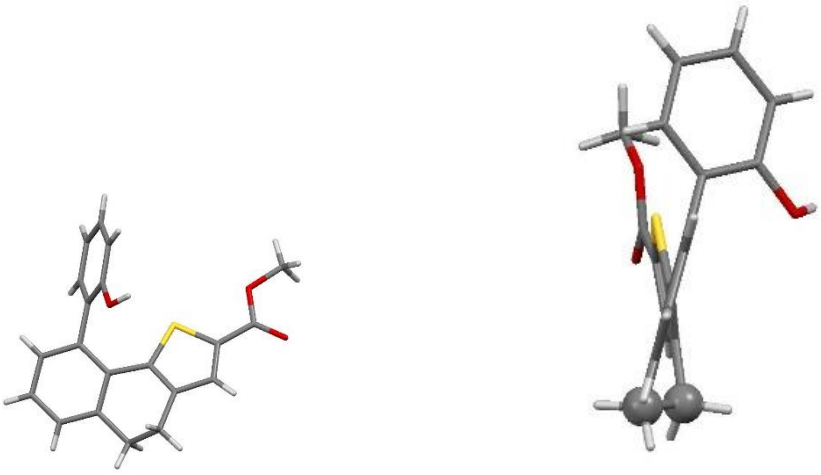


Figure S 2: X-ray structure of compounds **4c**.

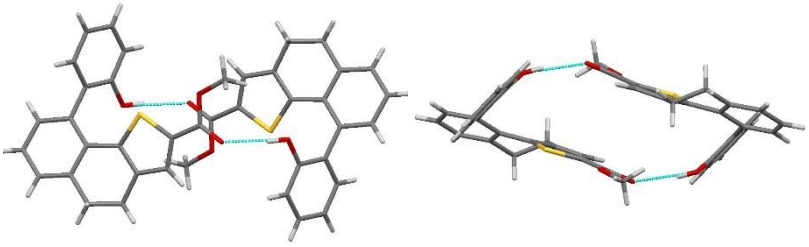


Figure S 3: dimer formed by **4c** in the crystal structure (blue lines show hydrogen bonding).

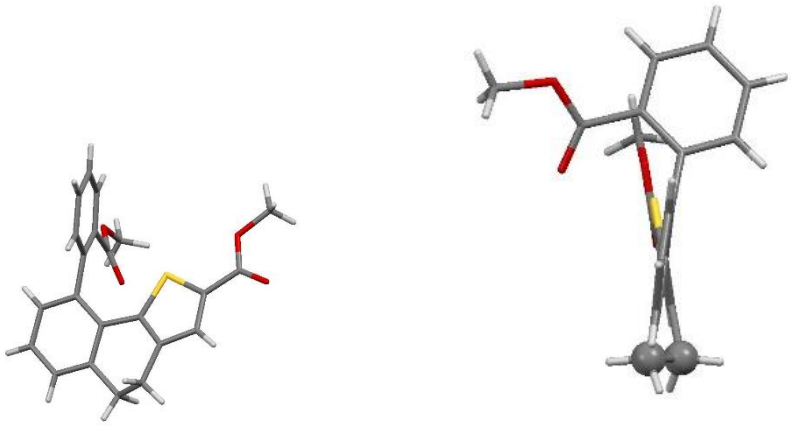


Figure S 4: X-ray structure of compounds **4d**.

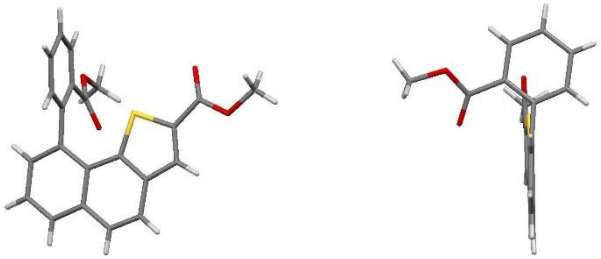


Figure S 5: X-ray structure of compounds **5c**.

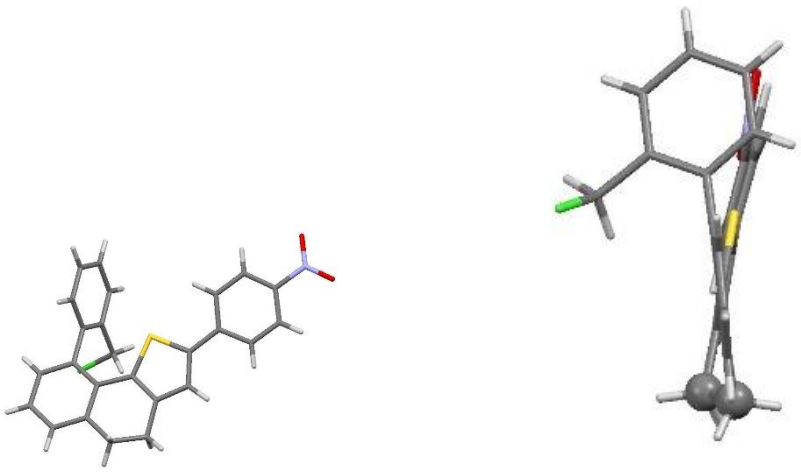


Figure S 6: X-ray structure of compounds **8**.

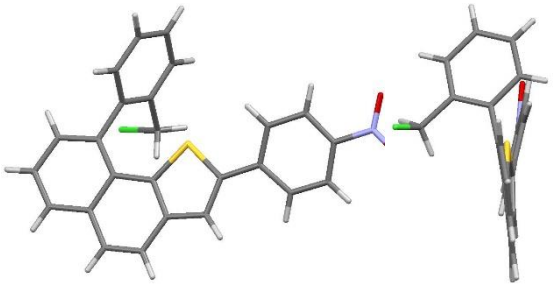


Figure S 7: X-ray structure of compounds **10**.

DFT Calculations

Optimized structures from DFT calculations

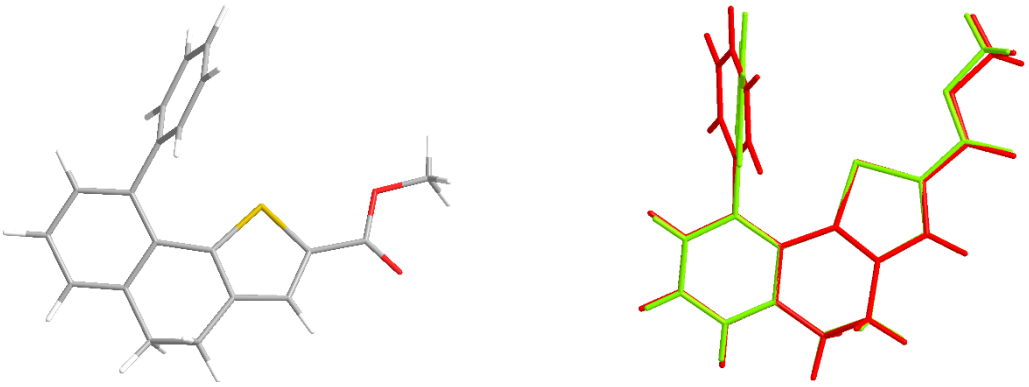


Figure S 8: optimized structure for **4a** (left) and overlay of calculated (red) and X-Ray (green) structures (right).

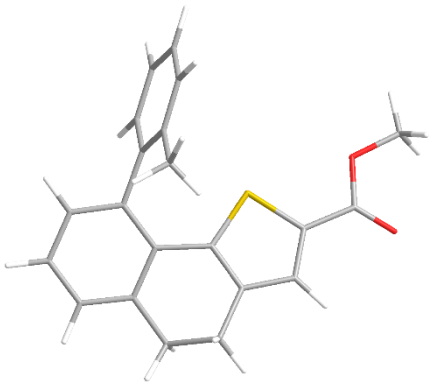


Figure S 9: optimized structure for **4b**.

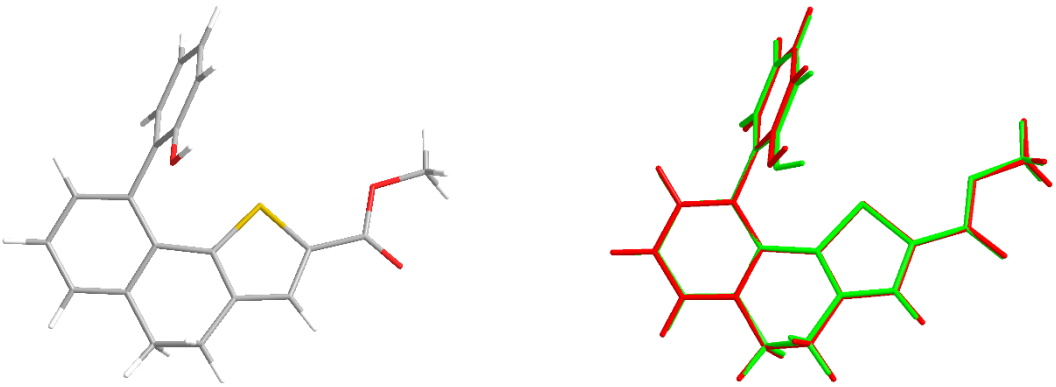


Figure S 10: optimized structure for **4c** (left) and overlay of calculated (red) and X-Ray (green) structures (right).

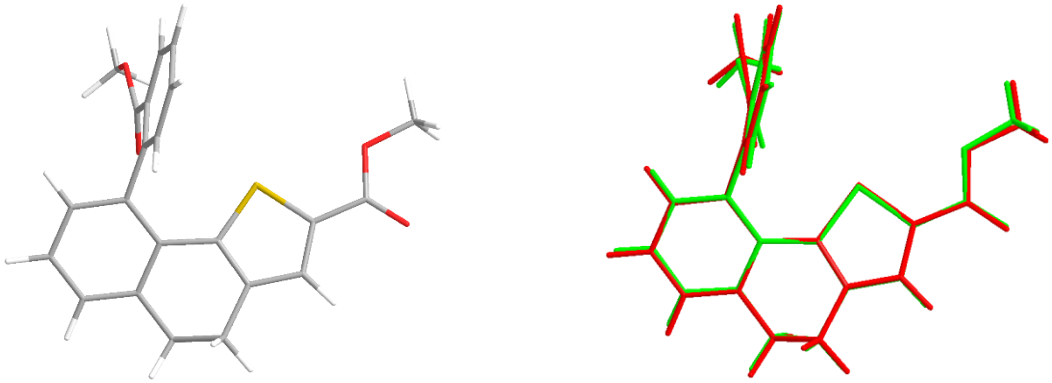


Figure S 11: optimized structure for **4d** (left) and overlay of calculated (red) and X-Ray (green) structures (right).

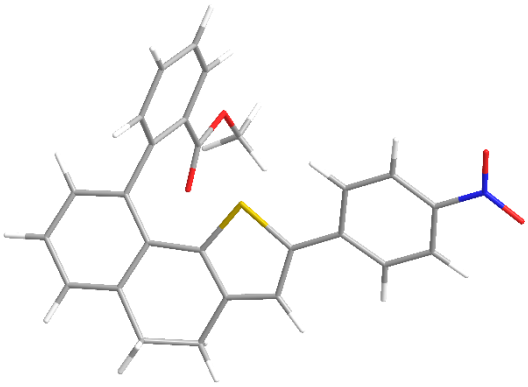


Figure S 12: optimized structure for **4e**.

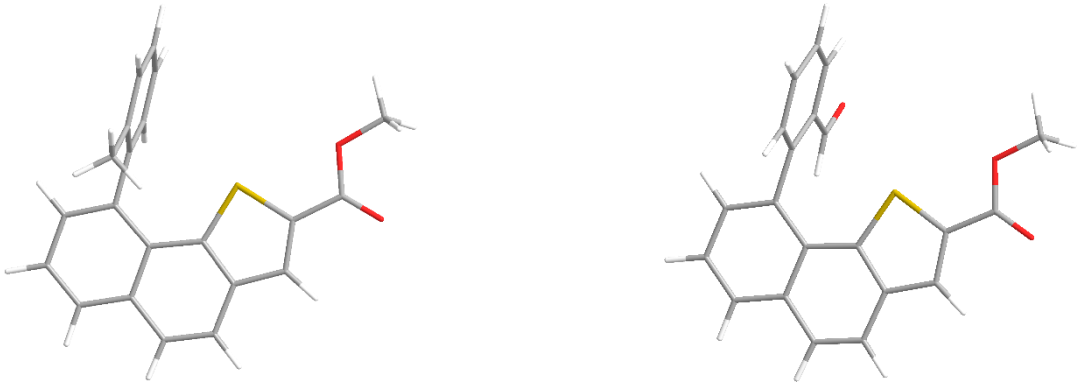


Figure S 13: optimized structure for **5a** (left) and **5b** (right).

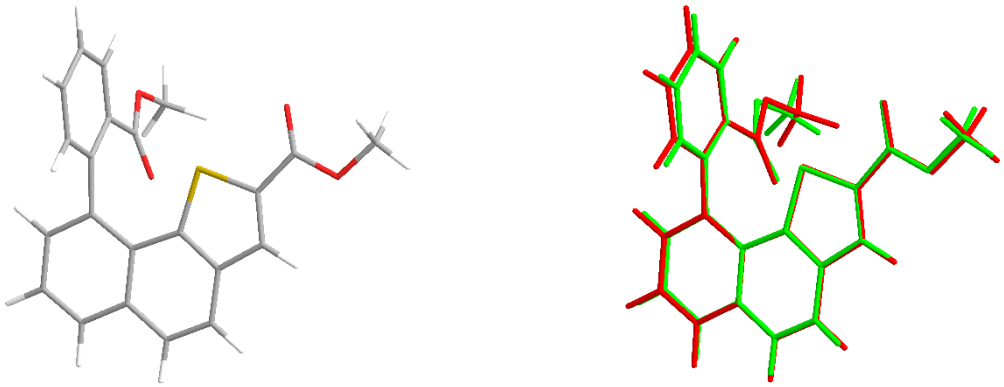


Figure S 14: optimized structure for **5c** (left) and overlay of calculated (red) and X-Ray (green) structures (right).

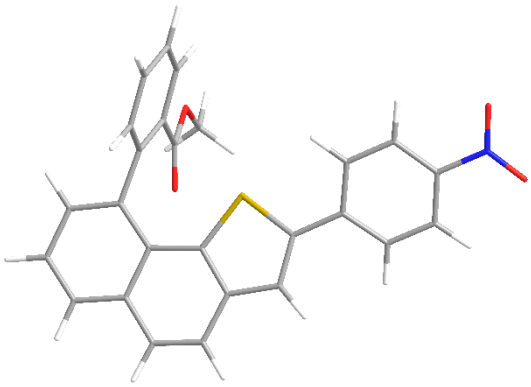


Figure S 15: optimized structure for **5d**.

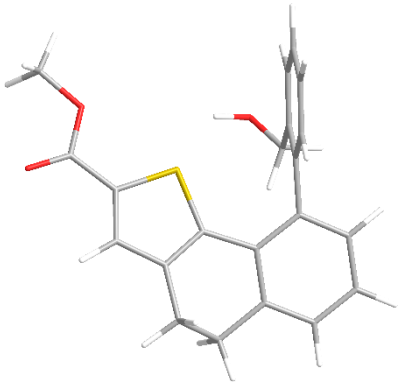


Figure S 16: optimized structure for **6a**.

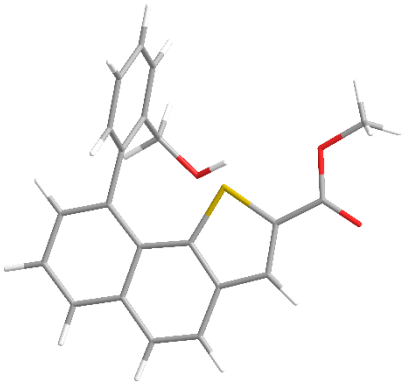


Figure S 17: optimized structure for **6b**.

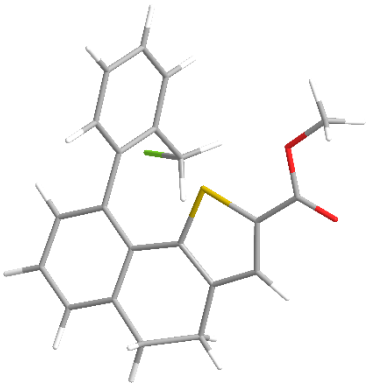
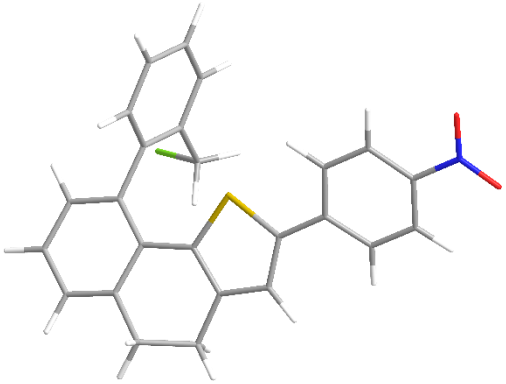
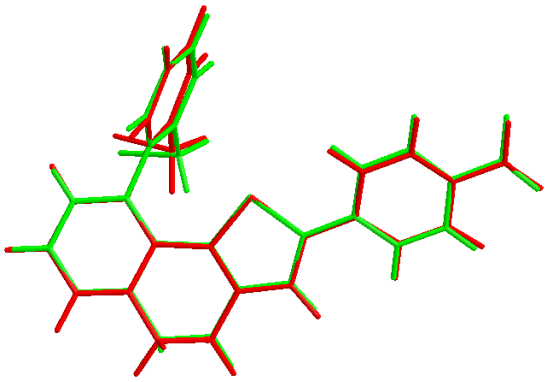


Figure S 18: optimized structure for **7**.



Optimized structure



Overlay of calculated (red) and X-Ray (green) structures

Figure S 19: optimized structure for **8** (left) and overlay of calculated (red) and X-Ray (green) structures (right).

9

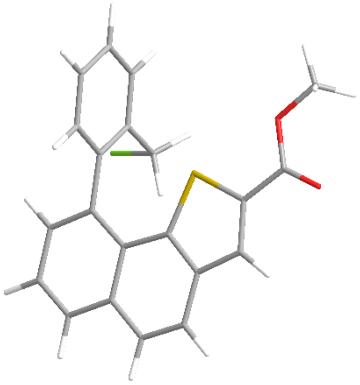
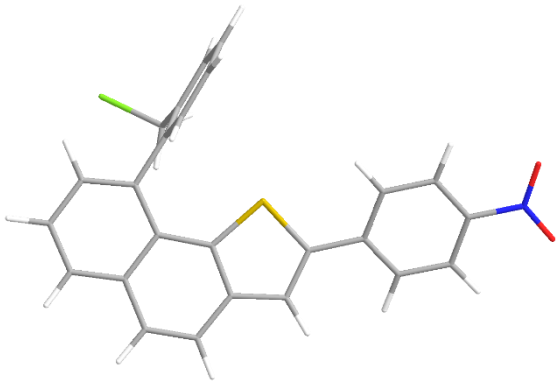
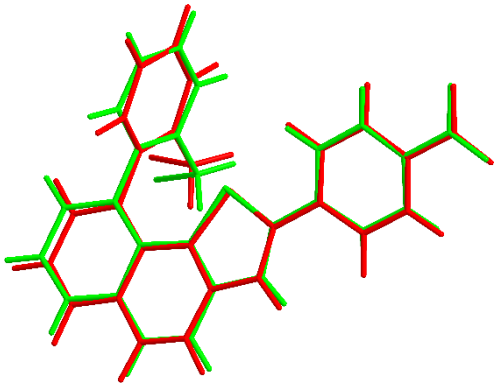


Figure S 20: optimized structure for **9**.



Optimized structure



Overlay of calculated (red) and X-Ray (green) structures

Figure S 21: optimized structure for **10** (left) and overlay of calculated (red) and X-Ray (green) structures (right).

Relative orientation of CH_2-CH_2 bridge

The inversion of the relative orientation of the CH_2-CH_2 bridge was studied by scanning the dihedral angle depicted in red in the structure below. The scan were obtained at the B3LYP/6-31g(d) level of theory.

Compound **4a**

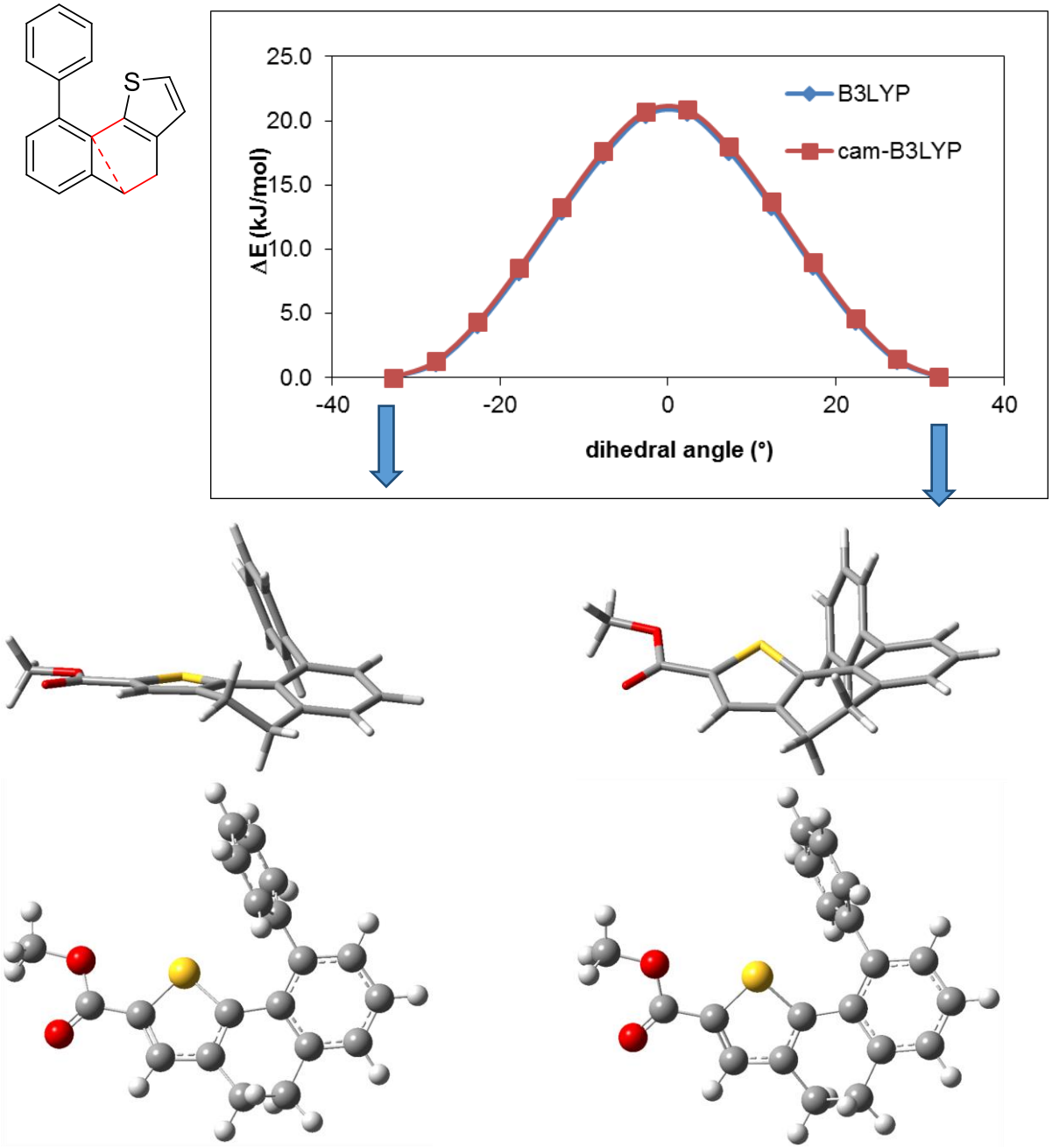


Figure S 22: structure (top left) and energy diagram (top right) for the scan on compound **4a**; starting geometry (based on crystal structure; bottom left) and final geometry ("opposite" to crystal structure; bottom right). Initial and final geometries have the same total energy. The energy of the interconversion barrier is 21 kJ/mol with both methods.

Compound **4c**

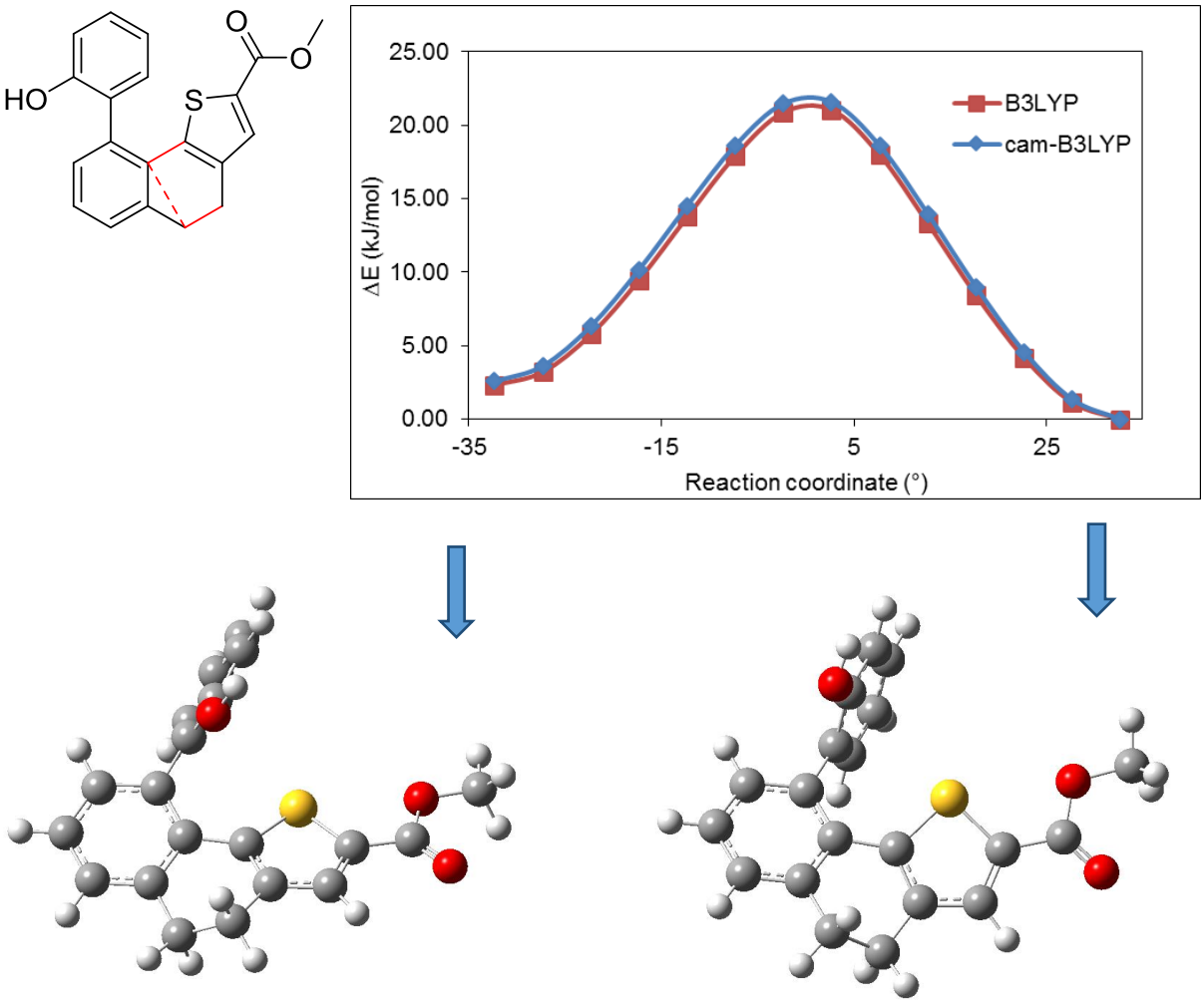
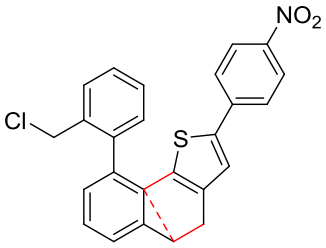
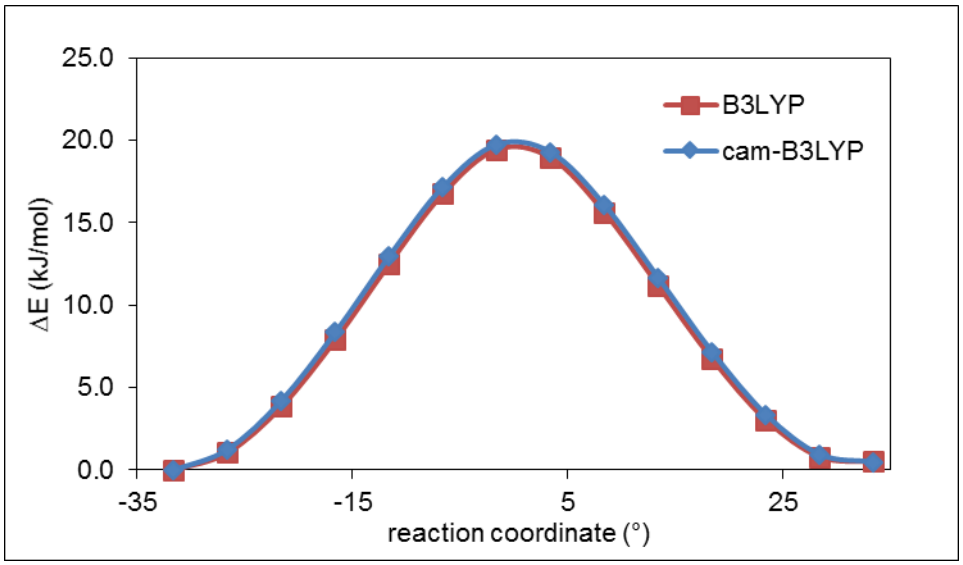


Figure S 23: structure (top left) and energy diagram (top right) for the scan on compound **4c**; starting geometry (based on crystal structure; bottom left) and final geometry ("opposite" to crystal structure; bottom right). Initial geometry is 2 kJ/mol higher in total energy. The energy of the interconversion barrier is 21 kJ/mol and 22 kJ/mol with b3lyp and cam-b3lyp respectively.

Compound **8**





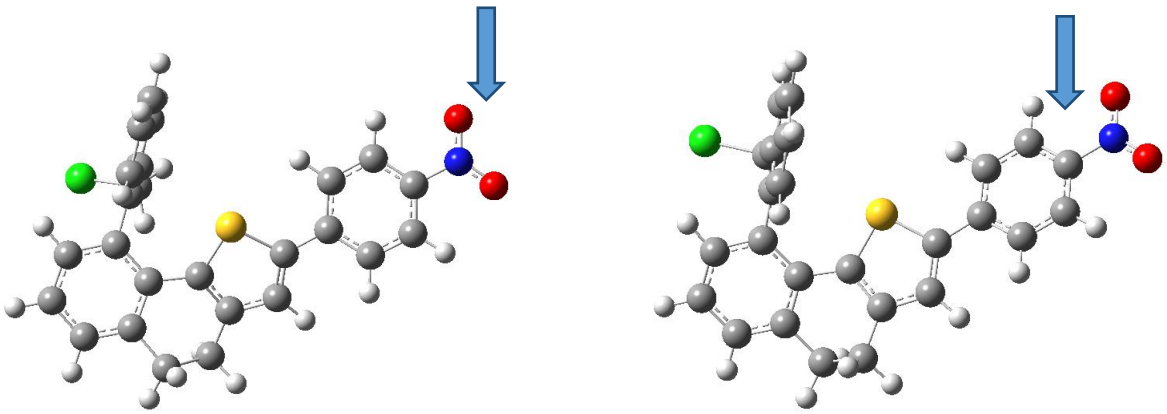
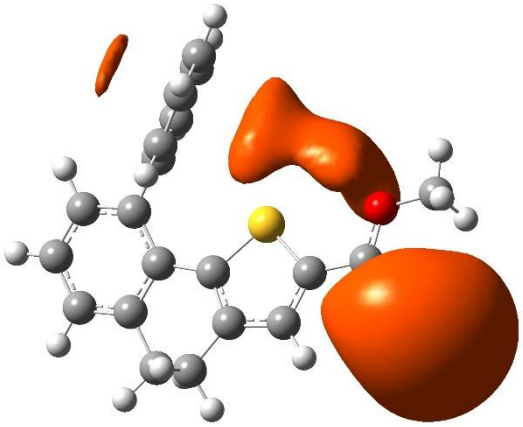


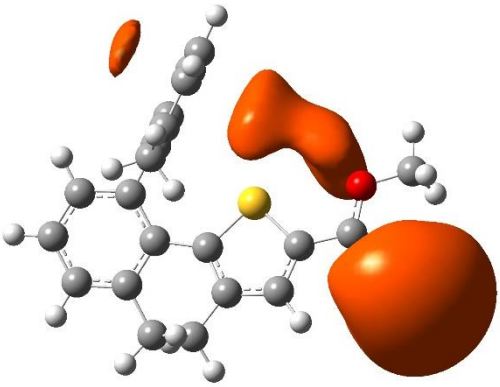
Figure S 24: structure (top left) and energy diagram (top right) for the scan on compound **8**; starting geometry (based on crystal structure; bottom left) and final geometry ("opposite" to crystal structure; bottom right). Final geometry is 0.5 kJ/mol higher in total energy with both methods. The energy of the interconversion barrier is 19 and 20 kJ/mol with b3lyp and cam-b3lyp respectively.

Electrostatic potential surfaces

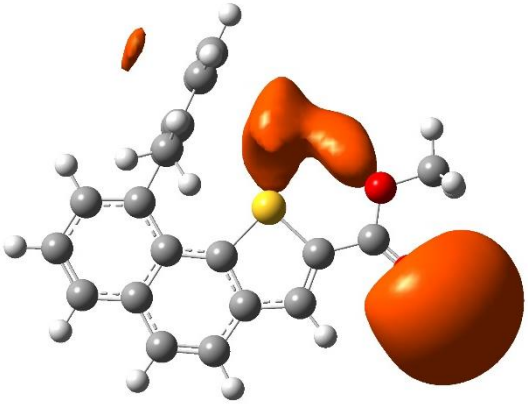
4a



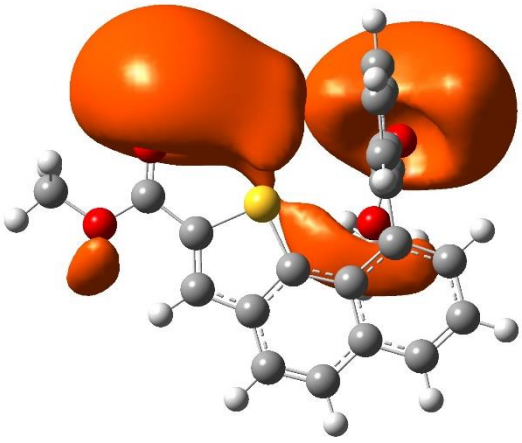
4b



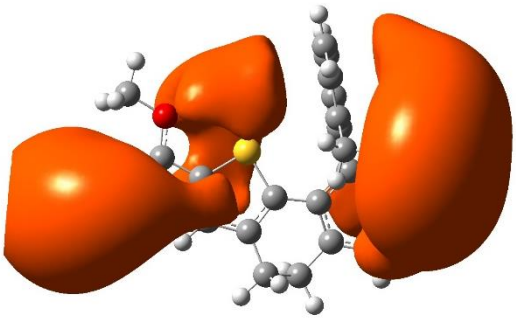
5a



5c



7



9

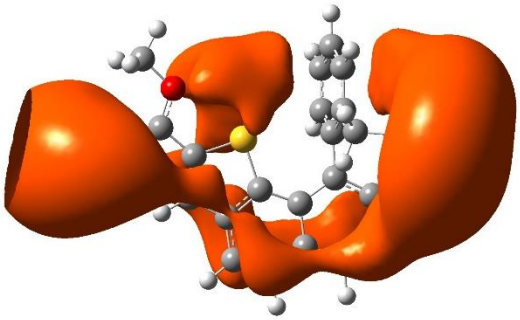


Figure S 25: electrostatic potential surfaces (orange = negative regions, positive regions have been omitted for clarity; isodensity = 0.02 for **4** and **5** series and 0.09 for **7** and **9**). Sulfur atom is in yellow.

Molecular orbitals of the carbocations

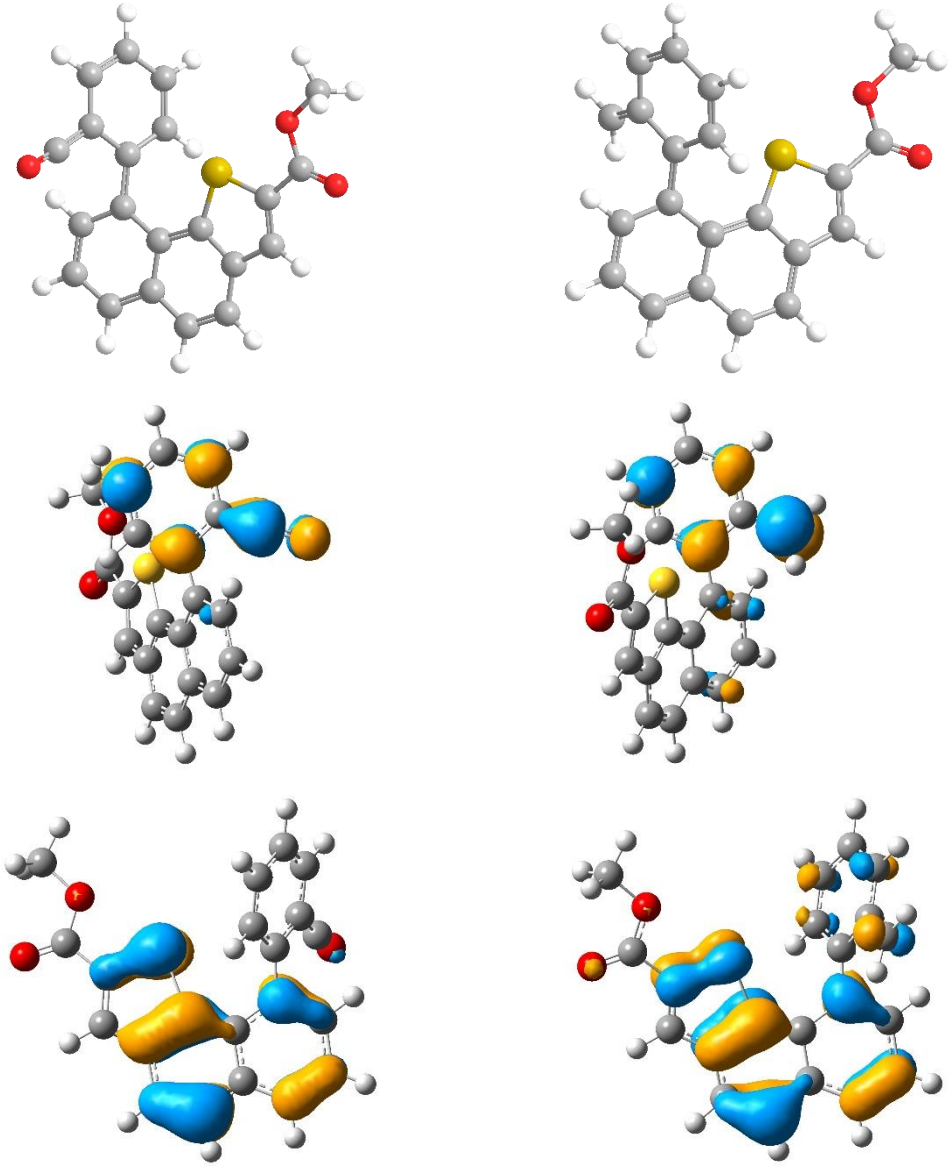


Figure S 26: optimized structures (top), LUMO (middle) and HOMO (bottom) of the carbocation of **5c** (left) and **9** (right); isodensity = 0.04.

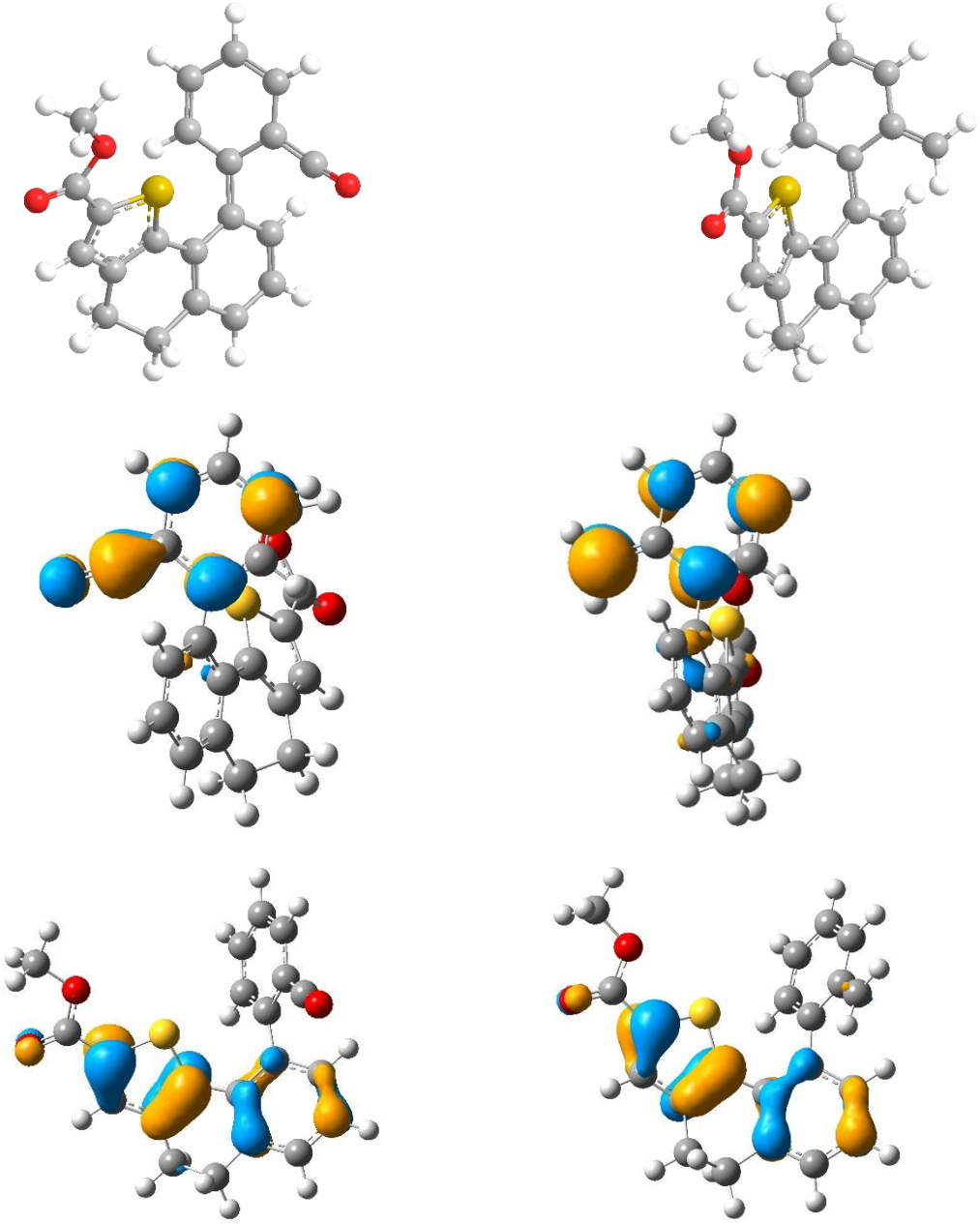


Figure S 27: optimized structures (top), LUMO (middle) and HOMO (bottom) of the carbocation of **4d** (left) and **7** (right); isodensity = 0.04.

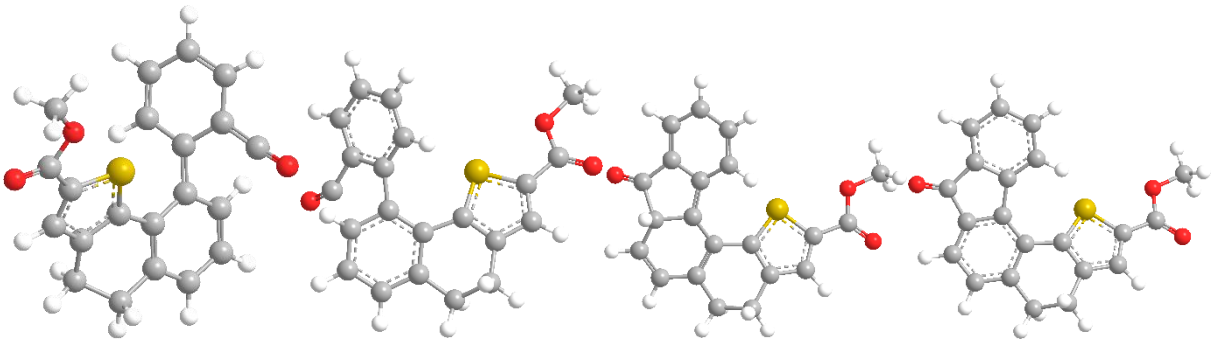


Figure S 28: optimized structures during cyclization of **4d**: carbocation (left), transition state (middle left), cyclized intermediate (middle right) and fluorenone (right).

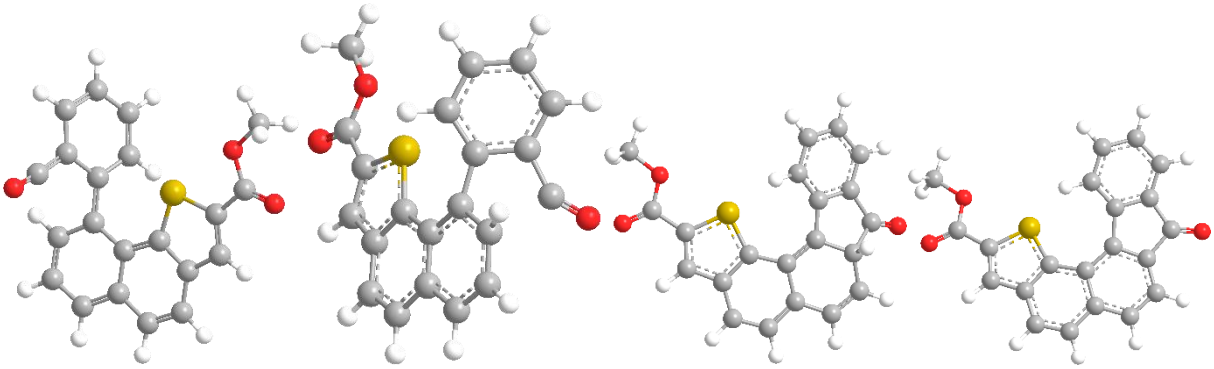


Figure S 29: optimized structures during cyclization of **5c**: carbocation (left), transition state (middle left), cyclized intermediate (middle right) and fluorenone (right).

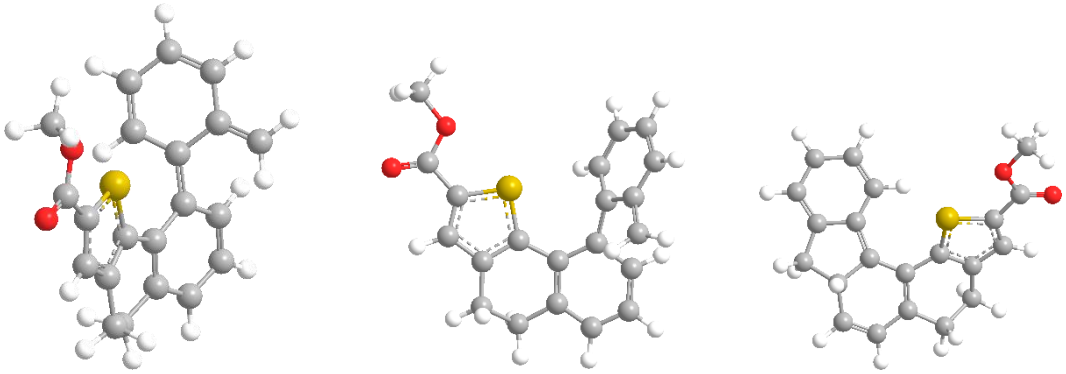


Figure S 30: optimized structures during cyclization of **6a**: carbocation (left), transition state (middle) and cyclized intermediate (right).

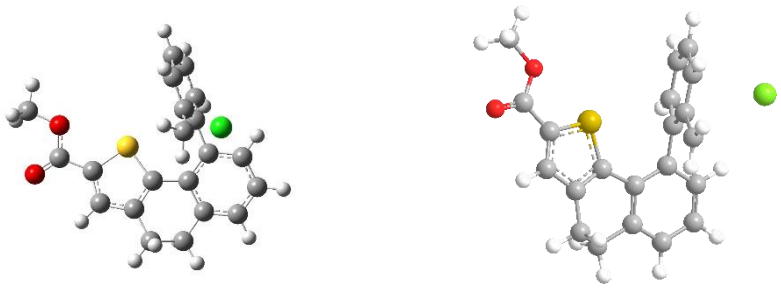


Figure S 31: optimized structures for chlorination of **6a**: reactant (left) and transition state (right). The product of reaction is compound **7**.

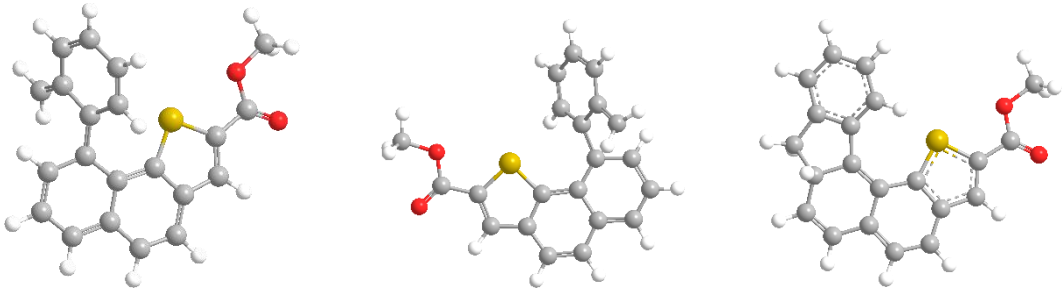


Figure S 32: optimized structures during cyclization of **6b**: carbocation (left), transition state (middle) and cyclized intermediate (right).

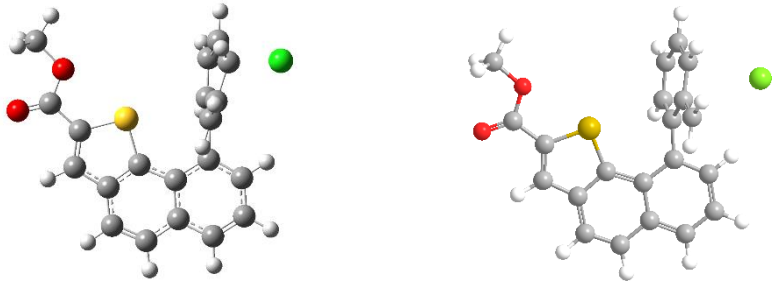


Figure S 33: optimized structures for chlorination of **6b**: reactant (left) and transition state (right). The product of reaction is compound **9**.

Standard orientations (energy from B3LYP/6-31g(d)

Compound **4a**; E= -1320.4256662

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.107132	2.099969	1.349702
2	6	0	-1.62432	1.746359	0.093175
3	6	0	-1.548024	2.678884	-0.952053
4	6	0	-0.953135	3.925746	-0.752515
5	6	0	-0.436427	4.262747	0.499057
6	6	0	-0.518391	3.347177	1.550687
7	1	0	-1.171843	1.390479	2.170151
8	1	0	-1.949284	2.417138	-1.927597
9	1	0	-0.894776	4.632976	-1.575704
10	1	0	0.025132	5.234028	0.655812
11	1	0	-0.124994	3.605572	2.530274
12	6	0	-2.318554	0.438078	-0.108015
13	6	0	-1.657862	-0.815418	-0.074866
14	6	0	-3.706156	0.476488	-0.305581
15	6	0	-2.429336	-2.004312	-0.192395
16	6	0	-4.452666	-0.690186	-0.437074
17	1	0	-4.199093	1.444224	-0.328793
18	6	0	-3.809801	-1.924778	-0.366883
19	1	0	-5.528742	-0.638219	-0.57813
20	1	0	-4.384784	-2.843579	-0.456204
21	6	0	-0.203748	-1.003988	0.050416
22	6	0	0.358839	-2.216855	0.429507
23	16	0	1.0352	0.167306	-0.328525
24	6	0	1.771743	-2.195353	0.428744
25	6	0	2.293223	-0.98331	0.034604
26	1	0	2.404527	-3.033698	0.698564
27	6	0	3.724166	-0.676584	-0.066022
28	8	0	4.616779	-1.464788	0.183894
29	8	0	3.941524	0.598021	-0.475355
30	6	0	5.319787	0.974819	-0.60028
31	1	0	5.827012	0.341823	-1.333579
32	1	0	5.309368	2.013455	-0.932178
33	1	0	5.832514	0.883385	0.361215
34	6	0	-1.743687	-3.357407	-0.181828
35	1	0	-1.39765	-3.590023	-1.200999
36	1	0	-2.464761	-4.136016	0.090536
37	6	0	-0.533467	-3.384219	0.760035
38	1	0	0.010667	-4.329612	0.659358
39	1	0	-0.87322	-3.321854	1.804886

Compound **4b**; E= -1359.7429226

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.168166	2.188627	1.132981
2	6	0	-1.549474	1.671569	-0.125664
3	6	0	-1.335947	2.436438	-1.281183
4	6	0	-0.727818	3.690019	-1.214698
5	6	0	-0.336645	4.196179	0.02332
6	6	0	-0.563241	3.449592	1.180257
7	1	0	-1.645834	2.033237	-2.241837
8	1	0	-0.564394	4.264186	-2.12262
9	1	0	0.137205	5.171864	0.09273
10	1	0	-0.267447	3.853837	2.145674
11	6	0	-2.254817	0.355115	-0.247699
12	6	0	-1.593366	-0.897079	-0.205461
13	6	0	-3.646985	0.388918	-0.409708
14	6	0	-2.363179	-2.088532	-0.305114
15	6	0	-4.394717	-0.780555	-0.510432
16	1	0	-4.140528	1.356155	-0.443925
17	6	0	-3.746998	-2.013312	-0.45137
18	1	0	-5.473765	-0.731926	-0.628273
19	1	0	-4.32119	-2.933933	-0.525953
20	6	0	-0.140915	-1.078942	-0.060046
21	6	0	0.422604	-2.287614	0.332921
22	16	0	1.096896	0.111962	-0.381883
23	6	0	1.834146	-2.248495	0.384349
24	6	0	2.354235	-1.026462	0.021
25	1	0	2.46684	-3.081375	0.670933
26	6	0	3.78434	-0.702402	-0.025758
27	8	0	4.676601	-1.482203	0.250384
28	8	0	4.000961	0.577834	-0.416929
29	6	0	5.378091	0.971996	-0.489592
30	1	0	5.918826	0.350894	-1.208988
31	1	0	5.366803	2.013015	-0.813878
32	1	0	5.857262	0.879159	0.488934
33	6	0	-1.671259	-3.438171	-0.303127
34	1	0	-1.320757	-3.660089	-1.323137
35	1	0	-2.388352	-4.223269	-0.039313
36	6	0	-0.463737	-3.465684	0.641669
37	1	0	0.088304	-4.405506	0.531376
38	1	0	-0.806834	-3.419599	1.686411
39	6	0	-1.399685	1.408311	2.405843
40	1	0	-2.440353	1.075582	2.491555
41	1	0	-0.773425	0.508348	2.443419
42	1	0	-1.162008	2.015902	3.284457

Compound **4c**; E= -1395.6410055

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.525272	2.545718	-1.177667
2	6	0	-1.589325	1.657144	-0.09645
3	6	0	-1.073699	2.085217	1.143236
4	6	0	-0.499869	3.352424	1.274335
5	6	0	-0.434105	4.210567	0.176909
6	6	0	-0.948889	3.811013	-1.055569
7	1	0	-1.928137	2.222718	-2.133951
8	1	0	-0.107167	3.665851	2.240318
9	1	0	0.017752	5.192047	0.292258
10	1	0	-0.903007	4.474611	-1.913826
11	6	0	-2.270371	0.334826	-0.238955
12	6	0	-1.594065	-0.908805	-0.184249
13	6	0	-3.658508	0.351909	-0.430447
14	6	0	-2.348588	-2.108832	-0.281768
15	6	0	-4.390059	-0.826751	-0.541677
16	1	0	-4.164149	1.312524	-0.46814
17	6	0	-3.73051	-2.051029	-0.455677
18	1	0	-5.467119	-0.791081	-0.680488
19	1	0	-4.29294	-2.978981	-0.529697
20	6	0	-0.140573	-1.073888	-0.041563
21	6	0	0.435866	-2.269381	0.36934
22	16	0	1.083375	0.114347	-0.413956
23	6	0	1.847656	-2.22043	0.400404
24	6	0	2.355674	-1.004762	-0.000443
25	1	0	2.489602	-3.042491	0.697594
26	6	0	3.78151	-0.673386	-0.077224
27	8	0	4.684539	-1.438671	0.205642
28	8	0	3.984385	0.598491	-0.505309
29	6	0	5.357807	0.996121	-0.613272
30	1	0	5.889168	0.357513	-1.32432
31	1	0	5.336247	2.027589	-0.966572
32	1	0	5.855137	0.932857	0.358629
33	6	0	-1.643544	-3.451464	-0.2462
34	1	0	-1.284545	-3.694439	-1.258501
35	1	0	-2.355309	-4.236639	0.031833
36	6	0	-0.441968	-3.445593	0.707084
37	1	0	0.117431	-4.384061	0.625755
38	1	0	-0.792947	-3.371824	1.747398
39	8	0	-1.163827	1.216735	2.194794
40	1	0	-0.719818	1.608105	2.963105

Compound **4d**; E= -1548.2982598

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.855457	-1.716177	0.341705
2	6	0	1.594129	-0.546226	1.090224
3	6	0	1.201406	-0.686808	2.429023
4	6	0	1.053483	-1.941776	3.01623
5	6	0	1.313722	-3.092628	2.271692
6	6	0	1.717373	-2.975982	0.945234
7	1	0	1.013752	0.210205	3.012139
8	1	0	0.741441	-2.018752	4.054289
9	1	0	1.203484	-4.075596	2.720809
10	1	0	1.922519	-3.862634	0.356671
11	6	0	1.827291	0.842006	0.573071
12	6	0	0.788752	1.707125	0.156487
13	6	0	3.14523	1.313987	0.611756
14	6	0	1.110686	3.044282	-0.201422
15	6	0	3.454331	2.621322	0.251074
16	1	0	3.931268	0.640705	0.942369
17	6	0	2.432664	3.481043	-0.14835
18	1	0	4.482346	2.970728	0.291511
19	1	0	2.66196	4.507073	-0.426523
20	6	0	-0.630944	1.339676	0.062654
21	6	0	-1.645182	2.288935	0.011301
22	16	0	-1.282761	-0.275197	-0.046469
23	6	0	-2.932184	1.716566	-0.096951
24	6	0	-2.910402	0.340096	-0.144103
25	1	0	-3.858082	2.278988	-0.146969
26	6	0	-4.093897	-0.516171	-0.266078
27	8	0	-5.237674	-0.106662	-0.336392
28	8	0	-3.766944	-1.833133	-0.293499
29	6	0	-4.874318	-2.735479	-0.418429
30	1	0	-5.421751	-2.547434	-1.346182
31	1	0	-4.437391	-3.73462	-0.427161
32	1	0	-5.560336	-2.623497	0.425791
33	6	0	0.018748	3.978588	-0.685616
34	1	0	-0.151224	3.799805	-1.758559
35	1	0	0.348239	5.018796	-0.58707
36	6	0	-1.303134	3.754848	0.059811
37	1	0	-2.103067	4.354591	-0.388254
38	1	0	-1.202928	4.088116	1.104092
39	6	0	2.218458	-1.628622	-1.105513
40	8	0	2.013764	-0.67406	-1.826663
41	8	0	2.802447	-2.769476	-1.549574
42	6	0	3.128407	-2.780626	-2.947556
43	1	0	2.228445	-2.647774	-3.554085
44	1	0	3.834592	-1.980158	-3.183431
45	1	0	3.577712	-3.756597	-3.134365

Compound **4d^{+}(-MeO^{-})**; E= -1432.8838155

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.168059	-2.226979	0.268239
2	6	0	-1.739006	-1.130416	-0.549172
3	6	0	-1.077446	-1.472644	-1.734718
4	6	0	-0.900658	-2.804621	-2.100327
5	6	0	-1.353119	-3.866225	-1.289952
6	6	0	-1.985719	-3.59674	-0.097054
7	1	0	-0.737445	-0.677931	-2.389517
8	1	0	-0.412902	-3.031519	-3.043668
9	1	0	-1.203755	-4.894013	-1.602855
10	1	0	-2.335298	-4.390488	0.554538
11	6	0	-2.099325	0.253745	-0.185147
12	6	0	-1.157699	1.317537	-0.111527
13	6	0	-3.474736	0.512687	0.001704
14	6	0	-1.646165	2.638598	0.070187
15	6	0	-3.931128	1.807171	0.213766
16	1	0	-4.193015	-0.294751	-0.115939
17	6	0	-3.015336	2.8594	0.229256
18	1	0	-4.992899	1.999537	0.329263
19	1	0	-3.369855	3.876714	0.371777
20	6	0	0.298243	1.164238	-0.14598
21	6	0	1.146503	2.226445	-0.428413
22	16	0	1.207622	-0.269708	0.279822
23	6	0	2.514955	1.873694	-0.342588
24	6	0	2.715321	0.566098	0.033206
25	1	0	3.343227	2.547231	-0.531866
26	6	0	4.033059	-0.074051	0.222346
27	8	0	5.08548	0.50409	0.056797
28	8	0	3.911983	-1.363407	0.60007
29	6	0	5.155976	-2.05915	0.825898
30	1	0	5.726933	-1.565372	1.615473
31	1	0	4.873471	-3.067692	1.126191
32	1	0	5.750391	-2.0789	-0.090518
33	6	0	-0.670777	3.796539	0.147541
34	1	0	-0.344055	3.908926	1.192449
35	1	0	-1.181423	4.726297	-0.122592
36	6	0	0.566053	3.580814	-0.737238
37	1	0	1.303125	4.369016	-0.556727
38	1	0	0.287603	3.644217	-1.799043
39	6	0	-2.704316	-1.947572	1.509071
40	8	0	-3.106934	-1.7991	2.567046

Transition state for cyclization of **4d**$^{+}$; E= -1432.87315494; ν = -190.9140

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.658953	-1.836863	0.249233
2	6	0	-1.751435	-1.148169	-0.590729
3	6	0	-0.925012	-1.900396	-1.425819
4	6	0	-1.01969	-3.29521	-1.395982
5	6	0	-1.910483	-3.96061	-0.539278
6	6	0	-2.755415	-3.23662	0.294907
7	1	0	-0.238942	-1.415436	-2.109705
8	1	0	-0.388914	-3.878889	-2.059661
9	1	0	-1.942515	-5.045176	-0.528485
10	1	0	-3.461161	-3.727066	0.957068
11	6	0	-1.919049	0.312869	-0.46451
12	6	0	-0.929868	1.293119	-0.253807
13	6	0	-3.312479	0.636509	-0.3011
14	6	0	-1.375355	2.623456	0.029466
15	6	0	-3.708111	1.943873	0.071515
16	1	0	-4.032226	0.079569	-0.90326
17	6	0	-2.739186	2.914011	0.221536
18	1	0	-4.762155	2.1863	0.164989
19	1	0	-3.023446	3.9324	0.470008
20	6	0	0.523787	1.086511	-0.227384
21	6	0	1.413652	2.13797	-0.400241
22	16	0	1.372625	-0.396332	0.145975
23	6	0	2.767252	1.743166	-0.270017
24	6	0	2.909848	0.410791	0.030735
25	1	0	3.620444	2.403512	-0.375758
26	6	0	4.200022	-0.28044	0.247807
27	8	0	5.273162	0.276925	0.170312
28	8	0	4.022524	-1.583511	0.538646
29	6	0	5.231528	-2.334635	0.781803
30	1	0	5.776624	-1.907638	1.626553
31	1	0	4.901705	-3.348312	1.00637
32	1	0	5.869329	-2.320513	-0.10494
33	6	0	-0.364141	3.727307	0.216809
34	1	0	-0.073971	3.74006	1.279869
35	1	0	-0.835133	4.694523	0.013466
36	6	0	0.89452	3.529043	-0.639593
37	1	0	1.647489	4.277374	-0.376433
38	1	0	0.656309	3.678056	-1.70202
39	6	0	-3.534788	-0.958111	0.980285
40	8	0	-4.282597	-0.875025	1.867607

Compound **4e**; E= -1755.9794229

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.226466	-1.677291	-2.239654
2	6	0	-2.519932	-1.258323	-0.933414
3	6	0	-2.245791	-2.147727	0.133141
4	6	0	-1.674713	-3.400764	-0.1383
5	6	0	-1.372701	-3.787076	-1.441011
6	6	0	-1.654408	-2.92239	-2.497767
7	1	0	-2.45075	-1.003939	-3.061972
8	1	0	-1.469795	-4.070367	0.688231
9	1	0	-0.926403	-4.759612	-1.628176
10	1	0	-1.433411	-3.21397	-3.521026
11	6	0	-3.189606	0.075103	-0.778329
12	6	0	-2.497063	1.274576	-0.489865
13	6	0	-4.570575	0.112435	-1.004231
14	6	0	-3.230656	2.488287	-0.411442
15	6	0	-5.283218	1.30527	-0.924956
16	1	0	-5.087241	-0.815701	-1.231922
17	6	0	-4.607672	2.486285	-0.625363
18	1	0	-6.356579	1.312835	-1.092848
19	1	0	-5.153858	3.424433	-0.56036
20	6	0	-1.056674	1.377659	-0.228001
21	6	0	-0.486871	2.469458	0.408154
22	16	0	0.173384	0.209128	-0.650593
23	6	0	0.915116	2.359812	0.560042
24	6	0	1.447964	1.199146	0.035376
25	1	0	1.517564	3.136049	1.020471
26	6	0	-2.504911	3.791615	-0.137502
27	6	0	-1.357227	3.610626	0.863302
28	6	0	2.844708	0.774616	0.006912
29	6	0	3.292872	-0.242496	-0.863271
30	6	0	3.794506	1.379641	0.859593
31	6	0	4.622464	-0.638942	-0.886639
32	1	0	2.591484	-0.718091	-1.542053
33	6	0	5.12785	0.998893	0.839117
34	1	0	3.476728	2.144571	1.560172
35	6	0	5.531737	-0.010946	-0.035668
36	1	0	4.968857	-1.416934	-1.555735
37	1	0	5.857481	1.459653	1.493618
38	7	0	6.935805	-0.420982	-0.057614
39	8	0	7.715054	0.15568	0.704354
40	8	0	7.260552	-1.319778	-0.836728
41	1	0	-1.765101	3.393739	1.861888
42	1	0	-0.774351	4.534591	0.95041
43	1	0	-3.215532	4.54441	0.220638
44	1	0	-2.087562	4.174482	-1.081968
45	6	0	-2.54565	-1.766677	1.54788
46	8	0	-2.886657	-0.665874	1.929029
47	8	0	-2.391513	-2.813846	2.396465
48	6	0	-2.637766	-2.517998	3.778752
49	1	0	-3.667008	-2.178227	3.921745
50	1	0	-2.464485	-3.453179	4.312208
51	1	0	-1.956204	-1.74014	4.13338

Compound **5a**; E= -1358.5452755

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.263886	2.267694	0.988608
2	6	0	-1.577209	1.592769	-0.212681
3	6	0	-1.307113	2.207066	-1.44373
4	6	0	-0.713894	3.467582	-1.505153
5	6	0	-0.392902	4.131666	-0.322497
6	6	0	-0.671356	3.533147	0.906764
7	1	0	-1.562774	1.68106	-2.359791
8	1	0	-0.507581	3.925273	-2.46878
9	1	0	0.06879	5.115142	-0.353387
10	1	0	-0.426039	4.058354	1.826984
11	6	0	-2.26828	0.263008	-0.196744
12	6	0	-1.569355	-0.984658	-0.117164
13	6	0	-3.654231	0.265122	-0.269387
14	6	0	-2.340397	-2.200177	-0.093462
15	6	0	-4.403146	-0.926481	-0.253294
16	1	0	-4.167838	1.220255	-0.336333
17	6	0	-3.752525	-2.136061	-0.161597
18	1	0	-5.487277	-0.884965	-0.31035
19	1	0	-4.314594	-3.066556	-0.142961
20	6	0	-0.142189	-1.136582	-0.066397
21	6	0	0.464373	-2.408841	0.01887
22	16	0	1.079419	0.125908	-0.111716
23	6	0	1.888168	-2.342042	0.052614
24	6	0	2.364087	-1.062567	-0.008691
25	1	0	2.542813	-3.20388	0.116956
26	6	0	3.790588	-0.701227	0.00384
27	8	0	4.701554	-1.503261	0.073823
28	8	0	3.971245	0.638315	-0.07295
29	6	0	5.338383	1.075082	-0.069552
30	1	0	5.877044	0.65616	-0.923808
31	1	0	5.297005	2.162454	-0.137088
32	1	0	5.83811	0.764807	0.852078
33	6	0	-1.694921	-3.474168	-0.004825
34	1	0	-2.321135	-4.36237	0.013864
35	6	0	-0.336353	-3.585118	0.053467
36	1	0	0.145612	-4.556543	0.120739
37	6	0	-1.551104	1.647103	2.33625
38	1	0	-1.294182	2.336826	3.146016
39	1	0	-2.608449	1.378155	2.440355
40	1	0	-0.973028	0.726965	2.484537

Compound **5b**; E= -1432.5494717

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.483123	2.226082	0.589984
2	6	0	1.6278	1.328584	-0.49126
3	6	0	1.290939	1.770799	-1.778848
4	6	0	0.811481	3.06268	-1.991147
5	6	0	0.663495	3.94413	-0.915846
6	6	0	1.001366	3.524804	0.365015
7	1	0	1.409534	1.090177	-2.617186
8	1	0	0.556281	3.382416	-2.997913
9	1	0	0.290042	4.950857	-1.081213
10	1	0	0.90308	4.184248	1.221846
11	6	0	2.209892	-0.044291	-0.32634
12	6	0	1.410891	-1.222879	-0.170951
13	6	0	3.592584	-0.152482	-0.379389
14	6	0	2.084157	-2.492192	-0.078815
15	6	0	4.243779	-1.396333	-0.285938
16	1	0	4.18124	0.752513	-0.500813
17	6	0	3.497126	-2.543519	-0.140655
18	1	0	5.327991	-1.443505	-0.330718
19	1	0	3.982979	-3.513319	-0.068351
20	6	0	-0.022377	-1.255701	-0.088213
21	6	0	-0.726361	-2.468868	0.071807
22	16	0	-1.139871	0.099078	-0.148906
23	6	0	-2.138821	-2.284416	0.141248
24	6	0	-2.511969	-0.974151	0.041077
25	1	0	-2.858612	-3.086022	0.262192
26	6	0	-3.903435	-0.494097	0.082068
27	8	0	-4.873135	-1.215291	0.210354
28	8	0	-3.973942	0.851447	-0.040949
29	6	0	-5.298756	1.404173	-0.005281
30	1	0	-5.784645	1.172749	0.946308
31	1	0	-5.168208	2.480584	-0.118145
32	1	0	-5.904196	1.001055	-0.821462
33	6	0	1.340428	-3.704266	0.077997
34	1	0	1.8944	-4.63714	0.140947
35	6	0	-0.021904	-3.702897	0.15159
36	1	0	-0.578424	-4.627944	0.273302
37	6	0	1.813687	1.831162	1.983946
38	8	0	1.74299	2.587477	2.935609
39	1	0	2.136423	0.781063	2.121301

Compound **5c**; E= -1547.1010246

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.444142	-2.138394	0.118066
2	6	0	1.476802	-1.149009	-0.891973
3	6	0	1.115473	-1.521323	-2.196528
4	6	0	0.717715	-2.821203	-2.502582
5	6	0	0.690051	-3.792027	-1.501006
6	6	0	1.058573	-3.448325	-0.205082
7	1	0	1.154351	-0.769441	-2.979529
8	1	0	0.438916	-3.074322	-3.521893
9	1	0	0.387293	-4.810195	-1.728357
10	1	0	1.057207	-4.185925	0.590133
11	6	0	1.988758	0.248559	-0.70071
12	6	0	1.138394	1.372799	-0.456116
13	6	0	3.352852	0.439888	-0.856636
14	6	0	1.740251	2.677555	-0.380938
15	6	0	3.936848	1.717913	-0.774153
16	1	0	3.981987	-0.424368	-1.05051
17	6	0	3.139721	2.815751	-0.543064
18	1	0	5.010127	1.83023	-0.899486
19	1	0	3.572482	3.811271	-0.482448
20	6	0	-0.282403	1.316211	-0.264744
21	6	0	-1.045107	2.479529	-0.023804
22	16	0	-1.31338	-0.105298	-0.265614
23	6	0	-2.433474	2.204544	0.15059
24	6	0	-2.731397	0.874616	0.051911
25	1	0	-3.190092	2.956642	0.343706
26	6	0	-4.082395	0.307883	0.188908
27	8	0	-5.082542	0.962945	0.409079
28	8	0	-4.081006	-1.037796	0.040209
29	6	0	-5.363582	-1.6708	0.160843
30	1	0	-6.051795	-1.291254	-0.599239
31	1	0	-5.178144	-2.735122	0.014373
32	1	0	-5.790588	-1.486872	1.150387
33	6	0	0.93878	3.8387	-0.141687
34	1	0	1.439152	4.802625	-0.098514
35	6	0	-0.41202	3.753175	0.031044
36	1	0	-1.012284	4.640197	0.213679
37	6	0	1.786604	-1.917005	1.559711
38	8	0	2.015288	-2.819511	2.34254
39	8	0	1.784834	-0.619196	1.918676
40	6	0	2.092701	-0.359178	3.297231
41	1	0	1.355394	-0.834414	3.949528
42	1	0	3.086332	-0.74032	3.546923
43	1	0	2.057425	0.725344	3.401355

Compound **5c^{+}(-MeO^{-})**; E= -1431.684908

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	-2.628E-06	7.473E-06	-1.2097E-05	1
2	6	-1.1499E-05	5.703E-06	-1.3088E-05	2
3	6	2.5248E-05	-9.42E-07	7.682E-06	3
4	6	-1.6067E-05	-6.61E-07	0.00001795	4
5	6	-8.288E-06	-2.354E-06	-1.2963E-05	5
6	6	0.00001019	-5.859E-06	9.438E-06	6
7	1	-5.293E-06	1.54E-07	-1.87E-07	7
8	1	2.361E-06	-4.685E-06	-4.272E-06	8
9	1	2.706E-06	-2.98E-07	4.685E-06	9
10	1	-4.093E-06	9.88E-07	1.046E-06	10
11	6	-6.849E-06	-2.8292E-05	-0.00000459	11
12	6	1.086E-06	0.00001014	1.87E-07	12
13	6	1.018E-06	1.3133E-05	5.702E-06	13
14	6	-1.1682E-05	-8.609E-06	2.645E-06	14
15	6	-3.26E-07	3.525E-06	-0.0000008	15
16	1	2.319E-06	8.02E-07	-1.457E-06	16
17	6	3.293E-06	7.233E-06	-2.595E-06	17
18	1	-6.465E-06	2.601E-06	1.355E-06	18
19	1	-2.025E-06	-7.37E-07	-2.047E-06	19
20	6	1.853E-06	6.711E-06	5.48E-07	20
21	6	8.735E-06	-4.74E-07	5.174E-06	21
22	16	-9.88E-07	-0.00000078	-5.89E-07	22
23	6	-7.607E-06	-2.562E-06	-9.783E-06	23
24	6	8.216E-06	3.874E-06	2.765E-06	24
25	1	1.325E-06	4.06E-07	1.788E-06	25
26	6	2.485E-06	-1.3501E-05	2.345E-06	26
27	8	3.159E-06	4.977E-06	0.00000255	27
28	8	-0.00000098	2.671E-06	-4.917E-06	28
29	6	6.756E-06	-3.712E-06	5.006E-06	29
30	1	6.14E-07	-9.49E-07	0.00000089	30
31	1	3.295E-06	-0.00000256	1.275E-06	31
32	1	3.016E-06	-1.325E-06	-0.00000156	32
33	6	0.00000491	1.1964E-05	8.82E-07	33
34	1	-1.976E-06	2.646E-06	-3.79E-07	34
35	6	-4.528E-06	-6.909E-06	-3.237E-06	35
36	1	-5.31E-07	0.0000003	1.302E-06	36
37	6	2.9901E-05	-5.806E-06	1.3974E-05	37
38	8	-3.0661E-05	5.712E-06	-1.4631E-05	38

Transition state for cyclization of **5c**$^{+}$; E= -1431.6758566; ν = -192.8676

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.591315	1.822188	0.40166
2	6	0	-1.704337	1.207673	-0.513958
3	6	0	-0.893754	2.027082	-1.298708
4	6	0	-0.97634	3.4143	-1.138133
5	6	0	-1.841945	4.003057	-0.203483
6	6	0	-2.678518	3.211418	0.576609
7	1	0	-0.235228	1.605349	-2.048589
8	1	0	-0.359089	4.052984	-1.762703
9	1	0	-1.864112	5.082273	-0.092571
10	1	0	-3.370759	3.644008	1.291231
11	6	0	-1.906205	-0.258658	-0.523614
12	6	0	-0.945537	-1.287483	-0.331964
13	6	0	-3.305233	-0.554764	-0.487071
14	6	0	-1.454972	-2.641626	-0.212751
15	6	0	-3.773718	-1.887082	-0.294392
16	8	0	-4.183204	0.657748	1.924319
17	1	0	-3.973672	0.117786	-1.023992
18	6	0	-2.859842	-2.894108	-0.181896
19	1	0	-4.839715	-2.089167	-0.299882
20	1	0	-3.187712	-3.923866	-0.073697
21	6	0	0.477502	-1.123273	-0.188579
22	6	0	1.326397	-2.244853	-0.029342
23	16	0	1.417749	0.350921	-0.115838
24	6	0	2.702182	-1.892231	0.124967
25	6	0	2.906407	-0.546279	0.106631
26	1	0	3.510596	-2.602646	0.253581
27	6	0	4.223104	0.119884	0.253926
28	8	0	5.258556	-0.488605	0.406782
29	8	0	4.107073	1.458648	0.194845
30	6	0	5.342715	2.195758	0.332103
31	1	0	5.062077	3.245695	0.259543
32	1	0	5.801957	1.981726	1.299655
33	1	0	6.034443	1.921131	-0.46723
34	6	0	-0.57026	-3.739008	-0.068422
35	1	0	-0.991043	-4.73713	0.000723
36	6	0	0.78749	-3.553974	0.005125
37	1	0	1.456026	-4.402221	0.119022
38	6	0	-3.46168	0.866483	1.03642

Compound **5d**; E= -1754.782374

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.236885	-1.330872	-2.329356
2	6	0	-2.544499	-1.08806	-0.982575
3	6	0	-2.318837	-2.12324	-0.045474
4	6	0	-1.789426	-3.349051	-0.477298
5	6	0	-1.475423	-3.562215	-1.816539
6	6	0	-1.702085	-2.548491	-2.747287
7	1	0	-2.424315	-0.54403	-3.054326
8	1	0	-1.624244	-4.132643	0.252659
9	1	0	-1.061013	-4.515948	-2.130819
10	1	0	-1.469352	-2.70446	-3.797206
11	6	0	-3.19467	0.221733	-0.647394
12	6	0	-2.459339	1.40414	-0.317997
13	6	0	-4.575042	0.279028	-0.753063
14	6	0	-3.192189	2.622236	-0.098317
15	6	0	-5.287568	1.472405	-0.528866
16	1	0	-5.116835	-0.625933	-1.013682
17	6	0	-4.603453	2.622237	-0.208684
18	1	0	-6.370487	1.478603	-0.614555
19	1	0	-5.136576	3.553915	-0.036308
20	6	0	-1.036619	1.490162	-0.182061
21	6	0	-0.388554	2.696301	0.148767
22	16	0	0.143402	0.201802	-0.360307
23	6	0	1.029109	2.559681	0.245245
24	6	0	1.481791	1.289979	0.000106
25	1	0	1.683473	3.397082	0.463167
26	6	0	-2.508112	3.834837	0.22836
27	6	0	-1.149118	3.882036	0.348442
28	6	0	2.863302	0.806395	0.011234
29	6	0	3.241831	-0.361629	-0.681963
30	6	0	3.858043	1.508229	0.724716
31	6	0	4.55528	-0.812204	-0.669625
32	1	0	2.500501	-0.913231	-1.251872
33	6	0	5.175682	1.07388	0.737163
34	1	0	3.587132	2.391755	1.293071
35	6	0	5.511794	-0.08642	0.038794
36	1	0	4.851998	-1.70659	-1.203433
37	1	0	5.942567	1.607057	1.285386
38	7	0	6.900234	-0.554294	0.053996
39	8	0	7.72275	0.11043	0.686698
40	8	0	7.165636	-1.585099	-0.567039
41	1	0	-0.640005	4.808817	0.598562
42	1	0	-3.104657	4.730196	0.382828
43	6	0	-2.605134	-1.912719	1.406926
44	8	0	-2.791417	-0.838327	1.939529
45	8	0	-2.627017	-3.082294	2.092393
46	6	0	-2.856152	-2.955287	3.503989
47	1	0	-3.824183	-2.484548	3.694535
48	1	0	-2.840272	-3.973343	3.894365
49	1	0	-2.07177	-2.351695	3.968455

Compound **6a**; E= -1434.9462911

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.310085	1.747857	-1.909516
2	6	0	-1.574065	1.428138	-0.568391
3	6	0	-1.257203	2.362668	0.437733
4	6	0	-0.673733	3.583445	0.07481
5	6	0	-0.408817	3.886517	-1.258921
6	6	0	-0.729823	2.965405	-2.25753
7	1	0	-1.559817	1.023783	-2.680561
8	1	0	-0.419533	4.287702	0.861325
9	1	0	0.045094	4.839379	-1.51856
10	1	0	-0.529062	3.192451	-3.301071
11	6	0	-2.2486	0.125586	-0.254539
12	6	0	-1.547113	-1.091414	-0.066539
13	6	0	-3.648944	0.127693	-0.193441
14	6	0	-2.286551	-2.282351	0.176004
15	6	0	-4.366149	-1.041168	0.041921
16	1	0	-4.172725	1.067183	-0.346365
17	6	0	-3.678474	-2.24004	0.223
18	1	0	-5.451764	-1.019494	0.078752
19	1	0	-4.228459	-3.159785	0.408074
20	6	0	-0.083784	-1.238027	-0.106942
21	6	0	0.53836	-2.471204	-0.258501
22	16	0	1.100708	0.039218	0.051131
23	6	0	1.9495	-2.386093	-0.246565
24	6	0	2.413222	-1.101955	-0.07474
25	1	0	2.620772	-3.231136	-0.353575
26	6	0	-1.558157	-3.587178	0.434166
27	6	0	-0.289472	-3.719309	-0.416434
28	6	0	-1.525216	2.081897	1.908558
29	1	0	-1.599544	0.999793	2.081036
30	1	0	-2.486315	2.51663	2.208848
31	1	0	-0.562088	-3.859427	-1.473465
32	1	0	0.282586	-4.604584	-0.117672
33	1	0	-2.233239	-4.431518	0.257174
34	1	0	-1.271986	-3.629157	1.496636
35	6	0	3.827417	-0.716556	-0.010371
36	8	0	4.757987	-1.493829	-0.107145
37	8	0	3.979371	0.618426	0.17501
38	6	0	5.337258	1.077085	0.244596
39	1	0	5.869409	0.845077	-0.681943
40	1	0	5.273729	2.155822	0.390369
41	1	0	5.860014	0.605736	1.08132
42	8	0	-0.565308	2.676913	2.774323
43	1	0	0.297778	2.296004	2.543922

Compound **6b**; E= -1433.7478061

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.23253	1.968433	-1.675489
2	6	0	1.582099	1.487849	-0.406033
3	6	0	1.400287	2.322272	0.72007
4	6	0	0.85602	3.598086	0.534938
5	6	0	0.501845	4.063266	-0.732334
6	6	0	0.693048	3.244341	-1.843188
7	1	0	1.387606	1.327893	-2.539551
8	1	0	0.711346	4.238792	1.402321
9	1	0	0.082108	5.058872	-0.848533
10	1	0	0.427529	3.593755	-2.837213
11	6	0	2.224191	0.137083	-0.299504
12	6	0	1.48284	-1.085074	-0.216138
13	6	0	3.610281	0.094934	-0.338086
14	6	0	2.213397	-2.32437	-0.18296
15	6	0	4.320052	-1.119932	-0.294461
16	1	0	4.156765	1.03128	-0.411848
17	6	0	3.628164	-2.307035	-0.221735
18	1	0	5.405969	-1.11336	-0.325107
19	1	0	4.158547	-3.255624	-0.192572
20	6	0	0.053266	-1.191837	-0.161698
21	6	0	-0.595523	-2.442375	-0.085838
22	16	0	-1.127032	0.111774	-0.154393
23	6	0	-2.016171	-2.328446	-0.025243
24	6	0	-2.451427	-1.033879	-0.04731
25	1	0	-2.697661	-3.16959	0.034893
26	6	0	1.526486	-3.577314	-0.110684
27	1	0	2.123903	-4.485065	-0.090153
28	6	0	0.164784	-3.645322	-0.065516
29	1	0	-0.34911	-4.600825	-0.008333
30	6	0	1.749282	1.856006	2.120481
31	1	0	1.654391	2.706115	2.814403
32	1	0	2.786505	1.509935	2.167784
33	6	0	-3.863181	-0.624156	0.000937
34	8	0	-4.801427	-1.39481	0.059249
35	8	0	-3.997187	0.723797	-0.026323
36	6	0	-5.348331	1.206835	0.011228
37	1	0	-5.270406	2.293849	-0.021911
38	1	0	-5.912809	0.834846	-0.848023
39	1	0	-5.846136	0.883877	0.929537
40	8	0	0.97254	0.745949	2.560872
41	1	0	0.038922	0.961183	2.405595

Compound **7**; E= -1819.33562

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.206194	-1.756035	-1.96398
2	6	0	-1.485613	-1.139739	-0.735475
3	6	0	-1.424614	-1.911563	0.444653
4	6	0	-1.071154	-3.26409	0.361751
5	6	0	-0.784875	-3.861532	-0.863531
6	6	0	-0.8564	-3.103974	-2.032805
7	1	0	-1.259564	-1.161707	-2.871965
8	1	0	-1.028689	-3.854404	1.273963
9	1	0	-0.510089	-4.911807	-0.904997
10	1	0	-0.639277	-3.558344	-2.995599
11	6	0	-1.907382	0.298968	-0.727803
12	6	0	-1.023347	1.375876	-0.467843
13	6	0	-3.253648	0.565109	-1.011927
14	6	0	-1.532357	2.704019	-0.494263
15	6	0	-3.743275	1.867085	-1.037111
16	1	0	-3.919235	-0.271781	-1.200364
17	6	0	-2.878454	2.928198	-0.775421
18	1	0	-4.791888	2.052552	-1.251641
19	1	0	-3.251083	3.949741	-0.79083
20	6	0	0.406335	1.24003	-0.145761
21	6	0	1.135531	2.263282	0.448987
22	16	0	1.421238	-0.150724	-0.45149
23	6	0	2.490939	1.92479	0.663297
24	6	0	2.807827	0.658292	0.227383
25	1	0	3.227698	2.578535	1.117037
26	6	0	-0.598116	3.876226	-0.265026
27	6	0	0.465065	3.566557	0.79551
28	6	0	-1.731646	-1.318556	1.788191
29	1	0	-1.57209	-0.242292	1.818497
30	1	0	-1.153577	-1.795902	2.579884
31	17	0	-3.492449	-1.563788	2.268323
32	1	0	-0.006471	3.497819	1.787649
33	1	0	1.199618	4.377404	0.850747
34	1	0	-1.176566	4.763915	0.012955
35	1	0	-0.087732	4.114788	-1.211101
36	6	0	4.139371	0.047312	0.312441
37	8	0	5.118618	0.595198	0.7821
38	8	0	4.153366	-1.208984	-0.19754
39	6	0	5.423712	-1.874525	-0.152499
40	1	0	5.770818	-1.971315	0.879815
41	1	0	5.254073	-2.856937	-0.594141
42	1	0	6.169786	-1.318377	-0.726641

Compound **6a^{+} (-OH^{-})**; E= -1358.8538545

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.232336	1.734741	-1.384531
2	6	0	1.803066	1.323917	-0.171193
3	6	0	2.147318	2.36806	0.797157
4	6	0	2.032041	3.759722	0.419487
5	6	0	1.508657	4.106534	-0.794992
6	6	0	1.103207	3.084738	-1.69256
7	1	0	0.969243	0.989494	-2.127007
8	1	0	2.3421	4.516437	1.134039
9	1	0	1.405796	5.147996	-1.08064
10	1	0	0.714858	3.364426	-2.668
11	6	0	2.180159	-0.069809	0.046536
12	6	0	1.310302	-1.191061	-0.171429
13	6	0	3.550181	-0.29528	0.342814
14	6	0	1.898675	-2.483368	-0.251467
15	6	0	4.085605	-1.570243	0.319699
16	1	0	4.201916	0.559236	0.491454
17	6	0	3.259749	-2.650827	-0.006307
18	1	0	5.142823	-1.723522	0.510484
19	1	0	3.683372	-3.649475	-0.068708
20	6	0	-0.152264	-1.140676	-0.163685
21	6	0	-0.934513	-2.290248	-0.021984
22	16	0	-1.162512	0.294675	-0.094759
23	6	0	-2.313995	-2.011591	0.115421
24	6	0	-2.599577	-0.668588	0.096555
25	1	0	-3.087863	-2.762123	0.230573
26	6	0	1.041252	-3.669105	-0.639336
27	6	0	-0.31429	-3.656331	0.070637
28	6	0	2.422063	2.051171	2.099067
29	1	0	2.389143	1.028488	2.459384
30	1	0	2.647896	2.826447	2.826589
31	1	0	-0.193975	-3.921539	1.13216
32	1	0	-0.978324	-4.41124	-0.362956
33	1	0	1.574983	-4.602577	-0.438887
34	1	0	0.871738	-3.628048	-1.725727
35	6	0	-3.955771	-0.086812	0.20074
36	8	0	-4.956239	-0.757544	0.334978
37	8	0	-3.928036	1.258206	0.134643
38	6	0	-5.213561	1.908242	0.234829
39	1	0	-5.682106	1.671292	1.192737
40	1	0	-5.005073	2.974785	0.158669
41	1	0	-5.865974	1.580726	-0.577736

Transition state for cyclization of **6a**$^{+}$; E= -1358.8360353, ν=-321.9366

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.232336	1.734741	-1.384531
2	6	0	1.803066	1.323917	-0.171193
3	6	0	2.147318	2.36806	0.797157
4	6	0	2.032041	3.759722	0.419487
5	6	0	1.508657	4.106534	-0.794992
6	6	0	1.103207	3.084738	-1.69256
7	1	0	0.969243	0.989494	-2.127007
8	1	0	2.3421	4.516437	1.134039
9	1	0	1.405796	5.147996	-1.08064
10	1	0	0.714858	3.364426	-2.668
11	6	0	2.180159	-0.069809	0.046536
12	6	0	1.310302	-1.191061	-0.171429
13	6	0	3.550181	-0.29528	0.342814
14	6	0	1.898675	-2.483368	-0.251467
15	6	0	4.085605	-1.570243	0.319699
16	1	0	4.201916	0.559236	0.491454
17	6	0	3.259749	-2.650827	-0.006307
18	1	0	5.142823	-1.723522	0.510484
19	1	0	3.683372	-3.649475	-0.068708
20	6	0	-0.152264	-1.140676	-0.163685
21	6	0	-0.934513	-2.290248	-0.021984
22	16	0	-1.162512	0.294675	-0.094759
23	6	0	-2.313995	-2.011591	0.115421
24	6	0	-2.599577	-0.668588	0.096555
25	1	0	-3.087863	-2.762123	0.230573
26	6	0	1.041252	-3.669105	-0.639336
27	6	0	-0.31429	-3.656331	0.070637
28	6	0	2.422063	2.051171	2.099067
29	1	0	2.389143	1.028488	2.459384
30	1	0	2.647896	2.826447	2.826589
31	1	0	-0.193975	-3.921539	1.13216
32	1	0	-0.978324	-4.41124	-0.362956
33	1	0	1.574983	-4.602577	-0.438887
34	1	0	0.871738	-3.628048	-1.725727
35	6	0	-3.955771	-0.086812	0.20074
36	8	0	-4.956239	-0.757544	0.334978
37	8	0	-3.928036	1.258206	0.134643
38	6	0	-5.213561	1.908242	0.234829
39	1	0	-5.682106	1.671292	1.192737
40	1	0	-5.005073	2.974785	0.158669
41	1	0	-5.865974	1.580726	-0.577736

Reactant for SN1 **6a^{+} + Cl^{-}**; E= -1819.2842395

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.727267	-1.080697	-1.894595
2	6	0	-1.693218	-0.427569	-0.679409
3	6	0	-1.782899	-1.216679	0.533236
4	6	0	-1.896245	-2.652024	0.432534
5	6	0	-1.878528	-3.27263	-0.817469
6	6	0	-1.809604	-2.492025	-1.96228
7	1	0	-1.672385	-0.504431	-2.812981
8	1	0	-1.870946	-3.240111	1.33867
9	1	0	-1.93931	-4.353432	-0.887692
10	1	0	-1.808064	-2.968951	-2.938982
11	6	0	-1.663937	1.06422	-0.624776
12	6	0	-0.50717	1.813841	-0.296712
13	6	0	-2.869026	1.726478	-0.899168
14	6	0	-0.607619	3.229977	-0.222018
15	6	0	-2.954511	3.113606	-0.831328
16	1	0	-3.747461	1.134221	-1.137293
17	6	0	-1.825008	3.854688	-0.486361
18	1	0	-3.898178	3.611746	-1.033476
19	1	0	-1.885859	4.938576	-0.424421
20	6	0	0.820192	1.245137	-0.022465
21	6	0	1.809233	1.955023	0.645548
22	16	0	1.396244	-0.334902	-0.496621
23	6	0	3.009974	1.222412	0.792881
24	6	0	2.951964	-0.031661	0.229222
25	1	0	3.902451	1.58875	1.28806
26	6	0	0.622816	4.056034	0.099358
27	6	0	1.537109	3.359696	1.1163
28	6	0	-1.935619	-0.641602	1.77139
29	1	0	-1.972821	0.435435	1.895814
30	1	0	-2.032643	-1.253176	2.65951
31	17	0	-4.37895	-2.388398	1.544097
32	1	0	1.052676	3.342608	2.104321
33	1	0	2.472766	3.916845	1.233763
34	1	0	0.321836	5.044522	0.46259
35	1	0	1.192979	4.219952	-0.828035
36	6	0	4.051593	-1.005266	0.219052
37	8	0	5.143478	-0.810387	0.716833
38	8	0	3.70445	-2.152025	-0.413623
39	6	0	4.728796	-3.157109	-0.467542
40	1	0	5.026212	-3.456179	0.541042
41	1	0	4.284969	-3.997214	-1.002206
42	1	0	5.606452	-2.78177	-1.000454

Transition state for SN1 **6a$^+$ + Cl$^-$ -> 7**; E= -1819.2588642, ν=-283.9876

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000569	-0.027142	-0.064355
2	6	0	-0.059085	0.042044	1.312672
3	6	0	1.184068	0.083941	2.057023
4	6	0	2.435873	0.060166	1.338955
5	6	0	2.445516	0.038098	-0.056534
6	6	0	1.241373	-0.019501	-0.743126
7	1	0	-0.921776	-0.07043	-0.637094
8	1	0	3.355251	0.183281	1.893172
9	1	0	3.388388	0.045019	-0.592916
10	1	0	1.242837	-0.049527	-1.829636
11	6	0	-1.374101	-0.02463	2.016637
12	6	0	-2.004747	1.098467	2.607066
13	6	0	-1.980458	-1.286406	2.096435
14	6	0	-3.231801	0.908964	3.299553
15	6	0	-3.185837	-1.459521	2.769583
16	1	0	-1.476153	-2.137026	1.647835
17	6	0	-3.799061	-0.361906	3.372225
18	1	0	-3.636793	-2.445391	2.834499
19	1	0	-4.737566	-0.490677	3.906061
20	6	0	-1.493048	2.475744	2.564709
21	6	0	-1.92516	3.456529	3.447728
22	16	0	-0.335243	3.123807	1.427747
23	6	0	-1.310767	4.710424	3.223065
24	6	0	-0.427951	4.699655	2.167463
25	1	0	-1.50194	5.606741	3.802711
26	6	0	-3.940332	2.099885	3.915439
27	6	0	-2.954207	3.122539	4.495717
28	6	0	1.221964	-0.026145	3.425784
29	1	0	0.314735	-0.126862	4.012015
30	1	0	2.16533	-0.024427	3.957056
31	17	0	2.903322	-2.357278	2.524852
32	1	0	-2.465596	2.705403	5.389255
33	1	0	-3.484695	4.024649	4.818899
34	1	0	-4.640894	1.757915	4.684793
35	1	0	-4.541614	2.59653	3.138382
36	6	0	0.342603	5.858716	1.698404
37	8	0	0.288537	6.965167	2.199222
38	8	0	1.124753	5.548442	0.636418
39	6	0	1.911087	6.631807	0.116433
40	1	0	2.592199	7.013251	0.881763
41	1	0	2.469805	6.211195	-0.719955
42	1	0	1.265173	7.446107	-0.222481

Compound **8**; E= -2027.0167049

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.163783	-1.91629	1.907357
2	6	0	2.49215	-1.332086	0.675044
3	6	0	2.257624	-2.061757	-0.510338
4	6	0	1.686964	-3.33796	-0.428054
5	6	0	1.353389	-3.90172	0.80141
6	6	0	1.596966	-3.188533	1.975428
7	1	0	2.353245	-1.356542	2.819171
8	1	0	1.510606	-3.896804	-1.344024
9	1	0	0.910394	-4.892863	0.842291
10	1	0	1.347433	-3.619167	2.941303
11	6	0	3.14194	0.018908	0.665384
12	6	0	2.428644	1.229021	0.477014
13	6	0	4.527266	0.060333	0.873422
14	6	0	3.143448	2.458841	0.500847
15	6	0	5.219345	1.267028	0.892569
16	1	0	5.05989	-0.876338	1.006396
17	6	0	4.521372	2.458977	0.704671
18	1	0	6.294483	1.278071	1.046874
19	1	0	5.052336	3.407908	0.719239
20	6	0	0.982893	1.332216	0.231662
21	6	0	0.391695	2.470555	-0.29513
22	16	0	-0.22674	0.106835	0.544349
23	6	0	-1.00982	2.353042	-0.45013
24	6	0	-1.519142	1.13886	-0.036174
25	1	0	-1.628572	3.159874	-0.828914
26	6	0	2.394626	3.769658	0.358241
27	6	0	1.237381	3.667836	-0.642032
28	6	0	2.604975	-1.503106	-1.85875
29	1	0	2.610946	-0.414729	-1.873022
30	1	0	1.93302	-1.875126	-2.632682
31	17	0	4.289304	-2.006364	-2.404654
32	6	0	-2.90998	0.689933	-0.045288
33	6	0	-3.34413	-0.391789	0.749789
34	6	0	-3.863833	1.33776	-0.860151
35	6	0	-4.66719	-0.811301	0.736142
36	1	0	-2.638464	-0.900168	1.399787
37	6	0	-5.191027	0.934608	-0.874953
38	1	0	-3.554329	2.154176	-1.504132
39	6	0	-5.581312	-0.140302	-0.075387
40	1	0	-5.004326	-1.639593	1.347059
41	1	0	-5.925033	1.427312	-1.500625
42	7	0	-6.979663	-0.574712	-0.09193
43	8	0	-7.763692	0.04259	-0.815439
44	8	0	-7.29203	-1.532236	0.61843
45	1	0	1.63455	3.564712	-1.663436
46	1	0	0.636893	4.584287	-0.62872
47	1	0	3.088729	4.565431	0.067294
48	1	0	1.983131	4.052147	1.33971

Compound **9**; E= -1818.1382186

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.146778	-1.393099	2.052066
2	6	0	1.515279	-0.939346	0.776537
3	6	0	1.600103	-1.869049	-0.281435
4	6	0	1.302774	-3.216235	-0.036229
5	6	0	0.931747	-3.652333	1.232885
6	6	0	0.856847	-2.736181	2.283244
7	1	0	1.086931	-0.676022	2.866006
8	1	0	1.371837	-3.928738	-0.854697
9	1	0	0.704143	-4.701126	1.401913
10	1	0	0.572401	-3.065093	3.278931
11	6	0	1.87112	0.505599	0.595284
12	6	0	0.899849	1.522184	0.318526
13	6	0	3.206468	0.853222	0.741845
14	6	0	1.351914	2.885201	0.215288
15	6	0	3.641422	2.187365	0.636314
16	1	0	3.928969	0.067733	0.940888
17	6	0	2.725496	3.182621	0.381709
18	1	0	4.694881	2.422693	0.756858
19	1	0	3.043908	4.218883	0.299513
20	6	0	-0.506017	1.303155	0.120704
21	6	0	-1.389768	2.368888	-0.155513
22	16	0	-1.377828	-0.223242	0.156699
23	6	0	-2.738178	1.939219	-0.331479
24	6	0	-2.89049	0.588002	-0.199027
25	1	0	-3.570104	2.599208	-0.550005
26	6	0	0.428758	3.943567	-0.05806
27	1	0	0.81933	4.955764	-0.122566
28	6	0	-0.902012	3.703412	-0.23883
29	1	0	-1.595561	4.512786	-0.44908
30	6	0	1.992662	-1.446758	-1.666681
31	1	0	1.814263	-0.388155	-1.847575
32	1	0	1.483915	-2.038996	-2.427791
33	17	0	3.788047	-1.700758	-1.988892
34	6	0	-4.170176	-0.126874	-0.332393
35	8	0	-5.233689	0.409678	-0.573982
36	8	0	-4.02204	-1.460649	-0.154299
37	6	0	-5.226671	-2.233397	-0.268204
38	1	0	-4.926278	-3.267725	-0.099239
39	1	0	-5.957352	-1.916982	0.480975
40	1	0	-5.664432	-2.116675	-1.263214

Compound **6b^{+} (-OH^{-})**; E= -1357.6597198

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.223669	1.614178	-1.391192
2	6	0	1.857761	1.224716	-0.202157
3	6	0	2.314331	2.283033	0.699379
4	6	0	2.247947	3.662288	0.269842
5	6	0	1.657288	3.987987	-0.91953
6	6	0	1.140206	2.955463	-1.745378
7	1	0	0.873499	0.855019	-2.081375
8	1	0	2.643564	4.429252	0.92905
9	1	0	1.58578	5.021798	-1.240536
10	1	0	0.700577	3.218192	-2.70355
11	6	0	2.180705	-0.17448	0.060333
12	6	0	1.245525	-1.262774	-0.080768
13	6	0	3.541653	-0.45072	0.299041
14	6	0	1.777376	-2.599087	-0.104406
15	6	0	4.036184	-1.75879	0.299887
16	1	0	4.238852	0.376735	0.375293
17	6	0	3.167339	-2.8085	0.072521
18	1	0	5.097089	-1.937481	0.43989
19	1	0	3.542511	-3.82771	0.039242
20	6	0	-0.178586	-1.144051	-0.102601
21	6	0	-1.009754	-2.288022	-0.222064
22	16	0	-1.158156	0.297071	0.120311
23	6	0	-2.401963	-1.971834	-0.15892
24	6	0	-2.637874	-0.64448	0.036074
25	1	0	-3.202761	-2.698173	-0.236276
26	6	0	0.91898	-3.726505	-0.260071
27	1	0	1.367944	-4.714546	-0.294541
28	6	0	-0.441147	-3.580801	-0.332723
29	1	0	-1.090374	-4.444524	-0.438105
30	6	0	2.656555	2.001026	1.9946
31	1	0	2.568952	1.002013	2.407352
32	1	0	2.989076	2.787334	2.667271
33	6	0	-3.980987	-0.029914	0.157467
34	8	0	-5.00958	-0.666576	0.09722
35	8	0	-3.900992	1.300673	0.343786
36	6	0	-5.166262	1.983409	0.484588
37	1	0	-4.913798	3.033402	0.627285
38	1	0	-5.769716	1.846613	-0.41551
39	1	0	-5.709809	1.5933	1.34794

Transition state for cyclization of **6b**$^{+}$; E= -1357.6446606, ν= -320.5173

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.108583	1.973217	1.18237
2	6	0	-1.845761	1.222699	0.256857
3	6	0	-2.71786	1.891798	-0.65902
4	6	0	-2.919997	3.28773	-0.569304
5	6	0	-2.163138	4.010314	0.336086
6	6	0	-1.267383	3.354793	1.207255
7	1	0	-0.483844	1.48581	1.92185
8	1	0	-3.61894	3.783222	-1.236447
9	1	0	-2.269002	5.089138	0.391433
10	1	0	-0.726579	3.937539	1.946793
11	6	0	-2.068455	-0.223954	0.228942
12	6	0	-1.096101	-1.268301	0.208637
13	6	0	-3.464717	-0.543903	0.089308
14	6	0	-1.586934	-2.627564	0.140843
15	6	0	-3.908053	-1.884422	-0.051866
16	1	0	-4.18955	0.175831	0.45314
17	6	0	-2.985549	-2.890552	0.004797
18	1	0	-4.969233	-2.096473	-0.12862
19	1	0	-3.30305	-3.928399	-0.043548
20	6	0	0.330964	-1.100761	0.158224
21	6	0	1.196316	-2.224631	0.137653
22	16	0	1.263473	0.373674	0.021412
23	6	0	2.577264	-1.868831	0.036501
24	6	0	2.769319	-0.524351	-0.04788
25	1	0	3.396666	-2.577898	0.012921
26	6	0	-0.693288	-3.725003	0.147188
27	1	0	-1.104216	-4.729271	0.116178
28	6	0	0.668447	-3.535121	0.16336
29	1	0	1.345561	-4.384153	0.16002
30	6	0	-3.381466	1.034909	-1.580357
31	1	0	-2.841085	0.276712	-2.132721
32	1	0	-4.340601	1.323602	-2.008776
33	6	0	4.087686	0.142768	-0.176101
34	8	0	5.134782	-0.463811	-0.218474
35	8	0	3.958202	1.479849	-0.238539
36	6	0	5.193195	2.218889	-0.369433
37	1	0	4.899537	3.267059	-0.407326
38	1	0	5.838974	2.025773	0.48997
39	1	0	5.710479	1.926102	-1.285721

Reactant for SN1 **6b^{+} + Cl^{-}**; E= -1818.0866436

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.527634	-0.802493	1.548857
2	6	0	1.74089	-0.18358	0.358929
3	6	0	2.20032	-0.982283	-0.790483
4	6	0	2.763362	-2.351399	-0.506264
5	6	0	2.275661	-2.983478	0.746479
6	6	0	1.715557	-2.232749	1.714158
7	1	0	1.173754	-0.224484	2.397909
8	1	0	2.670932	-3.00514	-1.372425
9	1	0	2.450673	-4.046836	0.876715
10	1	0	1.400548	-2.689232	2.648725
11	6	0	1.549768	1.292222	0.212554
12	6	0	0.266213	1.92334	0.131739
13	6	0	2.701293	2.067727	0.188461
14	6	0	0.222101	3.361804	0.06685
15	6	0	2.64974	3.47134	0.121783
16	1	0	3.663987	1.566658	0.23755
17	6	0	1.427373	4.103068	0.07137
18	1	0	3.570945	4.046859	0.116432
19	1	0	1.367277	5.187574	0.024646
20	6	0	-1.001635	1.247551	0.081187
21	6	0	-2.215443	1.96026	-0.026782
22	16	0	-1.307063	-0.483306	0.085223
23	6	0	-3.355785	1.106898	-0.107441
24	6	0	-3.03332	-0.21973	-0.070922
25	1	0	-4.378872	1.45531	-0.193268
26	6	0	-1.027554	4.053614	-0.017138
27	1	0	-1.006702	5.139604	-0.054426
28	6	0	-2.214433	3.382996	-0.063187
29	1	0	-3.158573	3.915451	-0.136566
30	6	0	2.120861	-0.545275	-2.060913
31	1	0	1.745615	0.443446	-2.302676
32	1	0	2.441609	-1.167249	-2.891857
33	17	0	4.663093	-2.210518	-0.348048
34	6	0	-4.008145	-1.320644	-0.134687
35	8	0	-5.209776	-1.16852	-0.235553
36	8	0	-3.404698	-2.530905	-0.068277
37	6	0	-4.287834	-3.661471	-0.12398
38	1	0	-3.643447	-4.538243	-0.055601
39	1	0	-4.99514	-3.636936	0.709297
40	1	0	-4.846122	-3.665999	-1.063972

Transition state for SN1 **6b$^+$ + Cl$^-$ -> 7**; E= -1818.0613077, ν= -255.7235

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.301784	-0.938307	1.63034
2	6	0	1.619667	-0.385786	0.40352
3	6	0	2.194243	-1.245446	-0.612251
4	6	0	2.526242	-2.607673	-0.271718
5	6	0	2.170781	-3.127802	0.969722
6	6	0	1.559598	-2.298785	1.904219
7	1	0	0.876605	-0.30954	2.406186
8	1	0	2.941971	-3.245008	-1.039679
9	1	0	2.391979	-4.162118	1.210772
10	1	0	1.294444	-2.694334	2.881202
11	6	0	1.51799	1.085277	0.190892
12	6	0	0.281283	1.805305	0.13866
13	6	0	2.728517	1.768517	0.130795
14	6	0	0.341174	3.242366	0.089383
15	6	0	2.773386	3.173415	0.071383
16	1	0	3.652749	1.196492	0.161098
17	6	0	1.599178	3.892342	0.06764
18	1	0	3.733609	3.679541	0.041074
19	1	0	1.617877	4.978749	0.034388
20	6	0	-1.028829	1.221105	0.0815
21	6	0	-2.191107	2.018502	0.007602
22	16	0	-1.450432	-0.483993	0.013506
23	6	0	-3.387551	1.246858	-0.094226
24	6	0	-3.156604	-0.098477	-0.114723
25	1	0	-4.385504	1.665496	-0.158378
26	6	0	-0.856738	4.021979	0.042046
27	1	0	-0.759878	5.104099	0.020682
28	6	0	-2.089777	3.437525	0.007286
29	1	0	-2.994298	4.037285	-0.038654
30	6	0	2.515661	-0.787945	-1.865267
31	1	0	2.314115	0.232776	-2.17035
32	1	0	2.981576	-1.446579	-2.588481
33	17	0	5.13371	-1.71253	-0.553149
34	6	0	-4.203939	-1.129154	-0.216714
35	8	0	-5.392089	-0.88961	-0.298533
36	8	0	-3.682029	-2.377235	-0.210334
37	6	0	-4.639201	-3.444335	-0.309993
38	1	0	-4.053619	-4.36355	-0.289547
39	1	0	-5.336787	-3.412059	0.530986
40	1	0	-5.202592	-3.366472	-1.243505

Compound **10**; E= -2025.8197355

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.134565	-1.59632	-2.003583
2	6	0	-2.517868	-1.185765	-0.717644
3	6	0	-2.349837	-2.077691	0.36285
4	6	0	-1.79272	-3.341874	0.128557
5	6	0	-1.409081	-3.734111	-1.151338
6	6	0	-1.584541	-2.857716	-2.223543
7	1	0	-2.271015	-0.910294	-2.834902
8	1	0	-1.6684	-4.026262	0.964267
9	1	0	-0.979375	-4.718988	-1.311712
10	1	0	-1.295202	-3.154613	-3.2279
11	6	0	-3.15155	0.161783	-0.543644
12	6	0	-2.393633	1.359034	-0.329136
13	6	0	-4.534212	0.231473	-0.630298
14	6	0	-3.105857	2.605968	-0.220336
15	6	0	-5.224218	1.453634	-0.521044
16	1	0	-5.092065	-0.687115	-0.784007
17	6	0	-4.517447	2.617767	-0.322839
18	1	0	-6.307754	1.469737	-0.593328
19	1	0	-5.034215	3.570464	-0.237526
20	6	0	-0.966992	1.433877	-0.203904
21	6	0	-0.300131	2.655284	0.015275
22	16	0	0.195193	0.116237	-0.268636
23	6	0	1.116133	2.507278	0.121372
24	6	0	1.548888	1.21432	-0.008664
25	1	0	1.783684	3.351184	0.259619
26	6	0	-2.401007	3.831929	-0.008146
27	1	0	-2.982102	4.747559	0.063873
28	6	0	-1.041125	3.866613	0.106343
29	1	0	-0.516173	4.80378	0.269584
30	6	0	-2.747501	-1.70151	1.760178
31	1	0	-2.773128	-0.623719	1.912492
32	1	0	-2.092693	-2.16002	2.50176
33	17	0	-4.437224	-2.295157	2.184479
34	6	0	2.92419	0.713149	0.042387
35	6	0	3.28707	-0.506031	-0.564964
36	6	0	3.925713	1.451	0.707484
37	6	0	4.594685	-0.971761	-0.517067
38	1	0	2.539657	-1.08654	-1.096953
39	6	0	5.23771	1.001165	0.754496
40	1	0	3.664823	2.376209	1.210571
41	6	0	5.558767	-0.209779	0.140767
42	1	0	4.880887	-1.905311	-0.98551
43	1	0	6.010825	1.561492	1.265622
44	7	0	6.94202	-0.693793	0.192394
45	8	0	7.771501	0.00357	0.778419
46	8	0	7.193824	-1.769	-0.353673