

## SUPPORTING INFORMATION

### Push-pull 1,3-Thiazolium-5-thiolates. Formation *via* Concerted and Stepwise Pathways, and Theoretical Evaluation of NLO Properties

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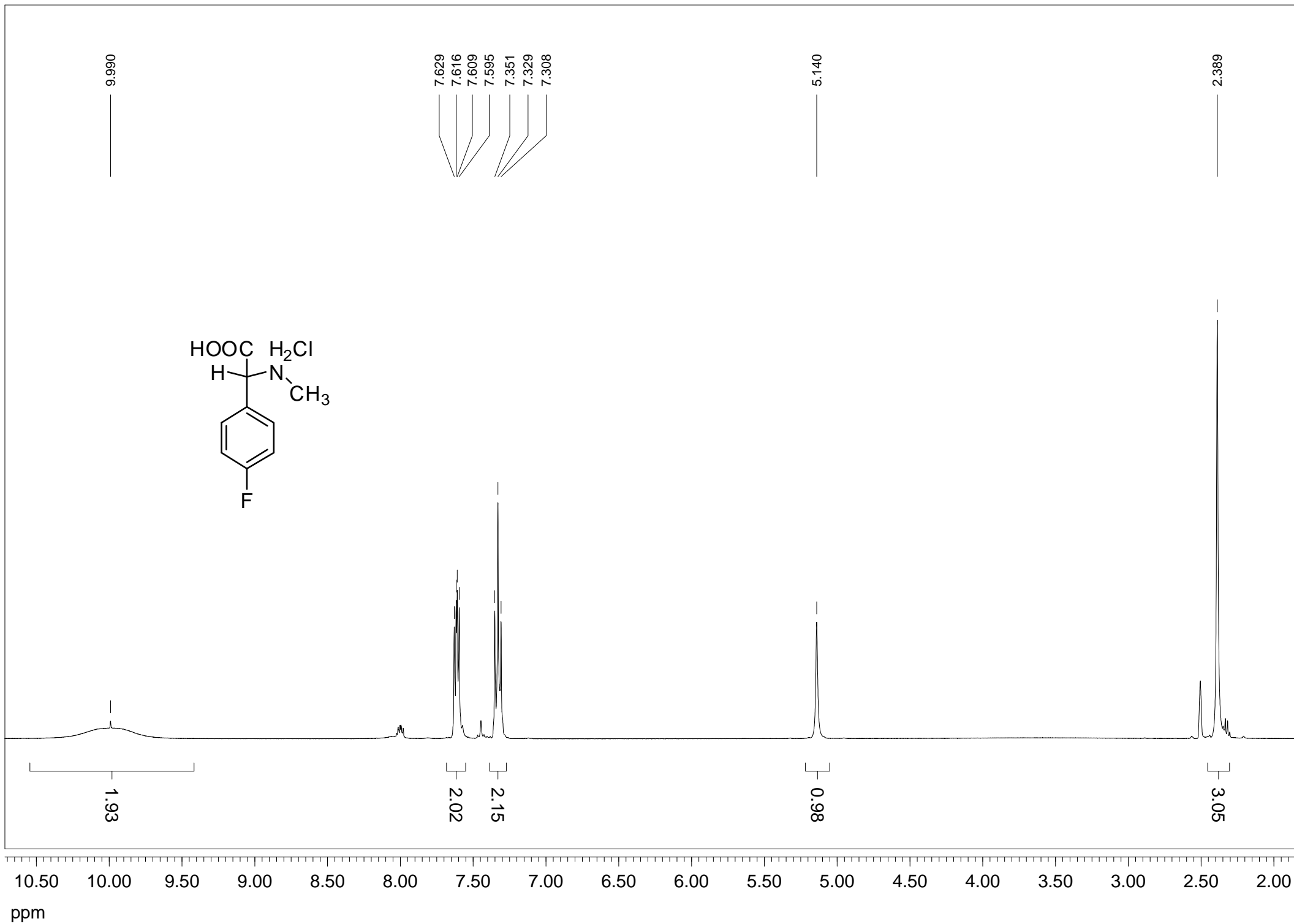
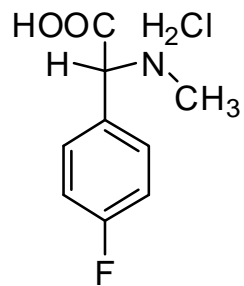
<sup>a</sup> *Departamento de Química Orgánica e Inorgánica, QUOREX Research Group, Facultad de Ciencias, Universidad de Extremadura, E-06006 Badajoz (Spain)*

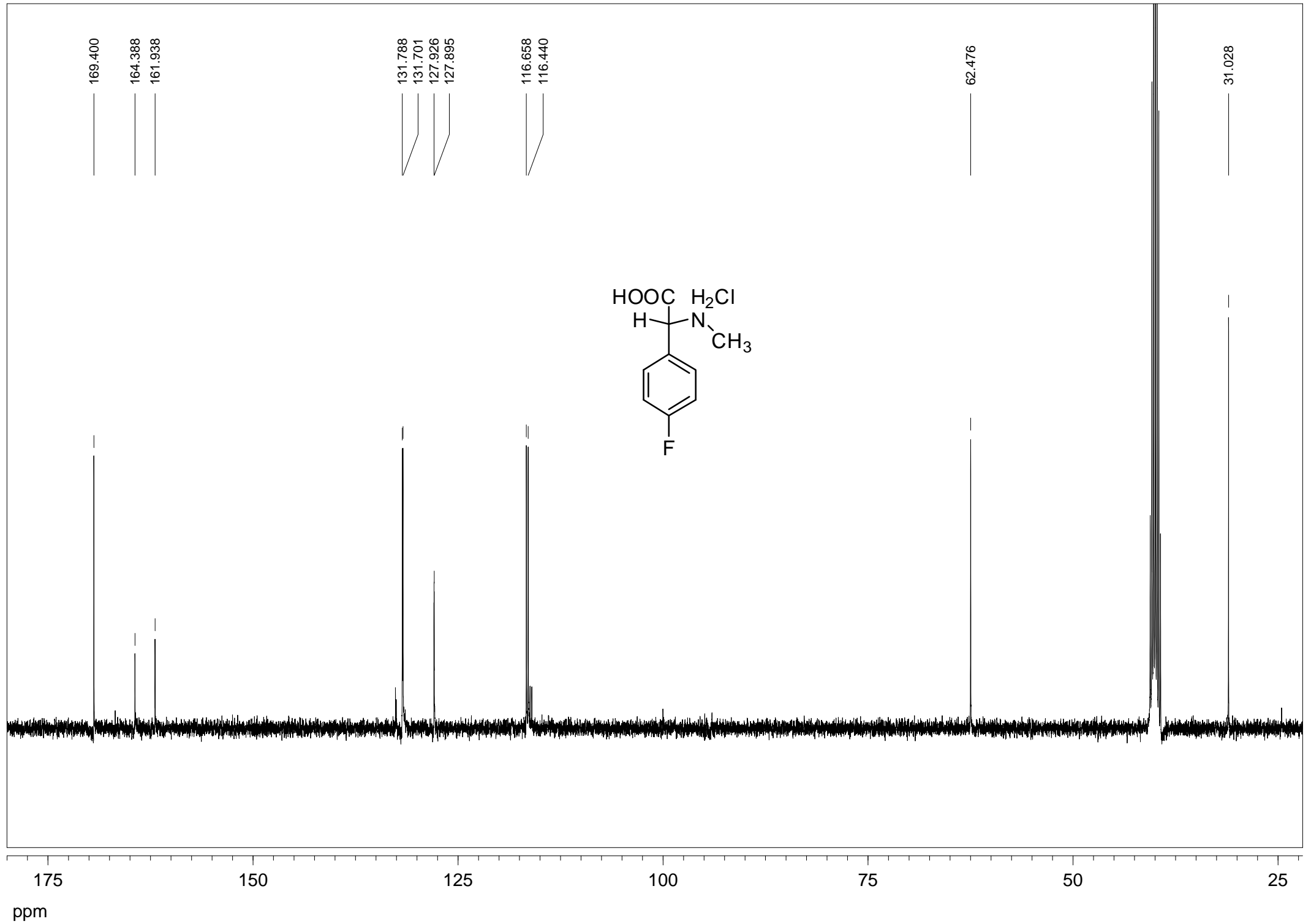
<sup>b</sup> *Department of Chemistry, University of Southampton, Highfield, Southampton SO17 1BJ, UK*

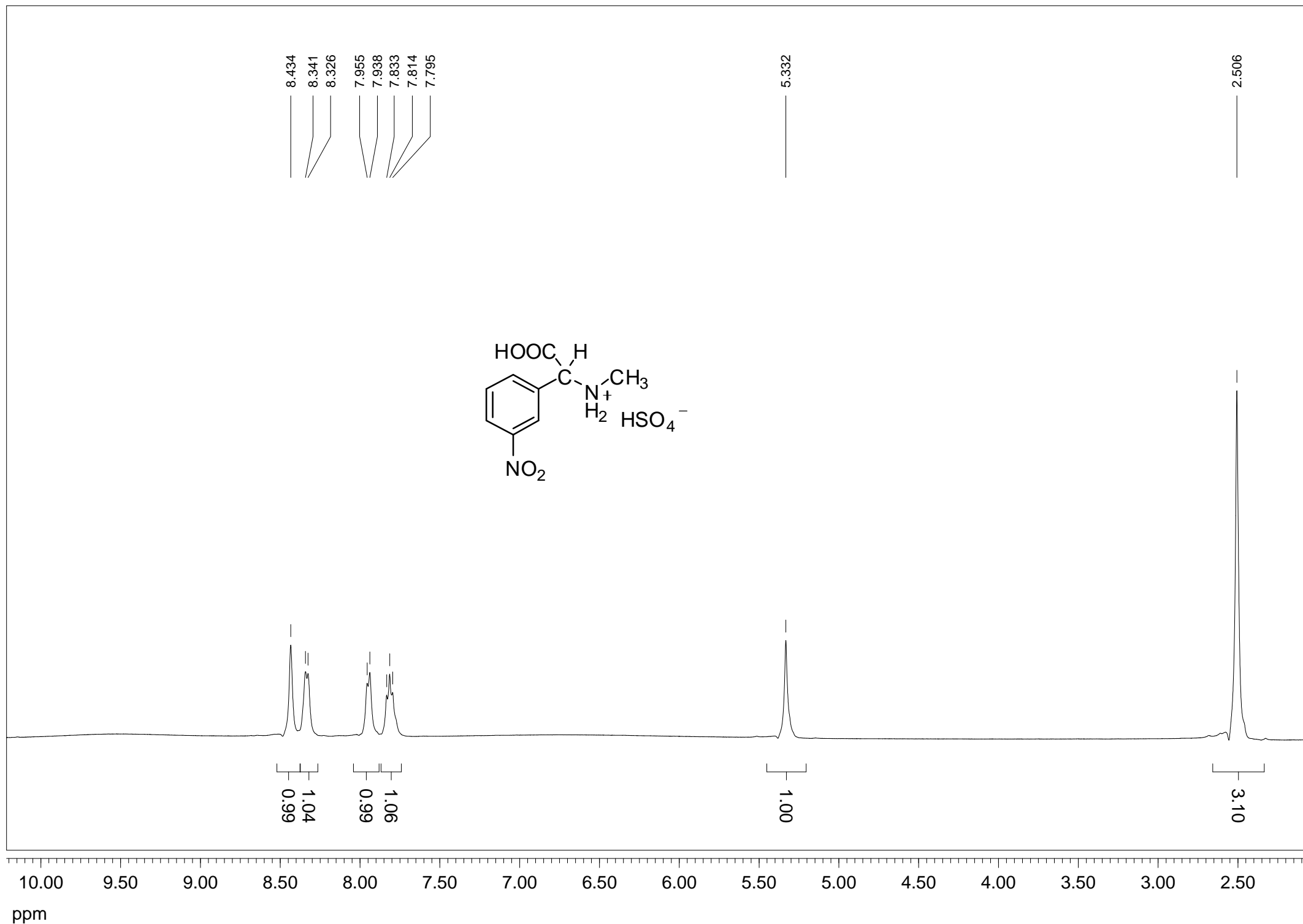
*dcannie@unex.es*

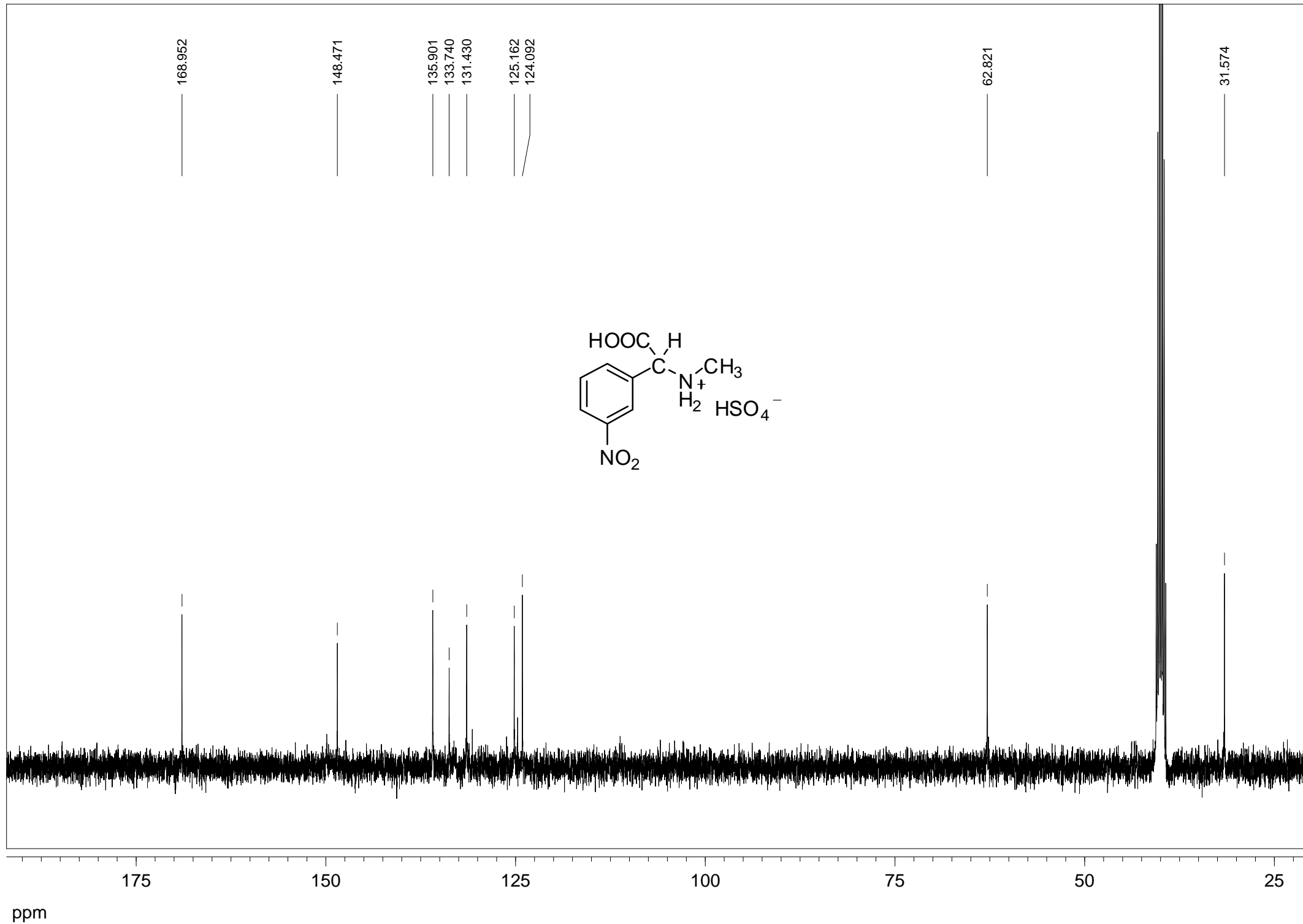
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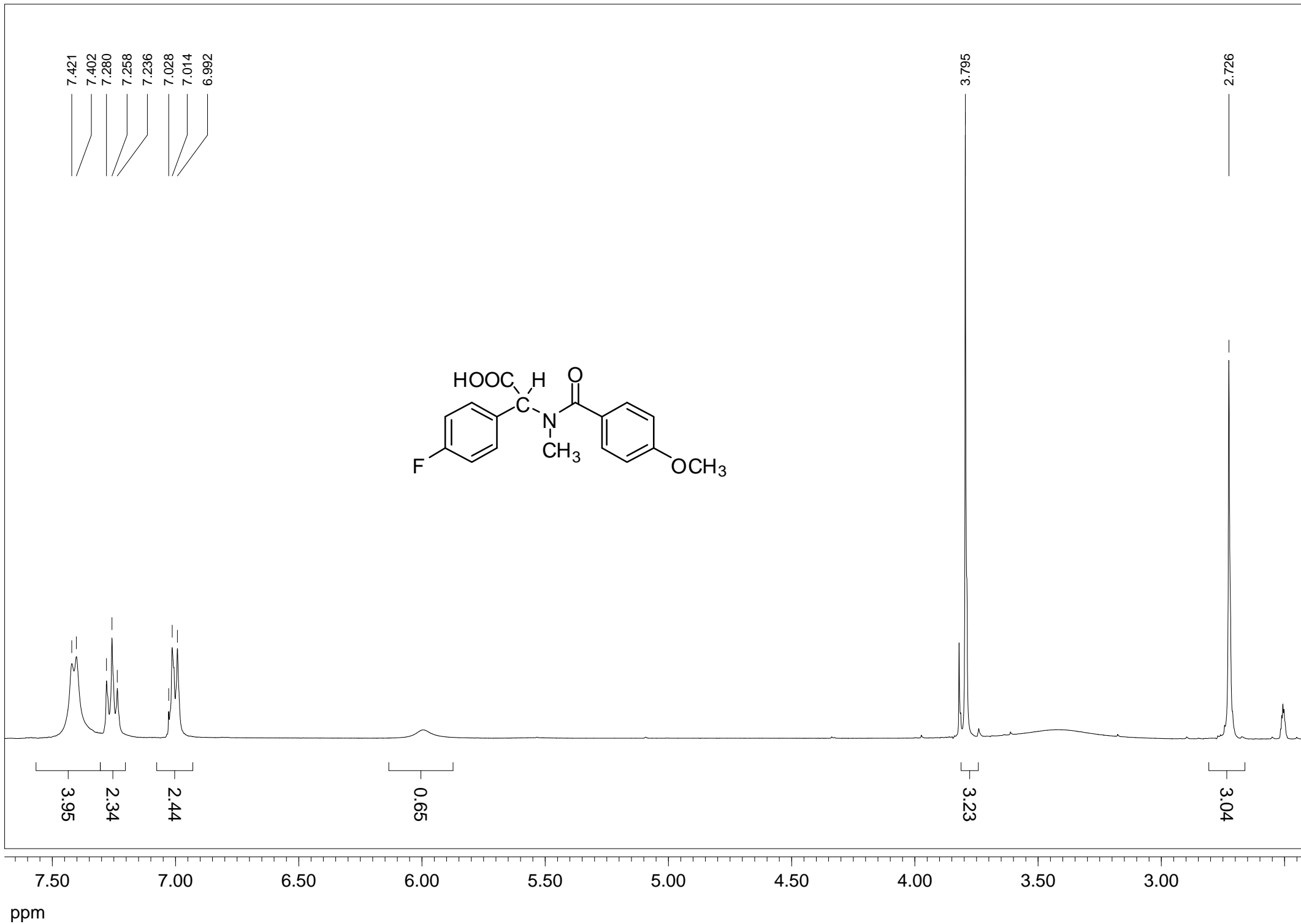
<sup>1</sup> H and <sup>13</sup> C NMR spectra of all new compounds .....	S2
UV spectra of 1,3-thiazolium-5-thiolate systems .....	S23
Cyclic voltammograms of 1,3-thiazolium-5-thiolate systems.....	S23
Computational data.....	S25

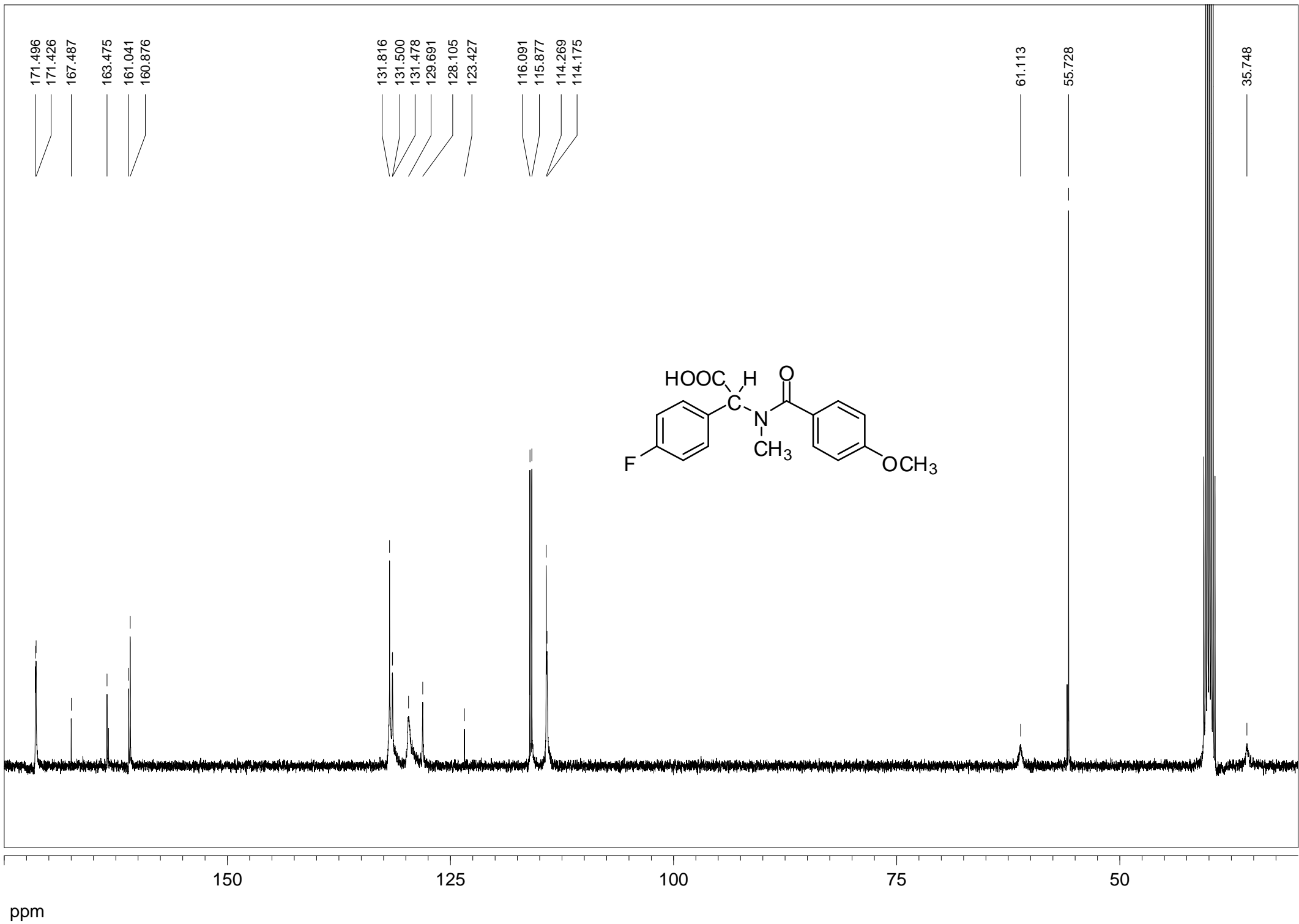


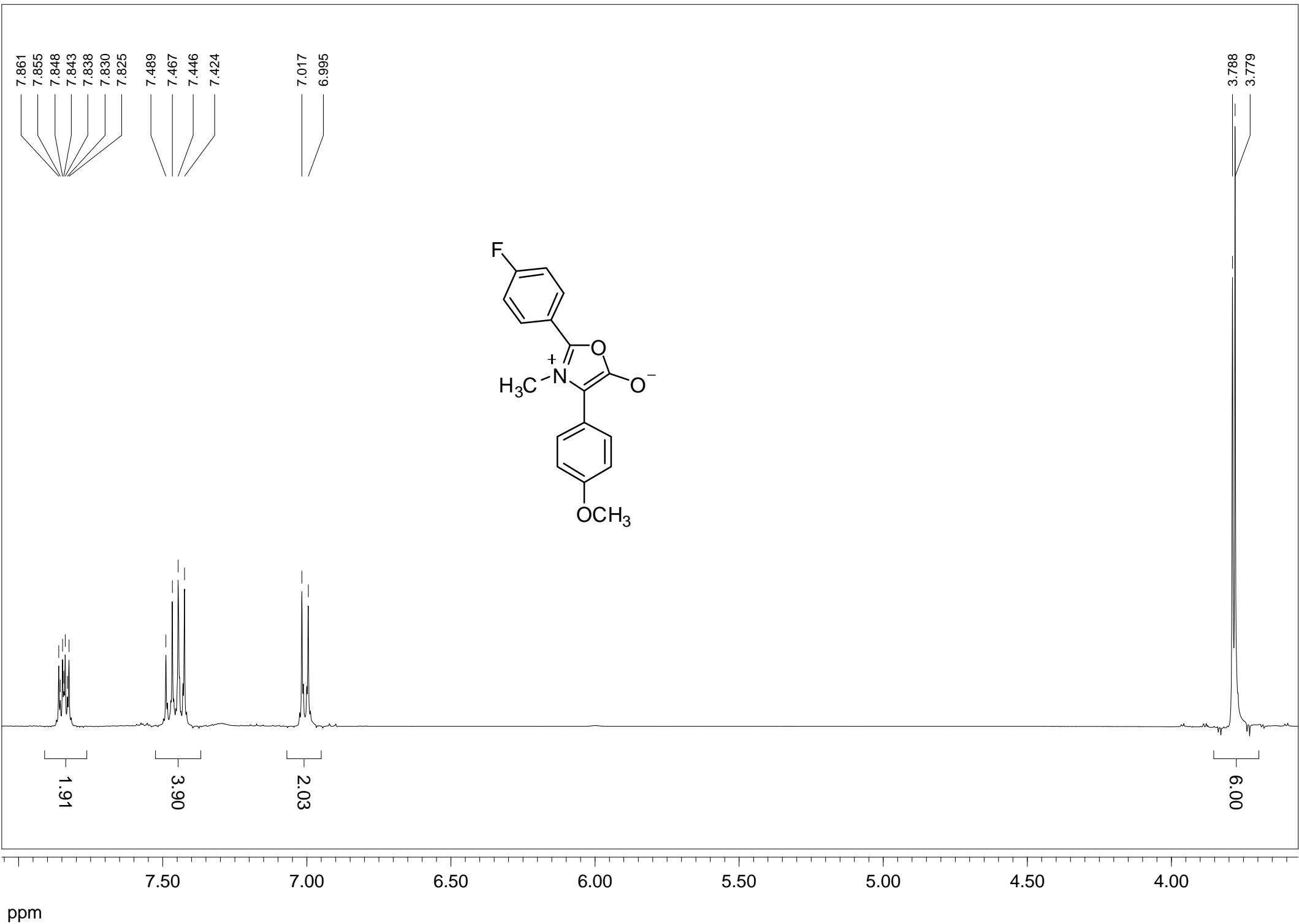




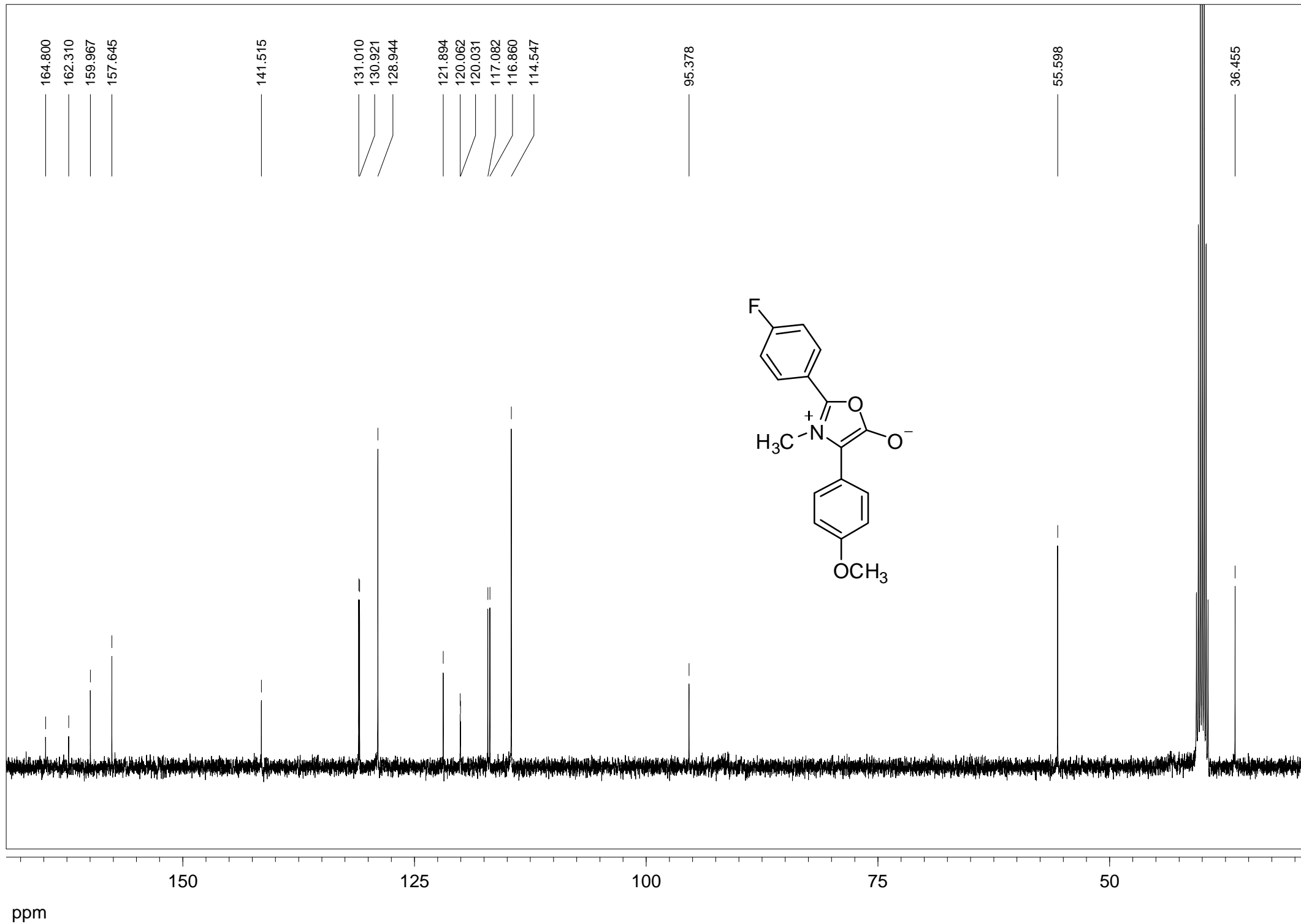


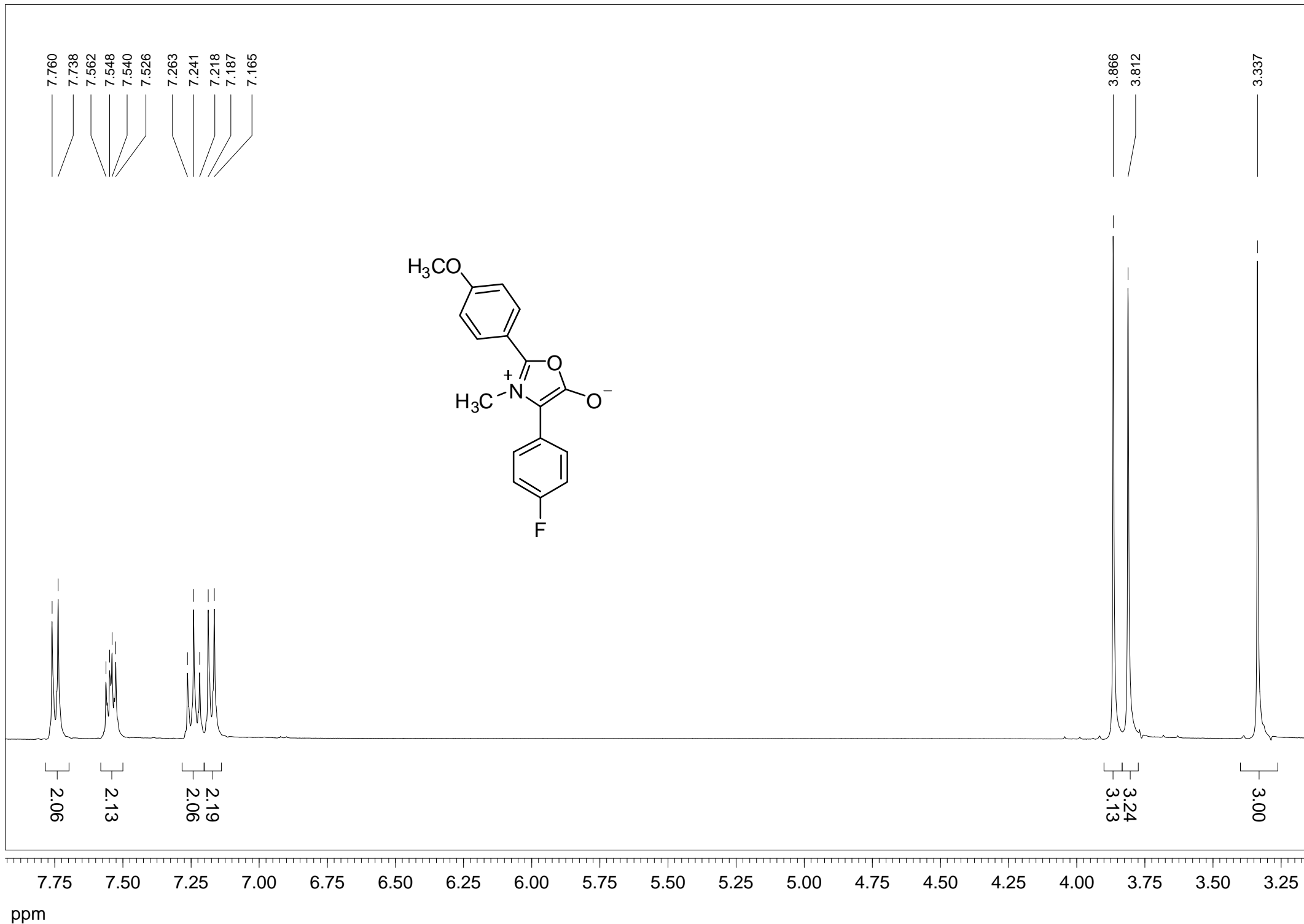


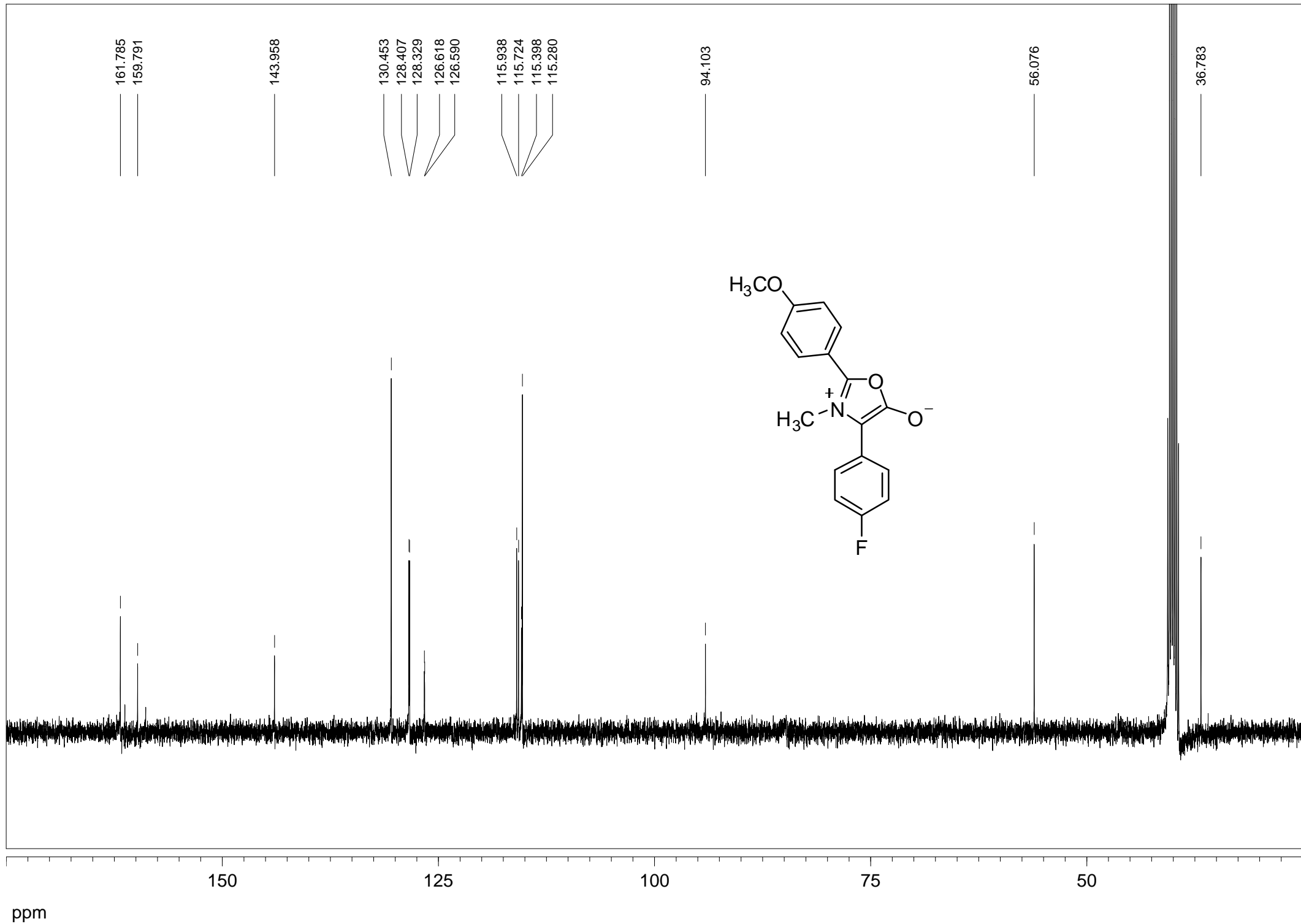


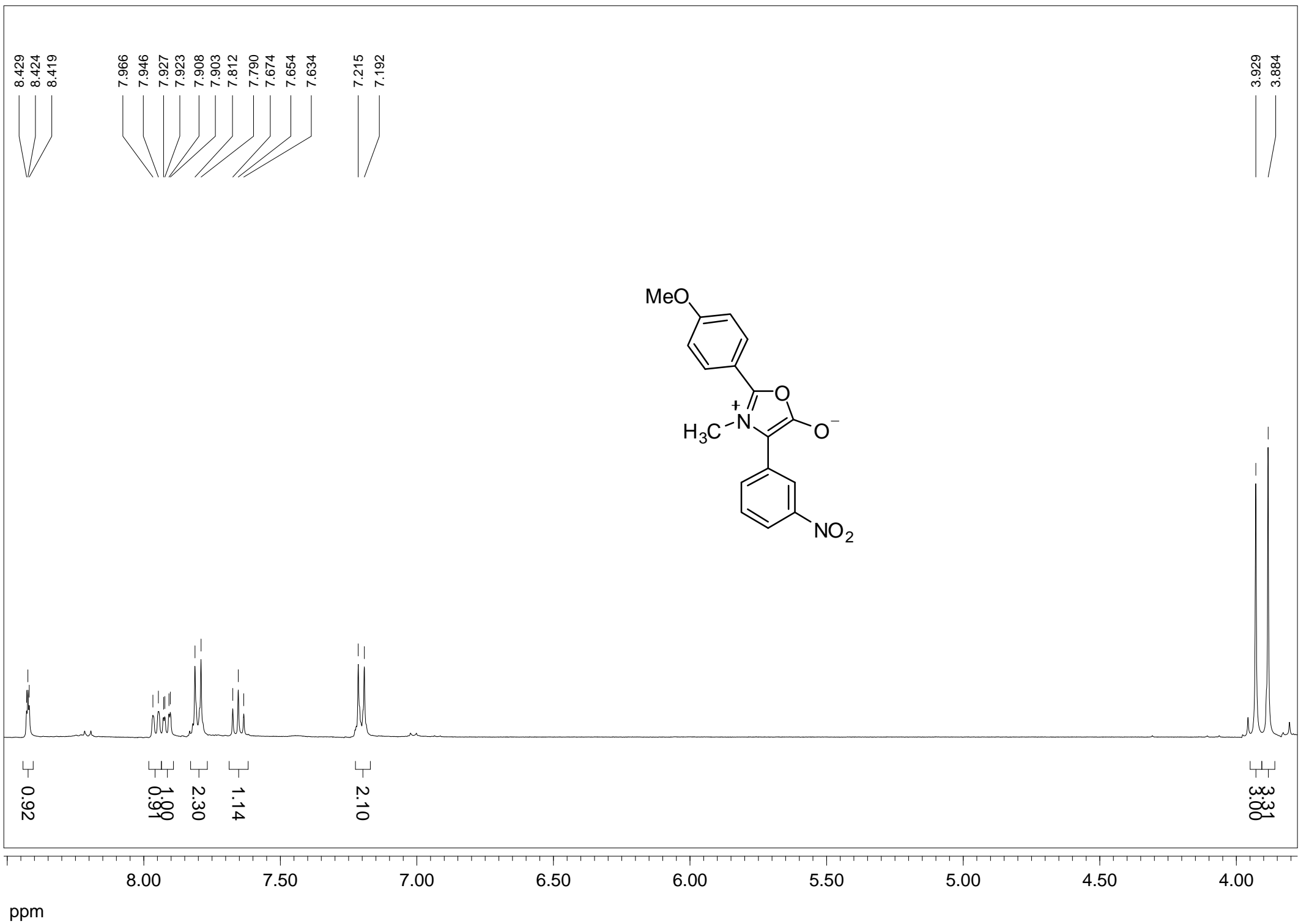


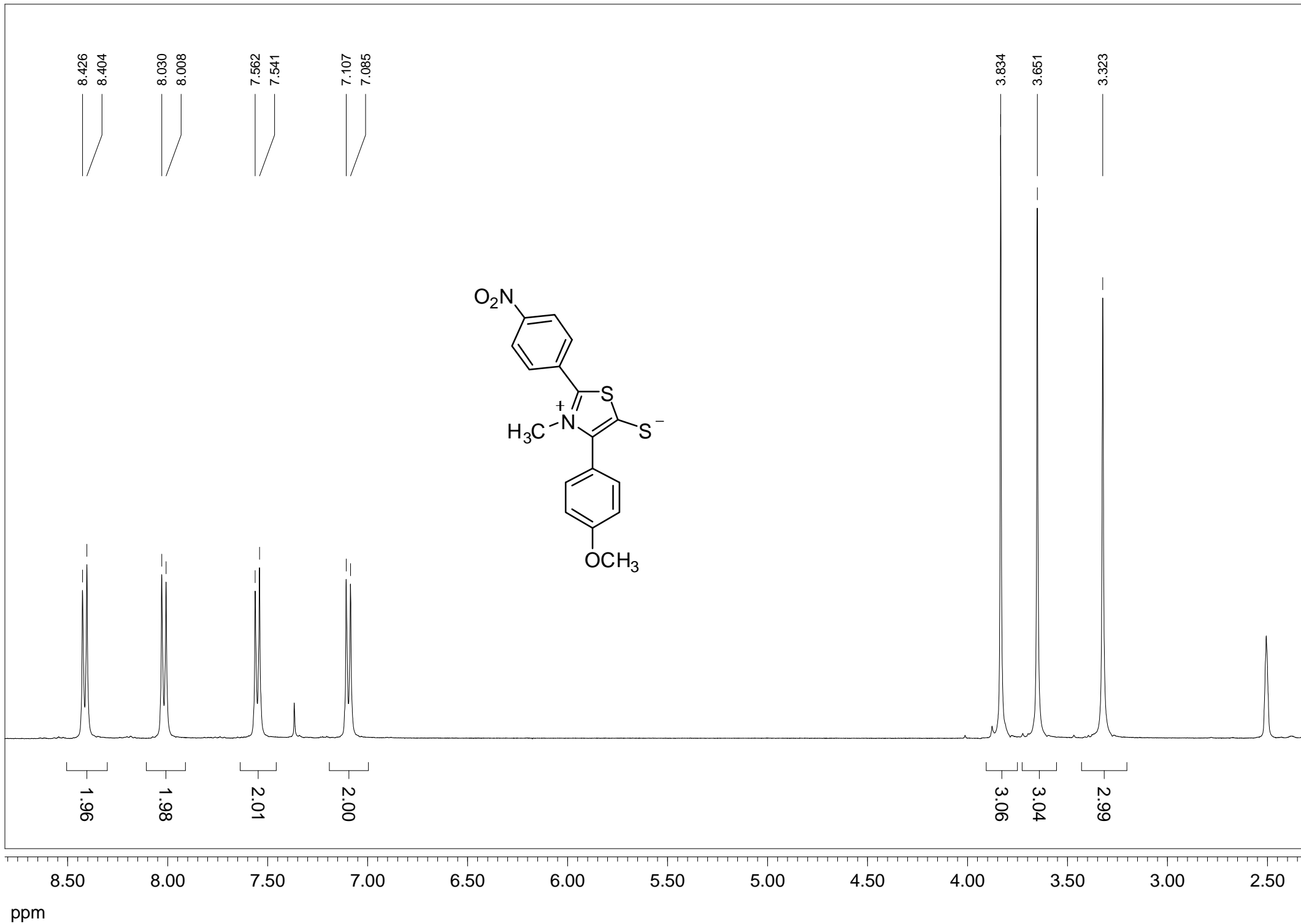


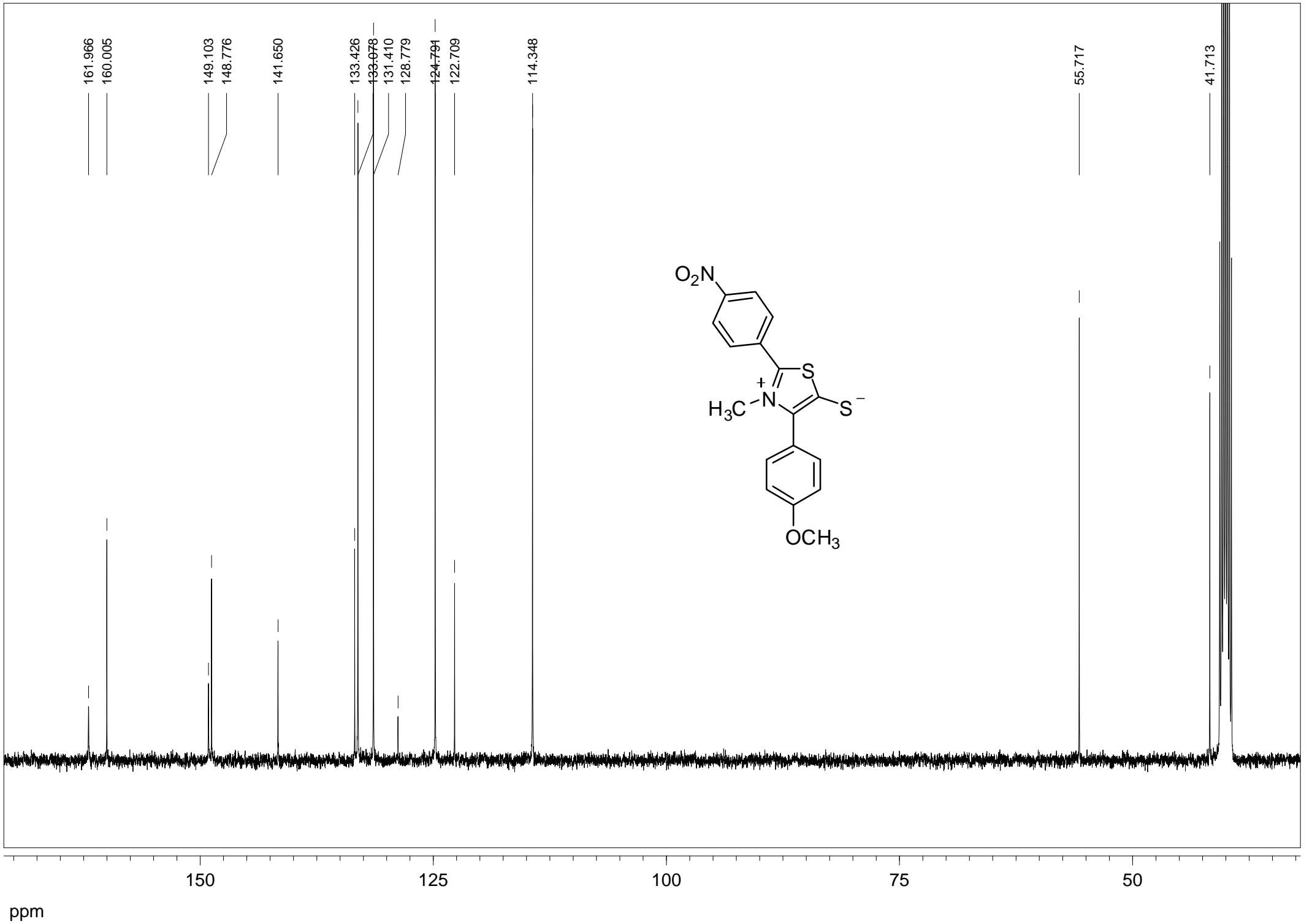


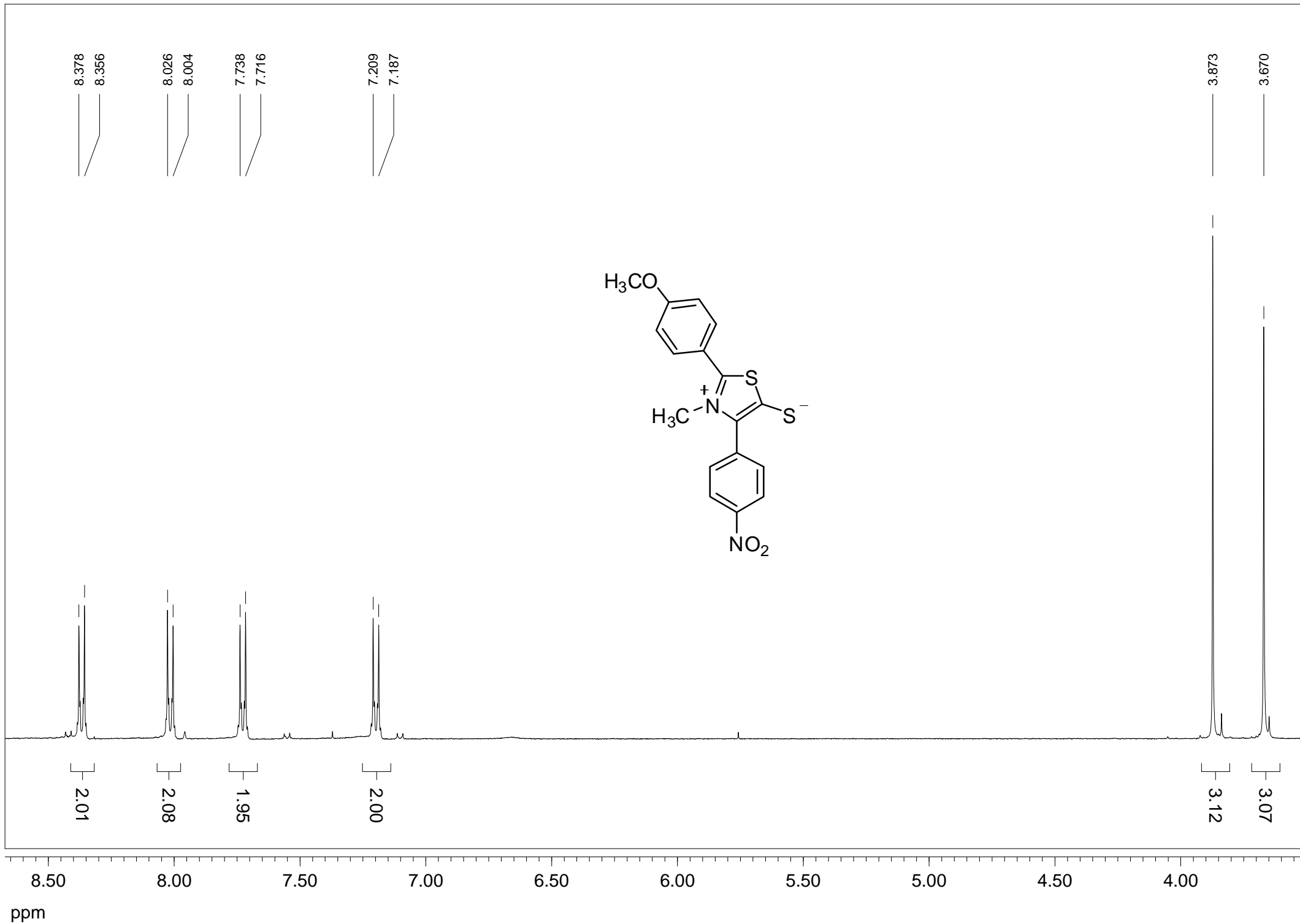


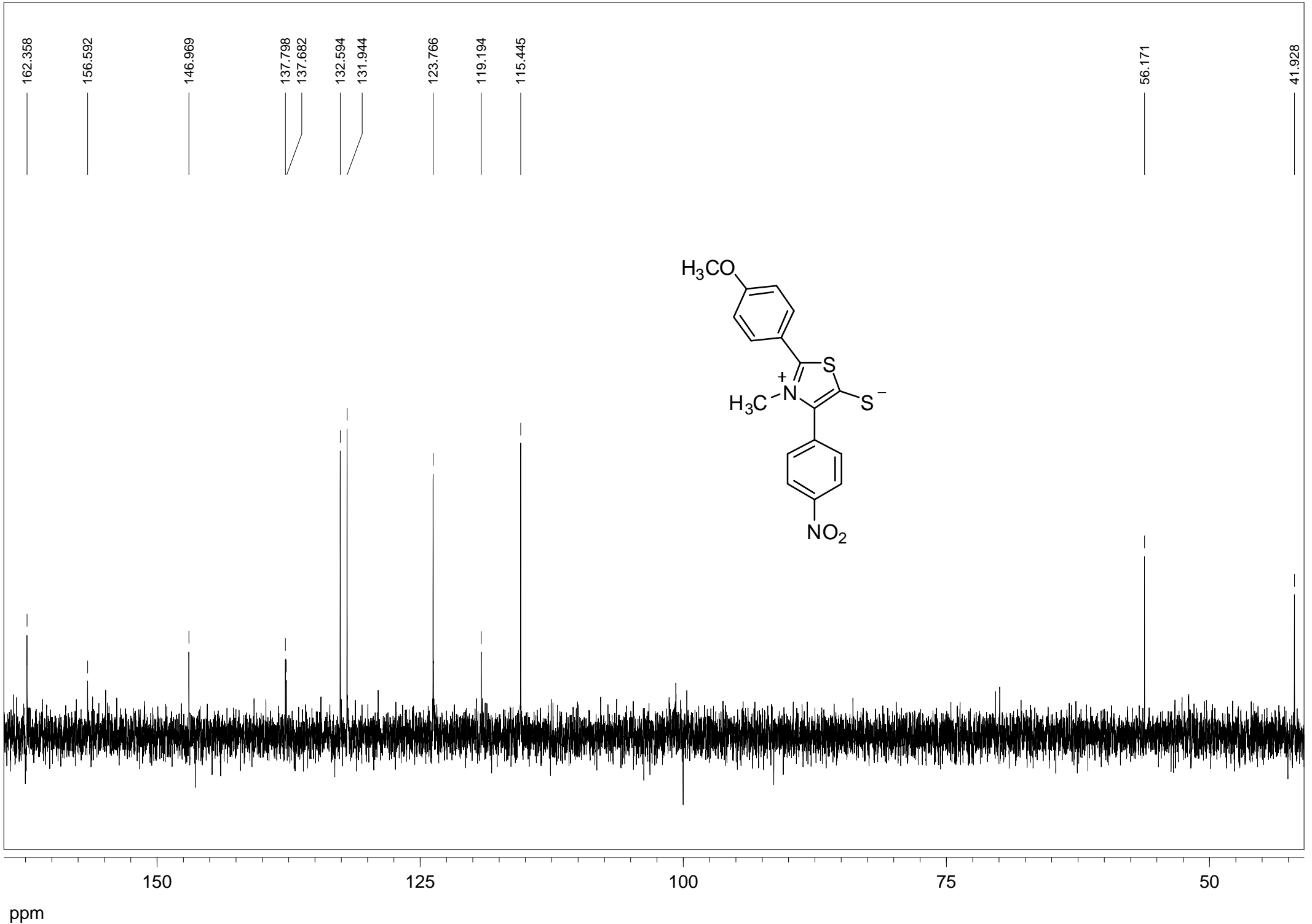




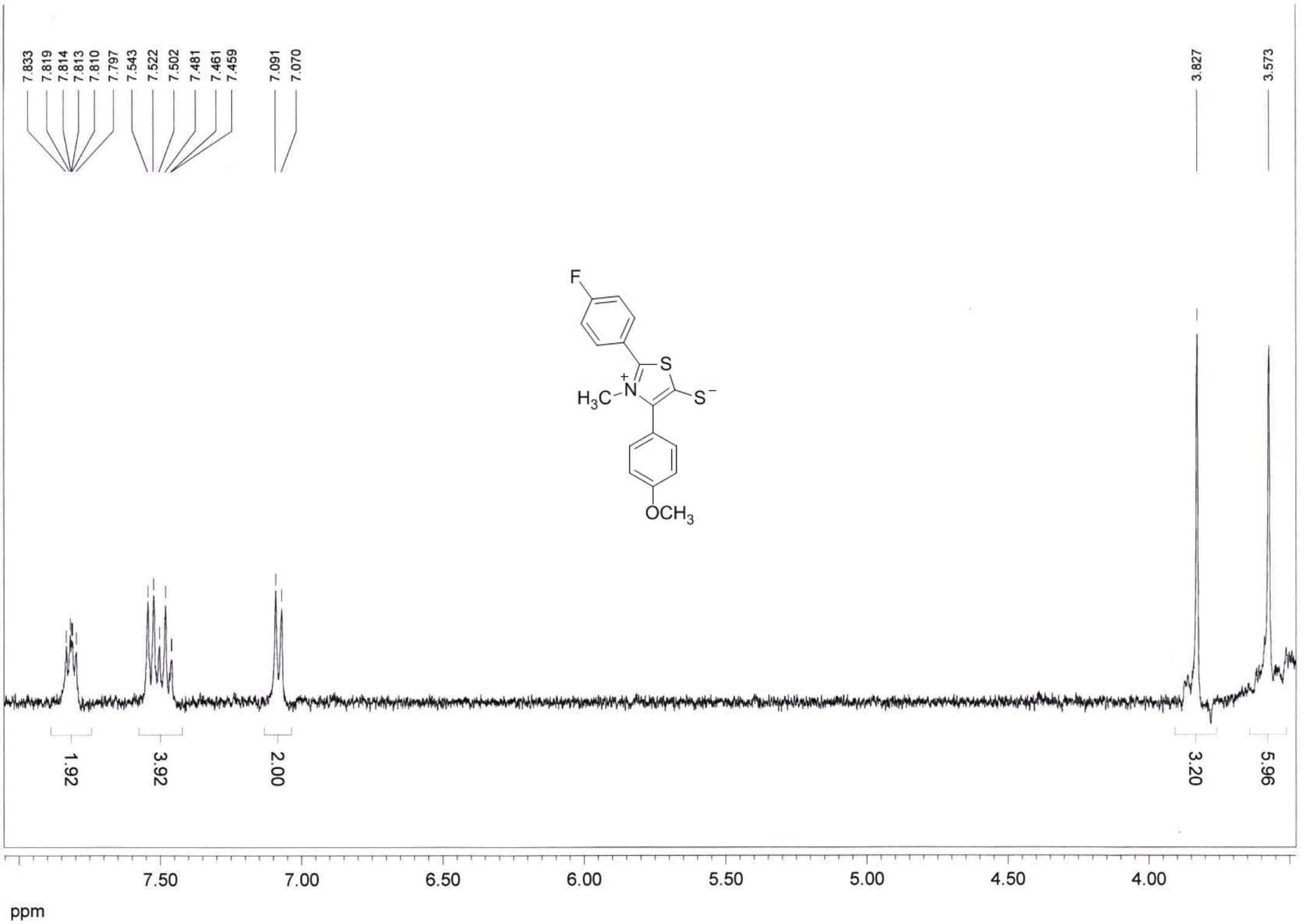


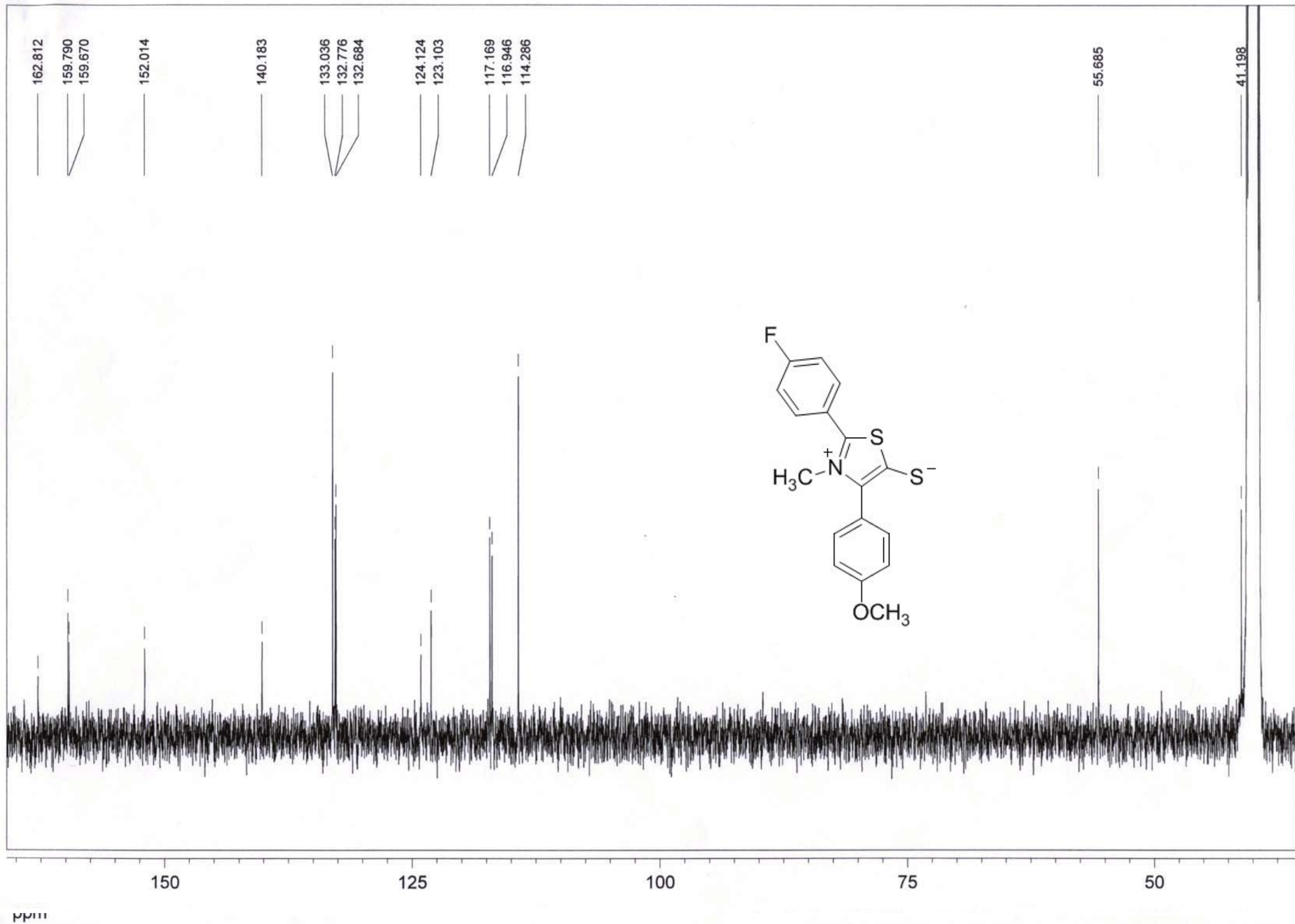


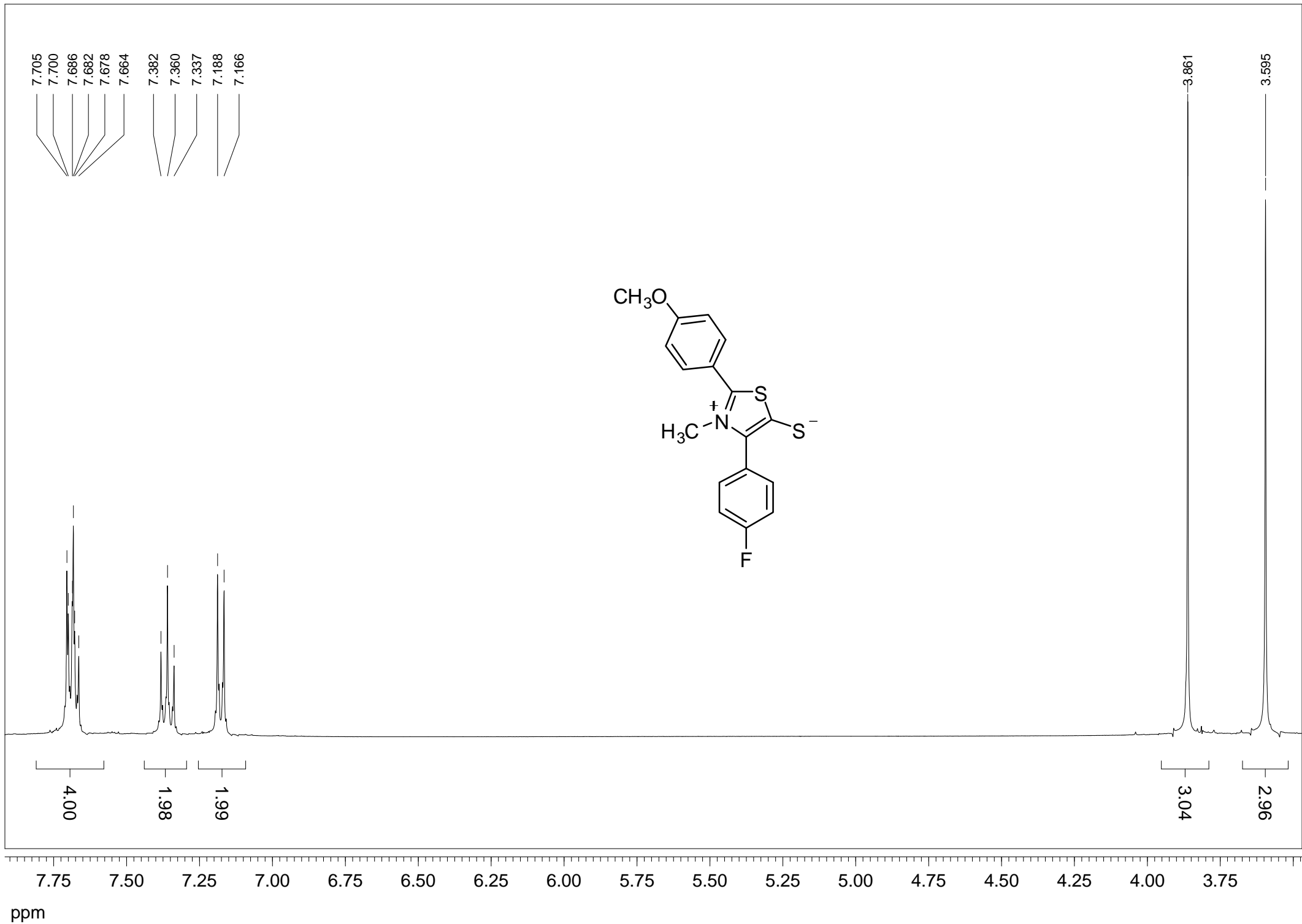


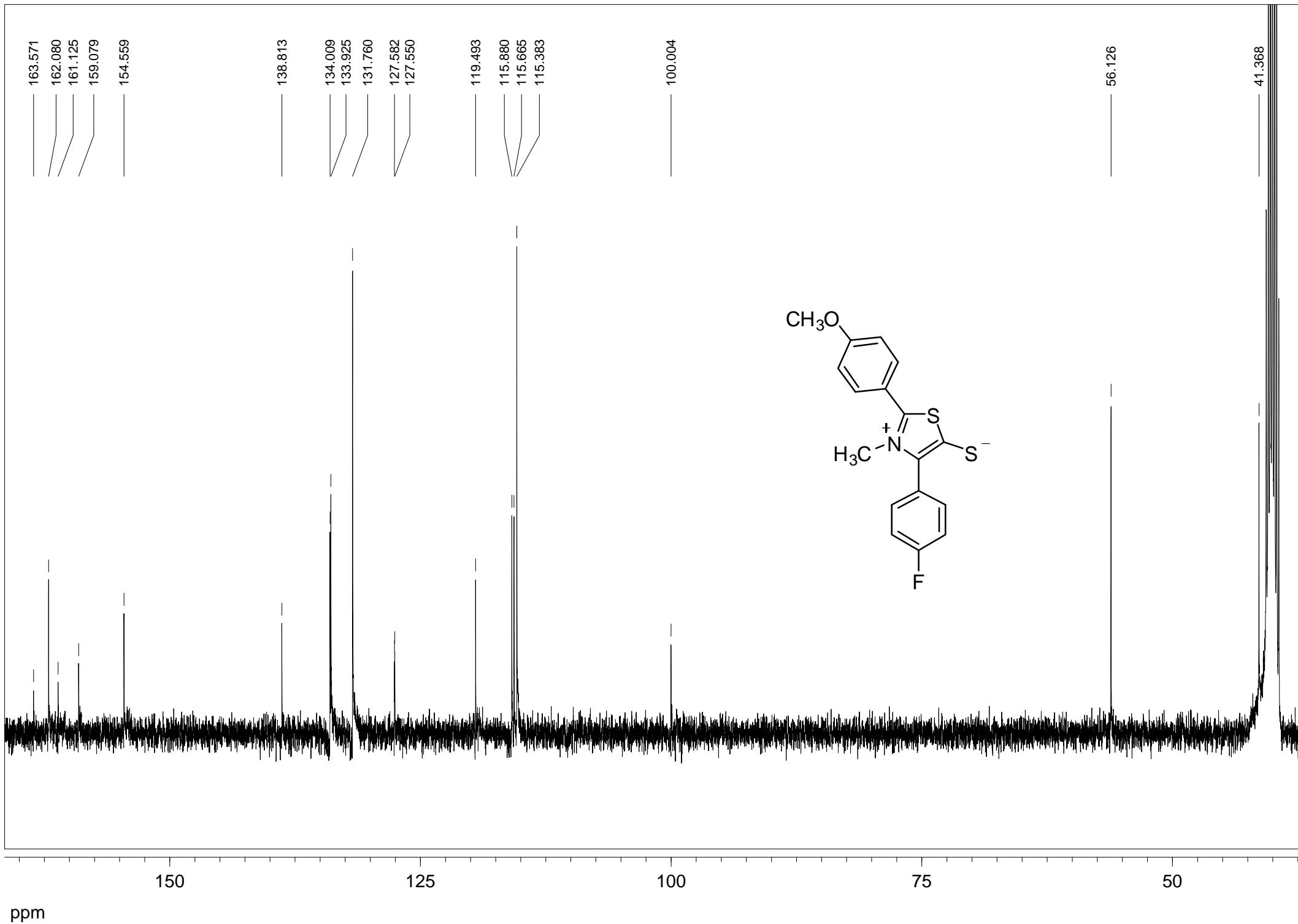


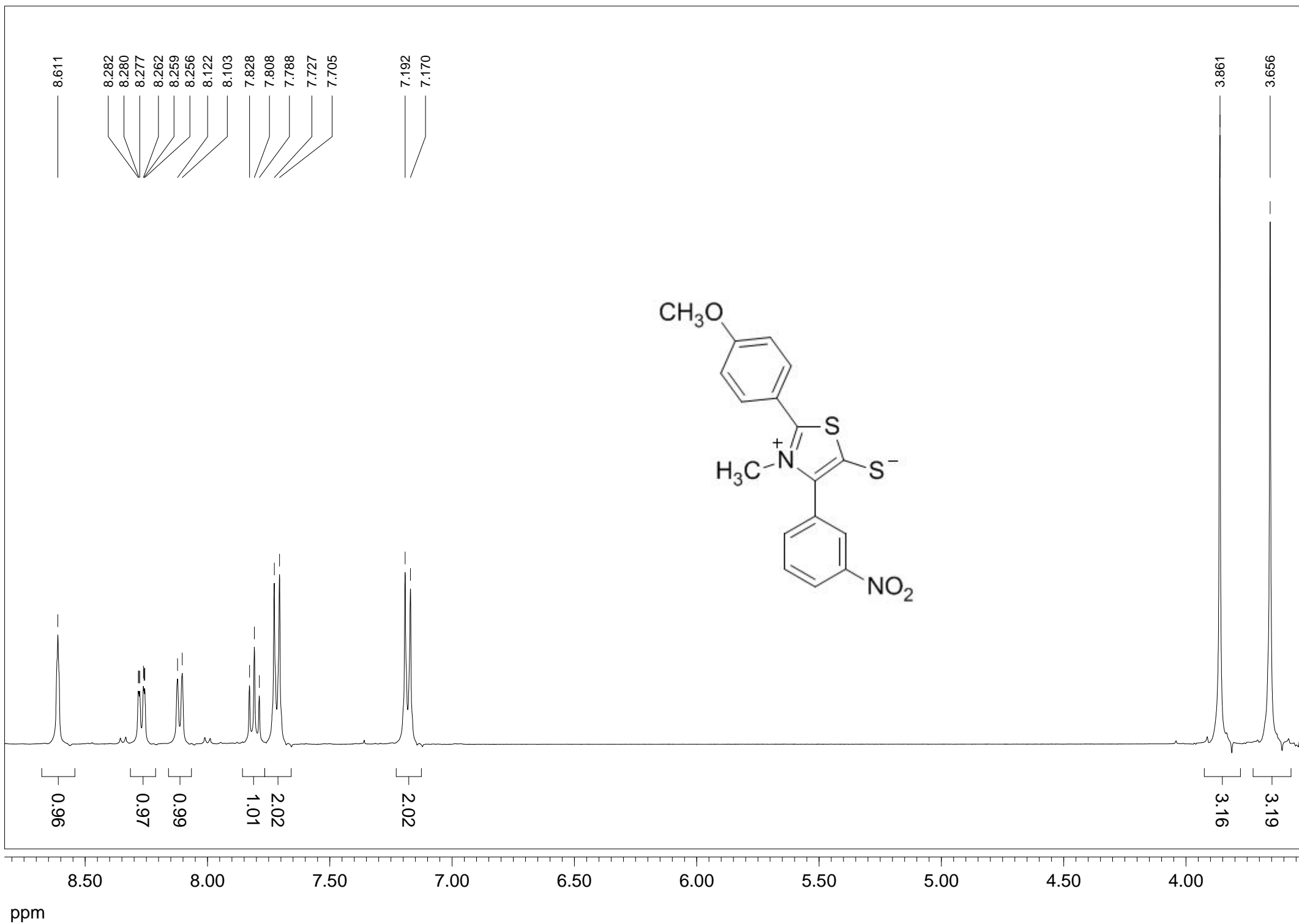


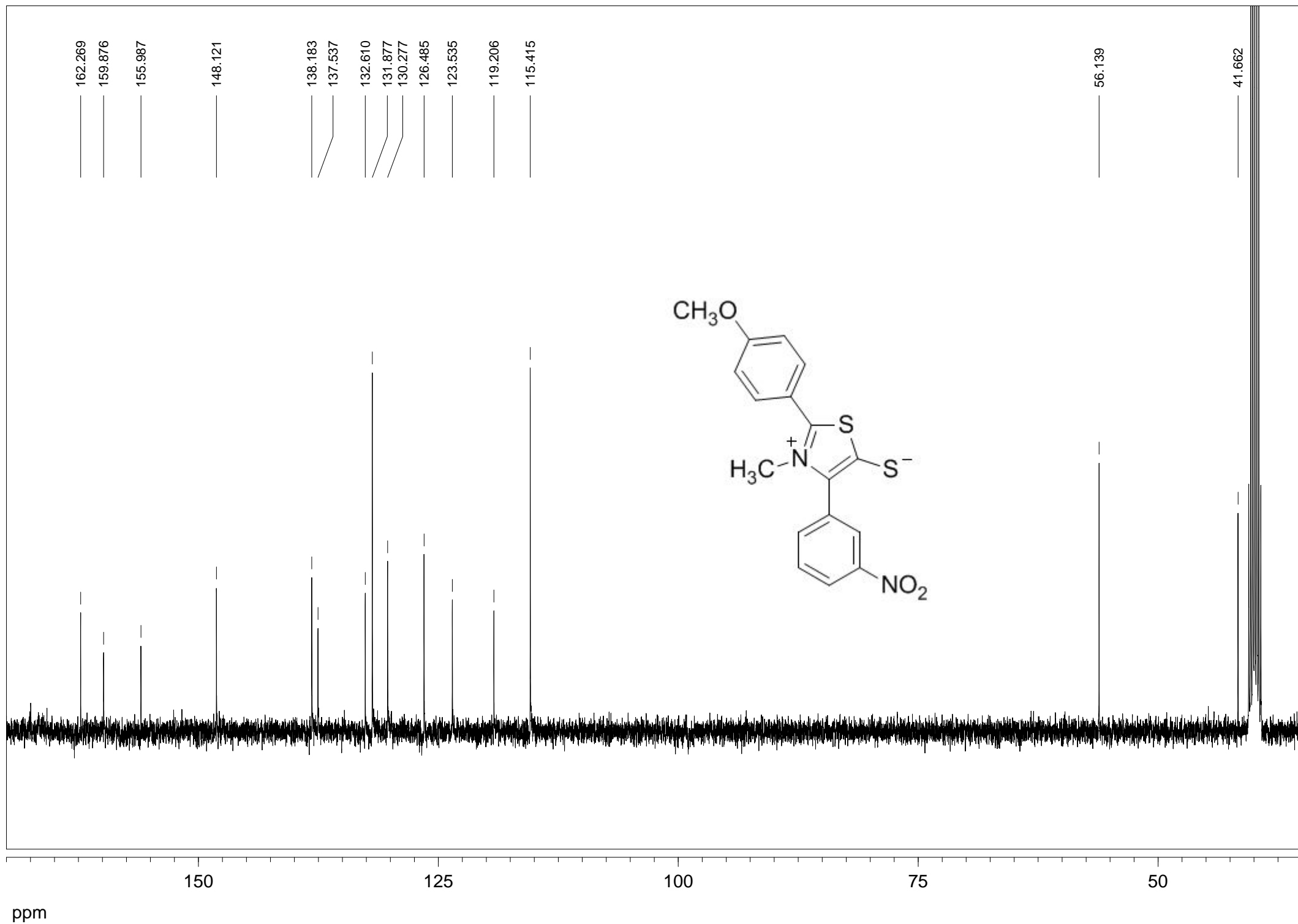




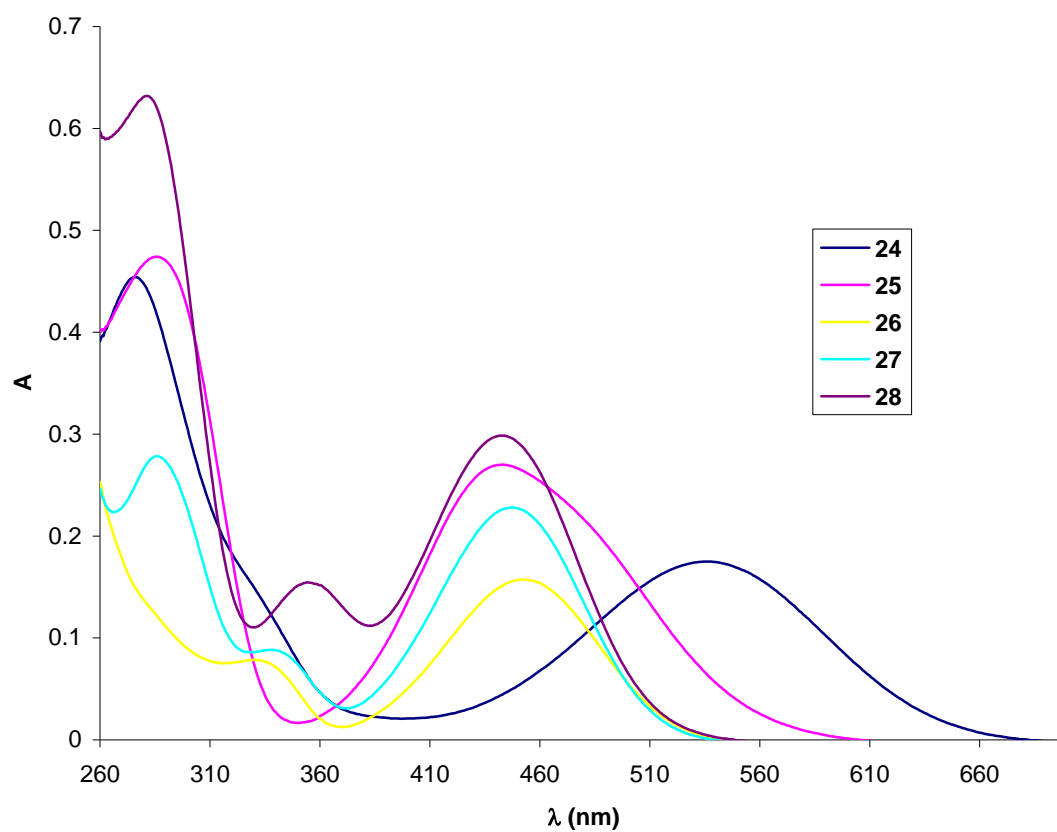




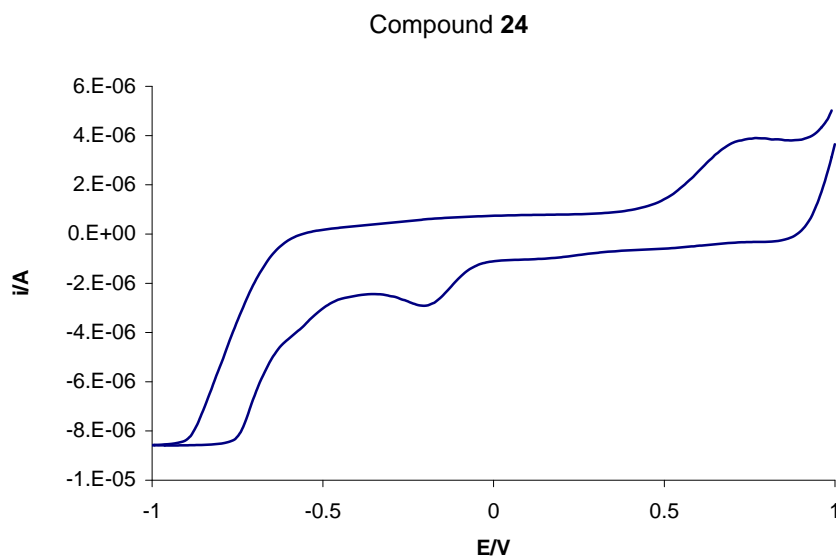




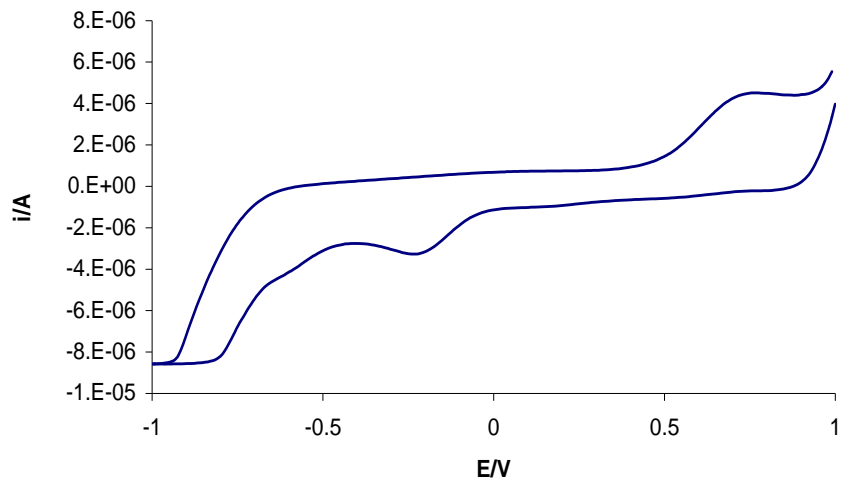
## UV Spectra of 1,3-thiazolium-5-thiolate systems



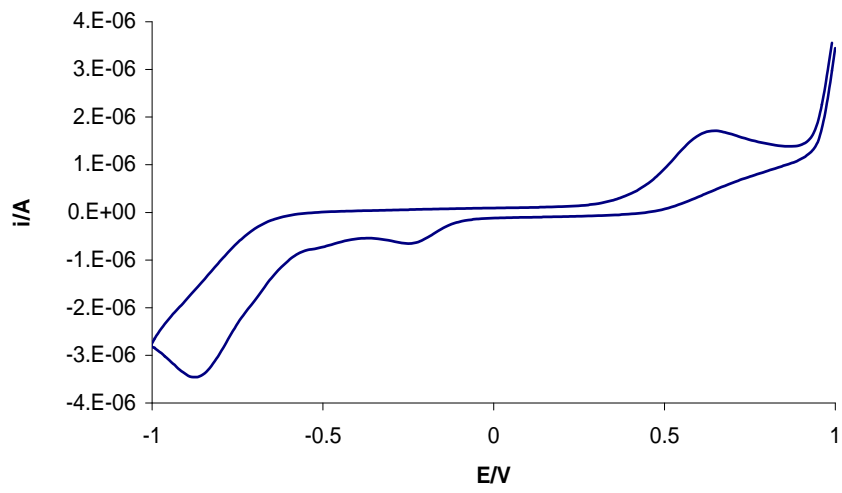
## Cyclic voltammograms of 1,3-thiazolium-5-thiolate systems



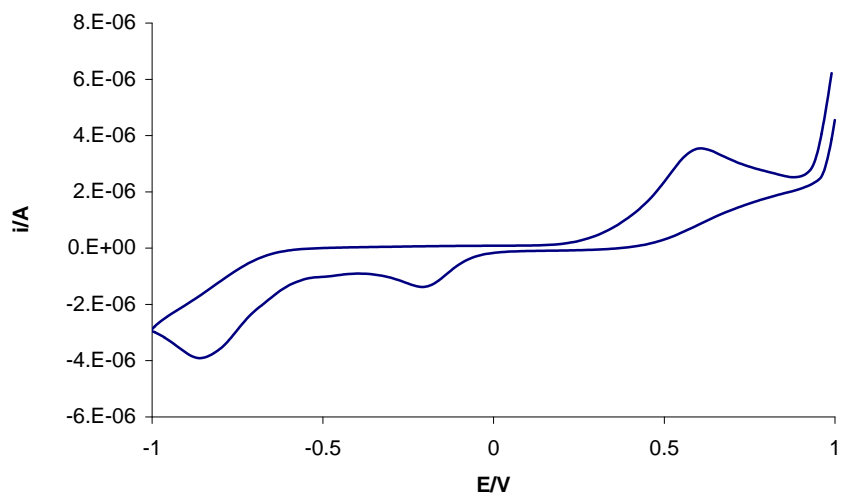
Compound 25



Compound 26

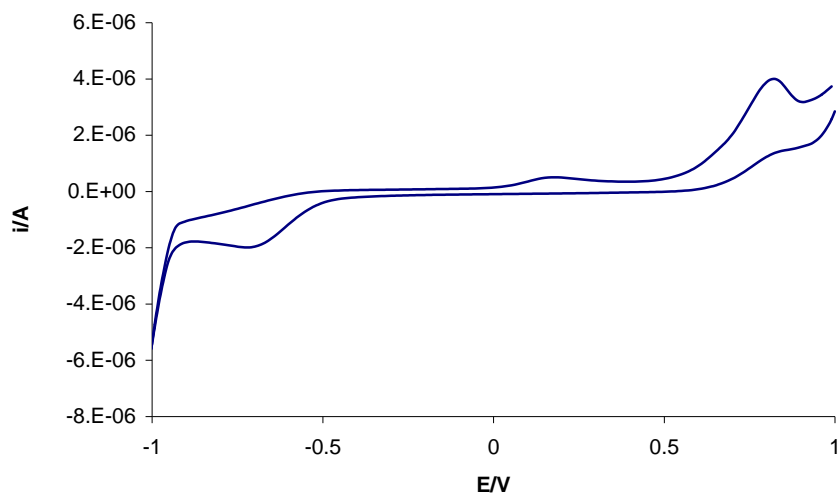


Compound 27



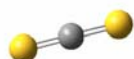


Compound 28



**Computational data: Cartesian coordinates, energies and imaginary frequencies (for transition structures) for all optimized geometries**

**CS<sub>2</sub>**

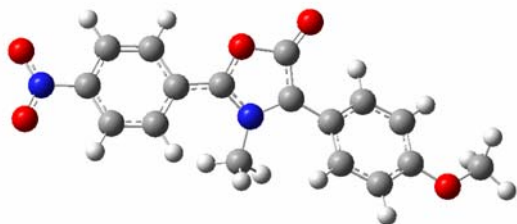


E = -834.488863669

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.005476
2	16	0	0.000000	1.563112	-0.001027
3	16	0	0.000000	-1.563112	-0.001027

**Structure 20**



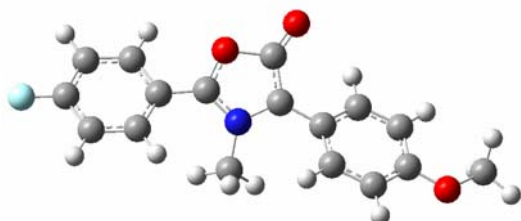
E = -1141.74207820

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.337898	0.541990	-0.125199
2	7	0	-0.189469	-0.229218	0.013507
3	6	0	0.907370	0.539578	-0.126672
4	8	0	0.528640	1.806479	-0.326324

5	6	0	-0.915203	1.890654	-0.312076
6	8	0	-1.470451	2.958996	-0.444613
7	6	0	-2.715880	0.078594	-0.082554
8	6	0	-0.181641	-1.612046	0.497796
9	6	0	2.308366	0.214098	-0.066151
10	6	0	3.222262	1.269916	0.179964
11	6	0	4.584266	1.031616	0.241678
12	6	0	5.059363	-0.269194	0.052533
13	6	0	-3.720045	0.964337	0.356969
14	6	0	-5.059647	0.587755	0.394307
15	6	0	-5.438798	-0.700082	-0.007049
16	6	0	-4.457027	-1.589681	-0.468114
17	6	0	-3.126350	-1.203149	-0.515323
18	6	0	4.190057	-1.326898	-0.217520
19	6	0	2.826266	-1.086035	-0.283929
20	7	0	6.495493	-0.527313	0.125481
21	8	0	7.239527	0.429636	0.351518
22	8	0	6.879102	-1.688113	-0.041439
23	6	0	-7.754250	-0.310047	0.433897
24	8	0	-6.715061	-1.175692	-0.000186
25	1	0	-1.091339	-1.773716	1.075518
26	1	0	0.688001	-1.761712	1.137567
27	1	0	-0.154005	-2.323571	-0.331886
28	1	0	2.840309	2.273462	0.326735
29	1	0	5.287502	1.831050	0.439865
30	1	0	-3.440699	1.967544	0.657931
31	1	0	-5.796259	1.303832	0.740354
32	1	0	-4.765775	-2.573918	-0.806085
33	1	0	-2.403289	-1.898429	-0.929839
34	1	0	4.595622	-2.316348	-0.388735
35	1	0	2.170145	-1.905510	-0.549704
36	1	0	-8.676264	-0.888537	0.355505
37	1	0	-7.608871	0.002165	1.476229
38	1	0	-7.828579	0.580522	-0.203360

## Structure 21



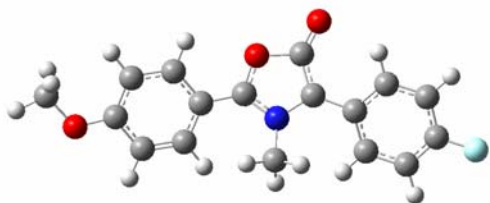
E = -1036.47315407

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.678620	0.525627	-0.128847
2	7	0	0.455410	-0.284685	0.017148
3	6	0	1.566942	0.449966	-0.124405
4	8	0	1.236130	1.721396	-0.335364
5	6	0	-0.224466	1.852781	-0.319382
6	8	0	-0.732341	2.945163	-0.458517
7	6	0	-2.068379	0.092184	-0.089576
8	6	0	0.426173	-1.660816	0.512841
9	6	0	2.964043	0.073214	-0.038363
10	6	0	3.900176	1.070197	0.317291
11	6	0	5.255480	0.780003	0.399640
12	6	0	5.686120	-0.514928	0.123435

13	6	0	-3.056184	1.001840	0.337054
14	6	0	-4.404843	0.655273	0.371680
15	6	0	-4.811009	-0.628198	-0.014343
16	6	0	-3.847156	-1.542648	-0.459780
17	6	0	-2.507316	-1.183869	-0.508901
18	6	0	4.798344	-1.517756	-0.250133
19	6	0	3.442001	-1.219824	-0.339685
20	6	0	-7.117434	-0.181572	0.415276
21	1	0	-0.469115	-1.784017	1.122358
22	1	0	1.311842	-1.840372	1.122976
23	1	0	0.397807	-2.381633	-0.309169
24	1	0	3.546693	2.073157	0.528775
25	1	0	5.979764	1.538296	0.677877
26	1	0	-2.756006	2.002135	0.628274
27	1	0	-5.126548	1.392135	0.706079
28	1	0	-4.174510	-2.525251	-0.785590
29	1	0	-1.798726	-1.900651	-0.911968
30	1	0	5.175318	-2.507442	-0.485368
31	1	0	2.762816	-1.991371	-0.683742
32	1	0	-8.054720	-0.736521	0.342884
33	1	0	-6.967172	0.141539	1.454097
34	1	0	-7.169491	0.703884	-0.232056
35	9	0	6.998906	-0.801672	0.208430
36	8	0	-6.101192	-1.077168	-0.005386

## Structure 22



E = -1036.47533550

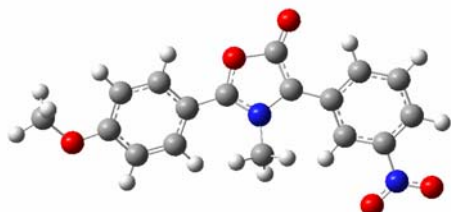
Standard orientation:

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			X	Y	Z
1	6	0	5.582581	-0.641291	0.108796
2	6	0	3.308658	-1.213540	-0.390485
3	6	0	0.347746	-1.664651	0.553008
4	6	0	5.203370	0.652373	0.451778
5	6	0	-0.757899	0.440511	-0.146818
6	6	0	1.487759	0.513629	-0.080691
7	6	0	-2.157382	0.064647	-0.096846
8	6	0	2.874313	0.076614	-0.017868
9	6	0	4.651788	-1.579486	-0.315842
10	6	0	1.044037	1.838482	-0.291219
11	6	0	-3.103758	1.051293	0.240036
12	6	0	-2.633018	-1.225530	-0.422143
13	6	0	-4.463823	0.765168	0.284622
14	6	0	-4.915925	-0.528652	-0.013680
15	6	0	-3.985899	-1.517738	-0.373224
16	6	0	3.860022	1.004627	0.392388
17	1	0	1.212451	-1.779254	1.207001
18	1	0	-2.759575	2.053786	0.470253
19	1	0	-5.159477	1.551316	0.553888
20	1	0	0.411608	-2.400552	-0.253596

21	1	0	-4.354130	-2.505770	-0.629906
22	1	0	-1.946540	-1.996967	-0.753320
23	1	0	3.555399	2.013010	0.647536
24	1	0	5.957822	1.366207	0.766834
25	1	0	4.982200	-2.572288	-0.604134
26	1	0	2.601160	-1.938866	-0.778041
27	1	0	-0.566143	-1.832272	1.123584
28	7	0	0.343939	-0.297345	0.032861
29	9	0	6.887147	-0.989748	0.178276
30	6	0	-7.210502	0.040156	0.339063
31	1	0	-8.163451	-0.488282	0.285246
32	1	0	-7.066873	0.428784	1.355241
33	1	0	-7.216395	0.875263	-0.372698
34	8	0	-6.216445	-0.920228	0.004577
35	8	0	-0.420674	1.708146	-0.356175
36	8	0	1.553073	2.931503	-0.420607

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### Structure 23



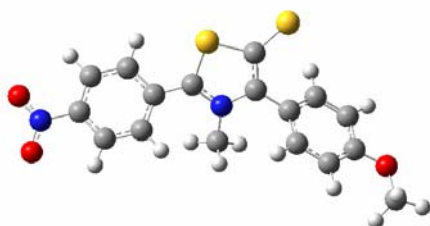
E = -1141.74713286

Standard orientation:

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1	6	0	5.273439	0.445295	0.248601
2	6	0	3.033436	-0.478266	-0.079252
3	6	0	0.130166	-1.219017	0.771875
4	6	0	4.698125	1.709705	0.384873
5	6	0	-1.191573	0.676020	-0.117778
6	6	0	1.021828	1.040253	0.001655
7	6	0	-2.534782	0.128136	-0.078665
8	6	0	2.447315	0.791053	0.089864
9	6	0	4.414076	-0.624349	0.016201
10	6	0	0.420253	2.279234	-0.317878
11	6	0	-3.605903	0.999704	0.192682
12	6	0	-2.830641	-1.224152	-0.359823
13	6	0	-4.919168	0.543904	0.217878
14	6	0	-5.193851	-0.808268	-0.036793
15	6	0	-4.136023	-1.684608	-0.332422
16	6	0	3.320724	1.886629	0.312789
17	1	0	0.946713	-1.166805	1.492399
18	1	0	-3.398342	2.046394	0.387544
19	1	0	-5.717010	1.243489	0.437472
20	1	0	0.353385	-1.993996	0.033805
21	1	0	-4.368821	-2.720451	-0.556487
22	1	0	-2.041260	-1.912691	-0.641143
23	1	0	2.894129	2.877934	0.411888
24	1	0	5.335864	2.571721	0.557972
25	1	0	2.452611	-1.357579	-0.315341
26	1	0	-0.794543	-1.469551	1.291748
27	7	0	-0.016791	0.095875	0.143582
28	6	0	-7.551603	-0.525588	0.239686
29	1	0	-8.425807	-1.175858	0.187098
30	1	0	-7.485811	-0.083549	1.241719
31	1	0	-7.645684	0.273048	-0.506620

32	8	0	-6.432193	-1.361066	-0.032966
33	8	0	-1.012512	1.957361	-0.410799
34	8	0	0.789181	3.415822	-0.519090
35	1	0	6.341472	0.282201	0.311068
36	7	0	4.982360	-1.971655	-0.153232
37	8	0	4.201960	-2.909000	-0.336372
38	8	0	6.205966	-2.090362	-0.099091

## Structure 24

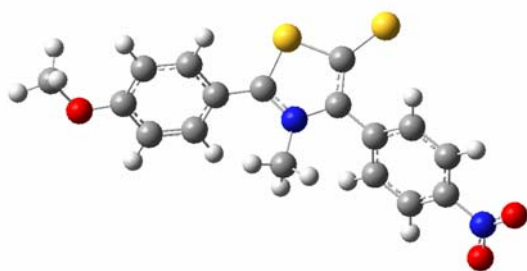


E = -1787.66633920

Standard orientation:

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			X	Y	Z
1	6	0	5.025362	-0.708612	0.033292
2	6	0	-2.628095	0.084649	0.085905
3	6	0	-2.980162	-0.989195	-0.744226
4	6	0	1.017816	0.703923	-0.048466
5	6	0	-1.108933	2.116488	-0.254679
6	6	0	4.034193	-1.535721	-0.494983
7	6	0	-3.589882	0.555750	1.001886
8	6	0	-0.154902	-1.376442	0.609290
9	6	0	3.410923	0.999220	0.510464
10	6	0	2.721364	-1.087409	-0.518360
11	6	0	4.726188	0.560770	0.530102
12	6	0	2.374581	0.183495	-0.002114
13	6	0	-1.310979	0.737605	-0.018741
14	6	0	-4.835947	-0.042477	1.096857
15	6	0	-5.168096	-1.126849	0.268659
16	6	0	-4.231674	-1.600019	-0.659390
17	6	0	-6.826255	-2.715666	-0.392153
18	1	0	-5.578048	0.316050	1.802915
19	1	0	-4.468233	-2.421809	-1.325314
20	1	0	-0.261993	-2.086075	-0.213726
21	1	0	-1.006189	-1.485503	1.279925
22	1	0	-3.350511	1.403276	1.634347
23	1	0	0.770951	-1.574735	1.146849
24	1	0	3.170092	1.976219	-0.917024
25	1	0	5.520558	1.176656	0.933308
26	1	0	4.307142	-2.504252	-0.895507
27	1	0	1.964849	-1.711953	-0.979522
28	1	0	-2.276848	-1.343371	-1.493696
29	1	0	-7.846984	-2.954224	-0.089121
30	1	0	-6.819336	-2.427942	-1.451322
31	1	0	-6.190331	-3.599683	-0.252350
32	7	0	6.411223	-1.181485	0.059424
33	7	0	-0.134494	0.012909	0.114075
34	8	0	6.637679	-2.312140	-0.376080
35	8	0	7.266204	-0.421370	0.516547
36	8	0	-6.415469	-1.641304	0.441047
37	16	0	0.661451	2.371240	-0.355013
38	16	0	-2.200985	3.369937	-0.451267

## Structure 25

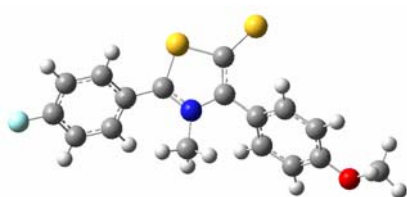


E = -1787.66980764

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-5.436103	-1.074844	-0.020098
2	6	0	2.187152	0.154317	0.004438
3	6	0	2.525236	-0.984404	-0.757536
4	6	0	-1.481947	0.572150	-0.127228
5	6	0	0.564733	2.112094	-0.227197
6	6	0	-5.152239	0.142345	0.615496
7	6	0	3.190850	0.752667	0.793219
8	6	0	-0.243380	-1.456942	0.506036
9	6	0	-3.124679	-1.241067	-0.719899
10	6	0	-3.857894	0.653636	0.583917
11	6	0	-4.407985	-1.759390	-0.690860
12	6	0	-2.814304	-0.025137	-0.070194
13	6	0	0.842213	0.741712	-0.048244
14	6	0	4.471962	0.217809	0.844290
15	6	0	4.762052	-0.922805	0.095784
16	6	0	3.801758	-1.529549	-0.712580
17	6	0	-7.746417	-1.017357	0.591784
18	1	0	5.244788	0.664380	1.457576
19	1	0	4.069769	-2.398291	-1.300996
20	1	0	-1.165740	-1.688839	1.037014
21	1	0	0.607012	-1.554402	1.179633
22	1	0	2.955839	1.642869	1.363072
23	1	0	-0.119721	-2.154168	-0.324973
24	1	0	-2.358667	-1.766421	-1.281476
25	1	0	-4.648933	-2.688532	-1.197008
26	1	0	-5.924457	0.692331	1.140181
27	1	0	-3.648777	1.589690	1.093142
28	1	0	1.789614	-1.427482	-1.421583
29	1	0	-8.610453	-1.663690	0.432524
30	1	0	-7.567805	-0.906557	1.668589
31	1	0	-7.941099	-0.032435	0.149632
32	7	0	6.109392	-1.497683	0.154547
33	7	0	-0.306747	-0.061581	0.032852
34	8	0	6.328291	-2.515225	-0.506546
35	8	0	6.943482	-0.934620	0.864836
36	8	0	-6.654942	-1.667199	-0.050709
37	16	0	-1.221475	2.258464	-0.384173
38	16	0	1.551438	3.462245	-0.349235

## Structure 26

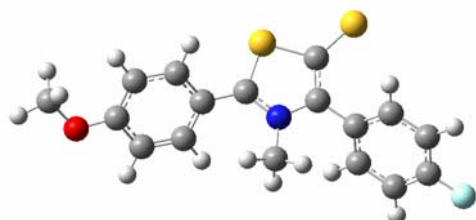


E = -1682.39932543

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.608529	-1.157014	-0.071832
2	6	0	3.634386	-1.621415	-0.968718
3	6	0	-0.391866	-1.604963	0.434495
4	6	0	-1.644618	0.467471	-0.041764
5	6	0	0.682914	0.590398	-0.084233
6	6	0	-2.984039	-0.113823	0.035900
7	6	0	2.021880	-0.026730	-0.074803
8	6	0	4.291126	-0.121312	0.815807
9	6	0	0.426026	1.968125	-0.221434
10	6	0	-3.994633	0.560072	0.753143
11	6	0	-3.328481	-1.299689	-0.645888
12	6	0	-5.292359	0.063096	0.806073
13	6	0	-5.585926	-1.120817	0.137063
14	6	0	-4.621669	-1.810402	-0.590604
15	6	0	2.367502	-1.056455	-0.972465
16	6	0	3.011552	0.432902	0.805729
17	6	0	6.865983	-1.306933	0.696296
18	9	0	-6.838295	-1.610084	0.189844
19	1	0	-1.301970	-1.874192	0.968586
20	1	0	-3.751099	1.473521	1.286737
21	1	0	-6.071326	0.572772	1.363078
22	1	0	-4.894556	-2.718700	-1.117391
23	1	0	-2.587372	-1.810606	-1.251745
24	1	0	1.639857	-1.400764	-1.702940
25	1	0	3.902590	-2.409273	-1.665529
26	1	0	5.027570	0.263680	1.511567
27	1	0	2.778993	1.245939	1.484316
28	1	0	0.474344	-1.732521	1.082792
29	1	0	-0.275390	-2.250611	-0.438649
30	1	0	7.739026	-1.915208	0.453454
31	1	0	7.094993	-0.250069	0.508799
32	1	0	6.615747	-1.439547	1.757101
33	7	0	-0.469705	-0.187270	0.041914
34	8	0	5.822806	-1.770661	-0.148366
35	16	0	-1.360949	2.157609	-0.260243
36	16	0	1.452254	3.289732	-0.360497

**Structure 27**

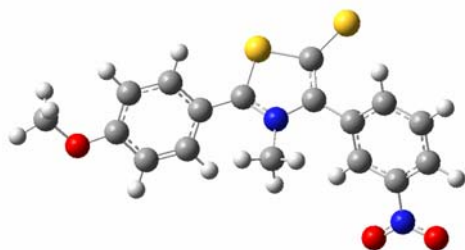


E = -1682.40090034

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.195002	-1.520102	0.167319
2	6	0	3.029740	-1.298054	-0.826495
3	6	0	0.185163	-1.627340	0.470329
4	6	0	4.944516	-0.450936	1.020274
5	6	0	-0.894434	0.514471	-0.100926
6	6	0	1.435577	0.479792	-0.040099
7	6	0	-2.272264	0.029040	-0.065193
8	6	0	2.728551	-0.226888	0.033773
9	6	0	4.256270	-1.956339	-0.760088
10	6	0	1.282667	1.866879	-0.210044
11	6	0	-3.261774	0.777605	0.596598
12	6	0	-2.678726	-1.142942	-0.742060
13	6	0	-4.595329	0.376450	0.607390
14	6	0	-4.974320	-0.799170	-0.054932
15	6	0	-4.001246	-1.553574	-0.731572
16	6	0	3.711954	0.192574	0.947843
17	1	0	1.008525	-1.801418	1.162357
18	1	0	-2.979072	1.682083	1.126982
19	1	0	-5.323589	0.978591	1.137771
20	1	0	0.293359	-2.300644	-0.382811
21	1	0	-4.314249	-2.449326	-1.258293
22	1	0	-1.954273	-1.718784	-1.309342
23	1	0	3.506633	1.037777	1.594532
24	1	0	5.708423	-0.134554	1.722806
25	1	0	4.497665	-2.780179	-1.423625
26	1	0	2.306770	-1.606036	-1.576848
27	1	0	-0.765612	-1.818601	0.965745
28	7	0	0.225838	-0.217543	0.046073
29	16	0	2.402145	3.114324	-0.322560
30	16	0	-0.485206	2.175998	-0.338090
31	9	0	6.386062	-2.150053	0.236644
32	6	0	-7.277082	-0.560348	0.540180
33	1	0	-8.192514	-1.125672	0.359976
34	1	0	-7.101267	-0.487676	1.620937
35	1	0	-7.382462	0.447449	0.119224
36	8	0	-6.240049	-1.287698	-0.106888

## Structure 28



E = -1787.67022290

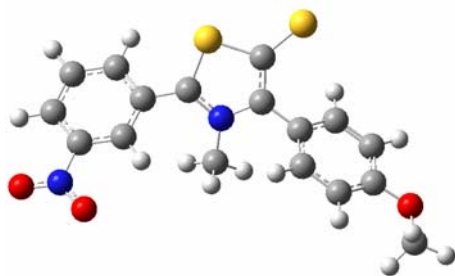
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-5.141920	-1.081706	-0.003757
2	6	0	2.420033	0.453824	0.343995
3	6	0	2.845300	-0.773869	-0.185269
4	6	0	-1.242072	0.689827	-0.104652
5	6	0	0.763489	2.265735	-0.349124



6	6	0	-4.945415	0.235746	0.433707
7	6	0	3.346480	1.219968	1.080026
8	6	0	0.007081	-1.146932	0.956665
9	6	0	-2.778372	-1.265487	-0.493889
10	6	0	-3.667858	0.788682	0.410030
11	6	0	-4.044321	-1.825329	-0.470213
12	6	0	-2.556714	0.054581	-0.041036
13	6	0	1.062214	0.965166	0.096488
14	6	0	4.646313	0.762221	1.293639
15	6	0	5.061606	-0.468215	0.788098
16	6	0	4.142449	-1.216745	0.056231
17	6	0	-7.493700	-1.021564	0.420878
18	1	0	5.341200	1.369771	1.865339
19	1	0	-0.947813	-1.330195	1.447504
20	1	0	0.800456	-1.087856	1.700812
21	1	0	3.037379	2.180345	1.474169
22	1	0	0.224819	-1.967108	0.269629
23	1	0	-1.954929	-1.844927	-0.899219
24	1	0	-4.216815	-2.835976	-0.825747
25	1	0	-5.772666	0.833000	0.798457
26	1	0	-3.526784	1.805125	0.765374
27	1	0	2.198628	-1.381812	-0.804544
28	1	0	-8.323549	-1.720823	0.310475
29	1	0	-7.403582	-0.726704	1.473893
30	1	0	-7.682197	-0.132119	-0.193120
31	7	0	-0.064697	0.144353	0.248330
32	8	0	-6.337053	-1.722217	-0.022297
33	16	0	-1.008891	2.313356	-0.643480
34	16	0	1.729703	3.607462	-0.645417
35	1	0	6.062910	-0.849203	0.945166
36	7	0	4.552413	-2.518832	-0.490782
37	8	0	3.703987	-3.182705	-1.090040
38	8	0	5.716615	-2.874911	-0.312611

## Structure 29



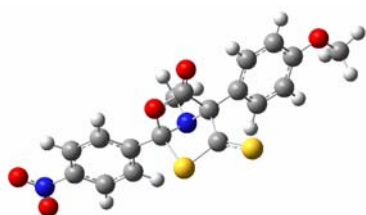
E = -1787.66526579

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.345602	-0.059022	0.497844
2	6	0	-2.379368	0.150409	0.089647
3	6	0	-2.606920	-1.025456	-0.639350
4	6	0	1.214438	1.029603	0.060617
5	6	0	-0.994016	2.247847	-0.388334
6	6	0	4.411532	-0.965627	0.002375
7	6	0	-3.421721	0.634769	0.904780
8	6	0	0.166058	-1.062725	0.864890
9	6	0	3.548767	1.548117	0.729704
10	6	0	3.066207	-0.652632	-0.149153
11	6	0	4.893393	1.211319	0.854957

12	6	0	2.604468	0.621036	0.232419
13	6	0	-1.108624	0.890180	-0.018684
14	6	0	-4.624796	-0.045799	1.002495
15	6	0	-4.830973	-1.231254	0.278623
16	6	0	-3.813278	-1.721133	-0.549285
17	6	0	-6.327479	-3.006858	-0.284534
18	1	0	-5.428760	0.323381	1.631178
19	1	0	-3.951703	-2.622392	-1.135153
20	1	0	0.180289	-1.849154	0.107305
21	1	0	-0.721061	-1.186772	1.484204
22	1	0	-3.279639	1.558246	1.454902
23	1	0	1.062124	-1.131168	1.480136
24	1	0	3.212959	2.534756	1.033435
25	1	0	5.594908	1.941795	1.245787
26	1	0	2.411441	-1.391263	-0.590689
27	1	0	-1.839457	-1.398539	-1.312886
28	1	0	-7.342320	-3.295026	-0.005477
29	1	0	-6.284420	-2.831540	-1.367255
30	1	0	-5.634908	-3.817150	-0.021156
31	7	0	0.110031	0.273868	0.244031
32	8	0	-6.045596	-1.822382	0.446005
33	16	0	0.760219	2.622682	-0.438512
34	16	0	-2.155830	3.395309	-0.761922
35	1	0	6.383819	-0.350735	0.591406
36	7	0	4.865493	-2.311293	-0.398233
37	8	0	6.063292	-2.563090	-0.288061
38	8	0	4.017067	-3.100400	-0.813374

### Cycloadduct 30



E = -1976.21047460

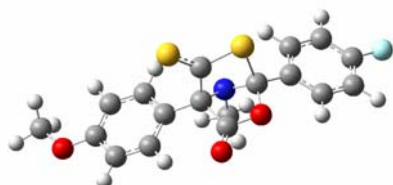
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-5.061248	-1.278604	0.252890
2	6	0	1.010670	0.681649	0.112061
3	6	0	2.829673	-0.614195	-1.012573
4	6	0	-0.656424	1.384674	1.476681
5	6	0	-1.200661	0.657717	0.200303
6	6	0	0.002718	-1.445702	0.803951
7	6	0	4.133491	-1.091138	-1.081242
8	6	0	2.420659	0.170824	0.076530
9	6	0	-2.922216	-0.855318	-0.783981
10	6	0	-1.055527	1.752149	-0.914246
11	6	0	-4.158186	-1.498311	-0.796515
12	6	0	-2.554398	0.000049	0.262311
13	6	0	3.327210	0.485446	1.095202
14	6	0	4.637344	0.014759	1.032711
15	6	0	5.018453	-0.766645	-0.053776
16	6	0	-3.467946	0.214719	1.304988
17	6	0	-4.705132	-0.417195	1.299447
18	1	0	2.121392	-0.849314	-1.800731
19	1	0	-0.878914	-2.059655	0.619253

20	1	0	0.039689	-1.191772	1.873568
21	1	0	0.892223	-2.024299	0.547554
22	1	0	3.006897	1.094425	1.931998
23	1	0	5.358637	0.243725	1.807287
24	1	0	-3.214350	0.883717	2.117788
25	1	0	-5.417734	-0.253837	2.101566
26	1	0	-4.406734	-2.154909	-1.622070
27	1	0	-2.229738	-1.025357	-1.603567
28	1	0	4.473463	-1.701388	-1.908571
29	7	0	-0.062540	-0.269840	-0.084833
30	8	0	-1.217643	1.914589	2.392658
31	8	0	0.715047	1.344364	1.369953
32	16	0	-2.254782	2.601181	-1.612839
33	16	0	0.661069	1.942286	-1.244621
34	7	0	6.403354	-1.268482	-0.121978
35	8	0	6.709278	-1.961689	-1.090828
36	8	0	7.164919	-0.963700	0.794038
37	6	0	-6.717520	-2.717015	-0.695406
38	1	0	-7.720651	-3.045877	-0.419077
39	1	0	-6.758851	-2.197473	-1.661419
40	1	0	-6.060307	-3.592150	-0.782692
41	8	0	-6.293734	-1.848591	0.345444

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### Cycloadduct 31



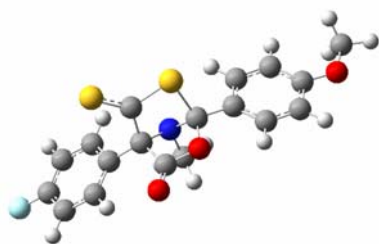
E = -1870.94505004

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.644850	-1.036457	0.198897
2	6	0	1.567810	0.442687	0.115161
3	6	0	3.283946	-0.893101	-1.119273
4	6	0	-0.030723	1.173751	1.549898
5	6	0	-0.640628	0.582988	0.233629
6	6	0	0.404411	-1.642979	0.669309
7	6	0	4.545636	-1.469263	-1.231403
8	6	0	2.931636	-0.171282	0.031083
9	6	0	-2.481248	-0.725372	-0.826352
10	6	0	-0.422487	1.741126	-0.802692
11	6	0	-3.766296	-1.262614	-0.869507
12	6	0	-2.041446	0.029404	0.268086
13	6	0	3.859907	-0.021745	1.067551
14	6	0	5.128038	-0.592799	0.963002
15	6	0	5.448944	-1.307406	-0.184463
16	6	0	-2.930361	0.249816	1.330447
17	6	0	-4.215282	-0.277495	1.295627
18	1	0	2.564190	-1.003722	-1.924747
19	1	0	-0.529072	-2.168632	0.466410

20	1	0	0.486248	-1.470984	1.752913
21	1	0	1.238559	-2.269933	0.349300
22	1	0	3.589889	0.539214	1.954538
23	1	0	5.862662	-0.489541	1.754424
24	1	0	-2.619005	0.842436	2.181566
25	1	0	-4.909452	-0.108307	2.112633
26	1	0	-4.070953	-1.842419	-1.733055
27	1	0	-1.807037	-0.898096	-1.660397
28	1	0	4.837674	-2.033160	-2.110827
29	7	0	0.419134	-0.405066	-0.131696
30	8	0	-0.543503	1.676307	2.509867
31	8	0	1.330178	1.039376	1.420770
32	16	0	-1.564090	2.726512	-1.417937
33	16	0	1.297563	1.821975	-1.143946
34	6	0	-6.423267	-2.254405	-0.832875
35	1	0	-7.451126	-2.512969	-0.572705
36	1	0	-6.420523	-1.663390	-1.757956
37	1	0	-5.847137	-3.175705	-0.990851
38	8	0	-5.921639	-1.506344	0.264449
39	9	0	6.671429	-1.860995	-0.289629

### Cycloadduct 32



E = -1870.94601657

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-5.009209	-1.710959	-0.135055
2	6	0	0.909328	0.575848	0.207494
3	6	0	2.874103	-0.463197	-0.936242
4	6	0	-0.857953	1.035982	1.555720
5	6	0	-1.300499	0.411191	0.189255
6	6	0	0.012597	-1.664679	0.639476
7	6	0	4.211342	-0.853523	-0.983281
8	6	0	2.345661	0.159926	0.199470
9	6	0	-2.862622	-1.121954	-1.010982
10	6	0	-1.186599	1.620229	-0.804260
11	6	0	-4.056902	-1.822926	-1.143505
12	6	0	-2.613900	-0.326712	0.119623
13	6	0	3.184291	0.399807	1.297959
14	6	0	4.517981	0.017576	1.258678
15	6	0	5.043088	-0.611235	0.119538
16	6	0	-3.594087	-0.230374	1.113990
17	6	0	-4.798299	-0.925063	0.989231
18	1	0	2.233351	-0.647823	-1.793866

19	1	0	-0.812680	-2.317221	0.352834
20	1	0	-0.012917	-1.519223	1.729739
21	1	0	0.953557	-2.148430	0.372257
22	1	0	2.786991	0.885686	2.181662
23	1	0	5.177279	0.197483	2.101610
24	1	0	-3.422286	0.392253	1.982880
25	1	0	-5.568239	-0.859549	1.750753
26	1	0	-4.260723	-2.442618	-2.010360
27	1	0	-2.109978	-1.191118	-1.790634
28	1	0	4.591759	-1.336577	-1.875530
29	7	0	-0.097627	-0.411815	-0.130789
30	8	0	-1.495615	1.428221	2.492988
31	8	0	0.510238	1.095384	1.509354
32	16	0	-2.419623	2.455731	-1.465316
33	16	0	0.520661	1.945755	-1.034081
34	6	0	6.956583	-1.573456	-0.943031
35	1	0	8.000694	-1.737768	-0.672391
36	1	0	6.482122	-2.538615	-1.162225
37	1	0	6.908321	-0.933969	-1.833665
38	8	0	6.359674	-0.943726	0.182674
39	9	0	-6.169364	-2.386834	-0.256864

### Cycloadduct 33



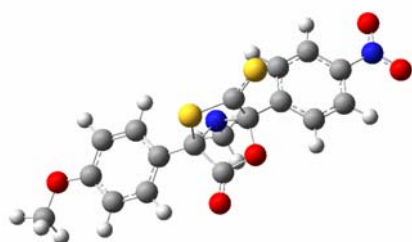
E = -1976.21332273

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.909210	0.639037	-1.045612
2	6	0	1.234519	-0.783578	0.033763
3	6	0	2.974269	0.917341	0.601912
4	6	0	-0.344879	-2.036001	-1.011452
5	6	0	-0.967983	-0.894069	-0.138994
6	6	0	0.212228	0.849388	-1.481804
7	6	0	4.263670	1.439541	0.518538
8	6	0	2.624106	-0.247454	-0.089998
9	6	0	-2.736232	0.852918	0.039927
10	6	0	-0.862375	-1.460132	1.319791
11	6	0	-4.004326	1.341332	-0.250782
12	6	0	-2.342286	-0.380133	-0.492711
13	6	0	3.594541	-0.898758	-0.865938
14	6	0	4.881875	-0.387554	-0.951471
15	6	0	5.227863	0.784667	-0.261686
16	6	0	-3.239049	-1.101270	-1.290651
17	6	0	-4.511912	-0.590259	-1.561025
18	1	0	2.230793	1.424654	1.210297
19	1	0	-0.680045	1.466343	-1.591668
20	1	0	0.302480	0.194231	-2.360885

21	1	0	1.084707	1.502796	-1.440114
22	1	0	3.336584	-1.804536	-1.402560
23	1	0	5.641877	-0.880938	-1.548518
24	1	0	-2.941505	-2.060202	-1.696303
25	1	0	-5.197144	-1.160685	-2.180447
26	1	0	-2.071860	1.430230	0.671087
27	1	0	4.504811	2.345073	1.062440
28	7	0	0.122175	0.118731	-0.202452
29	8	0	-0.857335	-2.894883	-1.674234
30	8	0	1.009594	-1.905250	-0.873050
31	16	0	-2.089908	-2.015443	2.236359
32	16	0	0.831900	-1.431608	1.761899
33	6	0	6.931170	2.377151	0.267588
34	1	0	7.982216	2.511306	0.007726
35	1	0	6.360710	3.255327	-0.060856
36	1	0	6.836502	2.267459	1.355345
37	8	0	6.512325	1.200379	-0.411967
38	1	0	-5.888312	1.057779	-1.242173
39	7	0	-4.401777	2.648467	0.300641
40	8	0	-5.537805	3.050037	0.051915
41	8	0	-3.573329	3.262288	0.972437

### Cycloadduct 34



E = -1976.21526471

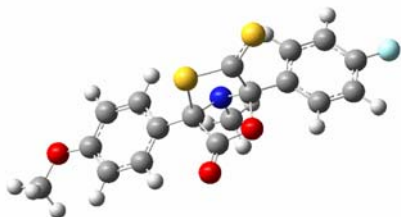
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.995343	-0.551454	0.787612
2	6	0	0.825361	0.650203	0.192641
3	6	0	-4.327048	-1.083459	-1.480467
4	6	0	-0.905173	0.992525	1.641212
5	6	0	-1.386858	0.570769	0.229176
6	6	0	-0.208897	-1.602214	0.288087
7	6	0	-3.076010	-0.542855	-1.237357
8	6	0	2.214067	0.075029	0.147700
9	6	0	-5.300835	-1.092259	-0.466203
10	6	0	-2.753512	-0.005698	0.024443
11	6	0	2.687047	-0.452340	-1.062945
12	6	0	3.032299	0.064245	1.281352
13	6	0	3.962993	-0.997513	-1.141421
14	6	0	4.758842	-1.000407	0.003259
15	6	0	4.315212	-0.475800	1.213053
16	6	0	-3.728858	-0.012480	1.025968
17	6	0	0.609462	1.964078	-0.624596
18	1	0	-1.108411	-2.122921	-0.041608

19	1	0	2.667554	0.478535	2.213367
20	1	0	-3.503217	0.406684	1.998940
21	1	0	-5.728723	-0.542230	1.585419
22	1	0	-4.581839	-1.502394	-2.448620
23	1	0	-2.330332	-0.533839	-2.027215
24	1	0	2.052368	-0.435022	-1.943108
25	1	0	4.349100	-1.411974	-2.064207
26	1	0	4.967800	-0.495469	2.076931
27	1	0	0.662307	-2.113306	-0.123980
28	1	0	-0.156335	-1.641386	1.385837
29	7	0	-0.246924	-0.229002	-0.252746
30	8	0	0.461975	1.015613	1.574572
31	8	0	-1.518017	1.275485	2.634799
32	16	0	-1.123401	2.186400	-0.747502
33	16	0	1.758756	2.962448	-1.201719
34	7	0	6.112114	-1.579155	-0.071185
35	8	0	6.475387	-2.040417	-1.152342
36	8	0	6.794232	-1.567989	0.952280
37	6	0	-7.528130	-1.674761	0.173317
38	1	0	-8.381804	-2.150774	-0.311431
39	1	0	-7.232181	-2.264184	1.050479
40	1	0	-7.808101	-0.663040	0.492958
41	8	0	-6.495815	-1.643545	-0.804023

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### Cycloadduct 35



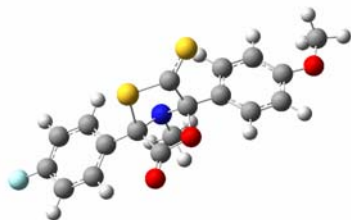
E = -1870.94895007

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.551286	-0.319014	0.779281
2	6	0	1.360065	0.378891	0.196452
3	6	0	-3.940257	-0.795347	-1.516617
4	6	0	-0.328676	0.784215	1.682610
5	6	0	-0.853606	0.487567	0.254486
6	6	0	0.134704	-1.776047	0.175406
7	6	0	-2.642238	-0.391628	-1.253523
8	6	0	2.691863	-0.309175	0.110630
9	6	0	-4.909310	-0.761207	-0.498740
10	6	0	-2.267776	0.046823	0.031596
11	6	0	3.122737	-0.804263	-1.128439
12	6	0	3.509733	-0.456692	1.234755
13	6	0	4.350342	-1.449438	-1.244699
14	6	0	5.143310	-1.583406	-0.108959
15	6	0	4.744584	-1.097175	1.129284
16	6	0	-3.237988	0.081896	1.037253
17	6	0	1.247585	1.753008	-0.540721
18	1	0	-0.808334	-2.199938	-0.171633
19	1	0	3.183292	-0.068899	2.192347

20	1	0	-2.971212	0.427397	2.028615
21	1	0	-5.279185	-0.279817	1.581221
22	1	0	-4.235549	-1.136638	-2.503622
23	1	0	-1.899666	-0.413070	-2.046002
24	1	0	2.493647	-0.683875	-2.005125
25	1	0	4.700663	-1.839451	-2.194357
26	1	0	5.393975	-1.219982	1.989471
27	1	0	0.958089	-2.331779	-0.274868
28	1	0	0.193350	-1.882615	1.268475
29	7	0	0.209299	-0.376164	-0.285086
30	8	0	1.032149	0.697436	1.602397
31	8	0	-0.911344	1.058579	2.697826
32	16	0	-0.461482	2.128375	-0.630855
33	16	0	2.469531	2.686775	-1.075469
34	6	0	-7.184481	-1.147070	0.120730
35	1	0	-8.083159	-1.505543	-0.383717
36	1	0	-6.953285	-1.808621	0.965432
37	1	0	-7.357689	-0.129580	0.493645
38	8	0	-6.154298	-1.173308	-0.858134
39	9	0	6.333701	-2.205567	-0.216060

### Cycloadduct 36



E = -1870.94815443

Standard orientation:

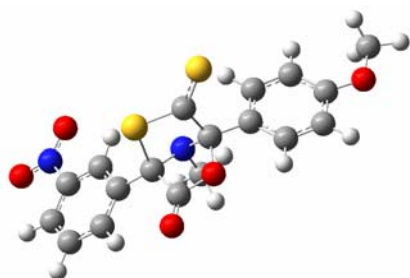
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-5.103128	-0.727242	0.815677
2	6	0	0.697895	0.575352	0.199404
3	6	0	-4.373191	-1.465681	-1.383582
4	6	0	-1.069661	0.997675	1.588895
5	6	0	-1.514504	0.431866	0.215737
6	6	0	-0.273186	-1.686168	0.497439
7	6	0	-3.137407	-0.866463	-1.164167
8	6	0	2.098581	0.041589	0.240422
9	6	0	-5.339242	-1.384864	-0.384310
10	6	0	-2.864103	-0.202230	0.043883
11	6	0	2.630063	-0.574848	-0.896152
12	6	0	2.893982	0.147427	1.389098
13	6	0	3.925153	-1.090926	-0.895764
14	6	0	4.713013	-0.982412	0.258420
15	6	0	4.186878	-0.358908	1.398945
16	6	0	-3.858877	-0.132763	1.028639
17	6	0	0.446094	1.798997	-0.740713
18	1	0	-1.143753	-2.272652	0.200764
19	1	0	2.497669	0.629554	2.275101



20	1	0	-3.659292	0.387166	1.957487
21	1	0	-5.884527	-0.684338	1.567014
22	1	0	-4.598673	-1.984761	-2.309128
23	1	0	-2.370427	-0.911773	-1.931554
24	1	0	2.027868	-0.655843	-1.796550
25	1	0	4.307854	-1.563526	-1.792701
26	1	0	4.811905	-0.281296	2.282710
27	1	0	0.628745	-2.195152	0.156112
28	1	0	-0.245156	-1.618790	1.594793
29	7	0	-0.347212	-0.373556	-0.172896
30	8	0	0.291174	1.064931	1.536703
31	8	0	-1.713187	1.345900	2.543461
32	16	0	-1.294082	1.952582	-0.903602
33	16	0	1.560995	2.781441	-1.403966
34	6	0	6.582431	-2.073206	-0.755248
35	1	0	7.588108	-2.357883	-0.441588
36	1	0	6.028377	-2.972008	-1.056089
37	1	0	6.648909	-1.386072	-1.608625
38	8	0	5.987433	-1.447116	0.372147
39	9	0	-6.538427	-1.961667	-0.591625

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### Cycloadduct 37



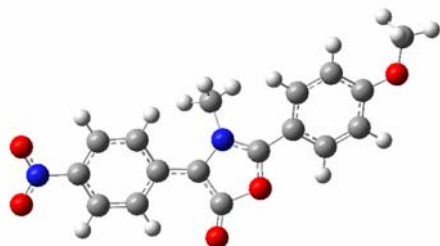
E = -1976.21413034

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.760793	-0.795771	-1.410095
2	6	0	1.048998	-0.770406	0.041840
3	6	0	-4.299748	1.122270	-0.060052
4	6	0	-0.506775	-2.073950	-1.014376
5	6	0	-1.147490	-0.939600	-0.172845
6	6	0	-0.049773	0.855041	-1.471338
7	6	0	-2.993094	0.701739	0.154792
8	6	0	2.399791	-0.163850	-0.189651
9	6	0	-5.200525	0.392443	-0.834924
10	6	0	-2.557924	-0.491283	-0.436842
11	6	0	2.736812	1.023214	0.467890
12	6	0	3.339762	-0.759355	-1.041337
13	6	0	3.981661	1.621125	0.278550
14	6	0	4.915953	1.019325	-0.575914
15	6	0	4.584412	-0.174692	-1.232854
16	6	0	-3.449982	-1.240855	-1.216883
17	6	0	0.784543	-1.350118	1.468803

18	1	0	-0.984320	1.406399	-1.582809
19	1	0	3.094740	-1.683236	-1.552217
20	1	0	-3.113396	-2.166055	-1.668863
21	1	0	-5.441937	-1.384077	-2.017080
22	1	0	-2.329489	1.296162	0.771110
23	1	0	2.020421	1.491406	1.136967
24	1	0	4.212410	2.541788	0.801288
25	1	0	5.320896	-0.627788	-1.888543
26	1	0	0.771713	1.568642	-1.404924
27	1	0	0.102188	0.224501	-2.359334
28	7	0	-0.102923	0.092426	-0.208188
29	8	0	0.837871	-1.931193	-0.857507
30	8	0	-1.011654	-2.942736	-1.675739
31	16	0	-0.948923	-1.609821	1.589732
32	16	0	1.883836	-1.704057	2.612686
33	6	0	6.561156	2.708131	-0.182131
34	1	0	7.579129	2.903475	-0.523019
35	1	0	5.917408	3.553012	-0.459419
36	1	0	6.559102	2.593267	0.909342
37	8	0	6.158279	1.510695	-0.832273
38	1	0	-6.210073	0.759761	-0.971225
39	7	0	-4.746506	2.386231	0.554102
40	8	0	-3.924829	3.023593	1.210970
41	8	0	-5.913831	2.726359	0.368654

### Structure 38



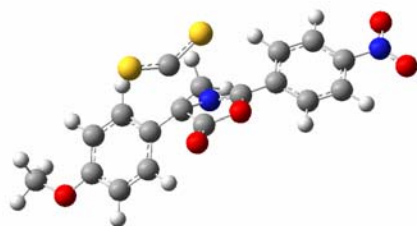
E = -1141.74833328

#### Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.841181	0.707867	-0.047634
2	7	0	0.315275	-0.093203	0.082255
3	6	0	1.406260	0.657336	-0.098399
4	8	0	1.063992	1.916616	-0.329250
5	6	0	-0.402953	2.037475	-0.270398
6	8	0	-0.914120	3.122807	-0.422113
7	6	0	-2.214907	0.264747	-0.030625
8	6	0	0.333796	-1.442984	0.650227
9	6	0	2.809736	0.297045	-0.027547
10	6	0	3.742600	1.296319	0.335021
11	6	0	5.093787	1.014458	0.396691
12	6	0	5.567187	-0.274348	0.089782
13	6	0	-3.234234	1.219793	0.226987
14	6	0	-4.569559	0.856507	0.249611
15	6	0	-4.926917	-0.474826	0.015425
16	6	0	-3.956785	-1.436697	-0.266214
17	6	0	-2.620500	-1.067435	-0.296531
18	6	0	4.658399	-1.270141	-0.295181
19	6	0	3.297698	-0.979546	-0.357301

20	1	0	-0.514864	-1.541903	1.327280
21	1	0	1.260898	-1.581092	1.207082
22	1	0	0.262071	-2.206743	-0.128862
23	1	0	3.385386	2.293195	0.569350
24	1	0	5.812759	1.775203	0.682508
25	1	0	-2.953146	2.251254	0.401126
26	1	0	-5.344179	1.585391	0.454682
27	1	0	-4.263516	-2.454282	-0.475252
28	1	0	-1.891058	-1.819657	-0.572242
29	1	0	4.998997	-2.262630	-0.565180
30	1	0	2.621123	-1.752292	-0.706159
31	7	0	-6.330094	-0.863542	0.050916
32	8	0	-7.166945	0.012397	0.287431
33	8	0	-6.606965	-2.049872	-0.155611
34	6	0	7.457846	-1.722869	-0.120505
35	1	0	8.533585	-1.625434	0.030876
36	1	0	7.064370	-2.499003	0.547842
37	1	0	7.260335	-2.002552	-1.162813
38	8	0	6.907704	-0.446755	0.186681

### Saddle Point 20→30



Imaginary Freq: -251.602  $\text{cm}^{-1}$   
 E = -1976.19376762

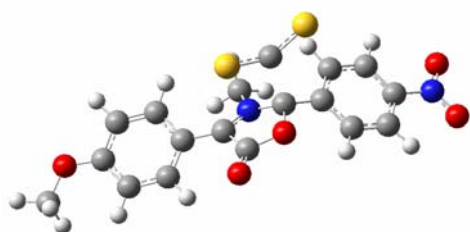
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.957288	-1.546827	0.127664
2	6	0	1.051401	0.236341	0.468446
3	6	0	3.010793	-0.192842	-1.044579
4	6	0	-0.689249	1.008010	1.662405
5	6	0	-1.175020	0.522731	0.344077
6	6	0	-0.056952	-1.012677	-1.360839
7	6	0	4.350053	-0.525777	-1.208672
8	6	0	2.458363	-0.105100	0.245404
9	6	0	-3.197828	-0.279659	-0.939090
10	6	0	-1.114652	2.171230	-0.568301
11	6	0	-4.405145	-0.971512	-1.024279
12	6	0	-2.507861	-0.157046	0.273769
13	6	0	3.273757	-0.317919	1.372327
14	6	0	4.612969	-0.653872	1.213342
15	6	0	5.127900	-0.759860	-0.076586
16	6	0	-3.077157	-0.739425	1.419497
17	6	0	-4.282874	-1.422052	1.351126
18	1	0	2.408296	0.050597	-1.911272

19	1	0	-0.030682	-0.347116	-2.230661
20	1	0	-0.976476	-1.597648	-1.371936
21	1	0	0.802712	-1.682936	-1.374397
22	1	0	2.852300	-0.221683	2.366476
23	1	0	5.257847	-0.832105	2.064735
24	1	0	-2.584240	-0.641856	2.380541
25	1	0	-4.726721	-1.864850	2.236876
26	1	0	-4.910337	-1.036711	-1.980675
27	1	0	-2.804628	0.191568	-1.833894
28	1	0	4.801008	-0.590649	-2.190942
29	7	0	-0.035530	-0.227977	-0.135026
30	8	0	-1.216662	1.477164	2.623120
31	8	0	0.741259	0.882792	1.596906
32	16	0	-2.545918	2.956954	-0.497741
33	16	0	0.403135	2.480815	-1.175392
34	7	0	6.548039	-1.120196	-0.250696
35	8	0	7.213347	-1.308263	0.765616
36	8	0	6.971709	-1.212686	-1.401075
37	6	0	-6.881574	-2.357437	-1.034971
38	1	0	-7.774492	-2.925374	-0.769113
39	1	0	-7.177523	-1.375281	-1.424793
40	1	0	-6.322319	-2.901287	-1.807375
41	8	0	-6.129105	-2.235206	0.164455

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### Saddle Point 20→34



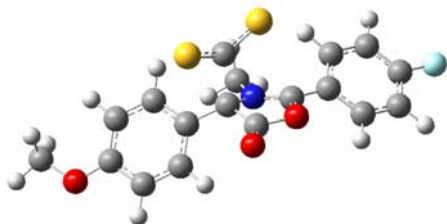
Imaginary Freq:  $-353.336 \text{ cm}^{-1}$   
 E = -1976.19671901

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.952187	-1.195368	0.670746
2	6	0	0.805197	0.440312	0.374965
3	6	0	-4.611310	-0.272177	-1.547860
4	6	0	-0.950439	0.279332	1.801303
5	6	0	-1.398888	-0.012085	0.422152
6	6	0	-0.226979	-0.546072	-1.713537
7	6	0	-3.296769	0.014350	-1.229999
8	6	0	2.181389	-0.085493	0.181484
9	6	0	-5.451488	-0.889949	-0.603471
10	6	0	-2.769376	-0.309148	0.041485
11	6	0	2.839478	0.001037	-1.058488
12	6	0	2.860607	-0.650803	1.275031
13	6	0	4.122748	-0.511938	-1.218375
14	6	0	4.758313	-1.086507	-0.121530
15	6	0	4.148226	-1.154326	1.128866
16	6	0	-3.630779	-0.897057	0.987307
17	6	0	0.640795	2.417865	-0.122153

18	1	0	-1.082665	-1.187281	-1.921970
19	1	0	2.373311	-0.695705	2.241261
20	1	0	-3.259764	-1.113788	1.981707
21	1	0	-5.582856	-1.656256	1.421597
22	1	0	-5.025150	-0.009550	-2.515844
23	1	0	-2.686403	0.543717	-1.953230
24	1	0	2.365561	0.492019	-1.898714
25	1	0	4.638946	-0.456205	-2.168523
26	1	0	4.678047	-1.601376	1.960733
27	1	0	-0.253028	0.329271	-2.371043
28	1	0	0.694849	-1.102558	-1.881914
29	7	0	-0.283323	-0.141242	-0.314345
30	8	0	0.413523	0.475165	1.704653
31	8	0	-1.551511	0.306744	2.844787
32	16	0	-0.938383	2.782238	0.106737
33	16	0	2.063526	3.090099	-0.521897
34	7	0	6.114411	-1.633740	-0.287645
35	8	0	6.621648	-1.570965	-1.407182
36	8	0	6.656390	-2.124835	0.701757
37	6	0	-7.635616	-1.723401	-0.102078
38	1	0	-8.577518	-1.810912	-0.644975
39	1	0	-7.300427	-2.719914	0.210667
40	1	0	-7.780589	-1.090874	0.782005
41	8	0	-6.717521	-1.131675	-1.016558

### Saddle Point 21→31 (gas phase)



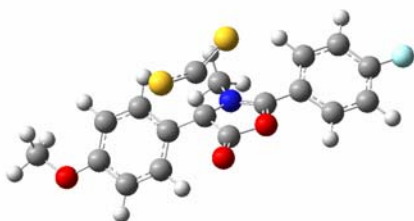
Imaginary Freq:  $-251.865 \text{ cm}^{-1}$   
 E = -1870.93072462

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.513443	-1.358985	0.100681
2	6	0	1.598247	-0.023445	0.437231
3	6	0	3.496630	-0.488057	-1.137699
4	6	0	-0.070371	0.839249	1.680278
5	6	0	-0.606302	0.460559	0.354843
6	6	0	0.374058	-1.054876	-1.452617
7	6	0	4.812048	-0.885293	-1.348116
8	6	0	2.969191	-0.442574	0.165512
9	6	0	-2.707881	-0.120189	-0.921219
10	6	0	-0.494487	2.179610	-0.479625
11	6	0	-3.957859	-0.730239	-1.020941
12	6	0	-1.978550	-0.134562	0.274327
13	6	0	3.794189	-0.766723	1.259490
14	6	0	5.108009	-1.169701	1.054910
15	6	0	5.594252	-1.227608	-0.248412
16	6	0	-2.552665	-0.768611	1.389712
17	6	0	-3.800562	-1.369687	1.308314
18	1	0	2.895822	-0.159469	-1.977378

19	1	0	0.428987	-0.355458	-2.293466
20	1	0	-0.584749	-1.573152	-1.466445
21	1	0	1.184832	-1.781140	-1.512611
22	1	0	3.397554	-0.703381	2.266811
23	1	0	5.757184	-1.432264	1.883028
24	1	0	-2.028336	-0.774691	2.339314
25	1	0	-4.247834	-1.851716	2.171682
26	1	0	-4.491873	-0.690226	-1.963067
27	1	0	-2.309334	0.395517	-1.788854
28	1	0	5.243450	-0.912728	-2.342747
29	7	0	0.476109	-0.325556	-0.196874
30	8	0	-0.543544	1.297357	2.674924
31	8	0	1.352493	0.609817	1.584660
32	16	0	-1.856087	3.044377	-0.223868
33	16	0	0.974092	2.407125	-1.214640
34	6	0	-6.514669	-1.959300	-1.058894
35	1	0	-7.434343	-2.491650	-0.810647
36	1	0	-6.758821	-0.933402	-1.362817
37	1	0	-6.011285	-2.472853	-1.888578
38	8	0	-5.725254	-1.977782	0.121887
39	9	0	6.863259	-1.613454	-0.450933

Saddle Point 21→31 (CPCM in DMF)



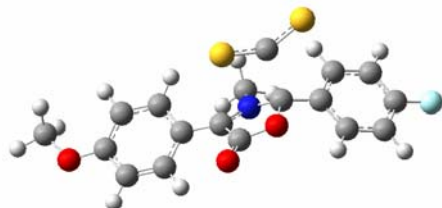
Imaginary Freq: -308.325  $\text{cm}^{-1}$   
 E = -1870.97313334

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.560249	-1.298066	0.171466
2	6	0	1.626799	-0.064876	0.431661
3	6	0	3.513255	-0.647703	-1.115227
4	6	0	-0.039267	0.879888	1.606126
5	6	0	-0.585229	0.349978	0.363999
6	6	0	0.395526	-1.292557	-1.340308
7	6	0	4.844794	-1.002782	-1.300822
8	6	0	3.005242	-0.459219	0.185013
9	6	0	-2.650491	-0.306093	-0.926824
10	6	0	-0.531905	2.207647	-0.599616
11	6	0	-3.930356	-0.855126	-1.000294
12	6	0	-1.964382	-0.200066	0.292183
13	6	0	3.859170	-0.608081	1.297249
14	6	0	5.188626	-0.970005	1.118448
15	6	0	5.653736	-1.162995	-0.179518
16	6	0	-2.613633	-0.649243	1.457341
17	6	0	-3.893449	-1.185899	1.402138
18	1	0	2.884080	-0.481175	-1.986442

19	1	0	0.391021	-0.716494	-2.274978
20	1	0	-0.540123	-1.850660	-1.239988
21	1	0	1.237185	-1.991221	-1.325311
22	1	0	3.473338	-0.451444	2.302547
23	1	0	5.863258	-1.102335	1.966480
24	1	0	-2.112741	-0.578946	2.420410
25	1	0	-4.393530	-1.533775	2.307880
26	1	0	-4.425220	-0.921945	-1.968366
27	1	0	-2.183405	0.053145	-1.842471
28	1	0	5.261945	-1.143073	-2.299823
29	7	0	0.509648	-0.387778	-0.194775
30	8	0	-0.508668	1.458613	2.555297
31	8	0	1.369578	0.683159	1.513741
32	16	0	-1.898612	3.031122	-0.257593
33	16	0	0.868563	2.363545	-1.429216
34	6	0	-6.530223	-1.994196	-1.007025
35	1	0	-7.483095	-2.454321	-0.732647
36	1	0	-6.712848	-1.020797	-1.481286
37	1	0	-5.991658	-2.647683	-1.706057
38	8	0	-5.806877	-1.843608	0.218506
39	9	0	6.942776	-1.509828	-0.358209

Saddle Point 21→35 (gas phase)



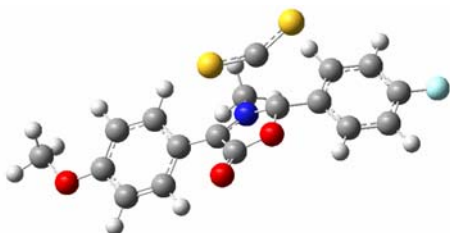
Imaginary Freq:  $-351.987 \text{ cm}^{-1}$   
 E = -1870.92969604

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.477810	-1.101861	1.057109
2	6	0	1.327269	0.182826	0.344593
3	6	0	-4.257665	-0.171019	-1.172472
4	6	0	-0.327767	0.148750	1.896978
5	6	0	-0.893046	-0.120268	0.559879
6	6	0	0.083538	-0.735797	-1.650387
7	6	0	-2.901384	0.033592	-0.938551
8	6	0	2.649221	-0.431051	0.056067
9	6	0	-5.055419	-0.751450	-0.174967
10	6	0	-2.304956	-0.333937	0.281023
11	6	0	3.234740	-0.376113	-1.220342
12	6	0	3.351558	-1.067202	1.093787
13	6	0	4.466060	-0.979345	-1.467751
14	6	0	5.124867	-1.611787	-0.420919
15	6	0	4.589452	-1.659748	0.861142
16	6	0	-3.130296	-0.888074	1.286434
17	6	0	1.240322	2.177148	-0.163260
18	1	0	-0.819506	-1.329580	-1.788891
19	1	0	2.923746	-1.094916	2.088862

20	1	0	-2.701075	-1.138107	2.249148
21	1	0	-5.113823	-1.534344	1.822537
22	1	0	-4.684351	0.141103	-2.118320
23	1	0	-2.313369	0.535858	-1.699026
24	1	0	2.746410	0.159791	-2.024751
25	1	0	4.926315	-0.942350	-2.449242
26	1	0	5.137170	-2.156365	1.655006
27	1	0	0.054227	0.138153	-2.309755
28	1	0	0.960698	-1.339744	-1.882826
29	7	0	0.155462	-0.325014	-0.255016
30	8	0	1.035647	0.261390	1.697130
31	8	0	-0.846442	0.222630	2.982475
32	16	0	-0.297464	2.634300	0.158022
33	16	0	2.676272	2.759192	-0.647151
34	6	0	-7.037425	-0.639704	-1.507382
35	1	0	-8.081250	-0.927972	-1.376251
36	1	0	-6.977585	0.440844	-1.687413
37	1	0	-6.616068	-1.177399	-2.366094
38	8	0	-6.382313	-1.000394	-0.296856
39	9	0	6.318511	-2.190501	-0.654411

Saddle Point 21→35 (CPCM in DMF)



Imaginary Freq:  $-376.872 \text{ cm}^{-1}$   
 E = -1870.96728006

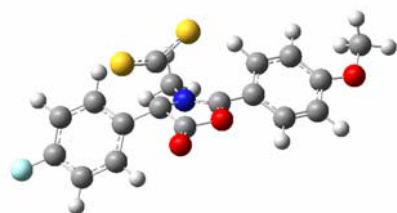
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.510101	-1.047457	1.112186
2	6	0	1.305846	0.128720	0.329638
3	6	0	-4.282518	-0.209624	-1.159317
4	6	0	-0.350274	0.253940	1.863842
5	6	0	-0.915892	-0.133539	0.564903
6	6	0	0.049605	-0.920679	-1.598857
7	6	0	-2.921933	-0.019533	-0.938738
8	6	0	2.628922	-0.479935	0.074332
9	6	0	-5.085466	-0.733733	-0.133005
10	6	0	-2.329201	-0.341086	0.297761
11	6	0	3.185803	-0.531540	-1.216417
12	6	0	3.372363	-0.986644	1.156178
13	6	0	4.434348	-1.112816	-1.431365
14	6	0	5.131930	-1.612575	-0.338887
15	6	0	4.627985	-1.555665	0.955370
16	6	0	-3.157529	-0.846364	1.326736
17	6	0	1.290151	2.197245	-0.272410
18	1	0	-0.881422	-1.489108	-1.676229



19	1	0	2.963832	-0.943802	2.162318
20	1	0	-2.727006	-1.092952	2.293517
21	1	0	-5.148209	-1.451087	1.900467
22	1	0	-4.707425	0.062917	-2.124836
23	1	0	-2.322600	0.419913	-1.733567
24	1	0	2.652759	-0.111029	-2.064519
25	1	0	4.871154	-1.164774	-2.430172
26	1	0	5.208883	-1.958168	1.787203
27	1	0	0.066429	-0.120262	-2.350753
28	1	0	0.901742	-1.591754	-1.743195
29	7	0	0.126759	-0.352682	-0.250040
30	8	0	1.009473	0.329336	1.667024
31	8	0	-0.863886	0.466974	2.943467
32	16	0	-0.217893	2.713210	0.053605
33	16	0	2.754963	2.680825	-0.782361
34	6	0	-7.069270	-0.667829	-1.481785
35	1	0	-8.117654	-0.938288	-1.333376
36	1	0	-6.991251	0.400652	-1.720784
37	1	0	-6.644095	-1.262174	-2.300842
38	8	0	-6.416381	-0.964600	-0.240805
39	9	0	6.348018	-2.170540	-0.541481

### Saddle Point 1 22→32



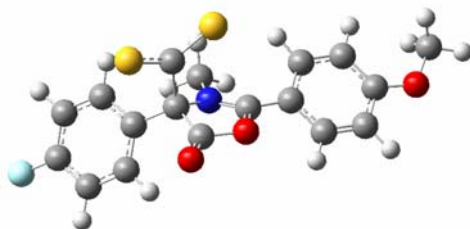
Imaginary Freq:  $-261.094 \text{ cm}^{-1}$   
 E =  $-1870.93347462$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.902164	-1.860958	-0.375175
2	6	0	0.972346	0.017347	0.542865
3	6	0	3.024188	-0.145885	-0.889152
4	6	0	-0.869639	0.627367	1.688276
5	6	0	-1.260779	0.291442	0.304278
6	6	0	0.014388	-0.982741	-1.509591
7	6	0	4.389748	-0.378824	-1.015816
8	6	0	2.392188	-0.233145	0.361657
9	6	0	-3.161666	-0.434918	-1.191680
10	6	0	-1.307904	2.075372	-0.415879
11	6	0	-4.329790	-1.154490	-1.427390
12	6	0	-2.552361	-0.434703	0.074418
13	6	0	3.174028	-0.524620	1.501035
14	6	0	4.529152	-0.765817	1.379648
15	6	0	5.150742	-0.700729	0.118878
16	6	0	-3.162079	-1.155336	1.111542
17	6	0	-4.340300	-1.868324	0.894780
18	1	0	2.459282	0.164605	-1.760588

19	1	0	0.051034	-0.225849	-2.299845
20	1	0	-0.872547	-1.604123	-1.633644
21	1	0	0.906103	-1.608649	-1.544621
22	1	0	2.702530	-0.564294	2.477036
23	1	0	5.138256	-1.001659	2.245851
24	1	0	-2.730342	-1.144319	2.105987
25	1	0	-4.822440	-2.421577	1.693731
26	1	0	-4.808600	-1.156247	-2.400789
27	1	0	-2.732674	0.152867	-1.996391
28	1	0	4.853182	-0.286043	-1.990562
29	7	0	-0.060887	-0.333159	-0.209006
30	8	0	-1.464795	0.965759	2.666579
31	8	0	0.569365	0.545232	1.700041
32	16	0	-2.774592	2.752873	-0.182082
33	16	0	0.157485	2.508397	-1.051488
34	6	0	7.184316	-0.879522	-1.127714
35	1	0	8.222170	-1.114068	-0.888661
36	1	0	6.800710	-1.612554	-1.847889
37	1	0	7.127502	0.126421	-1.560750
38	8	0	6.479485	-0.950796	0.108509
39	9	0	-6.037019	-2.553706	-0.594401

### Intermediate 22→32



E = -1870.93464747

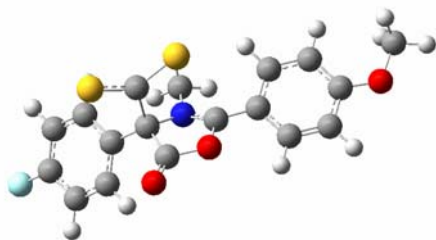
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.786341	-1.973313	-0.382722
2	6	0	0.940832	0.042570	0.528031
3	6	0	2.997070	-0.094036	-0.889391
4	6	0	-0.877646	0.671955	1.690902
5	6	0	-1.287775	0.438035	0.256920
6	6	0	-0.013257	-0.837201	-1.577442
7	6	0	4.358704	-0.342953	-1.016652
8	6	0	2.355298	-0.230546	0.352513
9	6	0	-3.239972	-0.321994	-1.168608
10	6	0	-1.320235	2.011325	-0.358840
11	6	0	-4.351641	-1.127537	-1.397958
12	6	0	-2.555953	-0.366325	0.057040
13	6	0	3.121365	-0.589272	1.483573
14	6	0	4.472088	-0.850536	1.359778
15	6	0	5.104404	-0.734347	0.107347
16	6	0	-3.019076	-1.234343	1.054098
17	6	0	-4.139683	-2.038019	0.843831
18	1	0	2.442617	0.273582	-1.744995
19	1	0	0.079721	-0.036454	-2.318653

20	1	0	-0.927765	-1.403251	-1.755138
21	1	0	0.845919	-1.506578	-1.630482
22	1	0	2.641743	-0.666912	2.453300
23	1	0	5.070620	-1.139366	2.217162
24	1	0	-2.524535	-1.274610	2.018425
25	1	0	-4.512672	-2.702518	1.615851
26	1	0	-4.890131	-1.094840	-2.339060
27	1	0	-2.915954	0.364488	-1.942840
28	1	0	4.832617	-0.208617	-1.981387
29	7	0	-0.087983	-0.261502	-0.242835
30	8	0	-1.473234	0.966607	2.676662
31	8	0	0.545440	0.527731	1.711789
32	16	0	-2.777554	2.772138	-0.138718
33	16	0	0.140777	2.568017	-0.983307
34	6	0	7.145488	-0.886996	-1.131367
35	1	0	8.176555	-1.150971	-0.894186
36	1	0	6.756152	-1.577490	-1.889198
37	1	0	7.109569	0.139797	-1.514308
38	8	0	6.427021	-1.006453	0.094352
39	9	0	-5.866221	-2.750012	-0.596776

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### Saddle Point 2 22→32



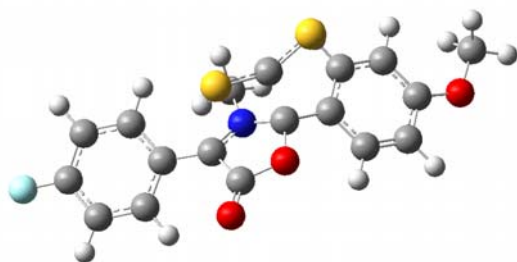
Imaginary Freq:  $-42.415 \text{ cm}^{-1}$   
 E = -1870.93457733

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.862751	-1.904539	-0.339498
2	6	0	0.932657	0.090160	0.499262
3	6	0	2.992220	-0.132230	-0.913020
4	6	0	-0.878131	0.680140	1.686470
5	6	0	-1.294440	0.412669	0.255817
6	6	0	-0.033026	-0.902896	-1.548100
7	6	0	4.350367	-0.404477	-1.029454
8	6	0	2.349786	-0.193769	0.333969
9	6	0	-3.240193	-0.353574	-1.173455
10	6	0	-1.251123	1.966146	-0.391632
11	6	0	-4.374817	-1.130926	-1.387307
12	6	0	-2.585973	-0.354252	0.069270
13	6	0	3.114350	-0.503364	1.479833
14	6	0	4.463084	-0.784876	1.368758
15	6	0	5.094837	-0.741947	0.112578
16	6	0	-3.103476	-1.149852	1.099621
17	6	0	-4.246776	-1.924716	0.904202
18	1	0	2.441757	0.191736	-1.788557

19	1	0	0.056607	-0.110579	-2.300373
20	1	0	-0.943362	-1.476763	-1.722371
21	1	0	0.829756	-1.568177	-1.598147
22	1	0	2.636018	-0.526545	2.452781
23	1	0	5.059002	-1.034523	2.240218
24	1	0	-2.632454	-1.155745	2.075906
25	1	0	-4.660042	-2.534088	1.700798
26	1	0	-4.889724	-1.130783	-2.342075
27	1	0	-2.875019	0.277391	-1.975835
28	1	0	4.822882	-0.329589	-2.001331
29	7	0	-0.109413	-0.323379	-0.217117
30	8	0	-1.478285	0.985838	2.667921
31	8	0	0.536113	0.560965	1.697482
32	16	0	-2.697500	2.773702	-0.353696
33	16	0	0.288398	2.483409	-0.857194
34	6	0	7.132420	-0.972943	-1.119163
35	1	0	8.162562	-1.230961	-0.871299
36	1	0	6.737950	-1.697734	-1.841679
37	1	0	7.101947	0.033681	-1.553067
38	8	0	6.415985	-1.026737	0.111741
39	9	0	-5.964551	-2.654053	-0.538550

### Saddle Point 22→36



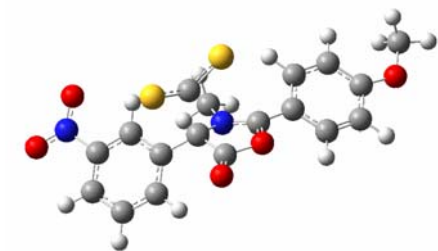
Imaginary Freq:  $-361.065 \text{ cm}^{-1}$   
 E =  $-1870.92851765$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-5.048433	-1.387852	0.705711
2	6	0	0.675034	0.343462	0.397774
3	6	0	-4.693326	-0.610709	-1.573241
4	6	0	-1.112397	0.288932	1.794180
5	6	0	-1.524977	-0.119131	0.436250
6	6	0	-0.295593	-0.822731	-1.617686
7	6	0	-3.389263	-0.258826	-1.244309
8	6	0	2.062168	-0.171971	0.278745
9	6	0	-5.501155	-1.179189	-0.592552
10	6	0	-2.886672	-0.479996	0.053769
11	6	0	2.766831	-0.158396	-0.932165
12	6	0	2.711923	-0.680857	1.419680
13	6	0	4.061186	-0.671622	-1.024167
14	6	0	4.687791	-1.185595	0.116856
15	6	0	4.001892	-1.180342	1.341601
16	6	0	-3.743817	-1.030301	1.028805
17	6	0	0.460230	2.255789	-0.270132

18	1	0	-1.124419	-1.508449	-1.791436
19	1	0	2.196279	-0.679401	2.372976
20	1	0	-3.383010	-1.163277	2.041374
21	1	0	-5.716007	-1.817958	1.444608
22	1	0	-5.095702	-0.433718	-2.564862
23	1	0	-2.774826	0.236708	-1.987435
24	1	0	2.322599	0.278300	-1.818616
25	1	0	4.572806	-0.641451	-1.978855
26	1	0	4.503268	-1.575206	2.219361
27	1	0	-0.337952	-0.001112	-2.340798
28	1	0	0.650595	-1.353511	-1.723304
29	7	0	-0.391561	-0.312682	-0.257387
30	8	0	0.250139	0.495723	1.710185
31	8	0	-1.739320	0.398199	2.818004
32	16	0	-1.138940	2.595327	-0.136348
33	16	0	1.875185	2.949878	-0.662846
34	6	0	6.703054	-1.707088	-1.056494
35	1	0	7.665021	-2.153739	-0.800034
36	1	0	6.219078	-2.310342	-1.835635
37	1	0	6.863619	-0.688936	-1.433305
38	8	0	5.944958	-1.703237	0.145091
39	9	0	-6.761488	-1.523261	-0.908579

### Saddle Point 23→33



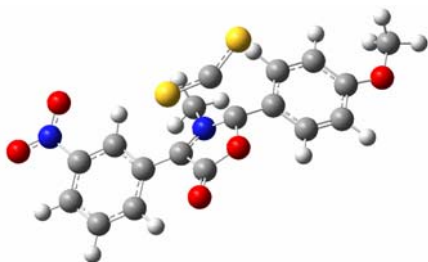
Imaginary Freq:  $-263.387 \text{ cm}^{-1}$   
 E =  $-1976.20038395$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.660906	0.707019	-1.667944
2	6	0	1.368005	-0.543903	-0.418659
3	6	0	3.225534	0.845874	0.530660
4	6	0	-0.300508	-1.998240	-0.819852
5	6	0	-0.869168	-0.776842	-0.206149
6	6	0	0.152825	1.553823	0.082077
7	6	0	4.560979	1.233241	0.531588
8	6	0	2.750366	-0.098855	-0.393569
9	6	0	-2.917013	0.666165	0.037836
10	6	0	-0.975241	-1.369500	1.594759
11	6	0	-4.118839	1.152699	-0.463819
12	6	0	-2.195878	-0.279864	-0.702832
13	6	0	3.662019	-0.681972	-1.301284
14	6	0	4.987941	-0.293604	-1.311053
15	6	0	5.450994	0.672550	-0.398356
16	6	0	-2.730368	-0.732949	-1.917925
17	6	0	-3.952951	-0.248533	-2.389259

18	1	0	2.563317	1.237709	1.294009
19	1	0	0.077434	1.653507	1.169788
20	1	0	-0.732890	1.978546	-0.390286
21	1	0	1.039016	2.071957	-0.283441
22	1	0	3.314308	-1.435442	-1.999746
23	1	0	5.695069	-0.725572	-2.011232
24	1	0	-2.204496	-1.488722	-2.489611
25	1	0	-4.351640	-0.620347	-3.328058
26	1	0	-2.573788	1.014825	1.002981
27	1	0	4.902155	1.949858	1.268819
28	7	0	0.243088	0.146170	-0.282024
29	8	0	-0.769047	-3.017836	-1.229462
30	8	0	1.119113	-1.799690	-0.802132
31	16	0	-2.426953	-2.056231	1.901593
32	16	0	0.442608	-1.100196	2.406380
33	6	0	7.310424	1.939342	0.413747
34	1	0	8.364449	2.025071	0.147760
35	1	0	6.823775	2.915617	0.300390
36	1	0	7.221938	1.601679	1.453253
37	8	0	6.763042	0.981463	-0.489108
38	1	0	-5.608164	1.104668	-2.010070
39	7	0	-4.844225	2.173908	0.310728
40	8	0	-5.943244	2.533146	-0.109759
41	8	0	-4.302651	2.615444	1.323855

### Saddle Point 23→37



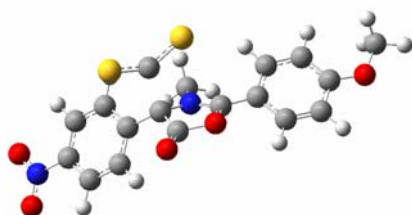
Imaginary Freq:  $-383.645 \text{ cm}^{-1}$   
 E = -1976.19350244

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.575388	-0.889205	-1.964302
2	6	0	1.064295	-0.664979	0.049754
3	6	0	-4.491929	0.883286	-0.362668
4	6	0	-0.514130	-2.091347	-0.733589
5	6	0	-1.102960	-0.752355	-0.521111
6	6	0	-0.152936	1.533712	-0.182415
7	6	0	-3.158120	0.618069	-0.080071
8	6	0	2.430826	-0.169386	-0.257352
9	6	0	-5.220364	0.150043	-1.297325
10	6	0	-2.504931	-0.414948	-0.771809
11	6	0	2.968071	0.972219	0.351622
12	6	0	3.227658	-0.866479	-1.185368
13	6	0	4.242208	1.436567	0.024149
14	6	0	5.017439	0.738743	-0.909576
15	6	0	4.499016	-0.420628	-1.508077
16	6	0	-3.235983	-1.176629	-1.707058
17	6	0	0.724568	-0.950342	2.007053

18	1	0	-0.967832	1.907591	-0.801883
19	1	0	2.842642	-1.765631	-1.652215
20	1	0	-2.748846	-2.000661	-2.213811
21	1	0	-5.121140	-1.483775	-2.690058
22	1	0	-2.668263	1.188246	0.697037
23	1	0	2.407103	1.501466	1.112628
24	1	0	4.623254	2.321862	0.519255
25	1	0	5.114599	-0.954757	-2.224599
26	1	0	-0.333853	1.799471	0.864844
27	1	0	0.788551	1.970951	-0.513963
28	7	0	-0.070283	0.087448	-0.338107
29	8	0	0.822229	-1.948613	-0.426453
30	8	0	-1.000556	-3.121774	-1.126671
31	16	0	-0.858568	-1.376549	2.138215
32	16	0	2.059236	-0.790955	2.919645
33	6	0	6.865724	2.238939	-0.701186
34	1	0	7.857137	2.325169	-1.148503
35	1	0	6.290317	3.148863	-0.915339
36	1	0	6.965513	2.119236	0.385020
37	8	0	6.270253	1.094219	-1.297321
38	1	0	-6.260049	0.393519	-1.477616
39	7	0	-5.158553	1.980378	0.363705
40	8	0	-6.351199	2.169787	0.135144
41	8	0	-4.477772	2.641638	1.146577

### Saddle Point 1 38→25



Imaginary Freq:  $-270.922 \text{ cm}^{-1}$   
 E = -1976.20030420

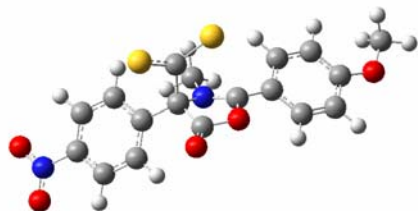
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.597688	-1.199562	-0.121351
2	6	0	1.451814	0.105807	0.560487
3	6	0	3.437607	-0.381650	-0.887210
4	6	0	-0.284255	1.010279	1.672772
5	6	0	-0.740512	0.607106	0.324952
6	6	0	0.348936	-0.967777	-1.378918
7	6	0	4.771319	-0.752139	-1.018240
8	6	0	2.832626	-0.304044	0.378168
9	6	0	-2.720722	-0.068773	-1.085685
10	6	0	-0.626635	2.297606	-0.548358
11	6	0	-3.959123	-0.678917	-1.245260
12	6	0	-2.109518	0.007763	0.178381
13	6	0	3.612721	-0.574977	1.524327
14	6	0	4.935234	-0.954141	1.399033
15	6	0	5.528264	-1.050483	0.126053
16	6	0	-2.785650	-0.515882	1.290359
17	6	0	-4.033181	-1.117949	1.147615
18	1	0	2.883158	-0.091726	-1.772173

19	1	0	0.430855	-0.297993	-2.240868
20	1	0	-0.590145	-1.519105	-1.426468
21	1	0	1.181069	-1.671427	-1.368993
22	1	0	3.165510	-0.489406	2.508805
23	1	0	5.541611	-1.176039	2.270756
24	1	0	-2.348933	-0.436462	2.278883
25	1	0	-4.565344	-1.524410	1.998618
26	1	0	-4.439492	-0.743171	-2.213530
27	1	0	-2.235006	0.376454	-1.947104
28	1	0	5.216176	-0.783526	-2.005410
29	7	0	0.369343	-0.193678	-0.144754
30	8	0	-0.820281	1.491427	2.624635
31	8	0	1.134145	0.772741	1.671948
32	16	0	-2.012379	3.141945	-0.356972
33	16	0	0.858247	2.521791	-1.243151
34	7	0	-5.907616	-1.851792	-0.281735
35	8	0	-6.453059	-2.293629	0.728827
36	8	0	-6.374693	-1.921010	-1.418221
37	6	0	7.505773	-1.515339	-1.137277
38	1	0	8.523133	-1.825244	-0.896588
39	1	0	7.039910	-2.264259	-1.789054
40	1	0	7.530112	-0.545420	-1.648161
41	8	0	6.826306	-1.423444	0.112759

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### Saddle Point 2 38→25



Imaginary Freq:  $-52.788 \text{ cm}^{-1}$   
 E = -1976.20123743

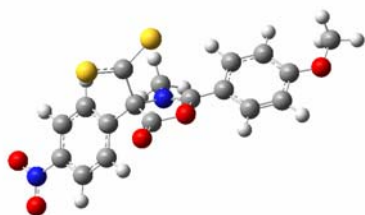
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.577258	-1.211438	-0.105657
2	6	0	1.418731	0.202762	0.493430
3	6	0	3.407944	-0.367302	-0.923626
4	6	0	-0.289005	1.061084	1.666768
5	6	0	-0.764768	0.731330	0.266078
6	6	0	0.303123	-0.857319	-1.442304
7	6	0	4.725243	-0.795668	-1.034689
8	6	0	2.792937	-0.244483	0.333040
9	6	0	-2.795458	0.053187	-1.086014
10	6	0	-0.571925	2.205870	-0.501948
11	6	0	-4.009680	-0.608109	-1.226616
12	6	0	-2.141491	0.104369	0.156936
13	6	0	3.549080	-0.528965	1.491580
14	6	0	4.856347	-0.964758	1.386897
15	6	0	5.457573	-1.107395	0.122866
16	6	0	-2.738953	-0.513084	1.263885
17	6	0	-3.962546	-1.168127	1.140649
18	1	0	2.874655	-0.067508	-1.817995
19	1	0	0.444078	-0.140738	-2.260085



20	1	0	-0.657192	-1.360846	-1.553675
21	1	0	1.101043	-1.600513	-1.453703
22	1	0	3.096041	-0.411952	2.469750
23	1	0	5.443359	-1.197705	2.268935
24	1	0	-2.266670	-0.468546	2.237798
25	1	0	-4.437555	-1.642360	1.990336
26	1	0	-4.523233	-0.652823	-2.178777
27	1	0	-2.364144	0.554381	-1.944756
28	1	0	5.178525	-0.861628	-2.016310
29	7	0	0.315862	-0.170909	-0.159657
30	8	0	-0.834883	1.499587	2.629590
31	8	0	1.100950	0.799288	1.661381
32	16	0	-1.926960	3.159681	-0.521011
33	16	0	1.007801	2.515846	-1.012267
34	7	0	-5.862184	-1.916475	-0.245888
35	8	0	-6.343127	-2.432847	0.762105
36	8	0	-6.373853	-1.951262	-1.364423
37	6	0	7.422844	-1.688317	-1.111967
38	1	0	8.421475	-2.042690	-0.854776
39	1	0	6.925875	-2.427641	-1.751540
40	1	0	7.499858	-0.732440	-1.643676
41	8	0	6.738195	-1.535461	0.129332

### Intermediate 38→25



E = -1976.20136436

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.522414	-1.257919	-0.133378
2	6	0	1.416270	0.134857	0.535198
3	6	0	3.404038	-0.352925	-0.904290
4	6	0	-0.284916	1.058002	1.677846
5	6	0	-0.755745	0.767703	0.272607
6	6	0	0.311759	-0.787562	-1.477928
7	6	0	4.728303	-0.753381	-1.032457
8	6	0	2.785692	-0.306351	0.356898
9	6	0	-2.798577	0.113354	-1.074292
10	6	0	-0.635093	2.276499	-0.464467
11	6	0	-3.997198	-0.572720	-1.228070
12	6	0	-2.118066	0.108357	0.155462
13	6	0	3.542921	-0.640539	1.502426
14	6	0	4.854955	-1.052980	1.378655
15	6	0	5.461478	-1.117061	0.109411
16	6	0	-2.672427	-0.591120	1.235744
17	6	0	-3.880761	-1.271486	1.100090
18	1	0	2.869754	-0.010437	-1.782477
19	1	0	0.459050	-0.059233	-2.282416
20	1	0	-0.656566	-1.275085	-1.590765
21	1	0	1.099655	-1.540763	-1.497282

22	1	0	3.085848	-0.579543	2.484095
23	1	0	5.443782	-1.324985	2.248129
24	1	0	-2.179402	-0.590997	2.200912
25	1	0	-4.323618	-1.808529	1.929539
26	1	0	-4.531321	-0.575132	-2.169919
27	1	0	-2.399947	0.678364	-1.909167
28	1	0	5.186229	-0.757608	-2.014040
29	7	0	0.336496	-0.107272	-0.190299
30	8	0	-0.819579	1.491396	2.647100
31	8	0	1.109542	0.752509	1.683461
32	16	0	-2.000199	3.199164	-0.269752
33	16	0	0.855769	2.617200	-1.162510
34	7	0	-5.789874	-1.990238	-0.288447
35	8	0	-6.232193	-2.581237	0.696172
36	8	0	-6.326729	-1.971900	-1.395538
37	6	0	7.442110	-1.590876	-1.146736
38	1	0	8.445961	-1.940019	-0.903570
39	1	0	6.963302	-2.300853	-1.831530
40	1	0	7.502299	-0.603649	-1.619684
41	8	0	6.747150	-1.525005	0.097465

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