Synthesis of Thiazolidine-Fused Heterocycles via *exo*-Mode Cyclizations of Vinylogous *N*-Acyliminium Ions

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Supplementary Data

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X, Y, Z Coordinates for the Optimized Structures of Products 19

19a-*cis*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.535252	0.444660	-1.629944
2	6	0	-3.414232	-1.067356	-1.476553
3	6	0	-3.250662	-1.413339	0.006763
4	6	0	-2.157243	-0.589333	0.717348
5	6	0	-2.143090	0.887743	0.267492
6	8	0	-2.366664	1.085480	-1.123941
7	1	0	-3.606027	0.747715	-2.678318
8	1	0	-4.433470	0.817834	-1.106230
9	1	0	-4.303165	-1.564424	-1.884537
10	1	0	-2.545924	-1.411042	-2.049461
11	1	0	-3.047571	-2.482388	0.144866
12	1	0	-4.200959	-1.215242	0.524292
13	6	0	-2.324216	-0.685649	2.241776
14	16	0	-0.452617	-1.184325	0.244888
15	7	0	-0.824341	1.382913	0.569470
16	1	0	-2.891362	1.463339	0.837047
17	1	0	1.827953	1.819883	0.194495
18	6	0	0.184870	0.469161	0.319921
19	6	0	-0.566467	2.811480	0.449948
20	6	0	2.507049	-0.233977	-0.034267
21	6	0	1.501538	0.788331	0.171873
22	8	0	2.301085	-1.438168	-0.133912
23	8	0	3.756412	0.303722	-0.116942
24	6	0	4.825365	-0.635565	-0.333316
25	6	0	6.121516	0.153563	-0.381759
26	1	0	4.643505	-1.179115	-1.266978
27	1	0	4.826729	-1.372411	0.477201
28	1	0	6.287263	0.689951	0.558366
29	1	0	6.102975	0.885806	-1.195645
30	1	0	6.966792	-0.523980	-0.546144
31	1	0	-3.302022	-0.289244	2.547685
32	1	0	-1.544532	-0.125328	2.764616
33	1	0	-2.266922	-1.730129	2.564061
34	1	0	-1.478980	3.352514	0.710376
35	1	0	-0.265416	3.092842	-0.567262
36	1	0	0.221662	3.105628	1.149737

19a-*trans*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.239042	0.763577	-0.619408
2	6	0	4.402773	-0.748207	-0.377805
3	6	0	3.075280	-1.530662	-0.546573
4	6	0	1.972649	-0.802205	0.238617
5	6	0	1.962344	0.636189	-0.284754
6	8	0	3.126203	1.328188	0.095696
7	1	0	5.118435	1.314805	-0.277427
8	1	0	4.105702	0.961661	-1.695287
9	1	0	5.154088	-1.132911	-1.078566

10	1	0	4.801645	-0.909969	0.629255
11	1	0	3.199805	-2.562727	-0.199850
12	1	0	2.799352	-1.576627	-1.607405
13	16	0	0.226709	-1.314765	-0.139320
14	6	0	2.198049	-0.876109	1.758313
15	7	0	0.750309	1.242011	0.235894
16	1	0	-1.901577	1.795876	0.206468
17	1	0	1.920819	0.613149	-1.394115
18	6	0	-2.700561	-0.210356	-0.057081
19	6	0	-0.319933	0.375981	0.093770
20	6	0	0.560867	2.677582	0.086572
21	1	0	1.535691	3.156771	0.184155
22	1	0	-0.092893	3.049325	0.880637
23	6	0	-1.629455	0.753907	0.096653
24	1	0	0.116731	2.937234	-0.886515
25	8	0	-2.566861	-1.413823	-0.245429
26	8	0	-3.922982	0.387029	0.017787
27	6	0	-5.054130	-0.488779	-0.143523
28	6	0	-6.306433	0.366159	-0.068317
29	1	0	-5.033379	-1.251241	0.642883
30	1	0	-4.972107	-1.009609	-1.103658
31	1	0	-6.311590	1.121486	-0.861027
32	1	0	-6.371286	0.880543	0.896123
33	1	0	-7.196391	-0.262343	-0.184681
34	1	0	1.418796	-0.332288	2.296864
35	1	0	3.161459	-0.443493	2.042760
36	1	0	2.173370	-1.921100	2.084028

19c-*cis*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.738885	0.110293	-1.626072
2	6	0	-3.321364	-1.325214	-1.319563
3	6	0	-3.077268	-1.538078	0.177025
4	6	0	-1.963837	-0.699744	0.837295
5	6	0	-1.979460	0.812727	0.531879
6	16	0	-2.400949	1.302398	-1.234293
7	1	0	-3.935117	0.250872	-2.693716
8	1	0	-4.654652	0.377903	-1.084201
9	1	0	-4.121416	-2.006380	-1.640403
10	1	0	-2.425055	-1.579251	-1.895493
11	1	0	-2.857836	-2.595726	0.370153
12	1	0	-4.011362	-1.324136	0.717998
13	6	0	-2.033948	-0.900909	2.364823
14	16	0	-0.277754	-1.238090	0.237614
15	7	0	-0.641412	1.277367	0.826334
16	1	0	-2.688659	1.321875	1.192410
17	1	0	1.994481	1.770067	0.396707
18	6	0	0.360639	0.401740	0.453738
19	6	0	-0.377126	2.703096	0.950815
20	6	0	2.669885	-0.250581	-0.044858
21	6	0	1.671238	0.742240	0.295003
22	8	0	2.461188	-1.441628	-0.246158
23	8	0	3.912819	0.299985	-0.131403
24	6	0	4.972965	-0.607490	-0.484807
25	6	0	6.257547	0.198713	-0.554474
26	1	0	4.736179	-1.081810	-1.443332

27	1	0	5.031193	-1.402723	0.266505
28	1	0	6.477567	0.667513	0.410318
29	1	0	6.182872	0.987564	-1.310142
30	1	0	7.095945	-0.455010	-0.819603
31	1	0	-3.003903	-0.560981	2.752339
32	1	0	-1.242578	-0.347714	2.876849
33	1	0	-1.922823	-1.961247	2.612556
34	1	0	-1.272107	3.192162	1.342160
35	1	0	-0.111460	3.165801	-0.009574
36	1	0	0.443481	2.863096	1.656669

19c-*trans*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.373534	0.243968	-0.799531
2	6	0	4.192119	-1.218975	-0.371536
3	6	0	2.743849	-1.740604	-0.503063
4	6	0	1.735720	-0.874948	0.273924
5	6	0	1.763510	0.556048	-0.281303
6	16	0	3.328559	1.431619	0.153347
7	1	0	5.404917	0.571379	-0.639306
8	1	0	4.148209	0.368895	-1.865638
9	1	0	4.844027	-1.840415	-1.000286
10	1	0	4.545752	-1.339788	0.658232
11	1	0	2.699510	-2.775996	-0.144887
12	1	0	2.457968	-1.760170	-1.562641
13	16	0	-0.033096	-1.349549	-0.102513
14	6	0	1.936921	-0.967475	1.795292
15	7	0	0.543526	1.200598	0.190974
16	1	0	-2.106642	1.796582	0.129880
17	1	0	1.756002	0.499629	-1.383397
18	6	0	-2.933109	-0.203969	-0.062994
19	6	0	-0.544145	0.347481	0.072676
20	6	0	0.340315	2.628844	-0.019517
21	1	0	1.294473	3.145899	0.090589
22	1	0	-0.349871	3.015724	0.735142
23	6	0	-1.847363	0.748656	0.058349
24	1	0	-0.070602	2.844303	-1.017292
25	8	0	-2.817399	-1.414799	-0.212839
26	8	0	-4.145690	0.413918	-0.005146
27	6	0	-5.291291	-0.448493	-0.135427
28	6	0	-6.529366	0.428495	-0.082007
29	1	0	-5.279275	-1.186489	0.674094
30	1	0	-5.221235	-0.999599	-1.079454
31	1	0	-6.525262	1.159645	-0.897063
32	1	0	-6.582366	0.972592	0.866718
33	1	0	-7.429726	-0.188710	-0.176528
34	1	0	1.237924	-0.312285	2.321361
35	1	0	2.949693	-0.680267	2.090299
36	1	0	1.754978	-1.995372	2.124721

19d-*cis*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-3.641144	0.377333	-1.624327
2	6	0	-3.515391	-1.131104	-1.377520
3	6	0	-3.273649	-1.399947	0.112756
4	6	0	-2.145409	-0.557297	0.745336
5	6	0	-2.143381	0.907881	0.237726
6	7	0	-2.452146	1.115025	-1.180261
7	1	0	-1.651243	0.789643	-1.723379
8	1	0	-3.800570	0.596321	-2.685939
9	1	0	-4.511157	0.777419	-1.083425
10	1	0	-4.422220	-1.656073	-1.704387
11	1	0	-2.682874	-1.525174	-1.974785
12	1	0	-3.077206	-2.464155	0.294091
13	1	0	-4.196672	-1.166226	0.663911
14	6	0	-2.249003	-0.608056	2.277556
15	16	0	-0.459244	-1.170474	0.226860
16	7	0	-0.804546	1.404368	0.523123
17	1	0	-2.874659	1.484765	0.821303
18	1	0	1.853476	1.816877	0.184178
19	6	0	0.196769	0.482215	0.302881
20	6	0	-0.533215	2.831102	0.425042
21	6	0	2.518409	-0.241032	-0.043247
22	6	0	1.519310	0.787669	0.158530
23	8	0	2.306223	-1.442945	-0.157075
24	8	0	3.772607	0.289361	-0.109874
25	6	0	4.836902	-0.654449	-0.328322
26	6	0	6.136491	0.128987	-0.378384
27	1	0	4.651470	-1.197104	-1.261805
28	1	0	4.836519	-1.391686	0.481916
29	1	0	6.305704	0.664988	0.561325
30	1	0	6.120139	0.861119	-1.192458
31	1	0	6.978670	-0.552188	-0.543635
32	1	0	-3.210104	-0.190888	2.608148
33	1	0	-1.444911	-0.039029	2.751953
34	1	0	-2.189635	-1.642213	2.631746
35	1	0	-1.455567	3.375510	0.635739
36	1	0	-0.176178	3.121189	-0.572166
37	1	0	0.220995	3.117601	1.165316

19d-*trans*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.298188	0.668817	-0.715060
2	6	0	4.403549	-0.826045	-0.372673
3	6	0	3.048322	-1.556239	-0.512729
4	6	0	1.975752	-0.773746	0.258727
5	6	0	1.961358	0.658109	-0.298515
6	7	0	3.208086	1.326699	0.039838
7	1	0	5.234838	1.178531	-0.466424
8	1	0	4.147016	0.770430	-1.806811
9	1	0	5.142714	-1.287937	-1.038067
10	1	0	4.784769	-0.937127	0.647884
11	1	0	3.129487	-2.584488	-0.141636
12	1	0	2.766601	-1.615939	-1.571606
13	16	0	0.226277	-1.299032	-0.098129
14	6	0	2.205129	-0.825387	1.779029
15	7	0	0.740710	1.254409	0.249576
16	1	0	-1.927506	1.797488	0.155601

17	1	0	1.846952	0.586852	-1.404031
18	6	0	-2.706832	-0.217367	-0.052993
19	6	0	-0.328910	0.386898	0.100439
20	6	0	0.524770	2.687671	0.167808
21	1	0	1.437256	3.207201	0.468807
22	1	0	-0.258038	2.977717	0.872999
23	6	0	-1.642328	0.756048	0.083867
24	1	0	0.227670	3.018767	-0.840293
25	8	0	-2.569125	-1.425284	-0.205394
26	8	0	-3.932727	0.378794	-0.009120
27	6	0	-5.059011	-0.504515	-0.159122
28	6	0	-6.314639	0.348185	-0.120617
29	1	0	-5.045171	-1.245727	0.647521
30	1	0	-4.965399	-1.050763	-1.104006
31	1	0	-6.312934	1.082300	-0.933079
32	1	0	-6.391703	0.887842	0.829034
33	1	0	-7.201630	-0.285731	-0.230170
34	1	0	1.435578	-0.260410	2.309697
35	1	0	3.174696	-0.401012	2.051680
36	1	0	2.163269	-1.864898	2.120901
37	1	0	3.172259	2.301023	-0.256695

X, Y, Z Coordinates for the Calculated Ground State (GS) and Transition State (TS) Structures 35-37

35a (GS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.161535	-0.570872	1.034530
2	6	0	0.811397	-1.924986	0.537547
3	16	0	-1.022525	-1.881556	0.234783
4	1	0	4.058577	-0.284459	-0.414837
5	6	0	-1.063704	-0.143575	0.526383
6	1	0	2.118721	-0.289306	1.472201
7	7	0	0.212561	0.316465	0.990710
8	8	0	3.153414	-0.568062	-0.663260
9	1	0	1.031067	-2.651029	1.330212
10	6	0	3.070212	-1.987074	-0.698666
11	6	0	-2.124252	0.675513	0.391096
12	1	0	-2.068099	1.735925	0.601865
13	6	0	0.418636	1.716393	1.413059
14	6	0	1.589564	-2.332666	-0.753171
15	1	0	3.561808	-2.392168	-1.594868
16	1	0	3.552206	-2.444395	0.179992
17	1	0	1.444729	-3.406008	-0.910540
18	1	0	1.145700	-1.809456	-1.605590
19	6	0	-3.412143	0.108440	-0.046563
20	1	0	1.446263	1.815338	1.764892
21	1	0	-0.288248	1.953560	2.210705
22	1	0	0.243513	2.369944	0.555678
23	8	0	-3.569940	-1.084198	-0.262823
24	8	0	-4.353683	1.046486	-0.166151
25	6	0	-5.672706	0.588971	-0.590703

26	6	0	-6.571630	1.805572	-0.670370
27	1	0	-6.027284	-0.146872	0.136946
28	1	0	-5.563217	0.084934	-1.555314
29	1	0	-6.191490	2.529611	-1.397551
30	1	0	-6.655218	2.298356	0.303127
31	1	0	-7.573637	1.496787	-0.985499
32	6	0	5.892710	1.812864	-0.497397
33	6	0	4.642430	2.618482	-0.792357
34	1	0	6.616813	2.401030	0.078190
35	1	0	6.374087	1.475793	-1.422728
36	1	0	3.923136	2.026274	-1.367340
37	1	0	4.166286	2.948961	0.137082
38	1	0	4.903829	3.505722	-1.377424
39	8	0	5.506888	0.646718	0.285478
40	1	0	6.307210	0.141162	0.503025

35a (TS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.292862	-0.838475	1.082343
2	6	0	0.909733	-2.124188	0.422012
3	16	0	-0.915382	-1.989091	0.093161
4	1	0	3.916203	0.149237	-0.165421
5	6	0	-0.915167	-0.295392	0.580807
6	1	0	2.185196	-0.692508	1.681404
7	7	0	0.341097	0.059669	1.158287
8	8	0	2.853496	-0.386607	-0.515380
9	1	0	1.084857	-2.938769	1.133834
10	6	0	3.084270	-1.754504	-0.810645
11	6	0	-1.949502	0.564421	0.493196
12	1	0	-1.874582	1.593215	0.821345
13	6	0	0.535568	1.366606	1.807288
14	6	0	1.707310	-2.394716	-0.890869
15	1	0	3.601525	-1.874623	-1.774146
16	1	0	3.700909	-2.245443	-0.038653
17	1	0	1.761835	-3.471696	-1.075977
18	1	0	1.163773	-1.937165	-1.722143
19	6	0	-3.229622	0.091524	-0.055277
20	1	0	1.525587	1.377000	2.265037
21	1	0	-0.237138	1.507144	2.566212
22	1	0	0.457420	2.154679	1.053904
23	8	0	-3.418662	-1.064534	-0.405866
24	8	0	-4.139037	1.070042	-0.115347
25	6	0	-5.447130	0.701807	-0.641060
26	6	0	-6.315470	1.942998	-0.610167
27	1	0	-5.849812	-0.105455	-0.022256
28	1	0	-5.310851	0.312883	-1.654554
29	1	0	-5.889087	2.737761	-1.230058
30	1	0	-6.428087	2.319346	0.411272
31	1	0	-7.310300	1.701416	-0.998423
32	6	0	5.291852	2.019367	-0.709971
33	6	0	4.047088	2.880044	-0.710556
34	1	0	6.168382	2.562497	-0.346357
35	1	0	5.504121	1.611915	-1.703195
36	1	0	3.180771	2.310075	-1.060324
37	1	0	3.842694	3.277021	0.289052
38	1	0	4.196870	3.726863	-1.387701

39	8	0	5.071450	0.888527	0.212697
40	1	0	5.859412	0.316003	0.207132

35b (GS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.153889	-1.015713	1.217764
2	1	0	2.994790	-0.907400	1.890347
3	6	0	2.129102	-2.001327	0.098474
4	16	0	0.389930	-1.955281	-0.554344
5	6	0	-0.111141	-0.851522	0.729673
6	7	0	0.987719	-0.528773	1.577096
7	16	0	3.480379	0.859846	-0.256890
8	1	0	2.301226	-2.992510	0.544175
9	6	0	3.184072	-0.380474	-1.590610
10	6	0	0.830600	0.426535	2.685795
11	1	0	0.599970	1.407756	2.259570
12	6	0	-1.354304	-0.368449	0.922990
13	1	0	-1.593959	0.307788	1.733317
14	1	0	1.764974	0.468810	3.245647
15	1	0	0.027320	0.090699	3.343666
16	6	0	3.202417	-1.786017	-0.988098
17	1	0	2.231474	-0.161923	-2.076939
18	1	0	3.981932	-0.277831	-2.329465
19	1	0	4.184089	-1.990619	-0.542528
20	1	0	3.059845	-2.531256	-1.779298
21	6	0	-2.423161	-0.761477	-0.009842
22	8	0	-2.232300	-1.512302	-0.956366
23	8	0	-3.590825	-0.195982	0.302465
24	6	0	-4.724070	-0.531144	-0.555067
25	6	0	-5.939612	0.183359	-0.001723
26	1	0	-4.840420	-1.618634	-0.553289
27	1	0	-4.481839	-0.218454	-1.575025
28	1	0	-5.795272	1.268175	-0.003536
29	1	0	-6.154121	-0.139248	1.021611
30	1	0	-6.810624	-0.047426	-0.623550
31	1	0	2.362034	1.627243	-0.376083
32	6	0	0.123813	3.744308	-0.505160
33	6	0	-0.834608	2.815320	-1.223873
34	1	0	0.737602	4.299988	-1.226133
35	8	0	0.982966	2.957372	0.356258
36	1	0	-0.428796	4.472335	0.102523
37	1	0	-1.469142	2.277804	-0.512192
38	1	0	-0.293637	2.083219	-1.833446
39	1	0	-1.482671	3.394818	-1.889257
40	1	0	1.565539	3.581926	0.819157

35b (TS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.218483	-1.339114	0.621137
2	1	0	2.967239	-1.909213	1.168541
3	6	0	2.128405	-1.616870	-0.871657
4	16	0	0.430630	-1.031215	-1.346353

5	6	0	-0.100062	-1.063251	0.349915
6	7	0	0.959490	-1.407315	1.195567
7	16	0	3.111057	0.529512	0.650127
8	1	0	2.179955	-2.700424	-1.027908
9	6	0	3.324549	0.552067	-1.188357
10	6	0	0.780449	-1.476682	2.642812
11	1	0	0.573070	-0.486831	3.069912
12	6	0	-1.363136	-0.811461	0.765617
13	1	0	-1.636222	-0.854222	1.812306
14	1	0	1.688663	-1.880927	3.093493
15	1	0	-0.051816	-2.144470	2.877471
16	6	0	3.246430	-0.911339	-1.638239
17	1	0	2.527077	1.148193	-1.633929
18	1	0	4.292331	1.003380	-1.414088
19	1	0	4.193730	-1.421324	-1.425460
20	1	0	3.088354	-0.967390	-2.720431
21	6	0	-2.400060	-0.481345	-0.211155
22	8	0	-2.177394	-0.300834	-1.404364
23	8	0	-3.611512	-0.379386	0.353357
24	6	0	-4.718443	-0.072907	-0.539245
25	6	0	-5.985397	-0.070905	0.292632
26	1	0	-4.742050	-0.826962	-1.331176
27	1	0	-4.526849	0.897933	-1.007304
28	1	0	-5.937189	0.683657	1.084053
29	1	0	-6.152614	-1.048725	0.754474
30	1	0	-6.843487	0.157470	-0.347941
31	1	0	1.840382	1.575680	0.877384
32	6	0	0.566858	3.360859	0.073965
33	6	0	-0.723750	2.900597	-0.561657
34	1	0	1.403912	3.397440	-0.628647
35	8	0	0.954934	2.405238	1.158284
36	1	0	0.467573	4.336499	0.554083
37	1	0	-1.533899	2.884073	0.172687
38	1	0	-0.634225	1.909078	-1.013260
39	1	0	-0.993577	3.608681	-1.353293
40	1	0	1.272028	2.898807	1.936843

35d (GS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.263094	0.206342	-0.775976
2	6	0	0.915108	1.655847	-0.715125
3	16	0	-0.890195	1.663468	-0.222276
4	1	0	2.802468	-0.913315	1.129172
5	6	0	-1.012265	-0.079059	-0.439804
6	7	0	0.263188	-0.635202	-0.764762
7	1	0	2.232633	-0.139345	-1.110147
8	8	0	2.121603	-0.213016	1.269823
9	6	0	1.064215	2.211995	-2.159215
10	6	0	2.676769	0.888652	2.002131
11	6	0	0.440090	-2.085364	-0.940142
12	1	0	1.504556	-2.298982	-1.037374
13	6	0	-2.127050	-0.828020	-0.329380
14	1	0	-2.122508	-1.899992	-0.480215
15	1	0	-0.101425	-2.415929	-1.829385
16	1	0	0.049693	-2.596547	-0.057689
17	6	0	1.822650	2.117769	1.731149

18	6	0	1.772744	2.516954	0.250200
19	1	0	0.459665	1.650557	-2.876805
20	1	0	2.680834	0.649871	3.073358
21	1	0	3.715966	1.069774	1.690219
22	1	0	2.243251	2.956167	2.298498
23	1	0	0.809886	1.954390	2.116479
24	1	0	1.380758	3.537226	0.165979
25	1	0	2.793087	2.555682	-0.157295
26	6	0	-3.398654	-0.171984	0.017753
27	8	0	-3.490478	1.028211	0.231832
28	8	0	-4.409559	-1.043157	0.070950
29	6	0	-5.716965	-0.495870	0.415086
30	6	0	-6.700556	-1.647859	0.436213
31	1	0	-5.975833	0.261671	-0.330440
32	1	0	-5.633320	0.000811	1.386153
33	1	0	-6.414715	-2.396164	1.181808
34	1	0	-6.759379	-2.134033	-0.542418
35	1	0	-7.696192	-1.271347	0.692441
36	1	0	2.112861	2.186685	-2.477747
37	1	0	0.728069	3.252725	-2.176225
38	6	0	5.116519	-2.303455	0.149472
39	1	0	5.688254	-2.231550	1.083096
40	6	0	5.412752	-1.125035	-0.757300
41	8	0	3.697029	-2.308971	0.449003
42	1	0	3.509912	-3.090347	0.994572
43	1	0	5.379679	-3.246684	-0.343512
44	1	0	5.152904	-0.177629	-0.270778
45	1	0	4.859717	-1.207051	-1.699662
46	1	0	6.480511	-1.095728	-0.995572

35d (TS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.504623	-0.573099	0.801143
2	6	0	1.046018	-2.000807	0.507535
3	16	0	-0.634510	-1.735452	-0.274572
4	1	0	2.301545	1.163625	-0.530515
5	6	0	-0.788725	-0.161386	0.527315
6	7	0	0.412880	0.194345	1.165107
7	1	0	2.341344	-0.492260	1.497401
8	8	0	2.093220	0.036105	-0.551816
9	6	0	0.880011	-2.744226	1.848133
10	6	0	3.092990	-0.746096	-1.282324
11	6	0	0.515017	1.400482	1.984120
12	1	0	1.473083	1.392971	2.508189
13	6	0	-1.904515	0.601195	0.535879
14	1	0	-1.931898	1.564467	1.030042
15	1	0	-0.287641	1.402956	2.726327
16	1	0	0.445892	2.313273	1.382048
17	6	0	2.451374	-2.062756	-1.670566
18	6	0	1.979825	-2.807096	-0.418588
19	1	0	0.191182	-2.224248	2.518580
20	1	0	3.369540	-0.136622	-2.146529
21	1	0	3.972850	-0.884584	-0.640717
22	1	0	3.185756	-2.668798	-2.212882
23	1	0	1.615073	-1.869539	-2.350308
24	1	0	1.469016	-3.734281	-0.700278

25	1	0	2.855312	-3.112437	0.171878
26	6	0	-3.112976	0.134820	-0.147509
27	8	0	-3.171204	-0.899609	-0.799294
28	8	0	-4.139954	0.983973	0.017633
29	6	0	-5.389421	0.612072	-0.624375
30	6	0	-6.404249	1.691534	-0.303969
31	1	0	-5.694063	-0.368652	-0.246806
32	1	0	-5.211021	0.515258	-1.699784
33	1	0	-6.078027	2.664551	-0.684692
34	1	0	-6.560625	1.775607	0.775988
35	1	0	-7.363030	1.443975	-0.771316
36	1	0	1.847130	-2.857652	2.354711
37	1	0	0.476680	-3.743735	1.663386
38	6	0	3.729685	3.158452	-0.737665
39	1	0	4.158740	2.881627	-1.706326
40	6	0	4.605129	2.727913	0.419595
41	8	0	2.416742	2.507089	-0.600482
42	1	0	1.799214	2.856842	-1.266785
43	1	0	3.547279	4.235936	-0.722484
44	1	0	4.791800	1.648227	0.407632
45	1	0	4.153305	3.003398	1.377024
46	1	0	5.574401	3.230433	0.342937

35e (GS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.755949	-1.596146	0.741371
2	6	0	1.781465	-1.654716	-0.756495
3	16	0	0.115589	-0.962651	-1.248109
4	6	0	-0.494485	-1.139740	0.397522
5	7	0	0.545655	-1.553492	1.274149
6	1	0	2.555445	-2.025803	1.332722
7	16	0	2.831178	0.691382	1.414411
8	1	0	1.793113	1.543031	1.161413
9	6	0	3.769990	1.089379	-0.121566
10	6	0	0.300702	-1.743336	2.709840
11	1	0	1.220718	-2.086045	3.183032
12	6	0	-1.757927	-0.911862	0.812905
13	1	0	-2.058839	-1.039597	1.845081
14	1	0	-0.013824	-0.797703	3.160395
15	1	0	-0.480802	-2.493524	2.848054
16	6	0	3.098295	0.580056	-1.394100
17	6	0	2.943765	-0.944281	-1.496162
18	1	0	4.760343	0.645721	0.019641
19	1	0	3.885669	2.175475	-0.145395
20	1	0	3.728946	0.900098	-2.233658
21	1	0	2.131999	1.077983	-1.528568
22	1	0	2.815504	-1.203661	-2.553268
23	1	0	3.879021	-1.432253	-1.187227
24	6	0	-2.764613	-0.462749	-0.160968
25	8	0	-2.498165	-0.220632	-1.330667
26	8	0	-3.975018	-0.346445	0.390920
27	6	0	-5.050538	0.094294	-0.489970
28	6	0	-6.316923	0.163170	0.338661
29	1	0	-5.128951	-0.619586	-1.315047
30	1	0	-4.771469	1.065390	-0.909531
31	1	0	-6.210611	0.875277	1.162819

32	1	0	-6.569369	-0.817048	0.754348
33	1	0	-7.148086	0.491775	-0.293679
34	6	0	-0.003734	3.980578	0.140722
35	1	0	-0.833585	3.959158	0.861182
36	1	0	0.239485	5.031602	-0.062330
37	8	0	1.153033	3.326461	0.705850
38	1	0	1.463922	3.869948	1.447277
39	6	0	-0.391007	3.273567	-1.144009
40	1	0	-0.667793	2.230038	-0.962281
41	1	0	-1.251280	3.774577	-1.600109
42	1	0	0.435481	3.298346	-1.862118
43	6	0	1.837909	-3.171607	-1.110514
44	1	0	1.740129	-3.286874	-2.193812
45	1	0	2.797423	-3.604649	-0.804868
46	1	0	1.027657	-3.731625	-0.636192

35e (TS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.844504	-1.445567	0.756446
2	6	0	1.859806	-1.555358	-0.746953
3	16	0	0.187675	-0.881595	-1.239547
4	6	0	-0.429074	-1.098999	0.401783
5	7	0	0.611909	-1.495158	1.276003
6	1	0	2.635397	-1.911580	1.334539
7	16	0	2.743195	0.727504	1.364261
8	1	0	1.650836	1.638620	1.029383
9	6	0	3.786772	1.141020	-0.098512
10	6	0	0.363448	-1.712394	2.704781
11	1	0	1.283367	-2.060286	3.175222
12	6	0	-1.704701	-0.911900	0.803524
13	1	0	-2.011762	-1.062299	1.830858
14	1	0	0.039425	-0.781050	3.179925
15	1	0	-0.412133	-2.471670	2.827459
16	6	0	3.181910	0.657883	-1.412985
17	6	0	3.008422	-0.862361	-1.518857
18	1	0	4.760618	0.680961	0.095824
19	1	0	3.918783	2.225896	-0.091023
20	1	0	3.864131	0.969819	-2.214053
21	1	0	2.231968	1.171502	-1.596354
22	1	0	2.856130	-1.118635	-2.573508
23	1	0	3.946067	-1.358114	-1.229843
24	6	0	-2.715385	-0.484347	-0.172779
25	8	0	-2.449872	-0.205893	-1.335255
26	8	0	-3.937395	-0.427013	0.366602
27	6	0	-5.018839	-0.016322	-0.519356
28	6	0	-6.298299	-0.022641	0.292248
29	1	0	-5.054869	-0.714179	-1.360974
30	1	0	-4.779726	0.975496	-0.914865
31	1	0	-6.235817	0.675713	1.132562
32	1	0	-6.510425	-1.021969	0.684329
33	1	0	-7.135589	0.280696	-0.344657
34	6	0	-0.302143	3.732219	0.262326
35	1	0	-1.077741	3.436770	0.981413
36	1	0	-0.252609	4.827476	0.245037
37	8	0	0.986144	3.226648	0.702072
38	1	0	1.256152	3.741120	1.480171

39	6	0	-0.604364	3.192815	-1.121297
40	1	0	-0.707163	2.103615	-1.119871
41	1	0	-1.548392	3.615407	-1.481243
42	1	0	0.184783	3.475956	-1.825372
43	6	0	1.916131	-3.078096	-1.061115
44	1	0	1.817473	-3.224726	-2.140518
45	1	0	2.876102	-3.503105	-0.744802
46	1	0	1.107562	-3.625513	-0.569979

36a (GS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.492785	-2.249592	0.531228
2	6	0	0.543593	-2.127574	-0.955451
3	16	0	-0.809873	-0.923600	-1.379322
4	6	0	-1.411042	-0.952632	0.281369
5	7	0	-0.572991	-1.759787	1.110233
6	1	0	1.129406	-2.923005	1.092187
7	1	0	0.282308	-3.105388	-1.383028
8	6	0	2.536840	-0.754178	-0.441798
9	1	0	3.942557	0.526402	-0.118768
10	8	0	2.094481	-0.741842	0.715323
11	8	0	3.531621	-0.037342	-0.871495
12	6	0	-0.840810	-1.901501	2.550691
13	6	0	-2.501384	-0.311878	0.743000
14	1	0	-0.092897	-2.565171	2.983748
15	1	0	-0.780917	-0.919893	3.026283
16	6	0	1.928663	-1.699477	-1.458072
17	1	0	-1.836627	-2.326013	2.692677
18	1	0	-2.817070	-0.370043	1.776963
19	6	0	-3.289231	0.506599	-0.195127
20	1	0	2.591990	-2.570269	-1.547634
21	1	0	1.883935	-1.239550	-2.448739
22	8	0	-2.973523	0.648576	-1.368606
23	8	0	-4.353574	1.055143	0.389551
24	6	0	5.298288	2.599475	0.686571
25	6	0	6.322857	2.309173	-0.392709
26	1	0	4.560919	3.338625	0.348025
27	1	0	5.781367	2.980392	1.593184
28	1	0	7.048867	1.566977	-0.047418
29	1	0	5.844900	1.935579	-1.304772
30	1	0	6.861607	3.227692	-0.646269
31	8	0	4.624036	1.356271	1.020444
32	1	0	4.011727	1.508242	1.757964
33	6	0	-5.204266	1.886291	-0.458098
34	1	0	-5.554132	1.271860	-1.292624
35	1	0	-4.590035	2.694135	-0.866256
36	6	0	-6.340666	2.398554	0.402237
37	1	0	-7.000184	3.027183	-0.204803
38	1	0	-6.932421	1.571874	0.806936
39	1	0	-5.964479	3.000470	1.235082

36a (TS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.825039	-1.840505	0.767188
2	6	0	0.630048	-2.190818	-0.703234
3	16	0	-0.847908	-1.198909	-1.240664
4	6	0	-1.278428	-0.844431	0.446563
5	7	0	-0.349140	-1.402834	1.335840
6	1	0	1.361516	-2.561688	1.382175
7	1	0	0.425289	-3.256759	-0.826265
8	6	0	2.438227	-0.652348	-0.515471
9	1	0	3.727573	1.048008	0.012751
10	8	0	1.910161	-0.657174	0.671191
11	8	0	3.308485	0.173732	-0.862610
12	6	0	-0.497746	-1.244623	2.782021
13	6	0	-2.369195	-0.140867	0.819433
14	1	0	0.264477	-1.844416	3.283010
15	1	0	-0.384590	-0.197011	3.082743
16	6	0	1.914874	-1.747445	-1.409080
17	1	0	-1.483956	-1.601776	3.089205
18	1	0	-2.588110	0.065839	1.859251
19	6	0	-3.282533	0.366587	-0.205347
20	1	0	2.662747	-2.551876	-1.440263
21	1	0	1.777229	-1.389151	-2.431638
22	8	0	-3.095407	0.224013	-1.408284
23	8	0	-4.333028	1.008377	0.324809
24	6	0	5.336637	2.563880	0.057546
25	6	0	6.424821	1.549285	-0.206884
26	1	0	4.967439	3.041020	-0.854097
27	1	0	5.637905	3.322596	0.781718
28	1	0	6.753852	1.073964	0.721365
29	1	0	6.093402	0.780831	-0.911780
30	1	0	7.281831	2.066051	-0.650842
31	8	0	4.184976	1.854434	0.694796
32	1	0	3.494878	2.487437	0.967910
33	6	0	-5.301131	1.545909	-0.617265
34	1	0	-5.685908	0.721041	-1.224426
35	1	0	-4.784195	2.240956	-1.285906
36	6	0	-6.390643	2.224553	0.188830
37	1	0	-7.143211	2.640419	-0.489049
38	1	0	-6.886084	1.513079	0.856772
39	1	0	-5.982884	3.041695	0.792090

36b (GS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.159008	-1.853148	1.023501
2	6	0	0.895558	-2.500102	-0.326111
3	16	0	-0.614539	-1.640849	-0.988487
4	6	0	-0.942684	-0.908664	0.597006
5	7	0	0.037923	-1.271484	1.537420
6	1	0	1.751303	-2.404225	1.750915
7	1	0	3.946277	0.666300	-0.760723
8	8	0	2.279625	-0.703014	0.584274
9	1	0	0.693755	-3.567685	-0.207568
10	6	0	2.701801	-0.972178	-0.599093
11	1	0	3.860339	-0.418176	-2.147092
12	6	0	-2.006403	-0.124123	0.865628
13	1	0	-2.164916	0.313463	1.842978

14	6	0	-0.031636	-0.800349	2.922405
15	1	0	0.095953	0.285964	2.974856
16	6	0	2.139805	-2.244331	-1.185068
17	7	0	3.567755	-0.200005	-1.202108
18	6	0	-2.974568	0.154455	-0.198614
19	8	0	-2.850404	-0.263496	-1.344299
20	1	0	2.882333	-3.044550	-1.059463
21	1	0	1.927027	-2.154593	-2.253694
22	8	0	-3.990203	0.914701	0.225261
23	6	0	-5.007564	1.243428	-0.762487
24	6	0	-6.056566	2.089766	-0.069945
25	1	0	-5.419111	0.309054	-1.155500
26	1	0	-4.525080	1.772446	-1.589951
27	1	0	-5.621309	3.014492	0.321543
28	1	0	-6.517917	1.543877	0.758759
29	1	0	-6.841801	2.355685	-0.785166
30	1	0	0.760167	-1.281895	3.498653
31	1	0	-0.998354	-1.073740	3.352042
32	6	0	4.034948	3.309283	0.286844
33	6	0	2.570482	3.276193	-0.107381
34	1	0	4.144461	3.308745	1.379134
35	1	0	4.521735	4.209475	-0.107622
36	1	0	2.459689	3.273577	-1.196639
37	1	0	2.073872	2.388979	0.301594
38	1	0	2.059645	4.161561	0.284091
39	8	0	4.684886	2.141895	-0.265410
40	1	0	5.620479	2.153186	-0.011255

36b (TS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.413672	-1.762650	0.932163
2	6	0	1.148890	-2.415998	-0.422008
3	16	0	-0.406148	-1.614015	-1.048536
4	6	0	-0.772999	-0.962166	0.565561
5	7	0	0.218859	-1.303639	1.486199
6	1	0	1.990804	-2.358647	1.640645
7	1	0	3.965195	1.424114	-0.439309
8	8	0	2.359582	-0.604827	0.577982
9	1	0	0.999392	-3.493135	-0.324869
10	6	0	2.837675	-0.759944	-0.649190
11	1	0	3.923762	-0.058144	-2.098053
12	6	0	-1.884278	-0.247991	0.856760
13	1	0	-2.065754	0.141262	1.850480
14	6	0	0.133169	-0.882943	2.881057
15	1	0	0.218579	0.205879	2.985048
16	6	0	2.372611	-2.057396	-1.270134
17	7	0	3.611730	0.136064	-1.150427
18	6	0	-2.873374	0.010268	-0.187192
19	8	0	-2.741433	-0.343997	-1.353497
20	1	0	3.165224	-2.809827	-1.157327
21	1	0	2.162936	-1.952351	-2.337479
22	8	0	-3.934972	0.688603	0.277365
23	6	0	-4.980154	0.984761	-0.686725
24	6	0	-6.086554	1.711893	0.051776
25	1	0	-5.323803	0.043437	-1.125878
26	1	0	-4.549958	1.590529	-1.490492

27	1	0	-5.720677	2.646662	0.488275
28	1	0	-6.495944	1.090913	0.854558
29	1	0	-6.896993	1.951700	-0.644404
30	1	0	0.939259	-1.358664	3.443539
31	1	0	-0.822575	-1.204484	3.303346
32	6	0	2.926727	3.039127	0.577847
33	6	0	2.226409	3.622860	-0.626312
34	1	0	2.337447	2.277553	1.094129
35	1	0	3.262768	3.802340	1.281248
36	1	0	2.861209	4.352738	-1.135670
37	1	0	1.928935	2.843835	-1.334335
38	1	0	1.318679	4.132626	-0.286692
39	8	0	4.184380	2.371124	0.105914
40	1	0	4.774533	2.162777	0.855682

37 (GS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.121846	0.523379	1.911170
2	6	0	-1.582146	-0.240836	0.753795
3	16	0	-0.059914	-0.615740	-0.235480
4	6	0	0.947780	0.271723	0.910358
5	7	0	0.146381	0.803486	1.977246
6	1	0	-1.784683	0.885657	2.692503
7	6	0	-2.417319	-1.482221	1.131206
8	1	0	-2.236987	0.436676	0.143547
9	6	0	0.745290	1.617124	3.053201
10	6	0	2.279602	0.470517	0.844562
11	1	0	2.823279	1.047471	1.582031
12	6	0	3.025880	-0.124998	-0.279211
13	8	0	2.480821	-0.790481	-1.147856
14	8	0	4.327540	0.151922	-0.215510
15	6	0	5.160245	-0.393590	-1.285331
16	6	0	6.582953	0.057667	-1.029205
17	1	0	-0.038132	1.909286	3.751944
18	1	0	1.503161	1.023715	3.568105
19	1	0	1.202311	2.505875	2.613592
20	1	0	4.768536	-0.027399	-2.238619
21	1	0	5.056270	-1.482405	-1.271718
22	1	0	6.946726	-0.310661	-0.065117
23	1	0	6.658370	1.149268	-1.038467
24	1	0	7.234910	-0.337392	-1.814988
25	6	0	-2.942581	-2.174698	-0.137496
26	1	0	-1.830578	-2.179888	1.739085
27	8	0	-3.004371	-1.583513	-1.213038
28	1	0	-3.284808	-1.166072	1.726770
29	7	0	-3.339277	-3.453720	0.022825
30	1	0	-3.720105	-3.943635	-0.776908
31	1	0	-3.258736	-3.953780	0.896121
32	6	0	-3.488876	2.169359	-1.937427
33	6	0	-3.450438	3.529425	-1.263854
34	1	0	-4.358179	2.101640	-2.605173
35	8	0	-3.590090	1.157910	-0.921760
36	1	0	-2.587088	2.012222	-2.546771
37	1	0	-2.571890	3.621618	-0.614435
38	1	0	-4.347829	3.683330	-0.656133
39	1	0	-3.401297	4.324561	-2.014808

40	1	0	-3.606818	0.279580	-1.348678

37 (TS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.327730	1.129771	-1.649988
2	6	0	1.751945	0.082736	-0.813543
3	16	0	0.248497	-0.744754	-0.166998
4	6	0	-0.772282	0.508450	-0.895777
5	7	0	0.027146	1.406162	-1.648641
6	1	0	1.990041	1.748034	-2.248865
7	6	0	2.916570	-0.807198	-1.258898
8	1	0	2.236814	0.805491	0.260758
9	6	0	-0.568548	2.553201	-2.346003
10	6	0	-2.112350	0.618789	-0.761053
11	1	0	-2.677162	1.421843	-1.217101
12	6	0	-2.820993	-0.404665	0.011980
13	8	0	-2.245940	-1.349400	0.542180
14	8	0	-4.137868	-0.187446	0.060136
15	6	0	-4.929704	-1.163714	0.797790
16	6	0	-6.380058	-0.735804	0.704627
17	1	0	0.217956	3.095195	-2.871457
18	1	0	-1.310852	2.195679	-3.063696
19	1	0	-1.049513	3.216361	-1.622285
20	1	0	-4.567053	-1.188319	1.829731
21	1	0	-4.755813	-2.149139	0.355680
22	1	0	-6.716819	-0.710524	-0.336258
23	1	0	-6.527485	0.255839	1.143376
24	1	0	-7.006065	-1.449104	1.250583
25	6	0	3.530618	-1.652342	-0.134869
26	1	0	2.597580	-1.451193	-2.086193
27	8	0	3.808020	-1.186218	0.978428
28	1	0	3.723248	-0.167687	-1.643081
29	7	0	3.791823	-2.934071	-0.440720
30	1	0	4.239898	-3.517098	0.255855
31	1	0	3.555705	-3.347428	-1.330932
32	6	0	2.116315	1.383562	2.509738
33	6	0	1.257482	2.624830	2.386623
34	1	0	2.848590	1.482886	3.315700
35	8	0	2.891561	1.208033	1.278269
36	1	0	1.517972	0.483063	2.682841
37	1	0	0.507879	2.516819	1.594346
38	1	0	1.872177	3.505482	2.177957
39	1	0	0.723215	2.792725	3.327137
40	1	0	3.444414	0.367050	1.347544

X, Y, Z Coordinates for the Calculated Ground State (GS) and Transition State (TS) for the Rotation around the C–C Bond of Structure 39

39 (GS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.105849	1.398078	-0.553539
2	6	0	-2.250655	0.081559	-1.213142
3	16	0	-0.590905	-0.738028	-1.035970
4	6	0	0.089643	0.716576	-0.305036
5	7	0	-0.922048	1.723319	-0.140613
6	1	0	-2.923826	2.102790	-0.441732
7	6	0	-0.612940	3.018599	0.497380
8	1	0	-2.423697	0.279798	-2.282799
9	8	0	-3.202953	0.095852	1.477084
10	6	0	-3.410831	-1.068816	0.767638
11	7	0	-3.583588	-2.241817	1.197785
12	6	0	1.366763	0.908585	0.076516
13	1	0	1.714917	1.833582	0.518931
14	1	0	-1.521999	3.617897	0.536075
15	1	0	-0.242668	2.834565	1.507553
16	6	0	-3.446196	-0.762199	-0.709393
17	1	0	0.147680	3.532794	-0.093084
18	1	0	-3.580516	-2.324160	2.218352
19	1	0	-3.208277	-0.089977	2.432728
20	1	0	-4.369987	-0.215306	-0.941589
21	1	0	-3.477939	-1.706304	-1.255304
22	6	0	2.328641	-0.195582	-0.114687
23	8	0	1.994658	-1.272450	-0.587741
24	8	0	3.552732	0.133347	0.286499
25	6	0	4.585487	-0.893474	0.139646
26	6	0	5.883801	-0.308476	0.653964
27	1	0	4.637036	-1.168294	-0.917644
28	1	0	4.266723	-1.773569	0.705230
29	1	0	5.801900	-0.031966	1.709498
30	1	0	6.172675	0.577250	0.080141
31	1	0	6.679235	-1.054272	0.556147

39 (TS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.131852	1.197158	-0.725488
2	6	0	-2.212983	-0.177395	-1.263332
3	16	0	-0.492342	-0.862216	-1.122372
4	6	0	0.084603	0.628011	-0.388104
5	7	0	-0.980474	1.587897	-0.280511
6	1	0	-2.984845	1.868051	-0.665268
7	6	0	-0.747578	2.926270	0.301510
8	1	0	-2.465930	-0.111325	-2.331573
9	8	0	-4.468261	-0.203925	1.321829
10	6	0	-3.362905	-0.905249	0.933371
11	7	0	-2.435822	-1.395570	1.644944
12	6	0	1.337838	0.899286	0.027572

13	1	0	1.621413	1.848394	0.464607
14	1	0	-1.683639	3.483615	0.288463
15	1	0	-0.395330	2.806678	1.327567
16	6	0	-3.333674	-1.018239	-0.580119
17	1	0	0.005105	3.444413	-0.295471
18	1	0	-2.571574	-1.255178	2.650611
19	1	0	-4.536267	-0.195837	2.293475
20	1	0	-4.299020	-0.701386	-0.984355
21	1	0	-3.178115	-2.063460	-0.859849
22	6	0	2.364544	-0.149749	-0.127737
23	8	0	2.112807	-1.231649	-0.638676
24	8	0	3.547203	0.233477	0.344276
25	6	0	4.636974	-0.737320	0.236762
26	6	0	5.876186	-0.095699	0.824292
27	1	0	4.755729	-0.992883	-0.819991
28	1	0	4.335635	-1.640987	0.774003
29	1	0	5.726784	0.160254	1.877603
30	1	0	6.148108	0.812112	0.277280
31	1	0	6.712585	-0.798930	0.758033

X, Y, Z Coordinates for the Calculated Ground State (GS) and Transition State (TS) Structures 49

49 (GS)

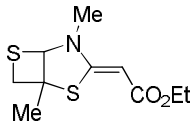
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.533907	1.260011	0.032768
2	6	0	-2.676263	-0.103856	-0.497144
3	16	0	-0.983305	-0.509777	-1.124420
4	6	0	-0.284084	0.801985	-0.187179
5	7	0	-1.329294	1.693506	0.243107
6	6	0	-2.965183	-1.031434	0.787355
7	6	0	1.012046	1.026509	0.104533
8	1	0	1.335308	1.922008	0.620564
9	6	0	-1.025231	2.961195	0.934236
10	1	0	-3.041583	-2.052780	0.392009
11	1	0	-3.941946	-0.737191	1.190546
12	6	0	2.043857	0.023244	-0.225098
13	1	0	-0.369372	3.563680	0.303488
14	1	0	-1.958133	3.493305	1.117993
15	1	0	-0.535855	2.734985	1.883804
16	8	0	1.789874	-1.099844	-0.649168
17	8	0	3.264402	0.488618	0.015570
18	6	0	4.384841	-0.411524	-0.260840
19	6	0	5.661336	0.355925	0.011336
20	1	0	4.303337	-0.740355	-1.300319
21	1	0	4.277093	-1.288308	0.384423
22	1	0	5.710499	0.685127	1.053601
23	1	0	5.740063	1.232680	-0.638326
24	1	0	6.520862	-0.293299	-0.184041
25	1	0	-3.378841	1.866529	0.347927
26	8	0	-0.083600	-2.692534	1.102313
27	1	0	0.595120	-2.356302	0.487390

28	6	0	-3.773413	-0.278401	-1.553371
29	1	0	-3.806116	-1.321211	-1.882517
30	1	0	-4.752981	-0.031573	-1.129253
31	1	0	-3.598134	0.352123	-2.428517
32	8	0	-1.997013	-0.882805	1.764168
33	1	0	-1.282425	-1.556209	1.620961
34	1	0	0.367754	-3.300714	1.706582

49 (TS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.561024	1.268047	-0.067610
2	6	0	-2.679423	-0.055334	-0.607542
3	16	0	-0.997967	-0.469157	-1.198841
4	6	0	-0.306396	0.780601	-0.167095
5	7	0	-1.349993	1.664941	0.249202
6	6	0	-2.897724	-1.002405	0.858957
7	6	0	0.988458	0.975646	0.169005
8	1	0	1.302960	1.879116	0.676579
9	6	0	-1.066423	2.866361	1.050164
10	1	0	-3.051962	-1.987677	0.389209
11	1	0	-3.845969	-0.632055	1.273574
12	6	0	2.028768	-0.026921	-0.095002
13	1	0	-0.384064	3.517845	0.500292
14	1	0	-2.002697	3.390757	1.239516
15	1	0	-0.617600	2.563371	1.998821
16	8	0	1.810847	-1.227058	-0.296797
17	8	0	3.242882	0.500071	-0.060351
18	6	0	4.378756	-0.400774	-0.271023
19	6	0	5.636103	0.441668	-0.229806
20	1	0	4.236995	-0.899808	-1.233134
21	1	0	4.355189	-1.159892	0.516082
22	1	0	5.746319	0.941261	0.737284
23	1	0	5.627813	1.199849	-1.018375
24	1	0	6.506979	-0.203515	-0.383942
25	1	0	-3.410053	1.876466	0.229069
26	8	0	-0.062953	-2.562571	1.125395
27	1	0	0.627815	-2.113402	0.553742
28	6	0	-3.813928	-0.362046	-1.575214
29	1	0	-3.838108	-1.431524	-1.804038
30	1	0	-4.775753	-0.096811	-1.122768
31	1	0	-3.707583	0.188238	-2.513949
32	8	0	-1.868767	-0.886812	1.690662
33	1	0	-0.948789	-1.754413	1.424405
34	1	0	0.376842	-2.923987	1.914400

X, Y, Z Coordinates for the Optimized Structures of the Expected Four-Membered Ring and the Obtained Tricyclic System 51 from the Reaction of Precursor 44



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.394060	0.704703	-0.379199
2	6	0	-2.397915	-0.837085	-0.291958
3	16	0	-0.603637	-1.303527	-0.082184
4	6	0	-0.046162	0.355234	-0.368453
5	7	0	-1.095065	1.190968	-0.698360
6	1	0	-3.131462	1.128713	-1.065487
7	6	0	-0.890701	2.621217	-0.865181
8	6	0	-3.013475	-1.573473	-1.479461
9	16	0	-3.037868	0.856943	1.409036
10	1	0	-1.809746	3.062103	-1.259300
11	6	0	1.259799	0.738173	-0.307484
12	1	0	1.543943	1.772075	-0.453244
13	1	0	-0.639496	3.113294	0.084820
14	1	0	-0.085256	2.801794	-1.582352
15	6	0	2.310187	-0.221155	-0.028887
16	6	0	-3.172707	-0.956847	1.043775
17	8	0	2.150530	-1.422056	0.158055
18	8	0	3.533203	0.372258	0.010356
19	1	0	-4.213799	-1.262114	0.901555
20	1	0	-2.705862	-1.588945	1.801626
21	6	0	4.643376	-0.502410	0.289930
22	6	0	5.899931	0.349138	0.306099
23	1	0	4.687953	-1.281880	-0.478474
24	1	0	4.474597	-1.000302	1.250728
25	1	0	5.838237	1.121542	1.079651
26	1	0	6.050704	0.841822	-0.660047
27	1	0	6.773941	-0.278099	0.513663
28	1	0	-2.481224	-1.334555	-2.405633
29	1	0	-4.068272	-1.295247	-1.598001
30	1	0	-2.964210	-2.658212	-1.332989

51

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.783119	0.959062	-0.968612
2	6	0	-1.706548	-0.588200	-0.940853
3	16	0	-1.019010	-1.379511	0.632658
4	6	0	0.733642	-1.698866	0.130172
5	6	0	1.783119	-0.959057	0.968622
6	6	0	1.706548	0.588206	0.940877
7	16	0	1.018987	1.379546	-0.632613
8	6	0	-0.733670	1.698847	-0.130110
9	16	0	3.454584	-1.336940	0.206516

10	6	0	4.051590	0.279205	0.621845
11	16	0	-3.454618	1.336960	-0.206592
12	6	0	-4.051594	-0.279215	-0.621853
13	6	0	5.337032	0.689754	0.429487
14	6	0	-5.337026	-0.689775	-0.429463
15	7	0	-3.050863	-1.047642	-1.181186
16	6	0	-3.290071	-2.438826	-1.535446
17	6	0	6.332319	-0.207385	-0.123349
18	8	0	6.131762	-1.360345	-0.489096
19	8	0	7.552583	0.387003	-0.207816
20	6	0	9.865956	0.419799	-0.789930
21	6	0	8.604125	-0.423663	-0.767505
22	7	0	3.050871	1.047638	1.181184
23	6	0	3.290110	2.438818	1.535445
24	6	0	-6.332324	0.207379	0.123328
25	8	0	-6.131785	1.360365	0.489002
26	8	0	-7.552575	-0.387029	0.207846
27	6	0	-9.865950	-0.419823	0.789952
28	6	0	-8.604127	0.423650	0.767498
29	6	0	1.766827	-1.439422	2.431293
30	6	0	-1.766743	1.439423	-2.431284
31	1	0	-1.053312	-0.944737	-1.741822
32	1	0	0.905005	-2.775771	0.225464
33	1	0	0.836954	-1.433936	-0.923537
34	1	0	1.053330	0.944737	1.741863
35	1	0	-0.905060	2.775755	-0.225326
36	1	0	-0.836980	1.433837	0.923580
37	1	0	5.639536	1.701954	0.663767
38	1	0	-5.639515	-1.701996	-0.663671
39	1	0	-4.164612	-2.502026	-2.189374
40	1	0	-2.421290	-2.816856	-2.078766
41	1	0	-3.453423	-3.068995	-0.652165
42	1	0	10.695696	-0.160156	-1.208982
43	1	0	9.726313	1.315325	-1.404189
44	1	0	10.142560	0.736359	0.221071
45	1	0	8.725786	-1.324722	-0.156748
46	1	0	8.311063	-0.747447	-1.771992
47	1	0	4.164527	2.501983	2.189546
48	1	0	3.453688	3.068937	0.652171
49	1	0	2.421245	2.816935	2.078567
50	1	0	-10.695695	0.160138	1.208983
51	1	0	-9.726298	-1.315327	1.404241
52	1	0	-10.142551	-0.736421	-0.221038
53	1	0	-8.311073	0.747477	1.771973
54	1	0	-8.725794	1.324683	0.156704
55	1	0	0.785833	-1.249561	2.884602
56	1	0	1.968601	-2.513769	2.483488
57	1	0	2.528847	-0.922210	3.020751
58	1	0	-0.785694	1.249651	-2.884510
59	1	0	-2.528665	0.922139	-3.020806
60	1	0	-1.968611	2.513750	-2.483499

X, Y, Z Coordinates for the Optimized Structures of *cis* and *trans* Isomers of Intermediate 50

50-*cis*

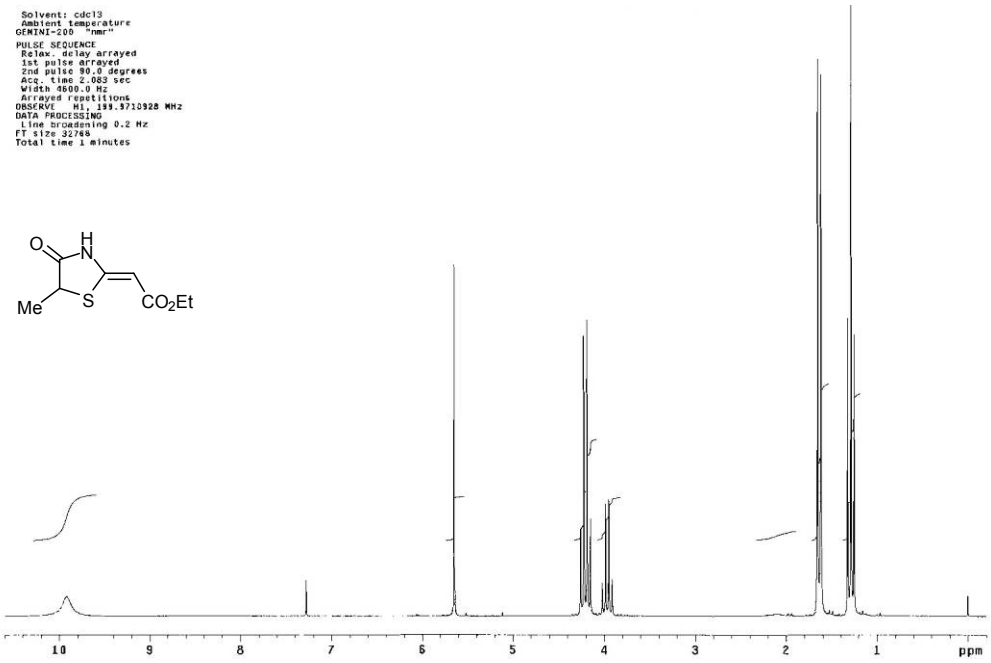
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.904658	1.039076	-0.024950
2	6	0	2.006237	-0.443910	0.398829
3	16	0	0.293716	-1.104089	0.006074
4	6	0	-0.410728	0.520531	0.181644
5	7	0	0.575440	1.468695	0.366873
6	1	0	2.648965	1.638982	0.504655
7	8	0	2.172517	1.276148	-1.399661
8	6	0	3.022217	-1.244667	-0.432977
9	6	0	2.273938	-0.561281	1.905932
10	1	0	1.523373	0.767517	-1.917223
11	6	0	-1.746967	0.781311	0.130958
12	1	0	-2.115696	1.795609	0.213208
13	6	0	0.251882	2.888275	0.329675
14	1	0	-0.156373	3.196219	-0.642134
15	6	0	-2.718115	-0.281213	-0.046088
16	8	0	-2.460221	-1.467638	-0.213133
17	8	0	-3.990878	0.197369	-0.019526
18	6	0	-5.031411	-0.781991	-0.205631
19	6	0	-6.360504	-0.052516	-0.131628
20	1	0	-4.942917	-1.550590	0.569536
21	1	0	-4.889487	-1.276125	-1.172937
22	1	0	-6.430399	0.712997	-0.911394
23	1	0	-6.484555	0.435527	0.840614
24	1	0	-7.184398	-0.761410	-0.269448
25	1	0	1.162719	3.458698	0.523110
26	1	0	-0.478387	3.123868	1.109747
27	16	0	4.768523	-0.654662	-0.328440
28	1	0	2.735307	-1.274259	-1.484790
29	1	0	3.049941	-2.277848	-0.073689
30	1	0	1.544969	0.019144	2.477876
31	1	0	3.279646	-0.195397	2.141487
32	1	0	2.203776	-1.605276	2.226604
33	1	0	4.591017	0.422775	-1.121513

50-*trans*

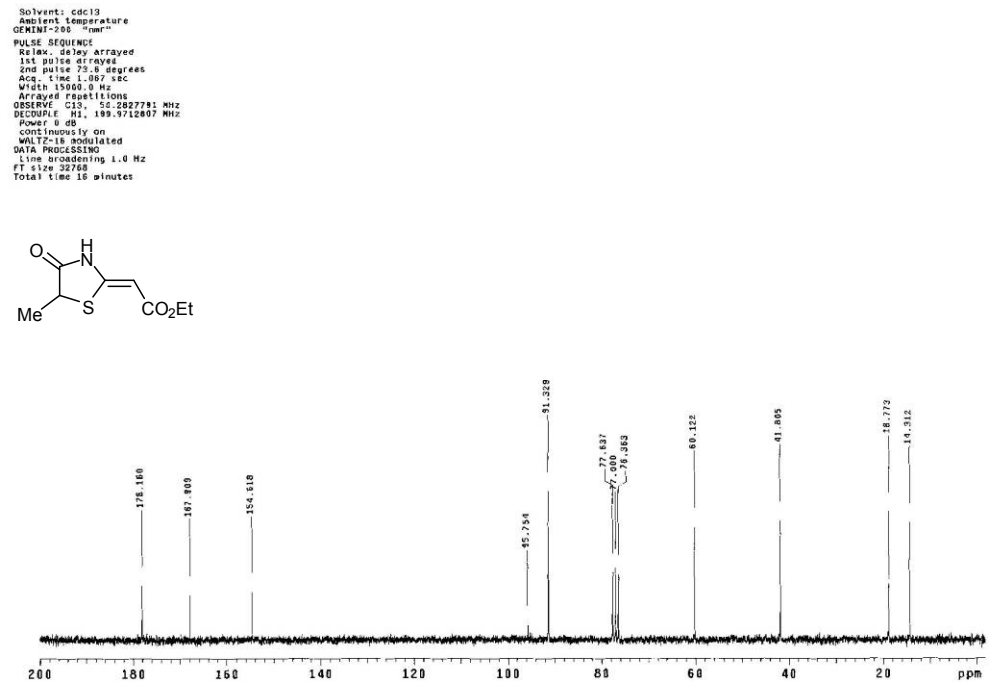
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.966582	0.993999	0.543856
2	6	0	-2.069628	-0.540896	0.407470
3	16	0	-0.292517	-1.095933	0.607444
4	6	0	0.301112	0.477239	0.017834
5	7	0	-0.743362	1.360894	-0.158204
6	1	0	-2.819800	1.477188	0.062292
7	8	0	-1.992079	1.465106	1.876931
8	6	0	-2.938044	-1.189941	1.485763
9	6	0	-2.507369	-0.949859	-1.018346
10	1	0	-1.258027	1.039211	2.354256

11	6	0	1.615251	0.755106	-0.211444
12	1	0	1.923627	1.741235	-0.533928
13	6	0	-0.480598	2.769590	-0.420185
14	1	0	0.065271	3.249670	0.402825
15	6	0	2.644125	-0.248116	-0.016579
16	8	0	2.465260	-1.387337	0.399264
17	8	0	3.875335	0.229266	-0.341672
18	6	0	4.970053	-0.690047	-0.160815
19	6	0	6.245482	0.041777	-0.537621
20	1	0	4.804491	-1.572113	-0.788830
21	1	0	4.985358	-1.029030	0.880542
22	1	0	6.394102	0.920183	0.098870
23	1	0	6.212051	0.374735	-1.580139
24	1	0	7.107811	-0.622891	-0.415258
25	1	0	-1.435233	3.282470	-0.553809
26	1	0	0.102573	2.874796	-1.340061
27	1	0	-3.970664	-0.834896	1.405834
28	1	0	-2.581625	-0.947743	2.488317
29	1	0	-2.937633	-2.280275	1.374819
30	1	0	-1.844465	-0.491779	-1.755898
31	16	0	-4.200609	-0.424356	-1.548412
32	1	0	-2.424722	-2.033027	-1.133668
33	1	0	-4.900495	-1.318769	-0.819028

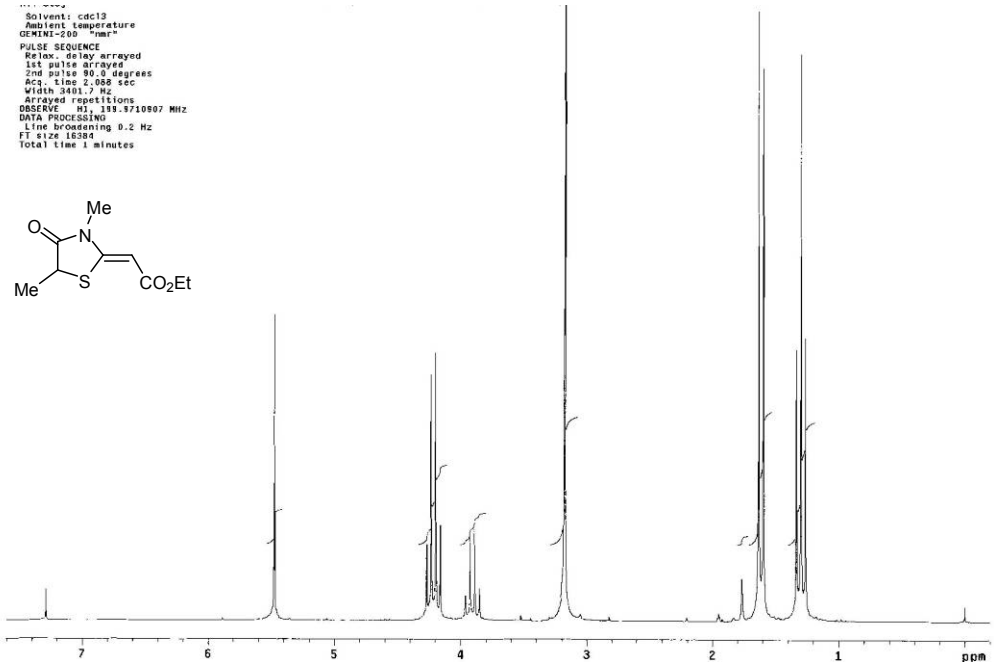
Copies of ^{1}H NMR, ^{13}C NMR and NOESY NMR Spectra for the Synthesized Compounds



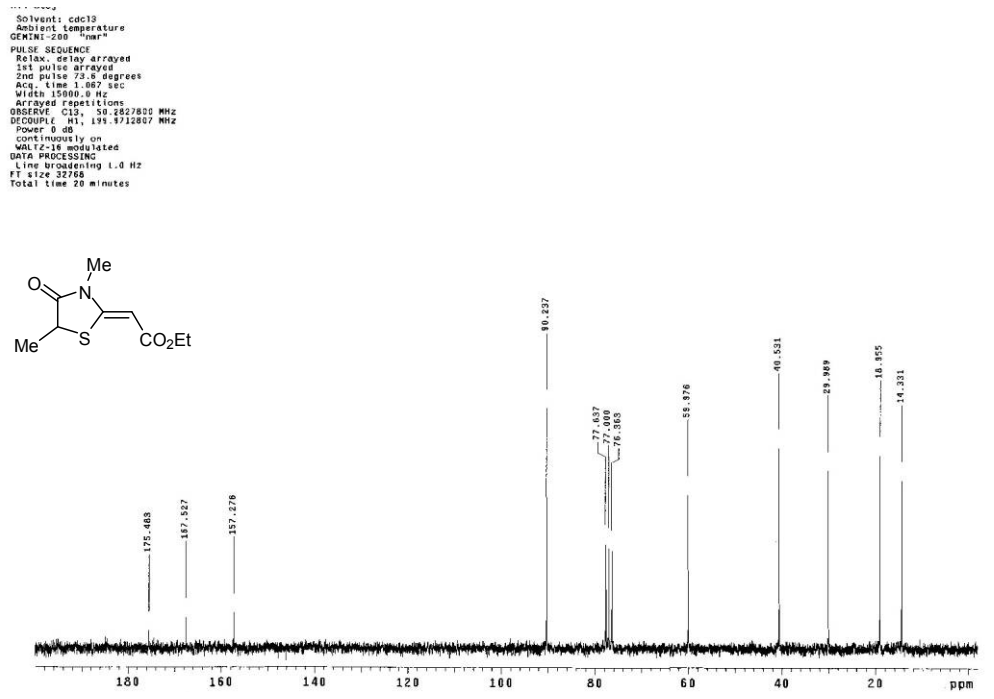
^{1}H NMR spectrum for **9a** (200 MHz, $CDCl_3$)



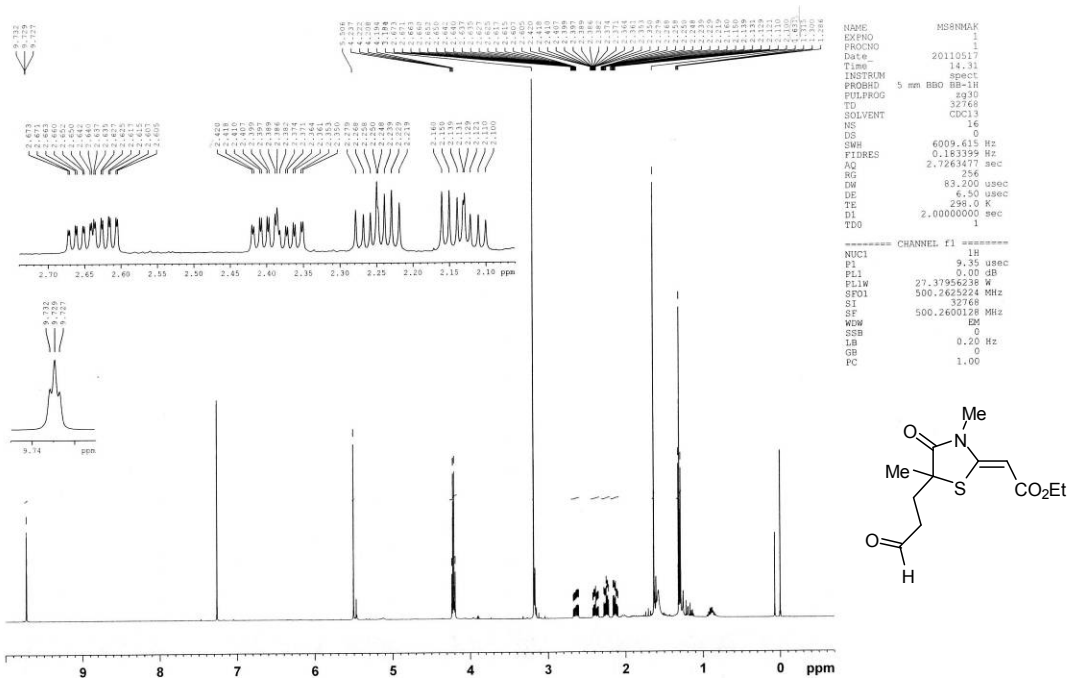
^{13}C NMR spectrum for **9a** (50 MHz, $CDCl_3$)



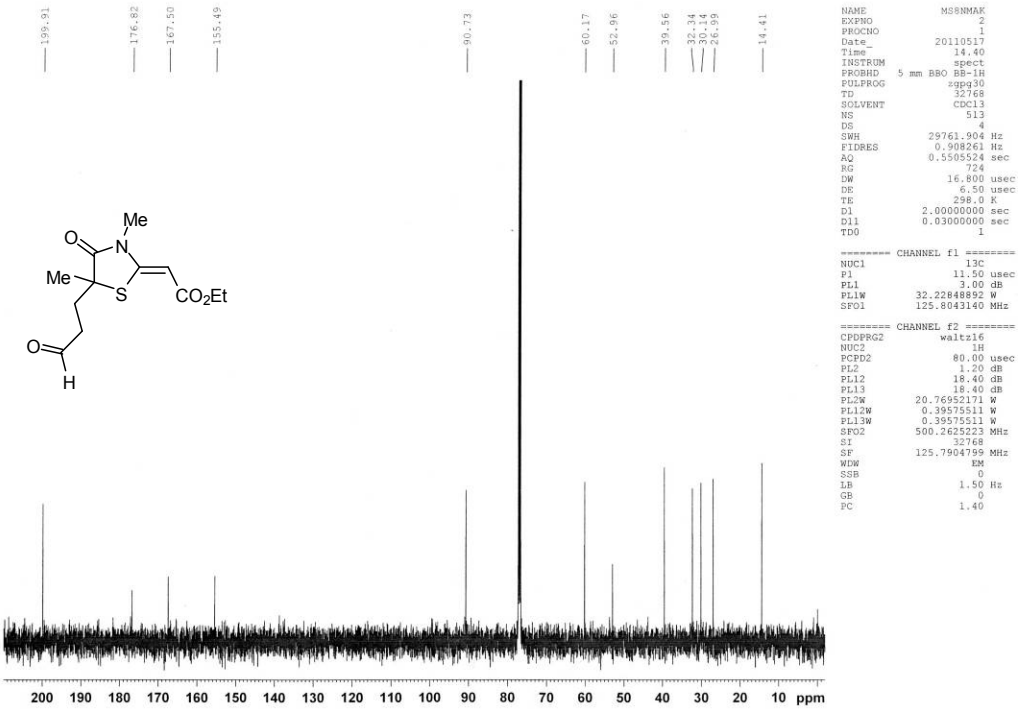
^{1}H NMR spectrum for **10** (200 MHz, $CDCl_3$)



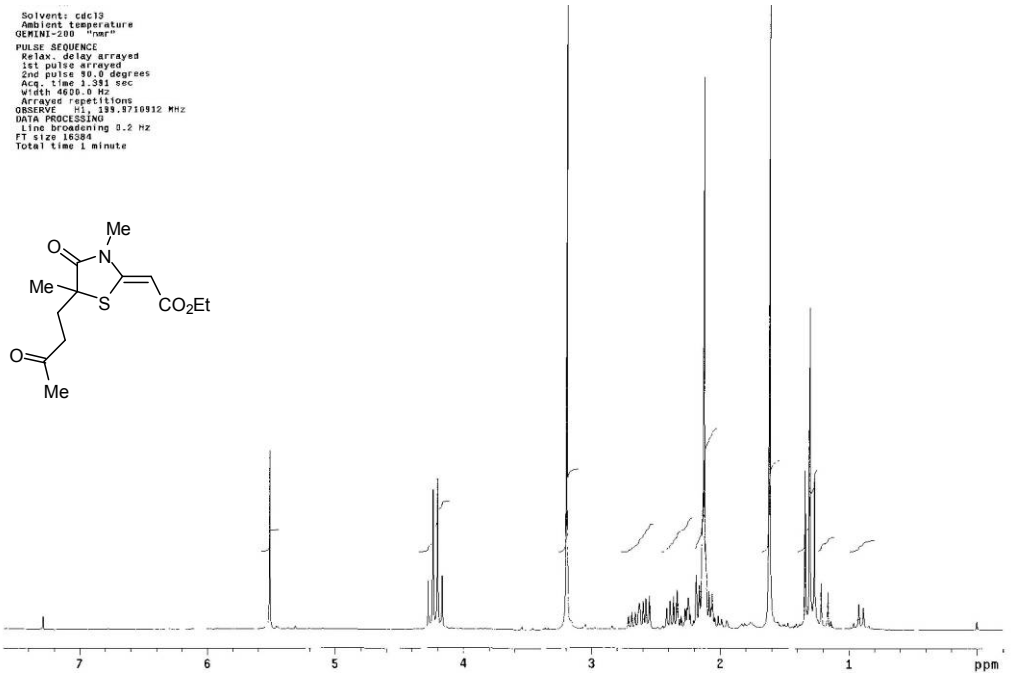
^{13}C NMR spectrum for **10** (50 MHz, $CDCl_3$)



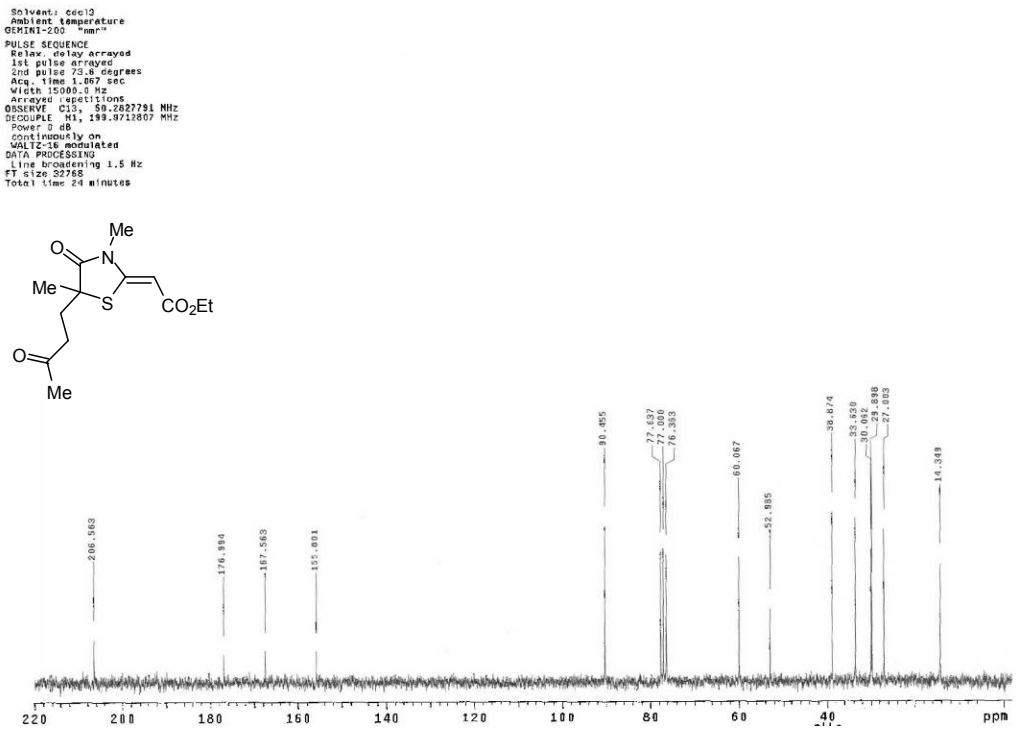
^{1}H NMR spectrum for **11a** (500 MHz, $CDCl_3$)



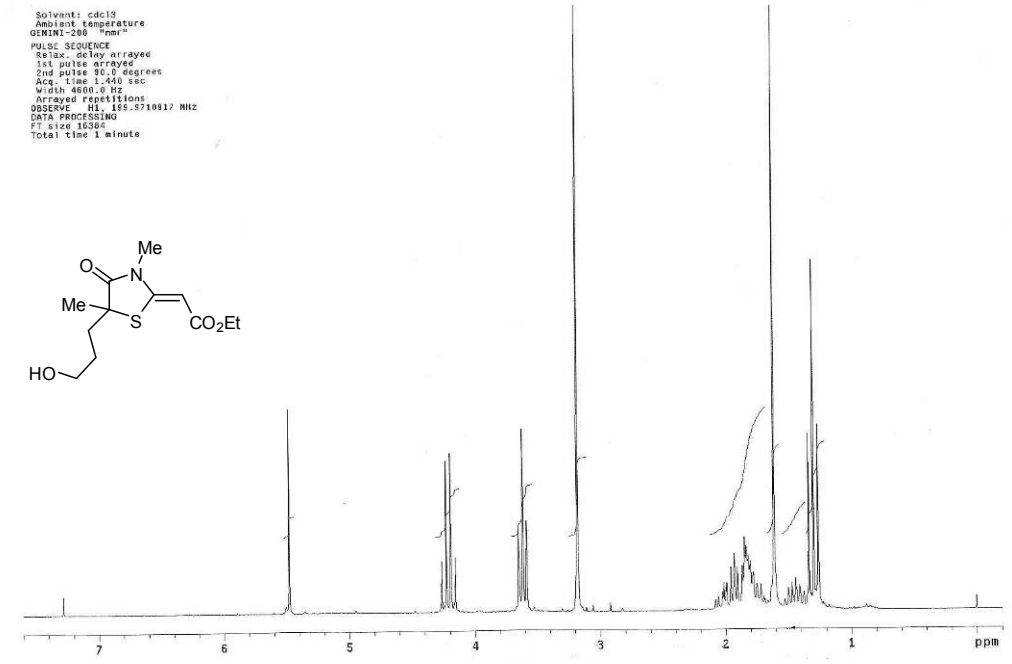
^{13}C NMR spectrum for **11a** (125 MHz, $CDCl_3$)



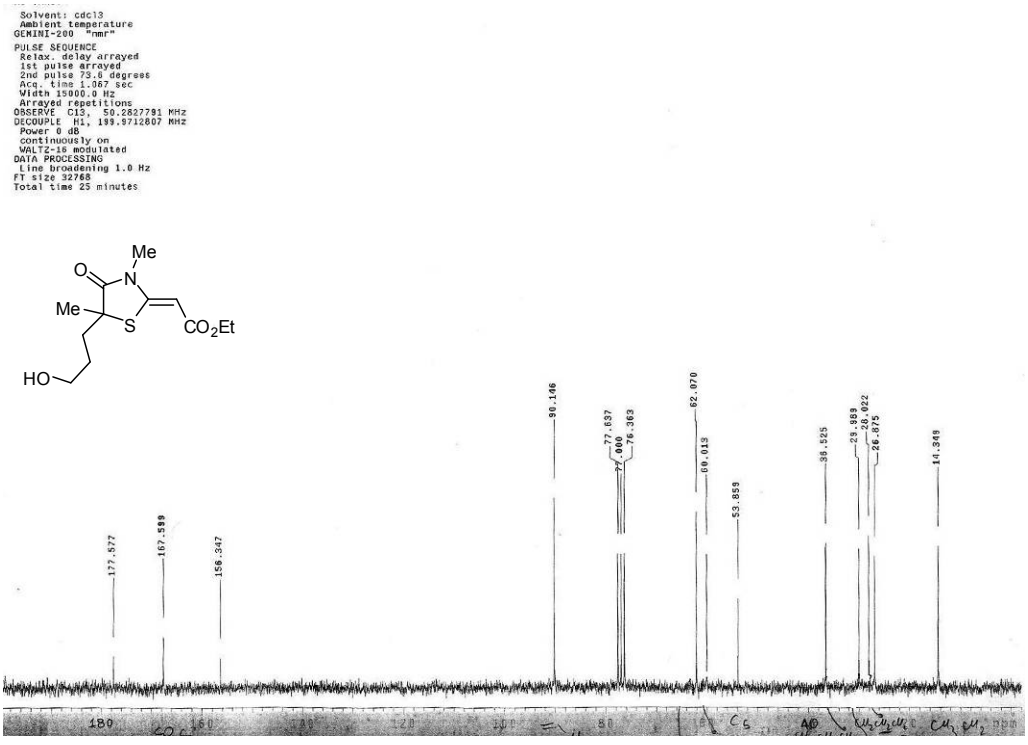
^{1}H NMR spectrum for **11b** (200 MHz, $CDCl_3$)



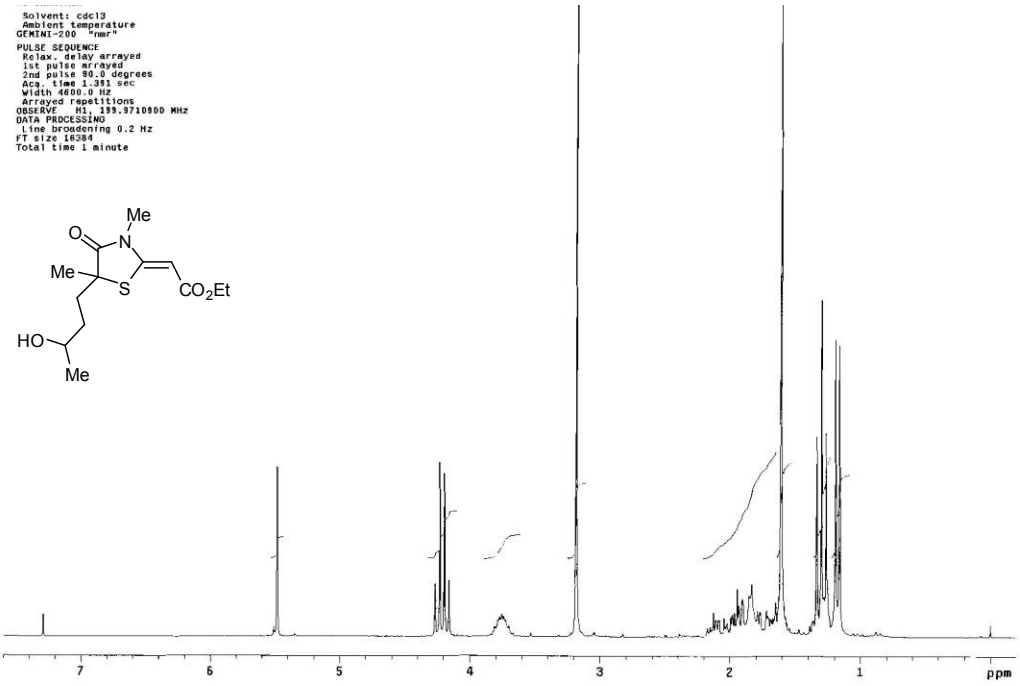
^{13}C NMR spectrum for **11b** (50 MHz, $CDCl_3$)



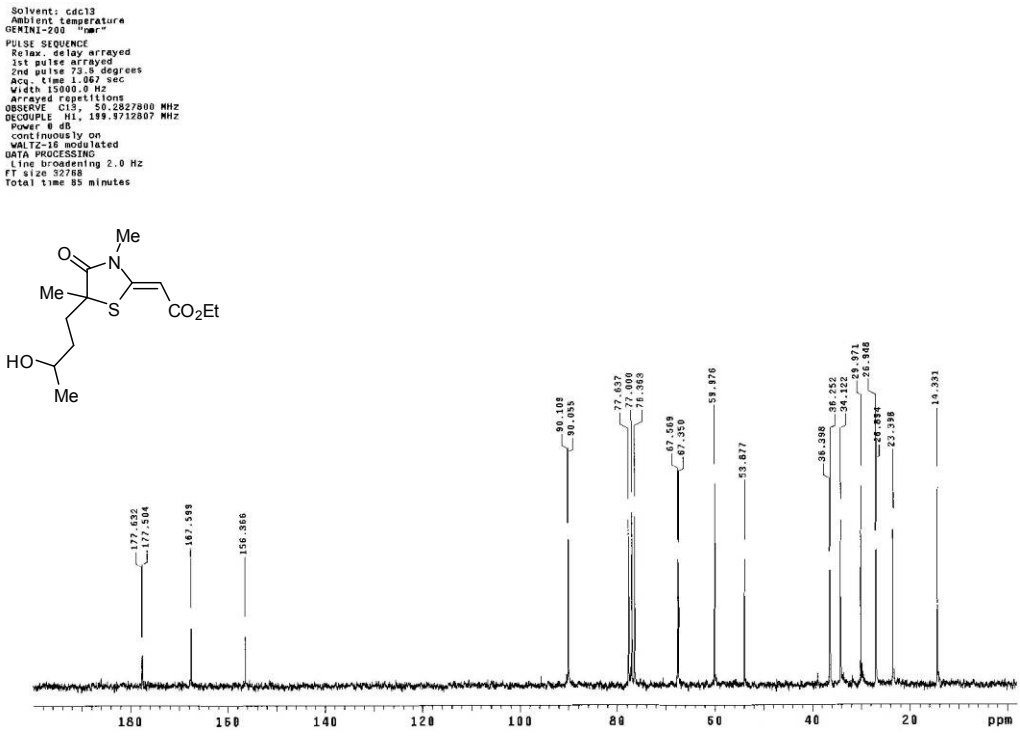
^{1}H NMR spectrum for **12a** (200 MHz, $CDCl_3$)



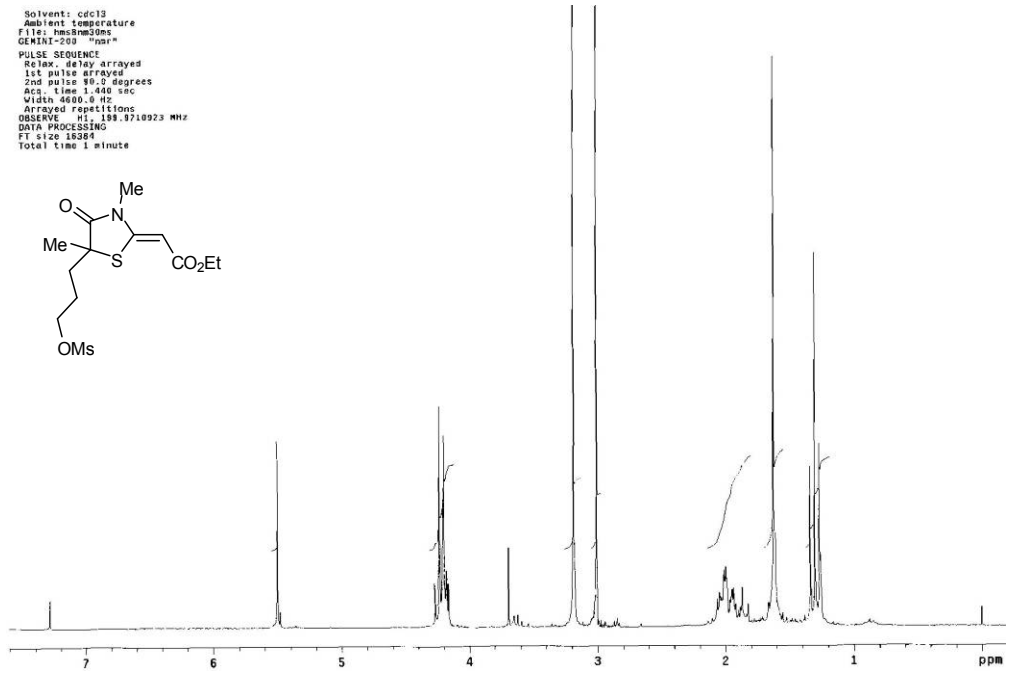
^{13}C NMR spectrum for **12a** (50 MHz, $CDCl_3$)



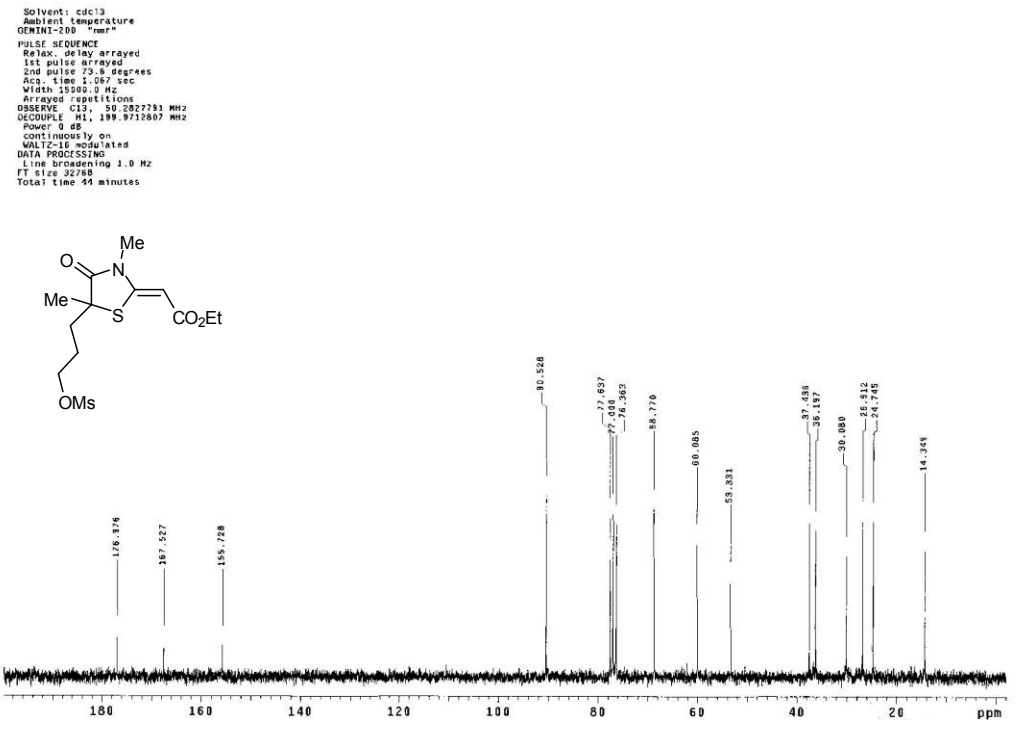
^{1}H NMR spectrum for **12b** (200 MHz, $CDCl_3$)



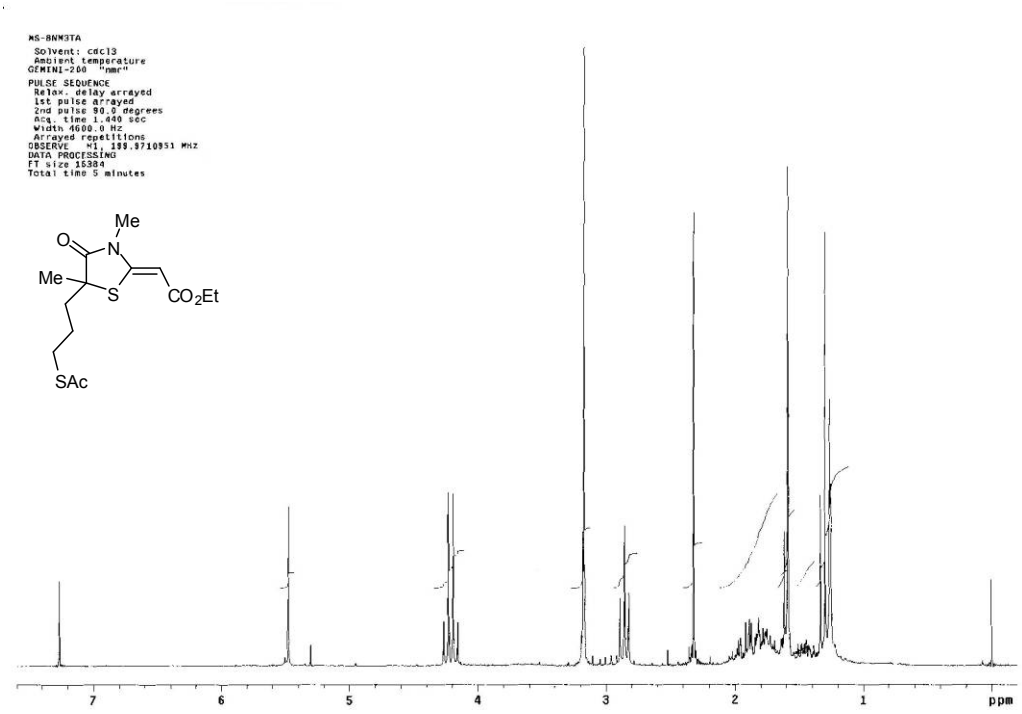
^{13}C NMR spectrum for **12b** (50 MHz, $CDCl_3$)



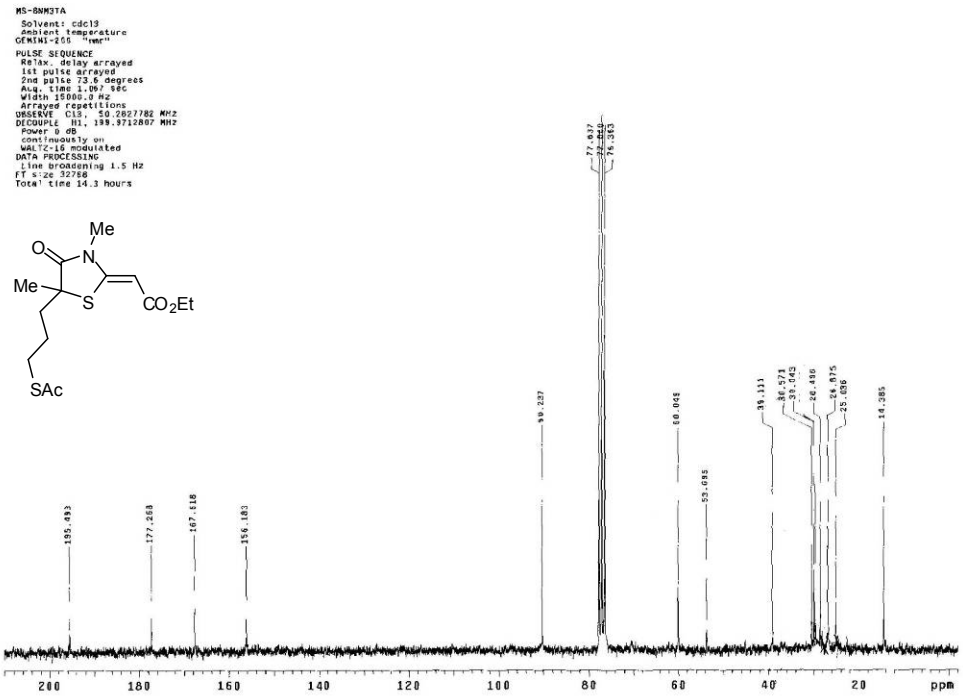
^{1}H NMR spectrum for **13** (200 MHz, $CDCl_3$)



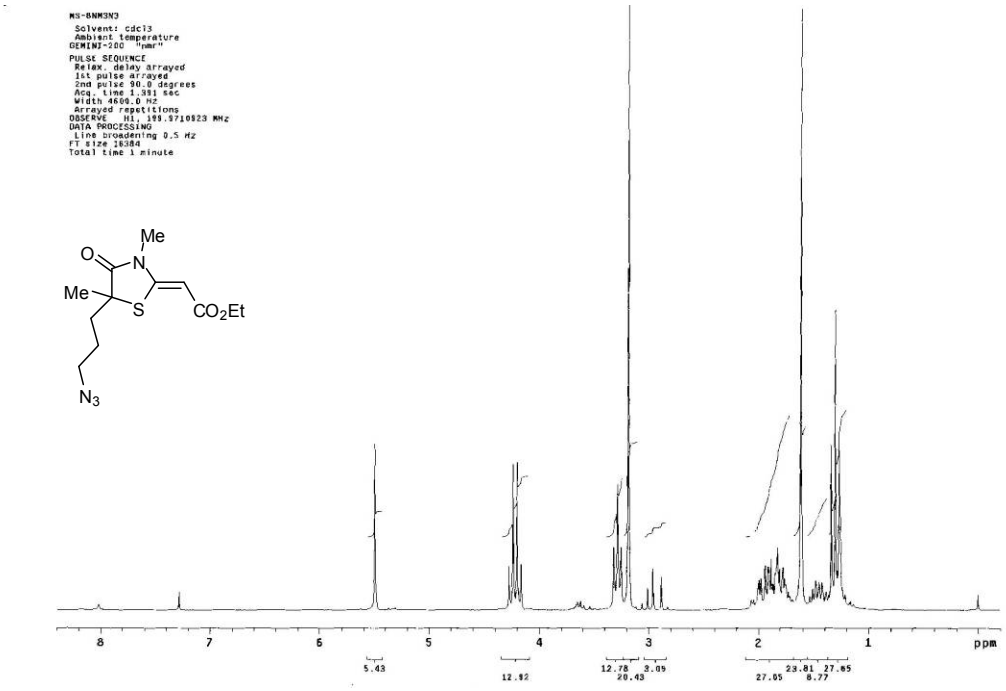
^{13}C NMR spectrum for **13** (50 MHz, $CDCl_3$)



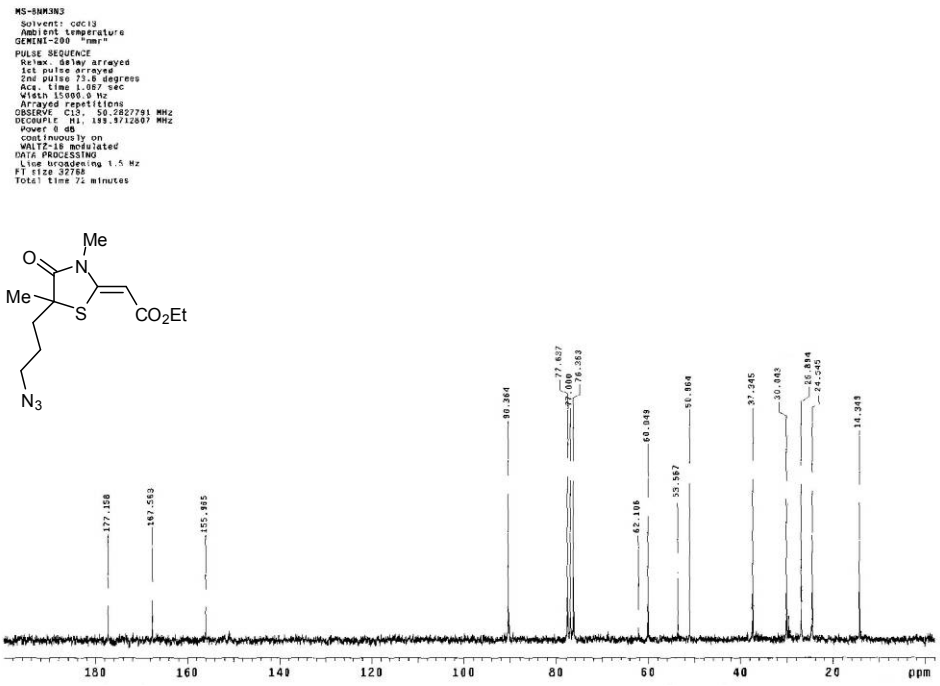
^{1}H NMR spectrum for **14** (200 MHz, $CDCl_3$)



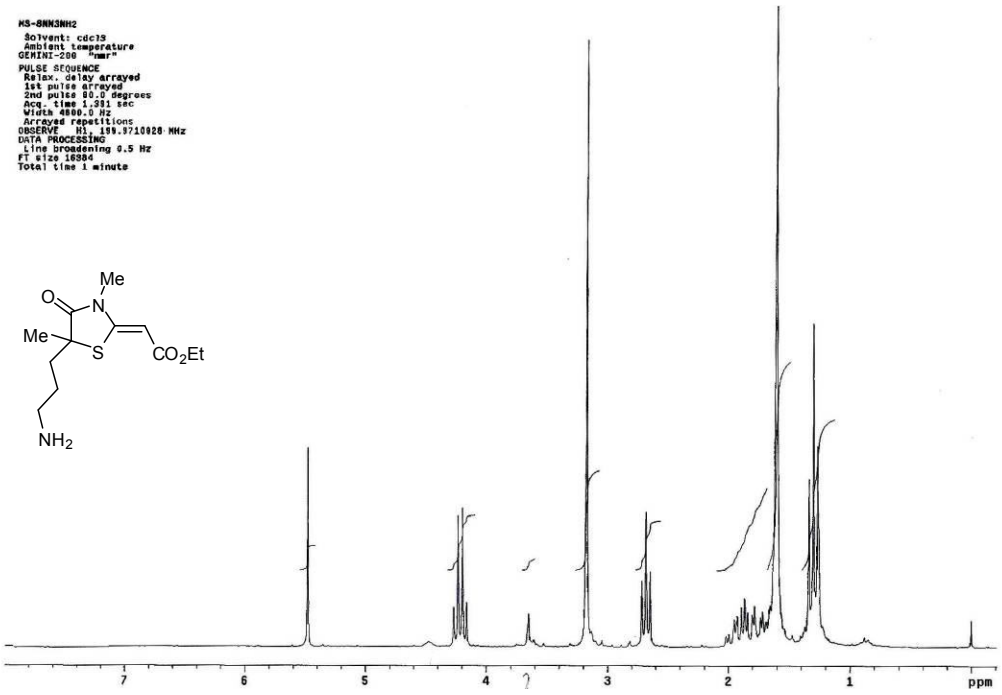
^{13}C NMR spectrum for **14** (50 MHz, $CDCl_3$)



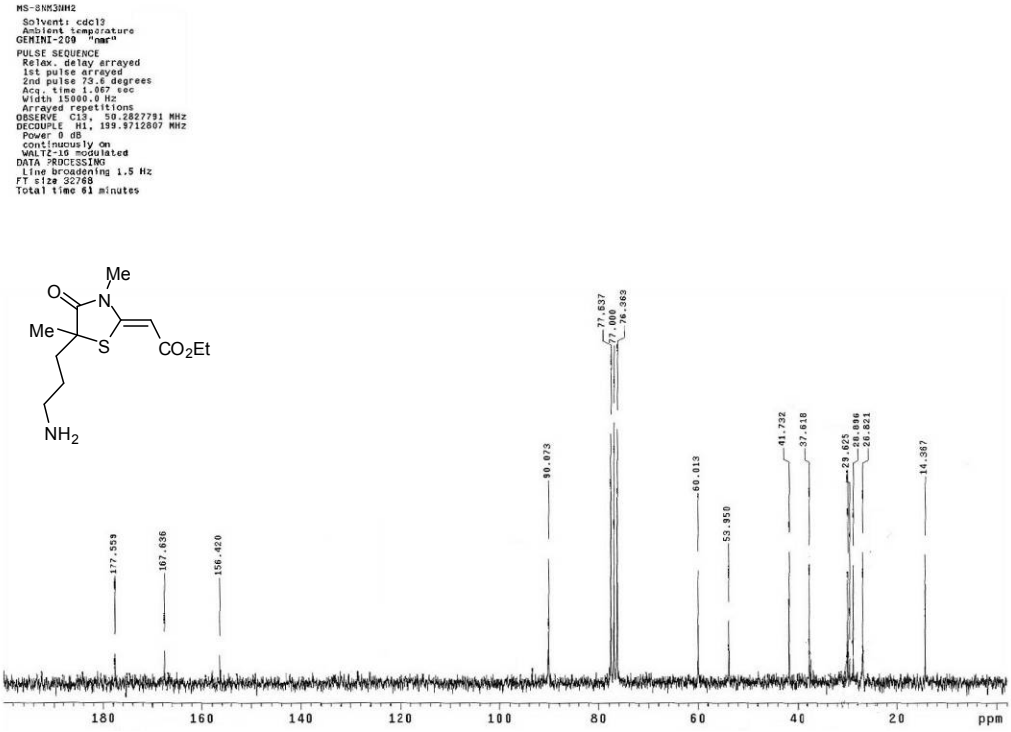
^{1}H NMR spectrum for **15** (200 MHz, $CDCl_3$)



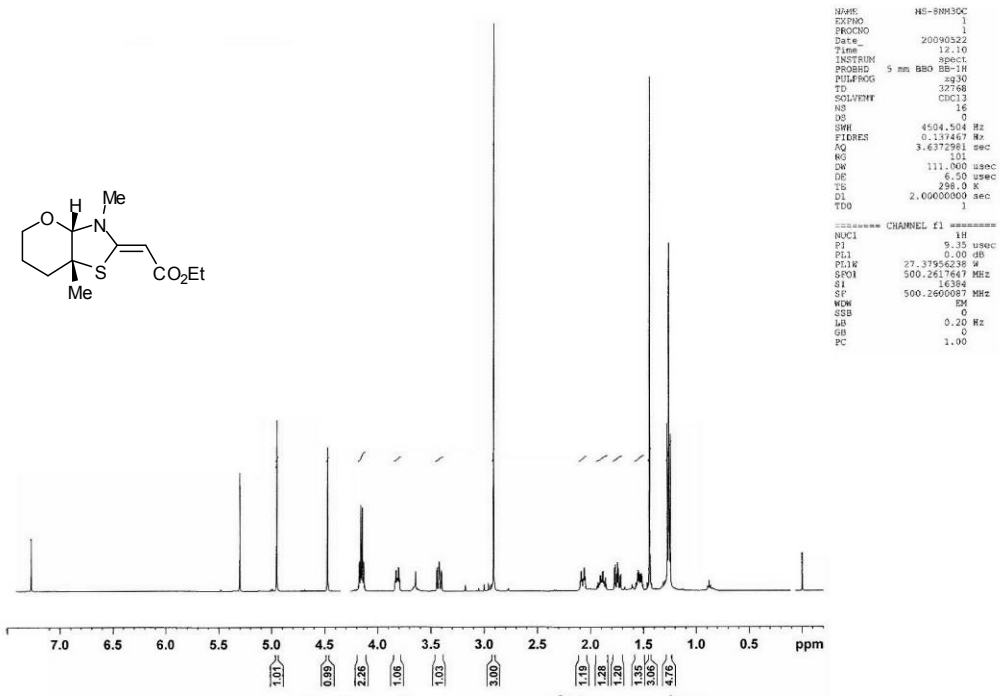
^{13}C NMR spectrum for **15** (50 MHz, $CDCl_3$)



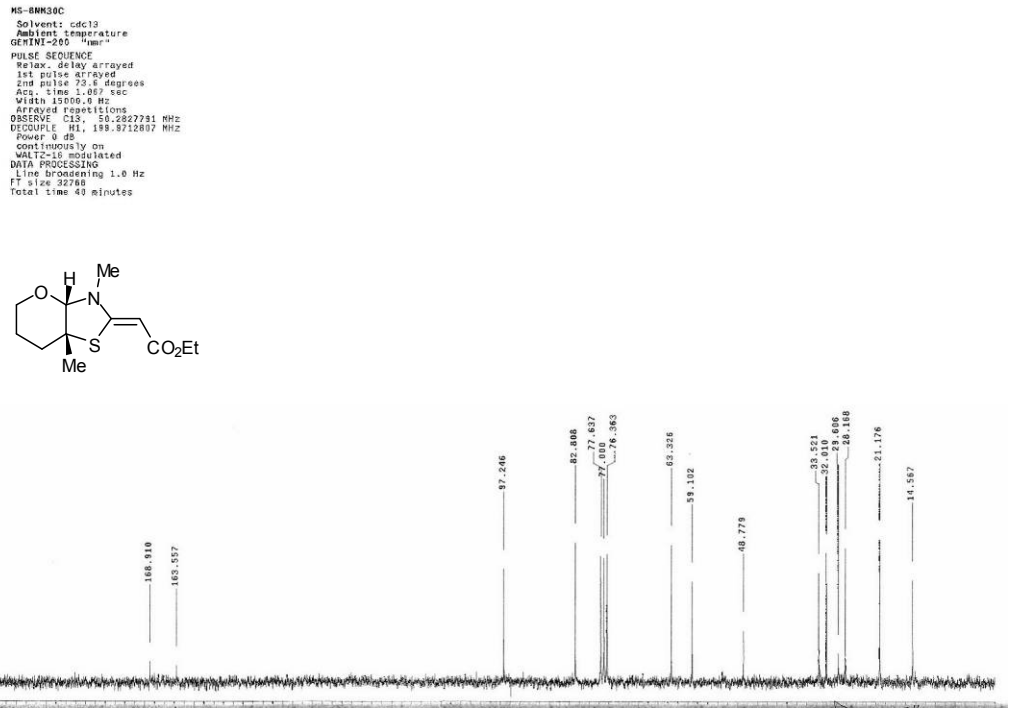
^{1}H NMR spectrum for **16** (200 MHz, $CDCl_3$)



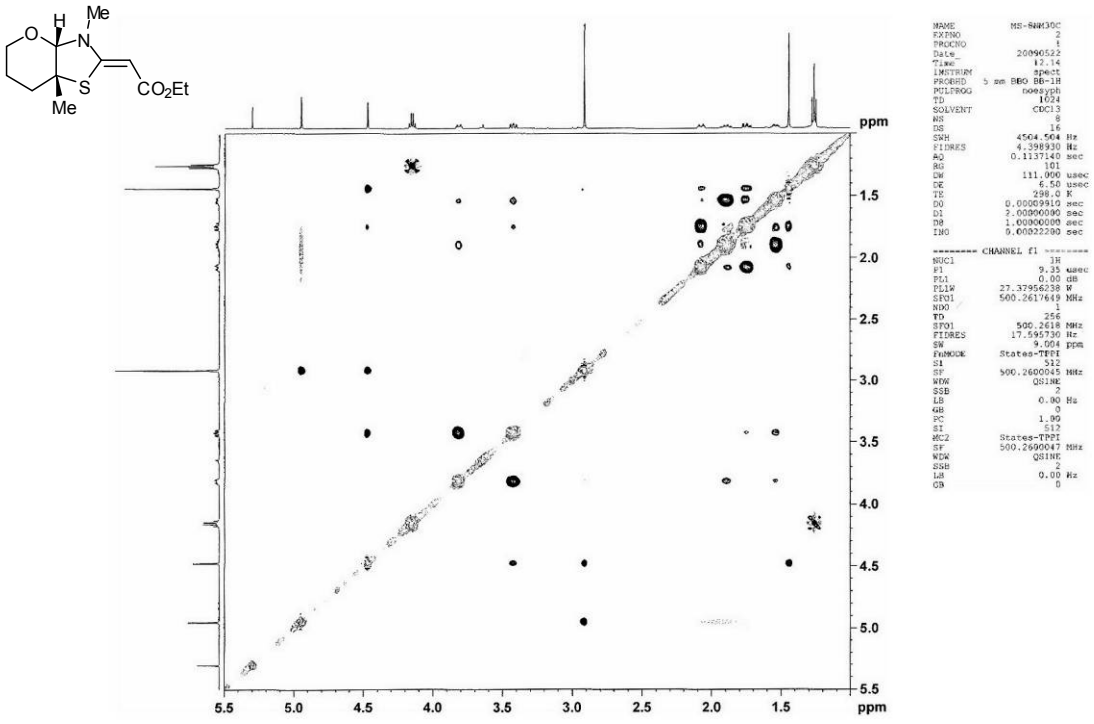
^{13}C NMR spectrum for **16** (50 MHz, $CDCl_3$)



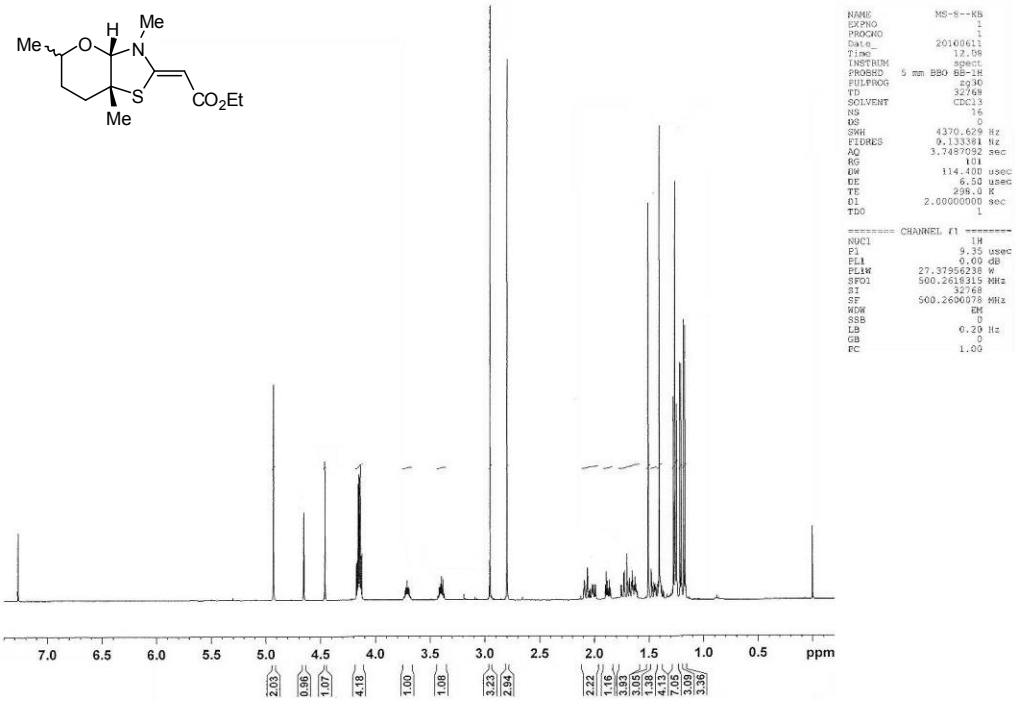
^{1}H NMR spectrum for **19a** (500 MHz, $CDCl_3$)



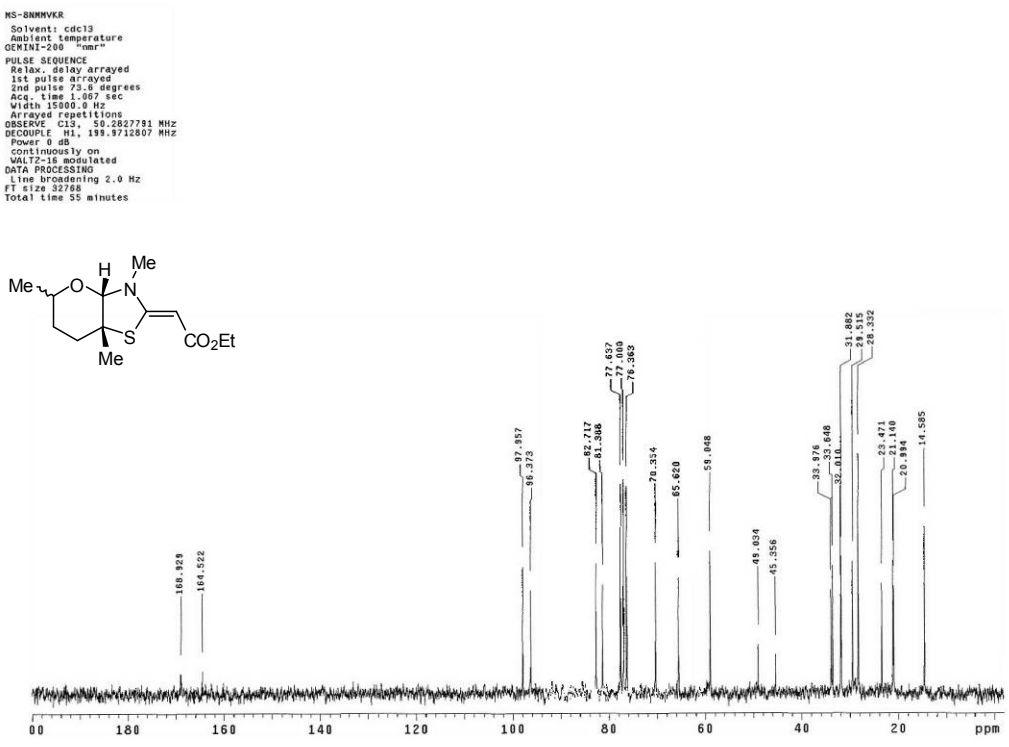
^{13}C NMR spectrum for **19a** (50 MHz, $CDCl_3$)



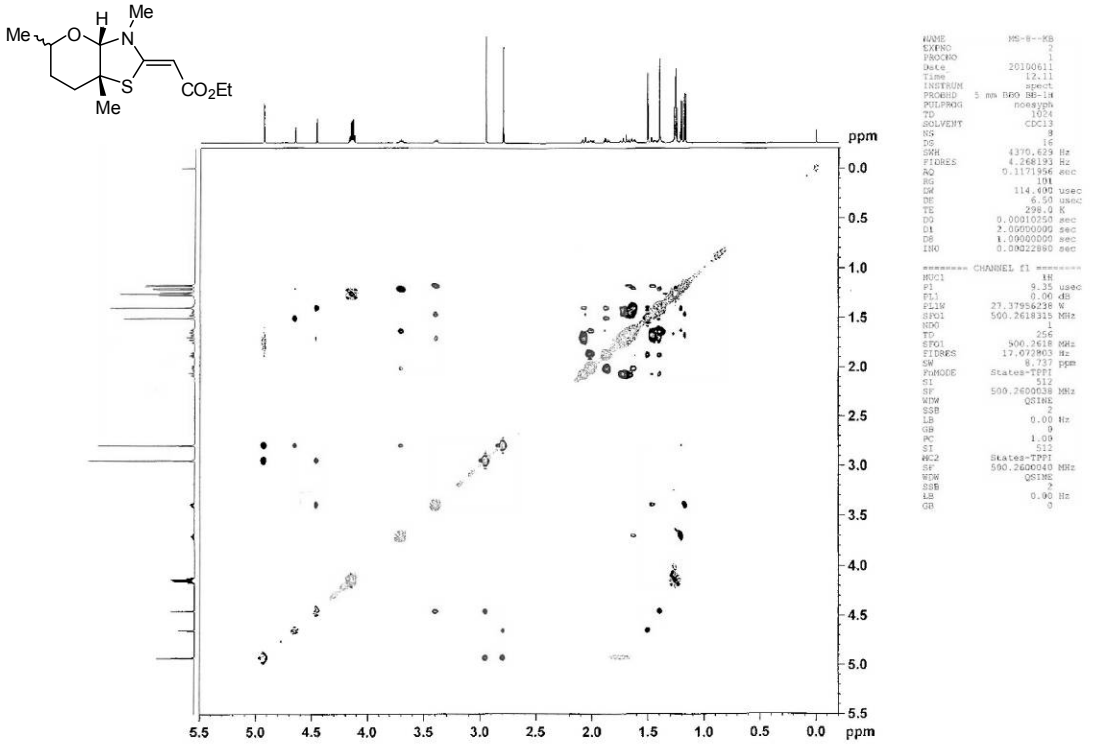
NOESY NMR spectrum for **19a** (500 MHz, $CDCl_3$)



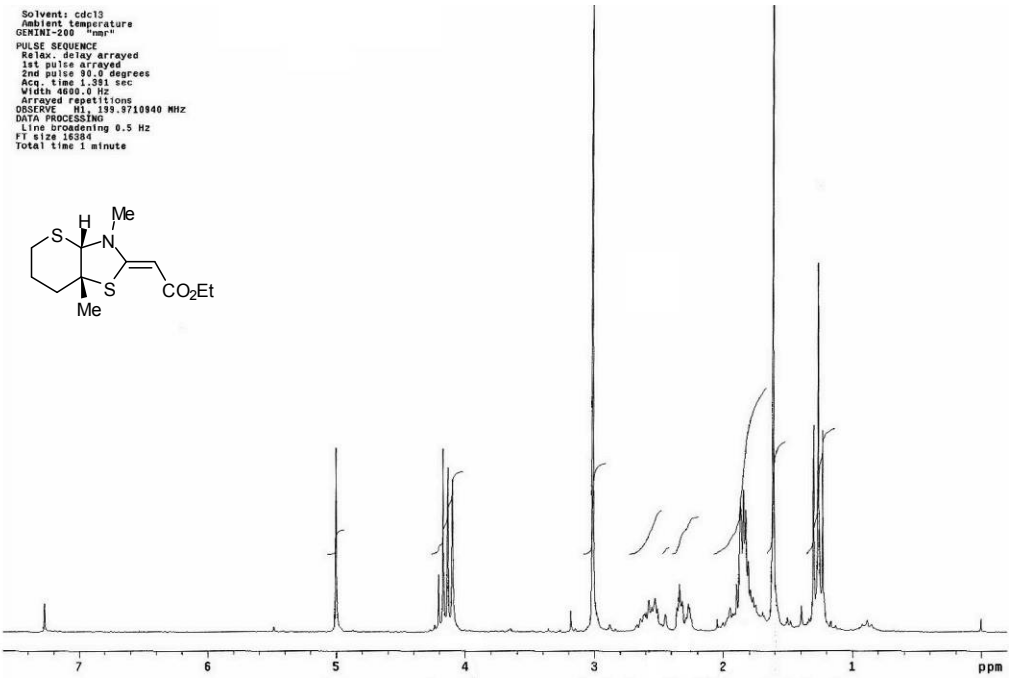
^{1}H NMR spectrum for mixture of ***cis***- and ***trans*-19b** (500 MHz, $CDCl_3$)



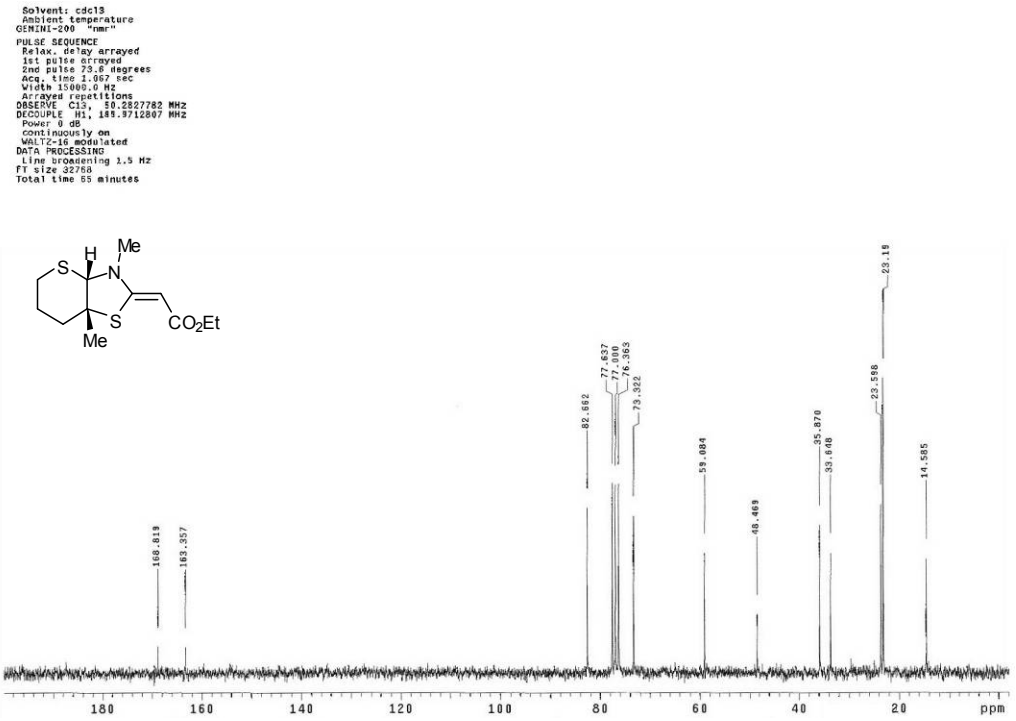
^{13}C NMR spectrum for mixture of ***cis*-** and ***trans*-19b** (50 MHz, $CDCl_3$)



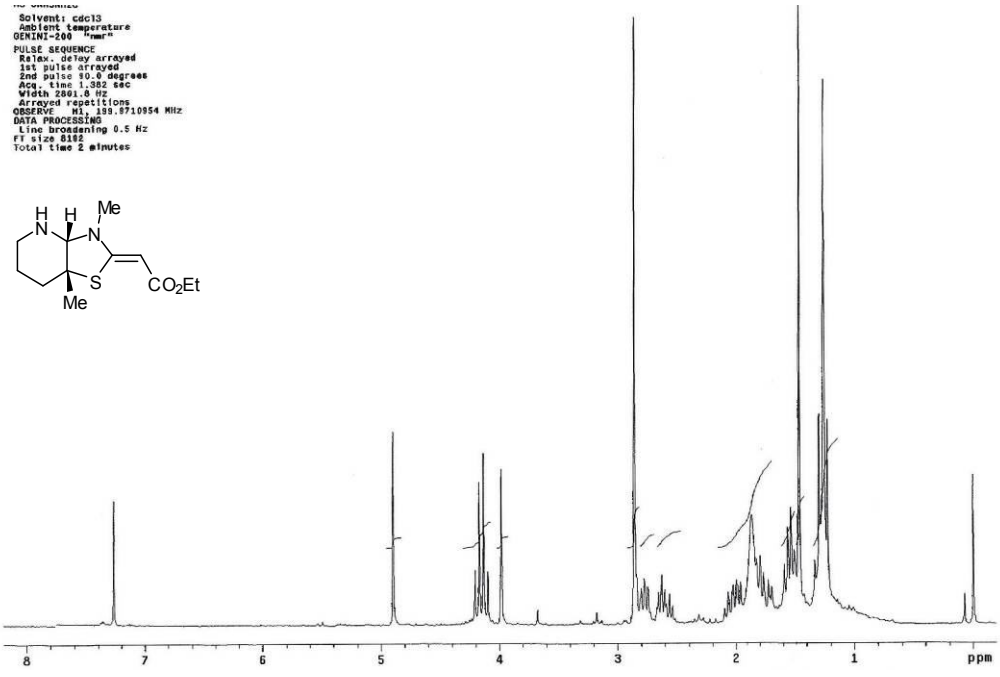
NOESY NMR spectrum for mixture of ***cis*-** and ***trans*-19b** (500 MHz, $CDCl_3$)



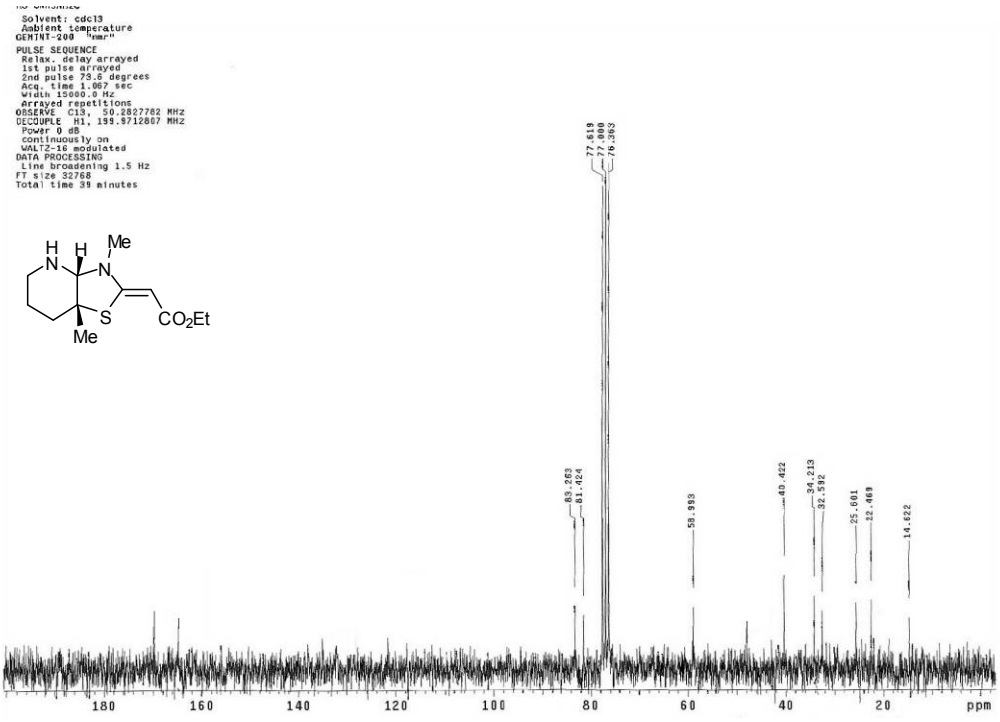
^{1}H NMR spectrum for **19c** (200 MHz, $CDCl_3$)



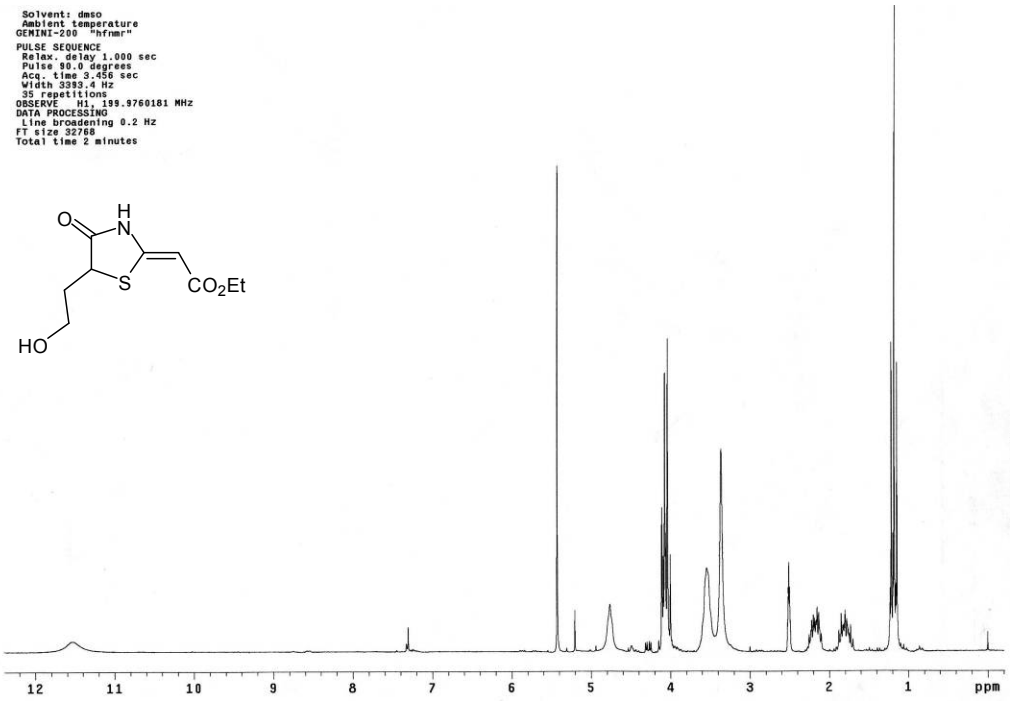
^{13}C NMR spectrum for **19c** (50 MHz, $CDCl_3$)



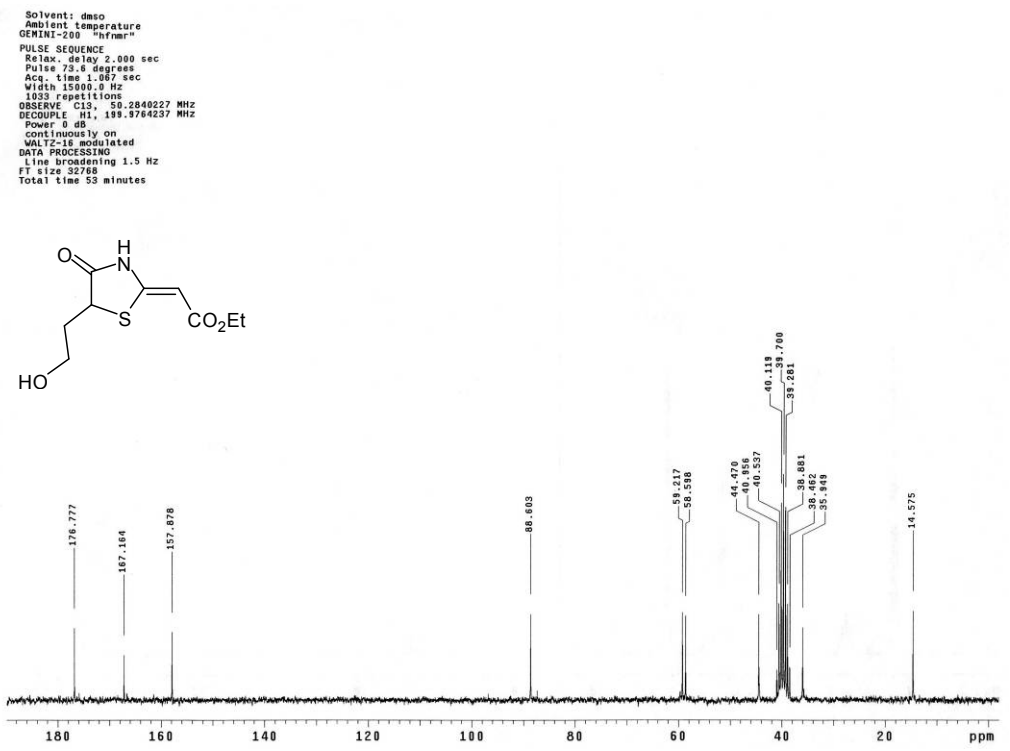
^{1}H NMR spectrum for **19d** (200 MHz, $CDCl_3$)



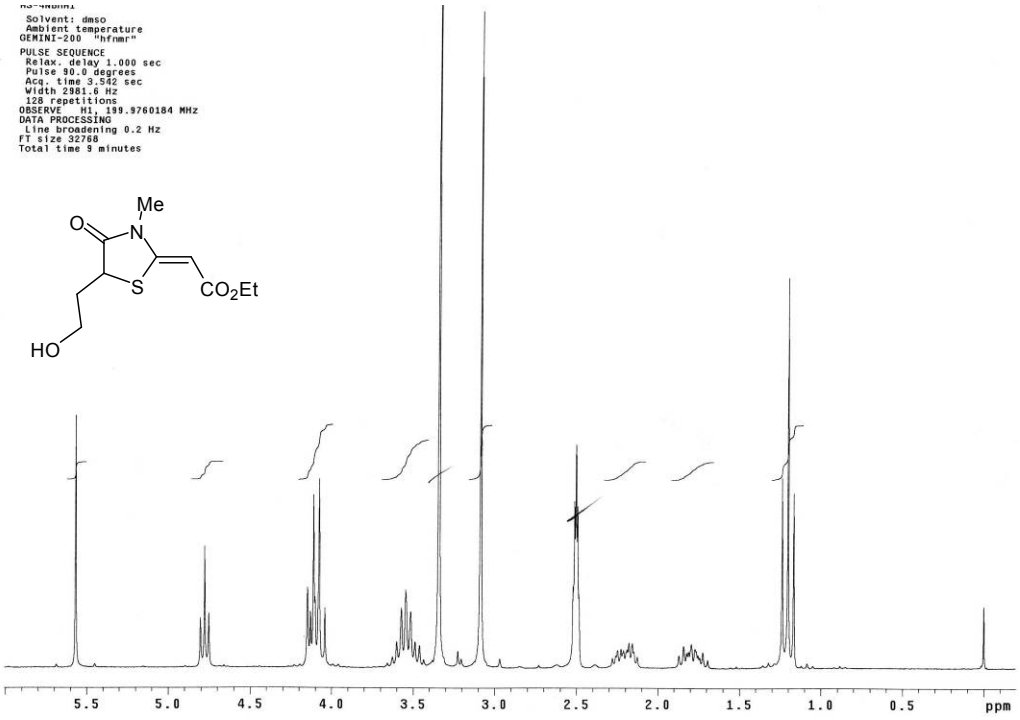
^{13}C NMR spectrum for **19d** (50 MHz, $CDCl_3$)



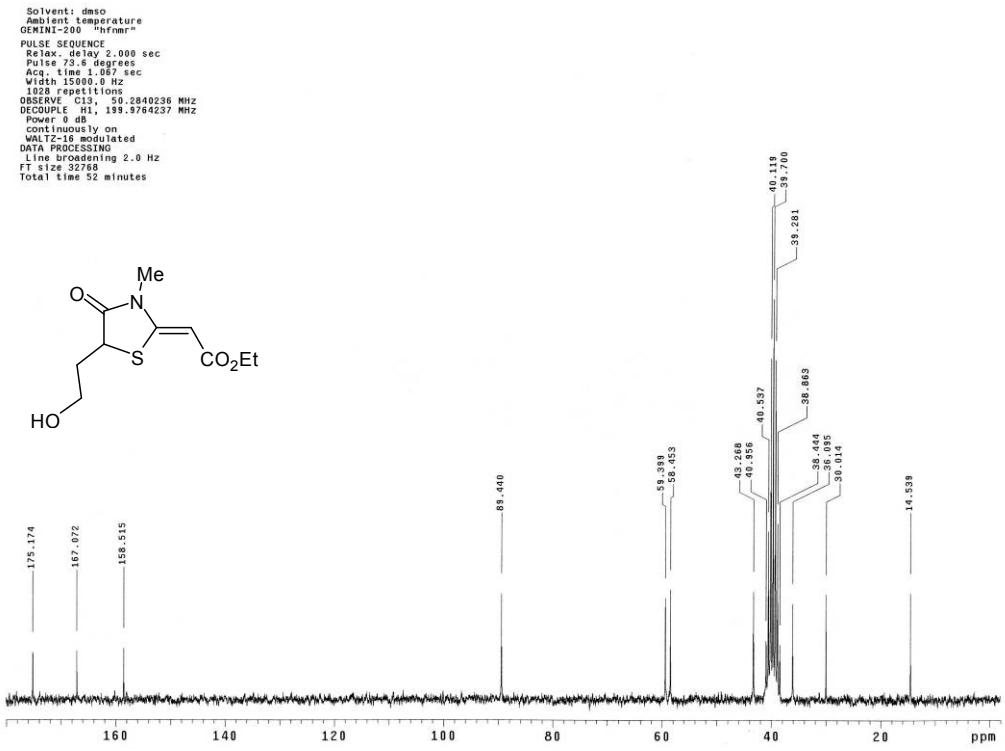
^{1}H NMR spectrum for **21** (200 MHz, DMSO-d_6)



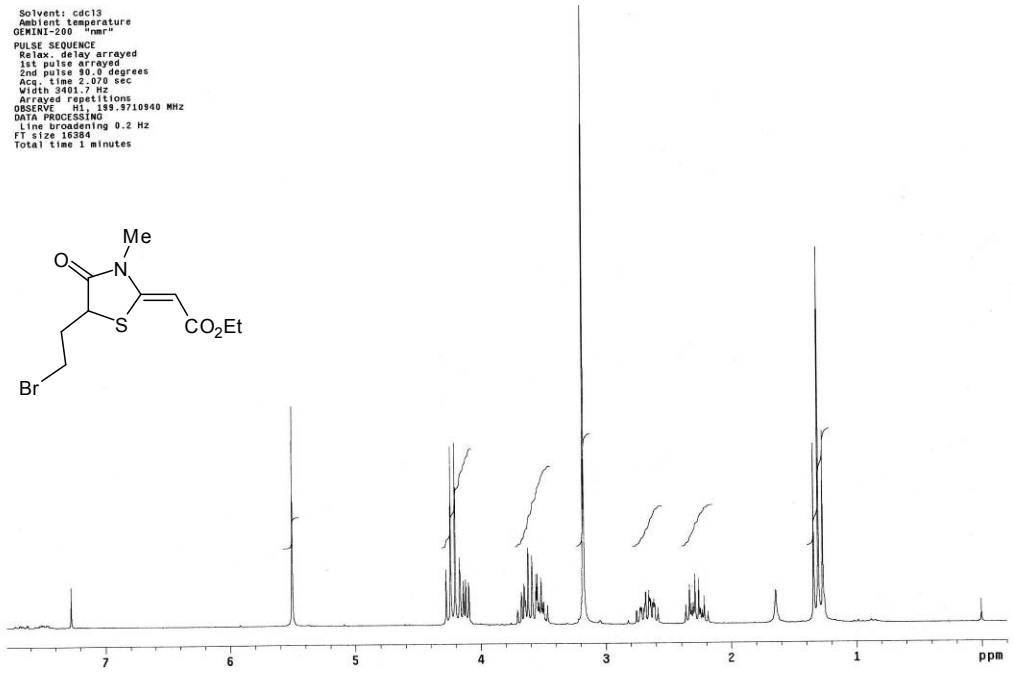
^{13}C NMR spectrum for **21** (50 MHz, DMSO-d_6)



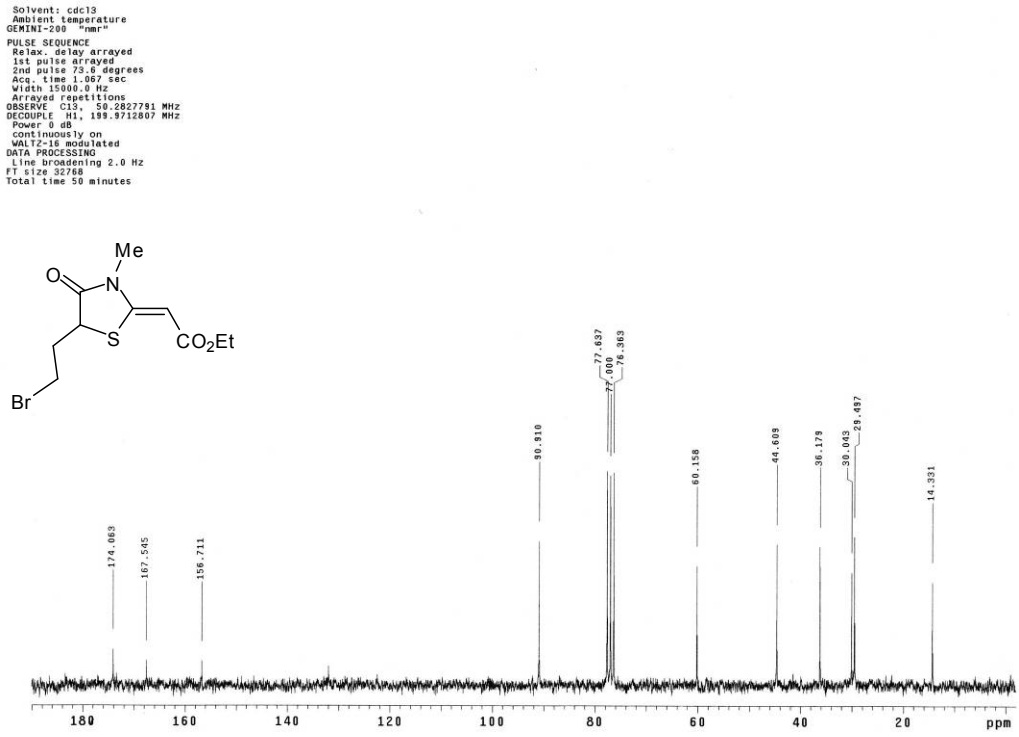
^{1}H NMR spectrum for **22** (200 MHz, DMSO-d_6)



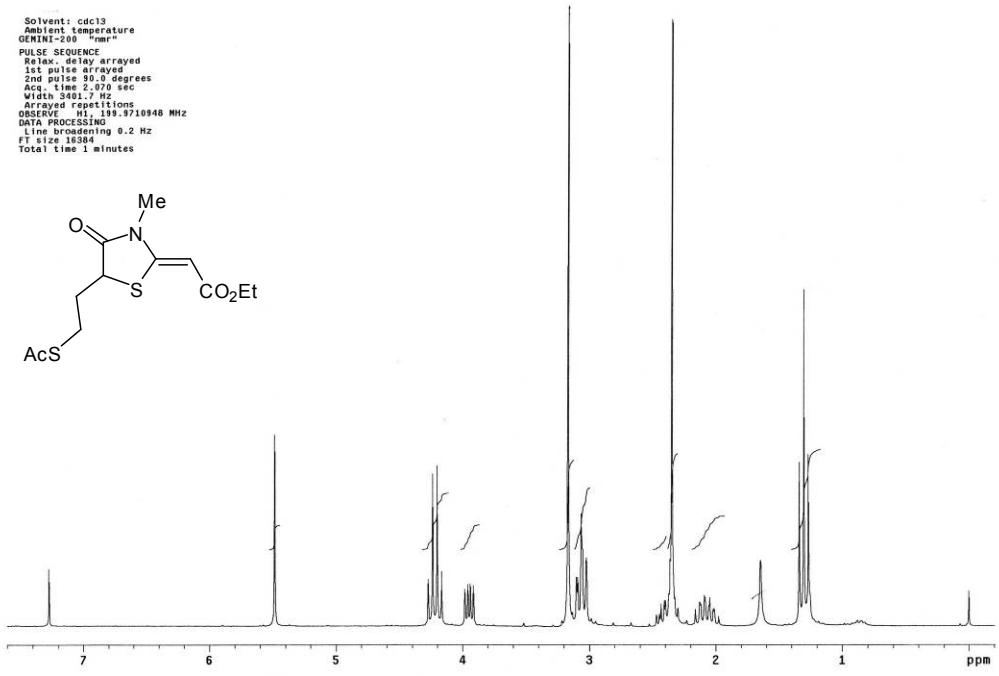
^{13}C NMR spectrum for **22** (50 MHz, DMSO-d_6)



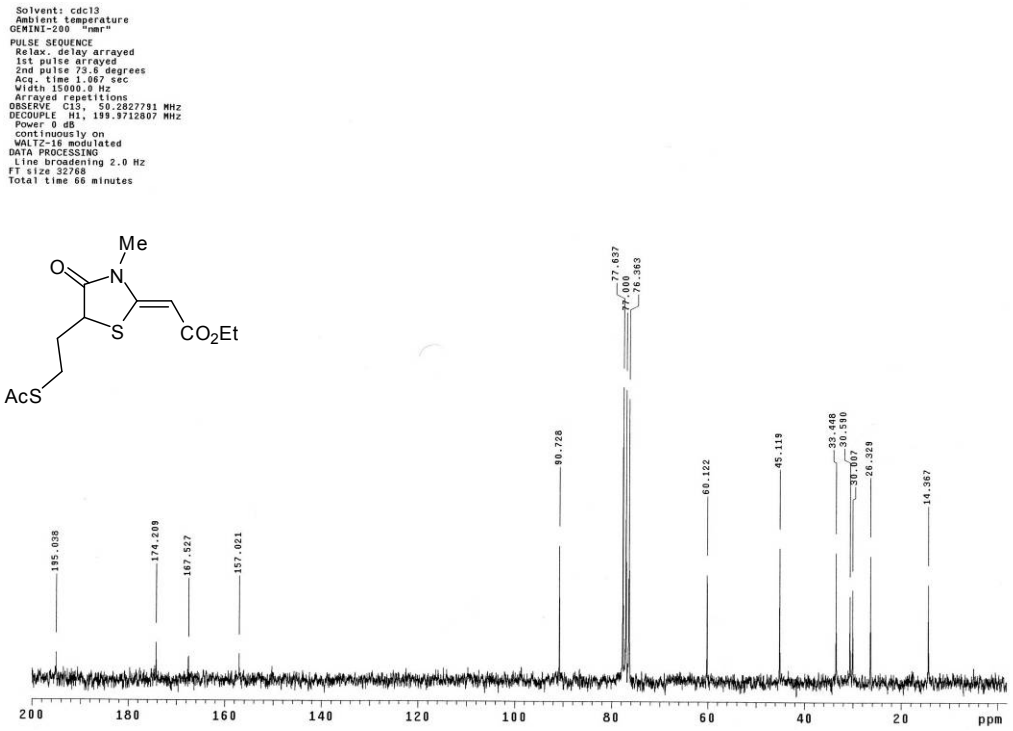
^{1}H NMR spectrum for **23** (200 MHz, $CDCl_3$)



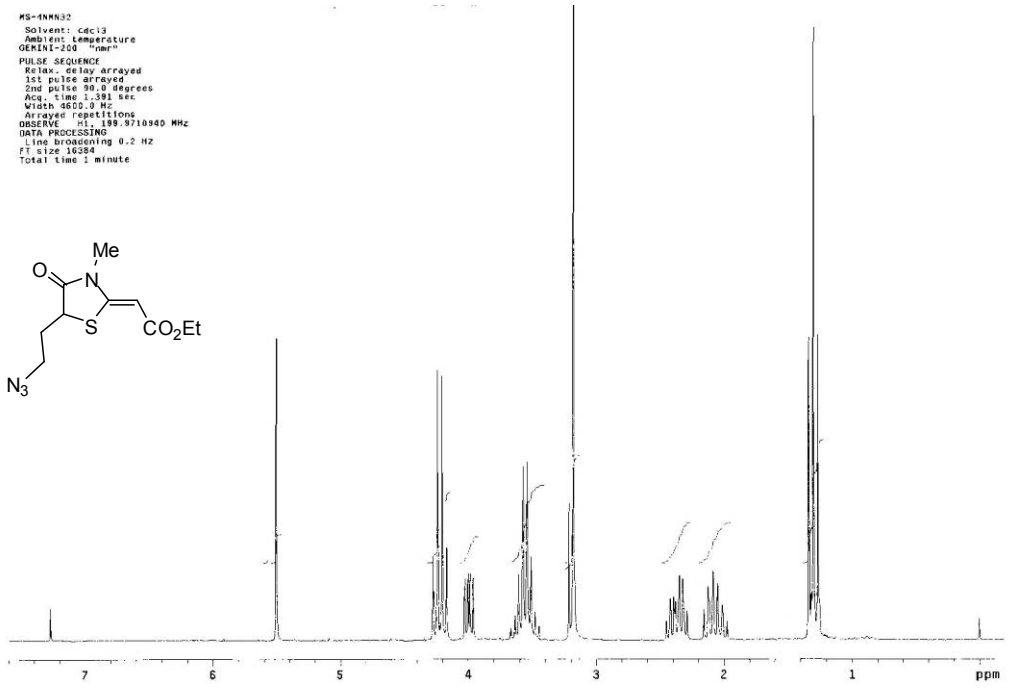
^{13}C NMR spectrum for **23** (50 MHz, $CDCl_3$)



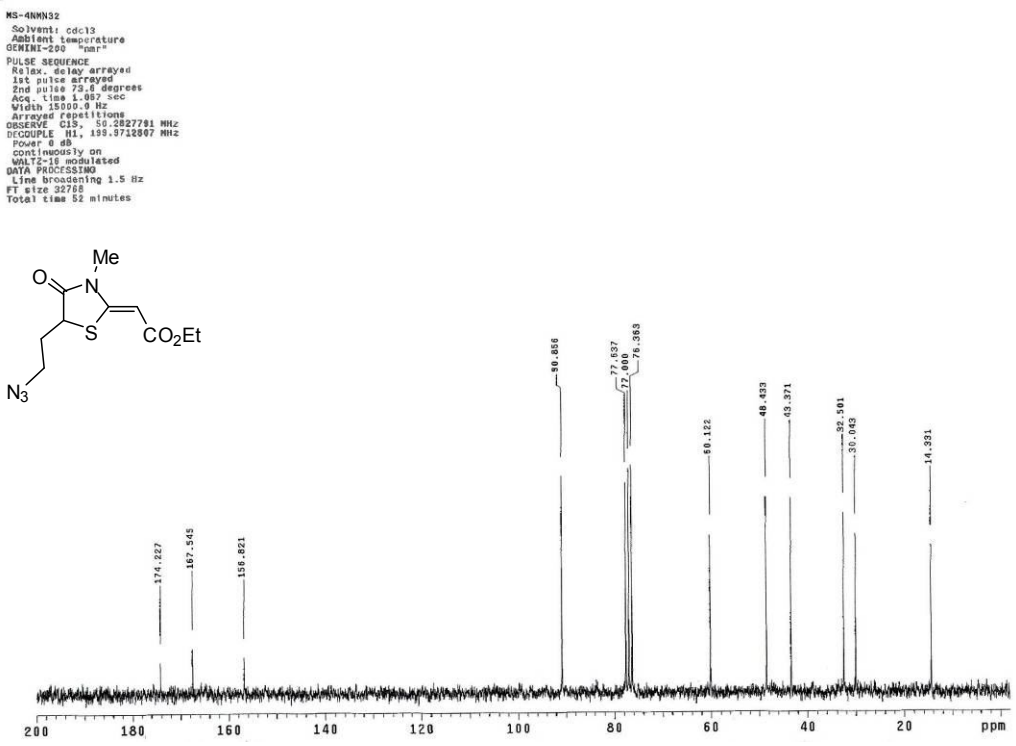
^{1}H NMR spectrum for **24** (200 MHz, $CDCl_3$)



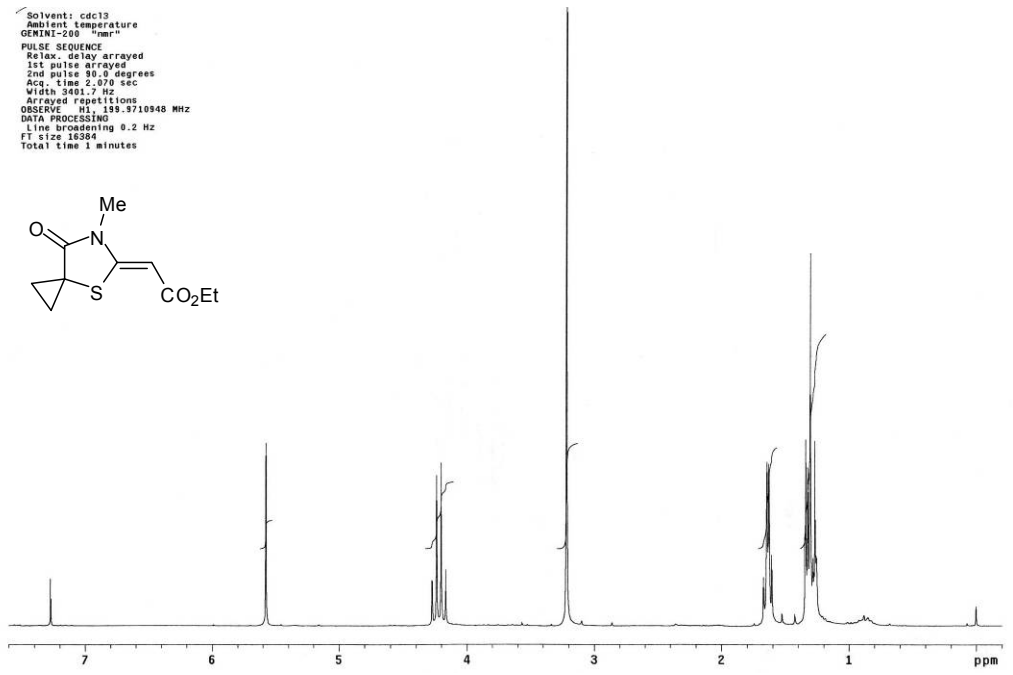
^{13}C NMR spectrum for **24** (50 MHz, $CDCl_3$)



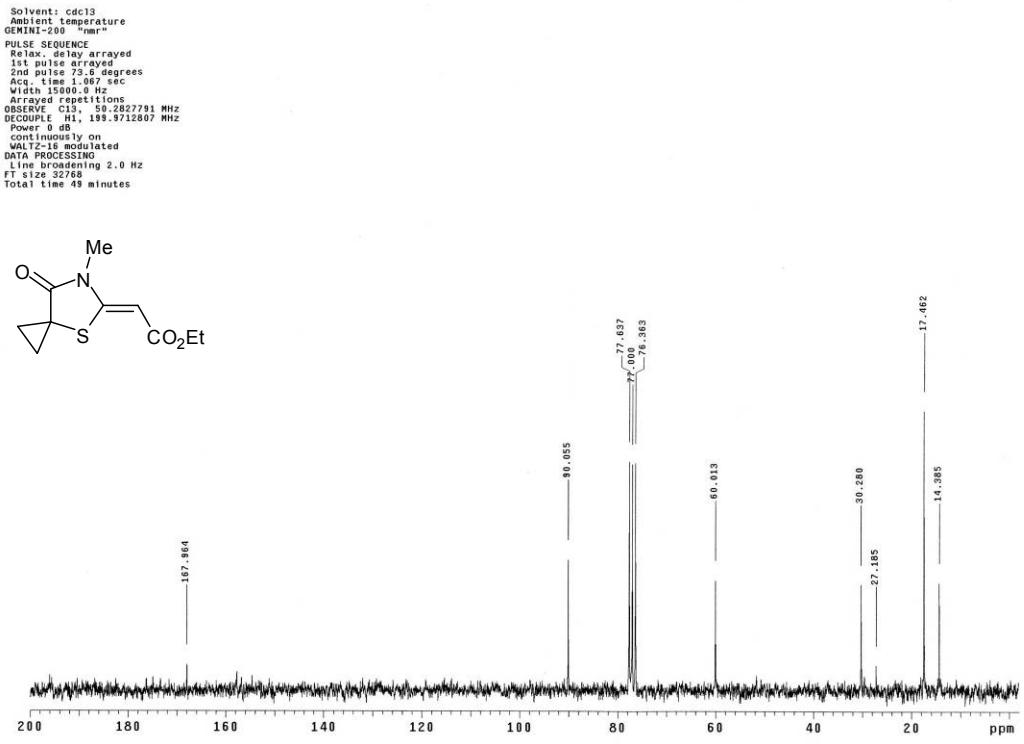
^{1}H NMR spectrum for **25** (200 MHz, $CDCl_3$)



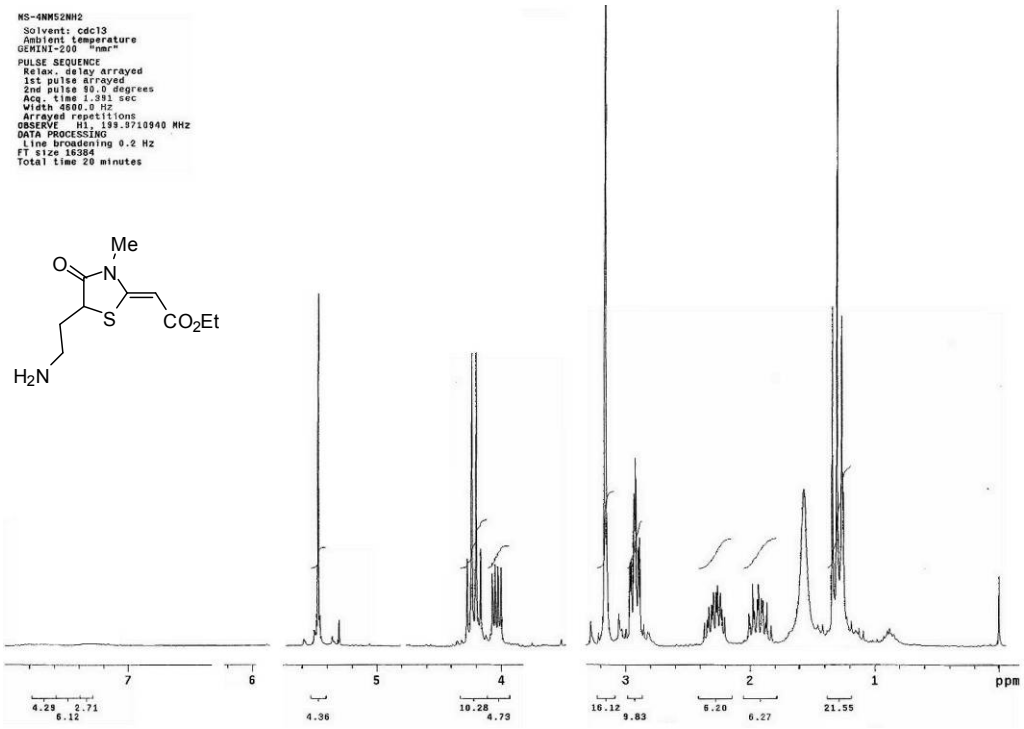
^{13}C NMR spectrum for **25** (50 MHz, $CDCl_3$)



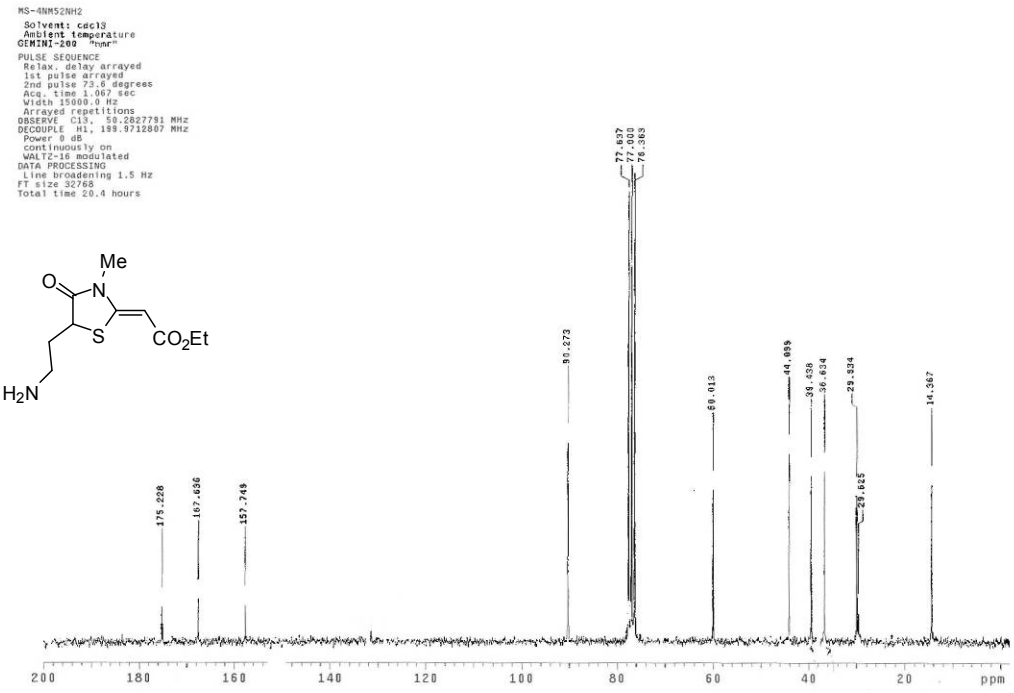
^{1}H NMR spectrum for **26** (200 MHz, $CDCl_3$)



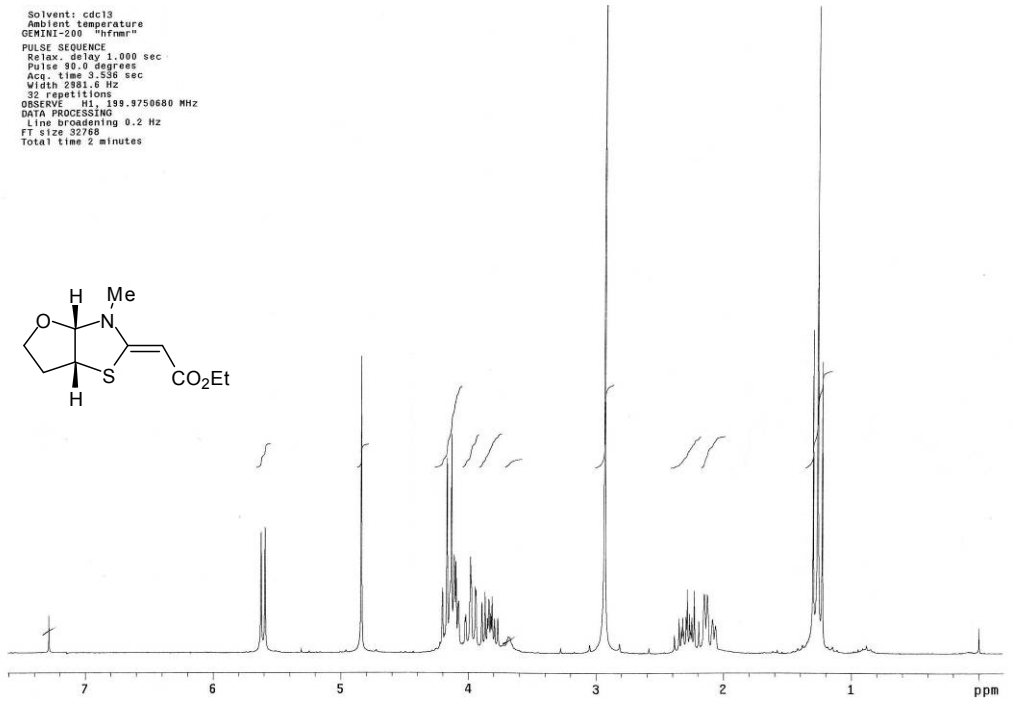
^{13}C NMR spectrum for **26** (50 MHz, $CDCl_3$)



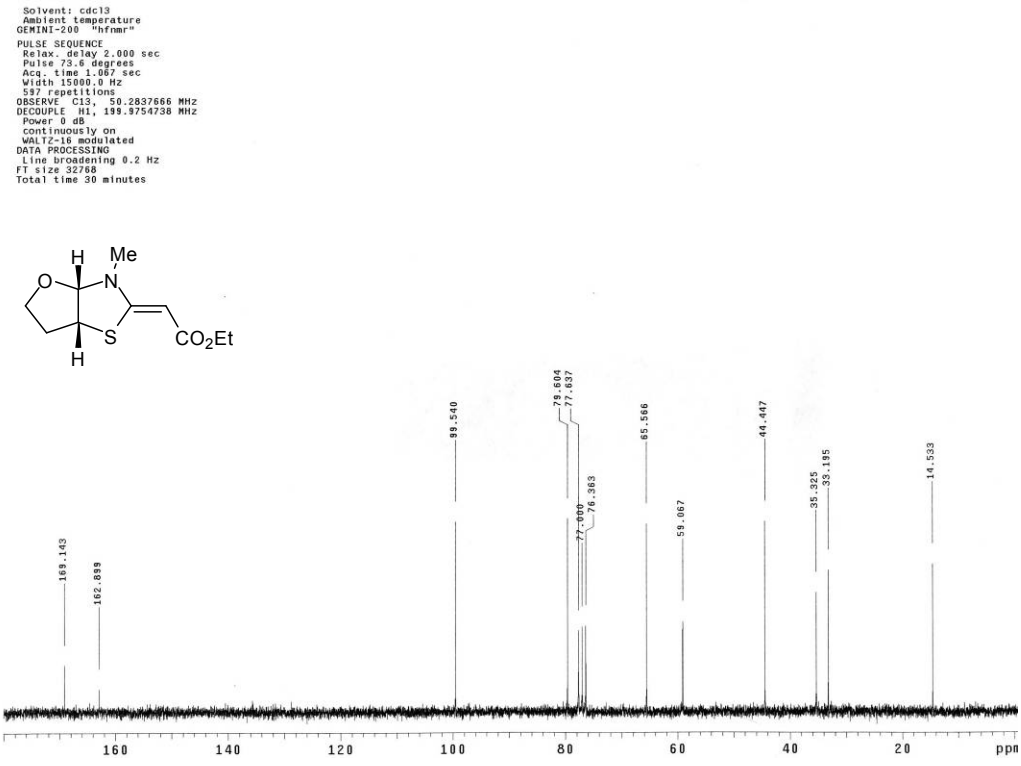
^{1}H NMR spectrum for **27** (200 MHz, $CDCl_3$)



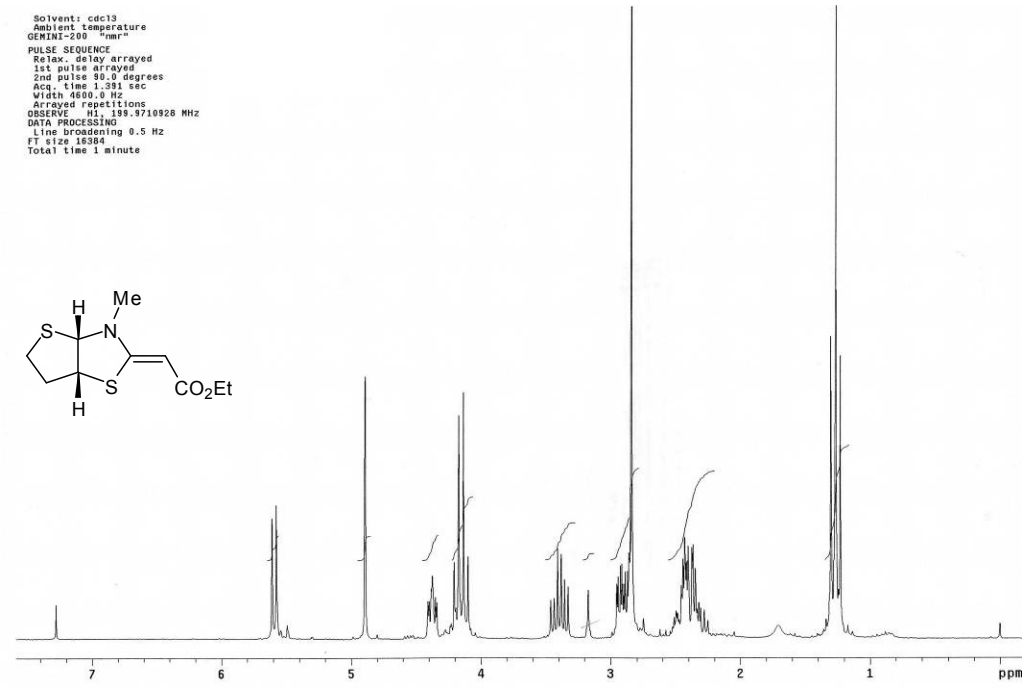
^{13}C NMR spectrum for **27** (50 MHz, $CDCl_3$)



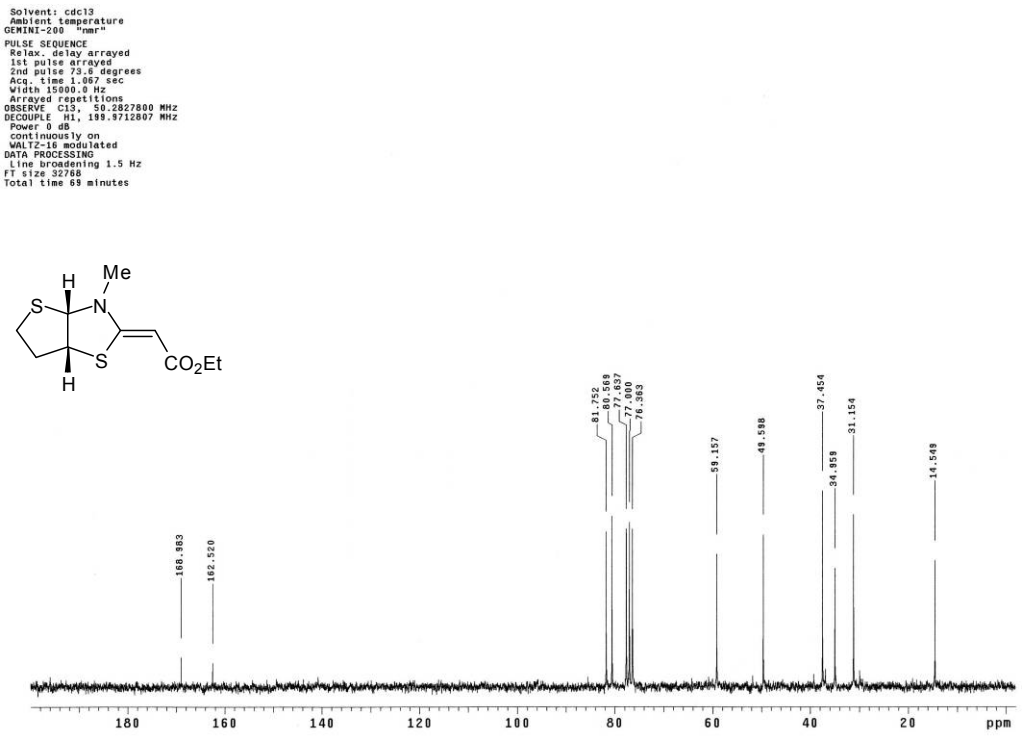
^{1}H NMR spectrum for **29a** (200 MHz, $CDCl_3$)



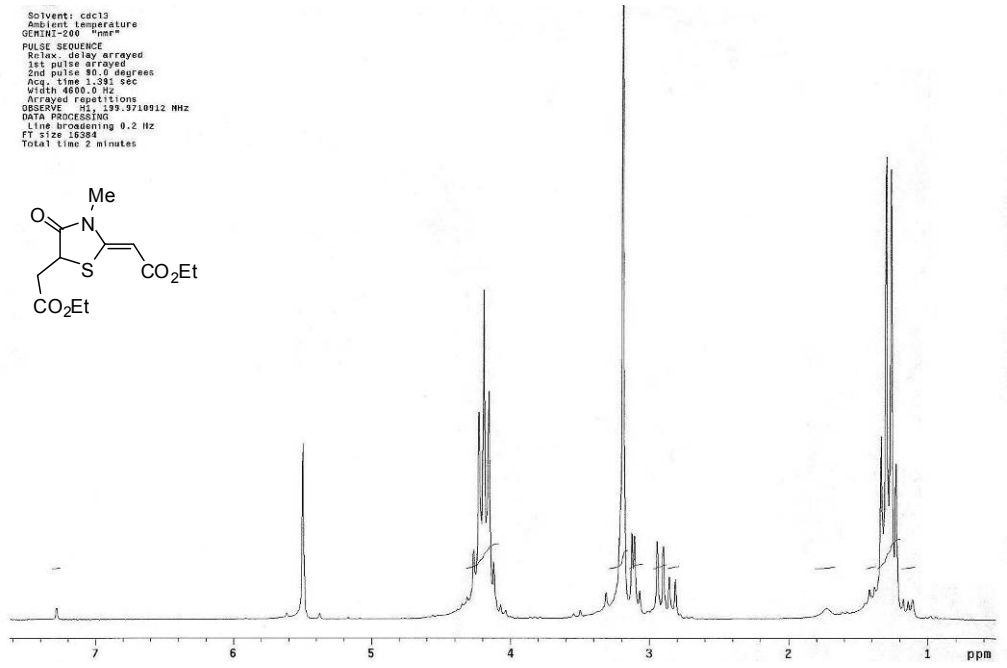
^{13}C NMR spectrum for **29a** (50 MHz, $CDCl_3$)



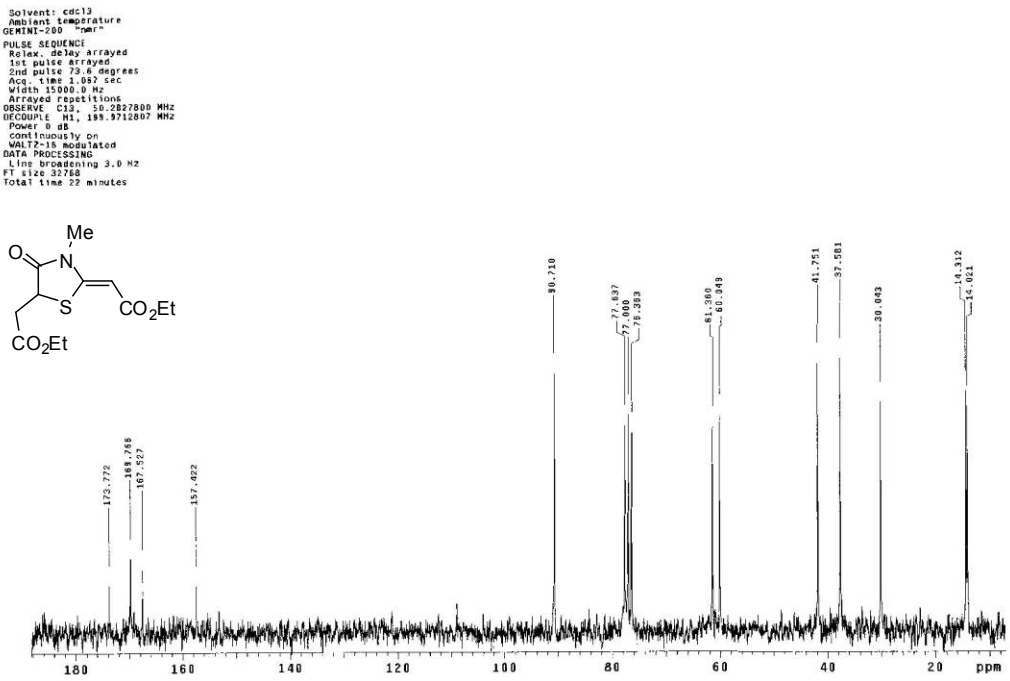
^{13}H NMR spectrum for **29b** (200 MHz, $CDCl_3$)



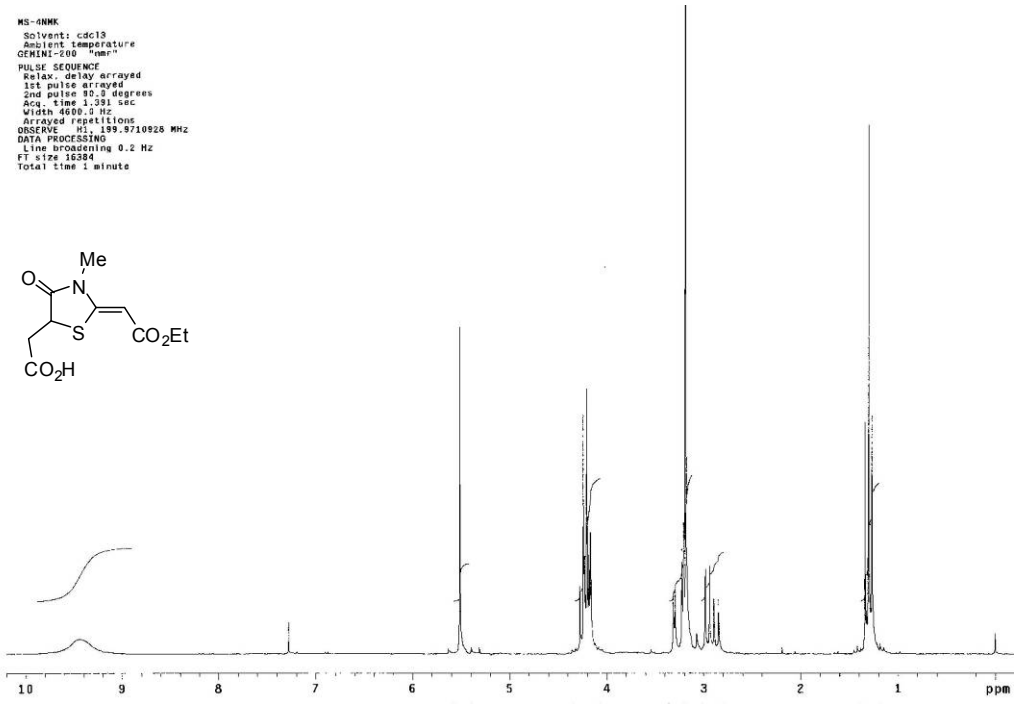
^{13}C NMR spectrum for **29b** (50 MHz, $CDCl_3$)



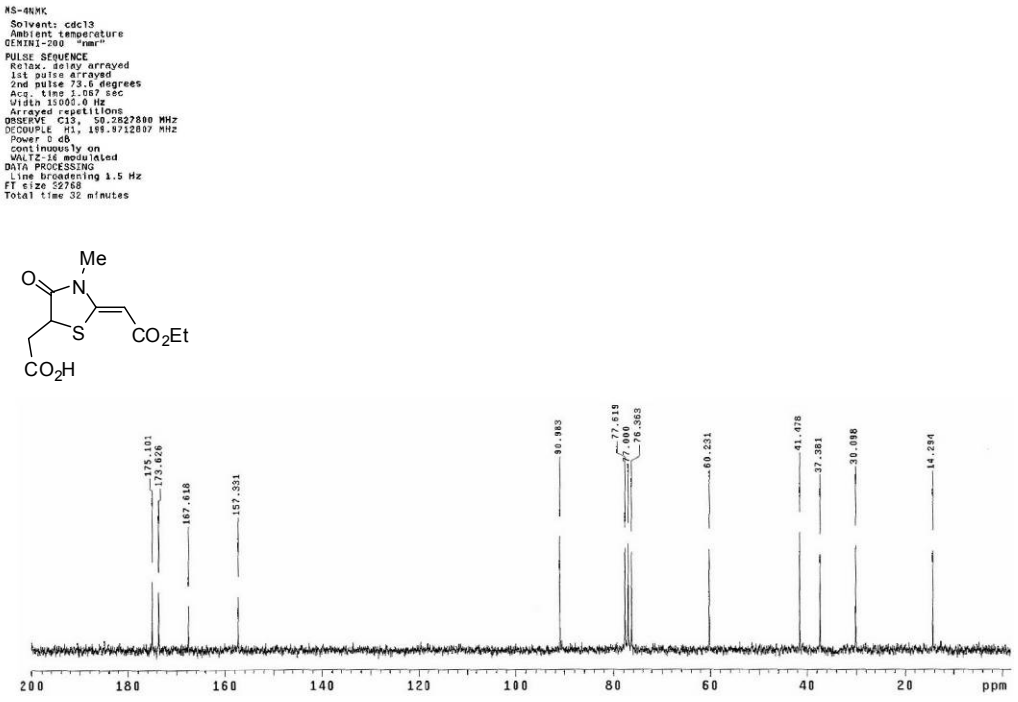
^{1}H NMR spectrum for **30** (200 MHz, $CDCl_3$)



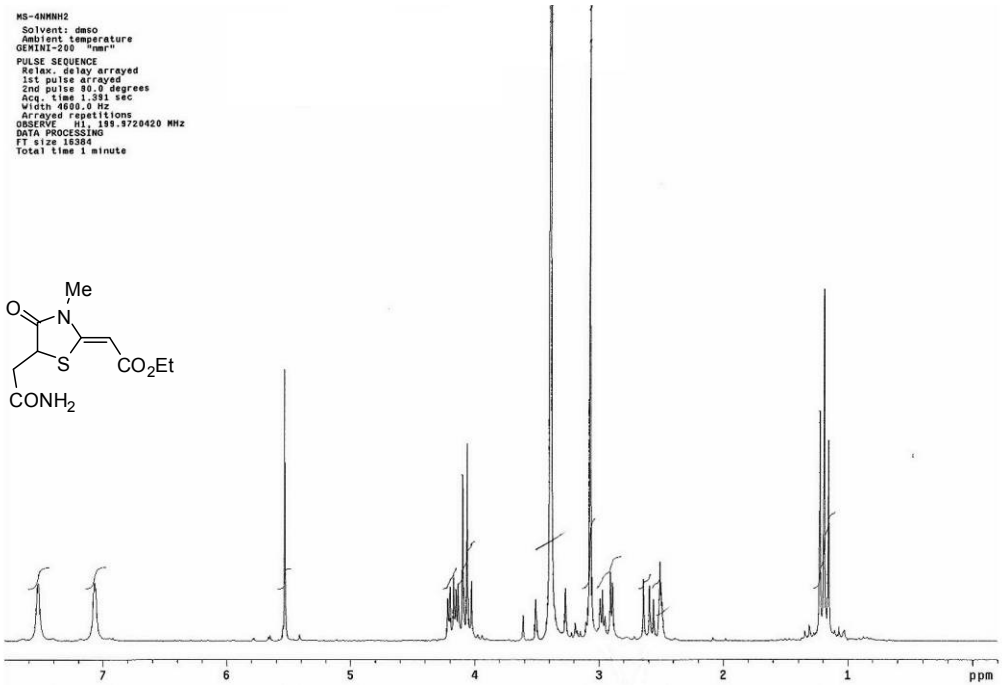
^{13}C NMR spectrum for **30** (50 MHz, $CDCl_3$)



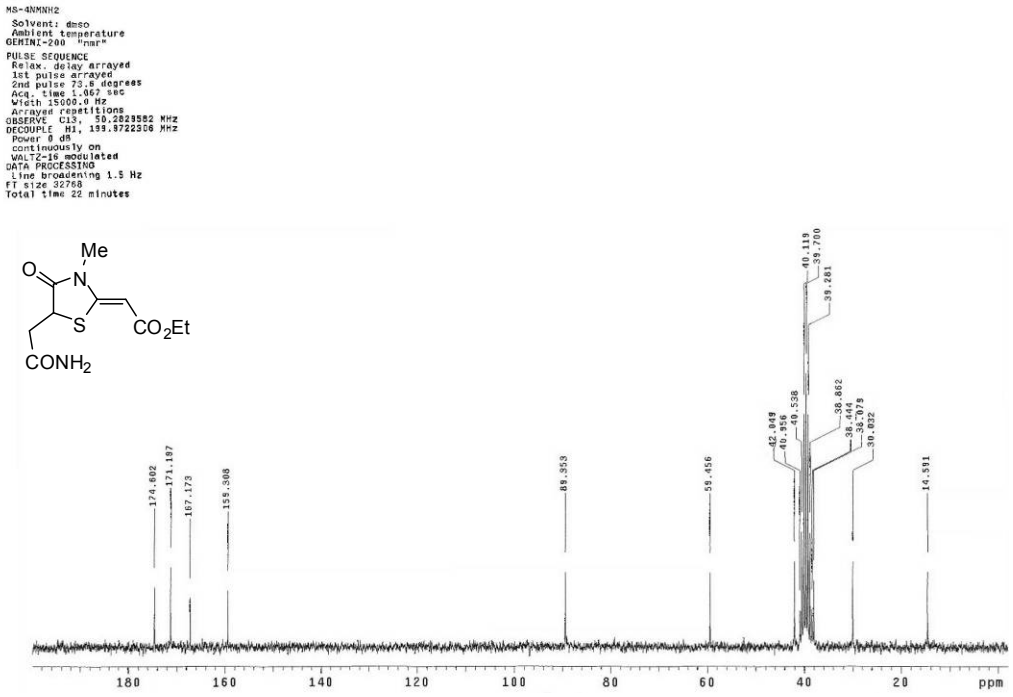
^{1}H NMR spectrum for **31** (200 MHz, $CDCl_3$)



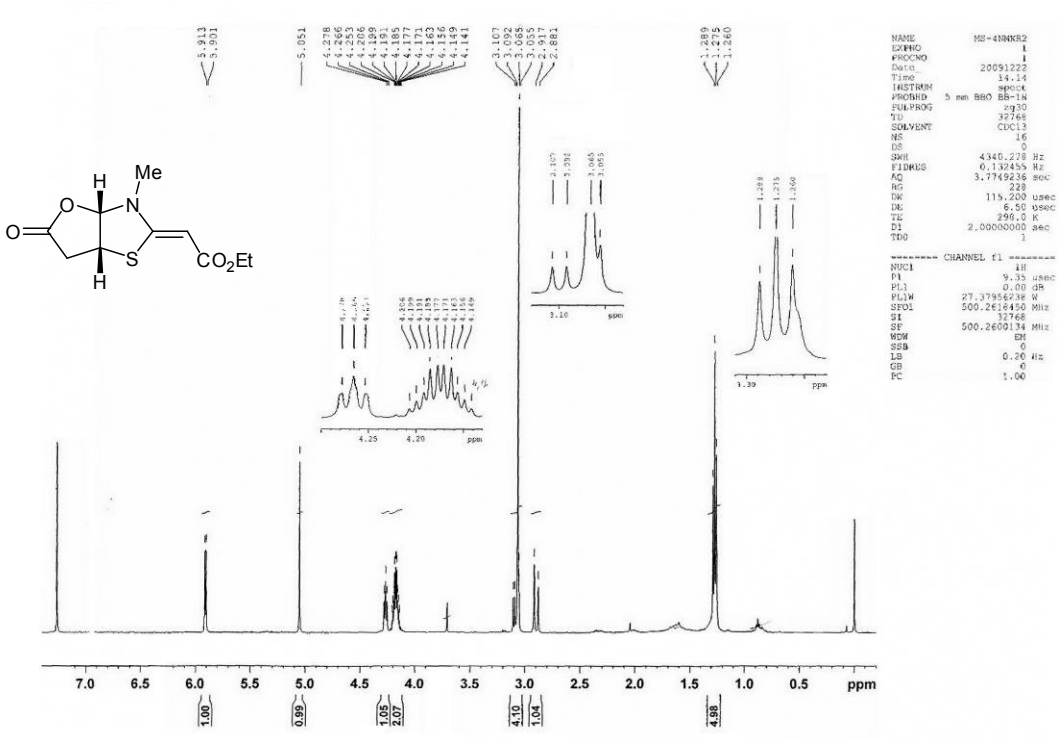
^{13}C NMR spectrum for **31** (50 MHz, $CDCl_3$)



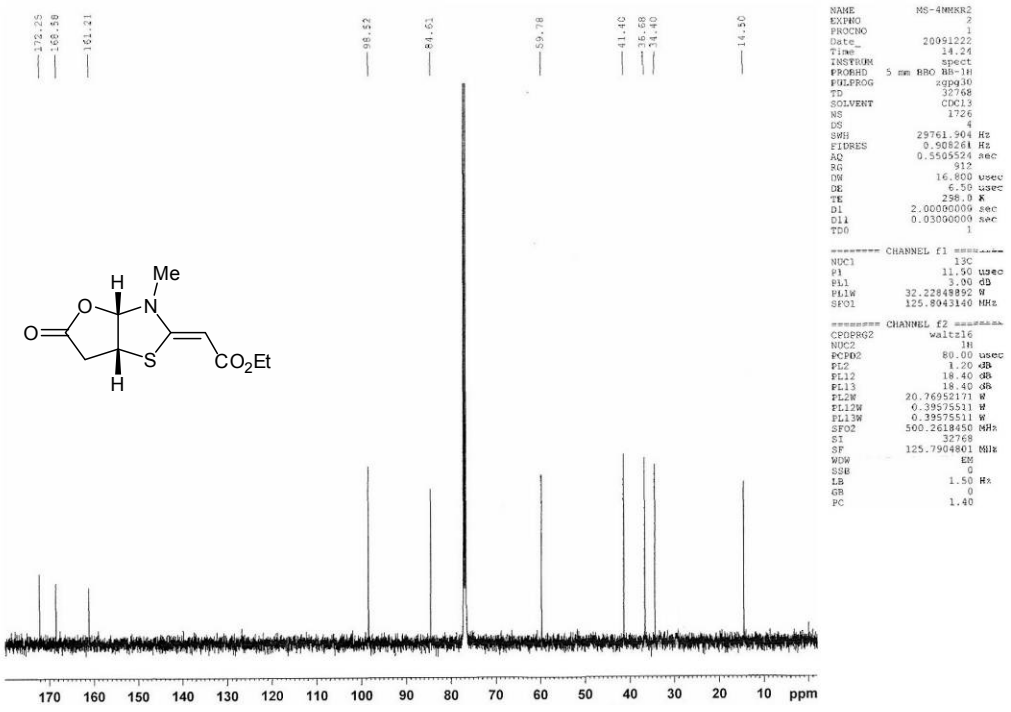
^{1}H NMR spectrum for **32** (50 MHz, DMSO-d_6)



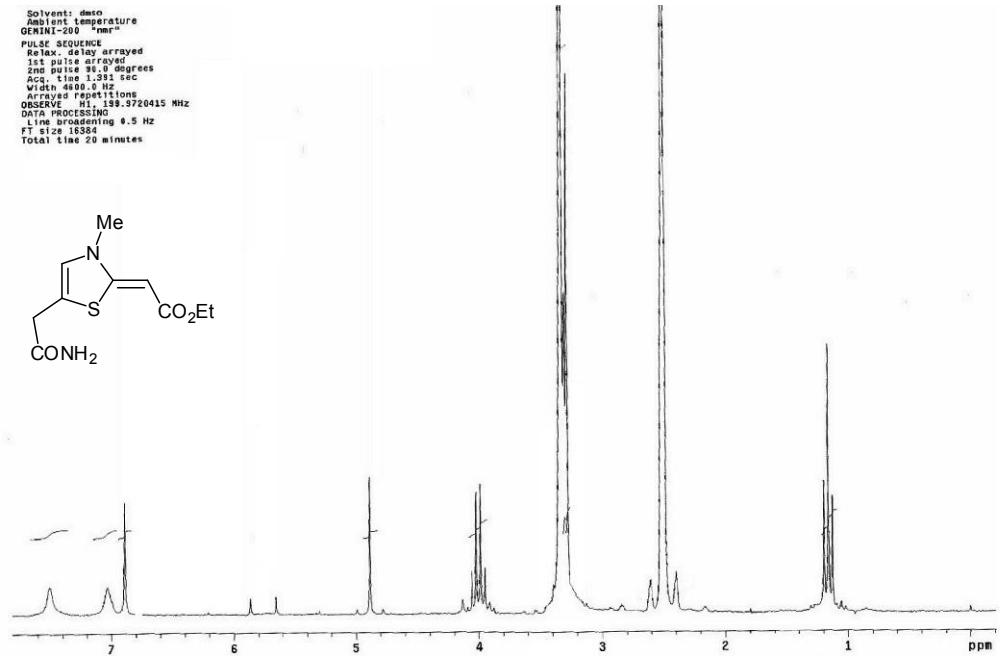
^{13}C NMR spectrum for **32** (50 MHz, DMSO-d_6)



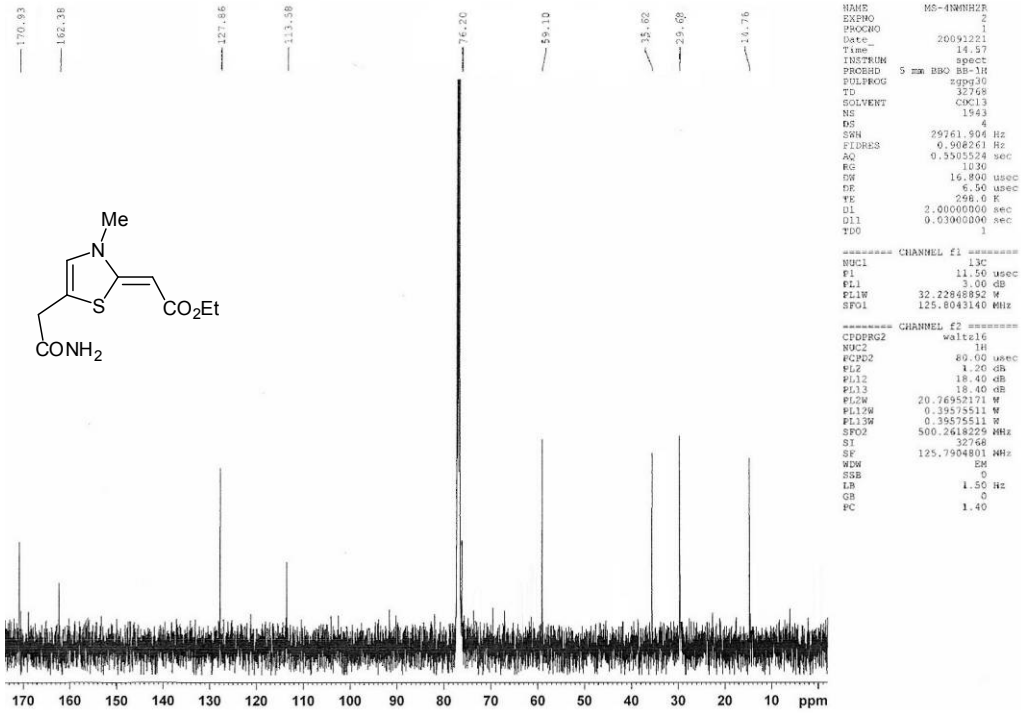
^{1}H NMR spectrum for **33** (500 MHz, $CDCl_3$)



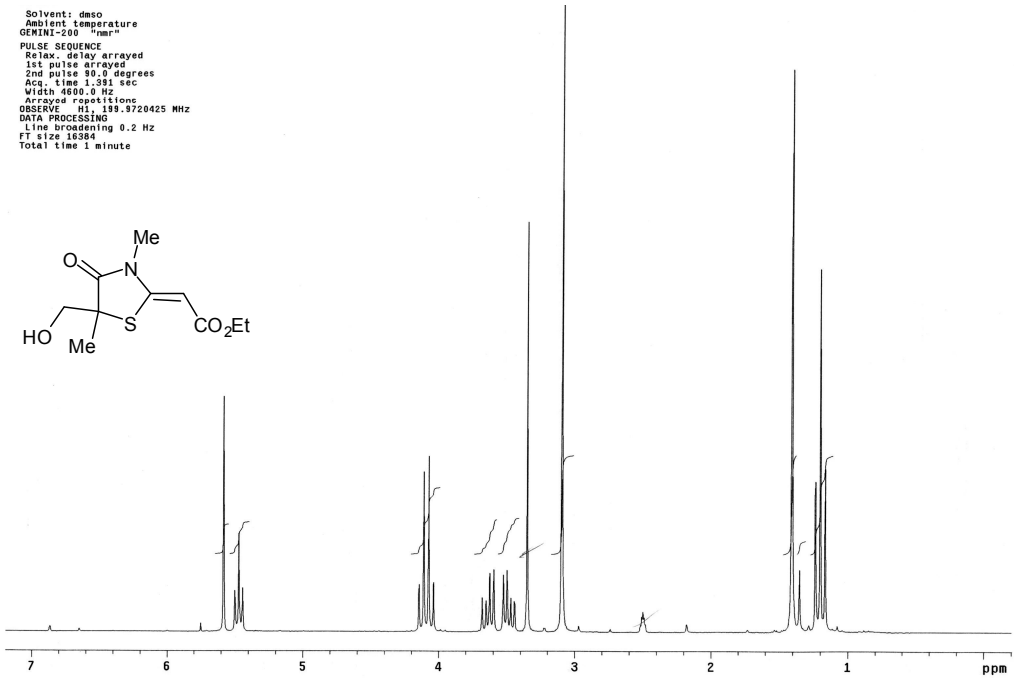
^{13}C NMR spectrum for **33** (125 MHz, $CDCl_3$)



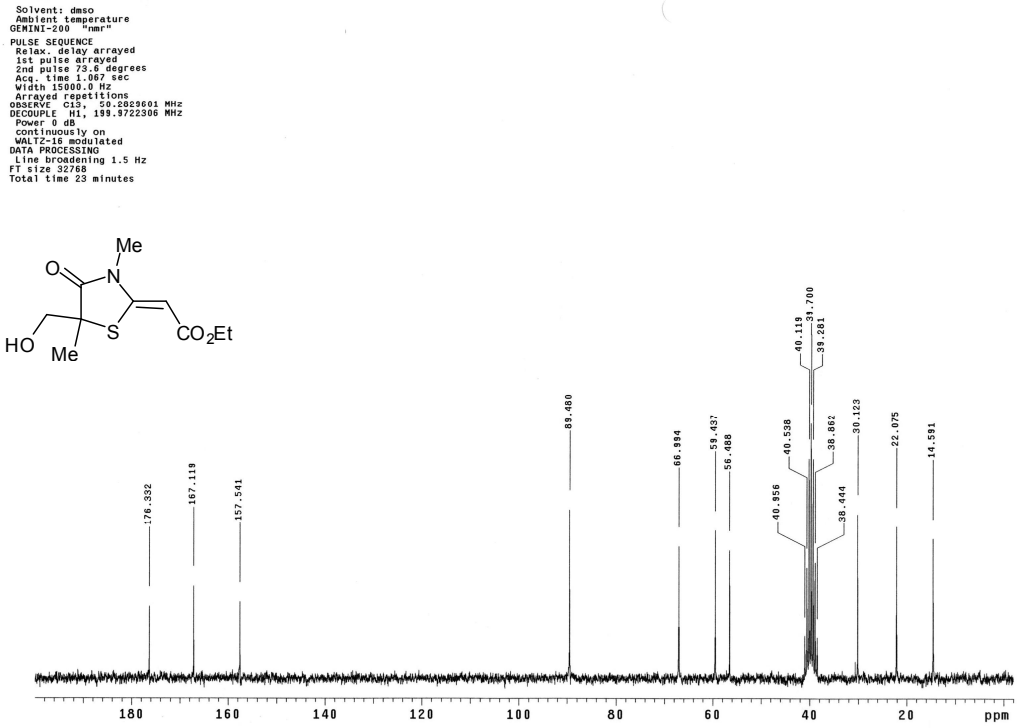
^{1}H NMR spectrum for **34** (200 MHz, DMSO-d_6)



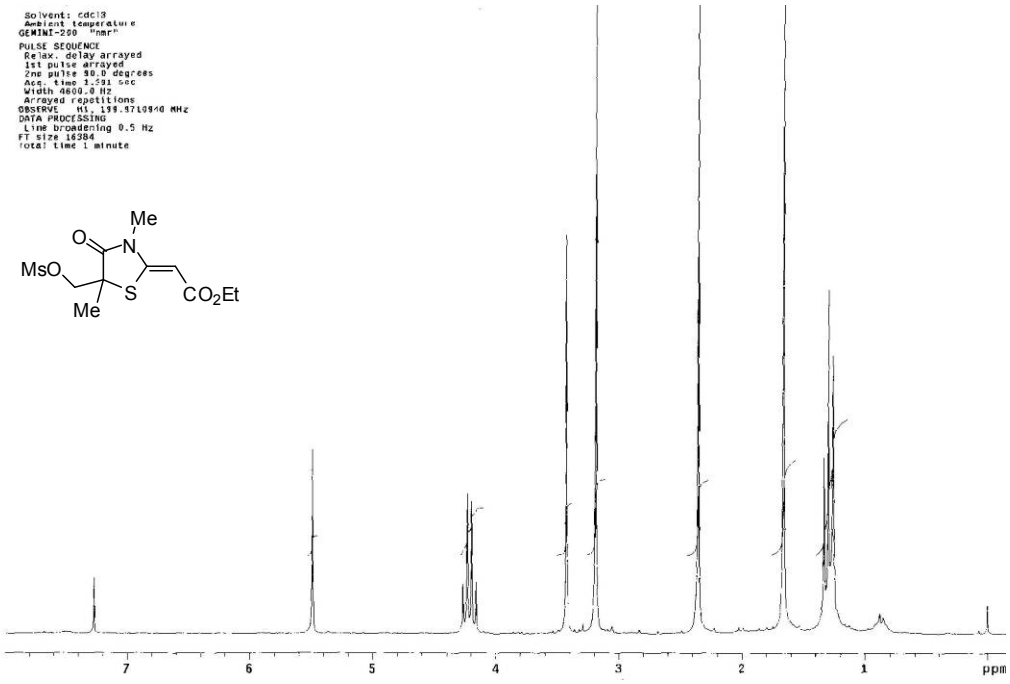
^{13}C NMR spectrum for **34** (125 MHz, $CDCl_3$)



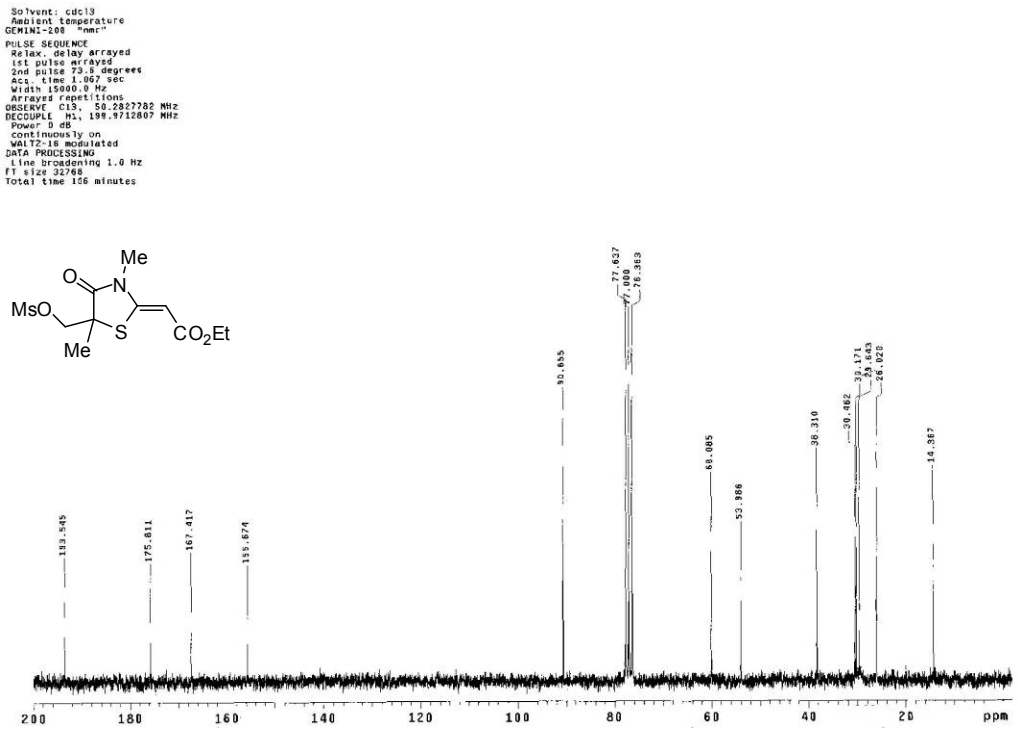
^{1}H NMR spectrum for **42** (200 MHz, DMSO-d_6)



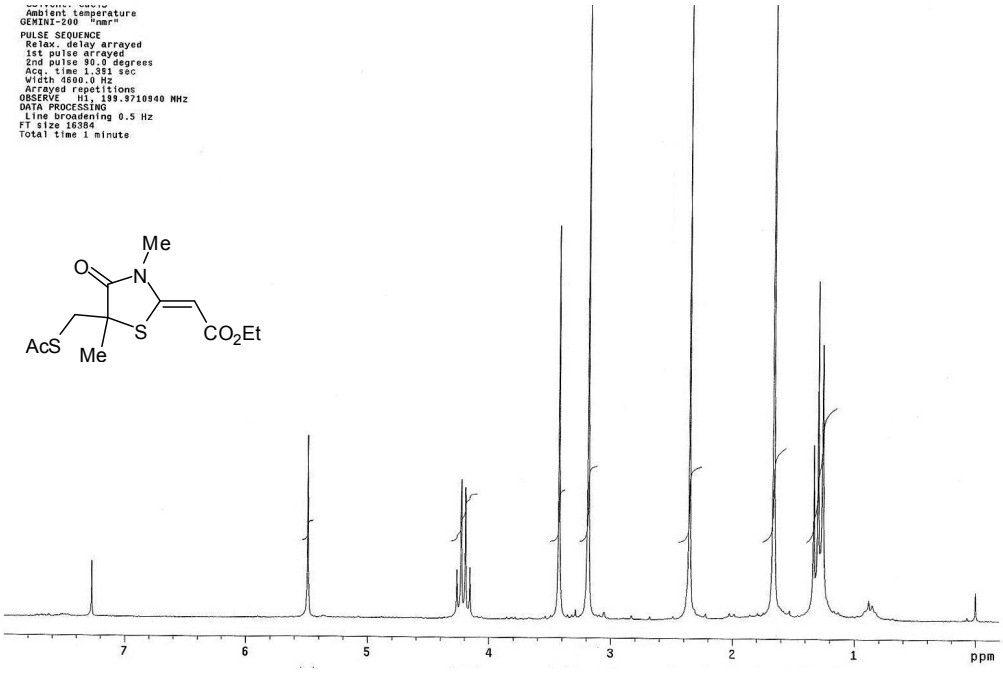
^{13}C NMR spectrum for **42** (50 MHz, DMSO-d_6)



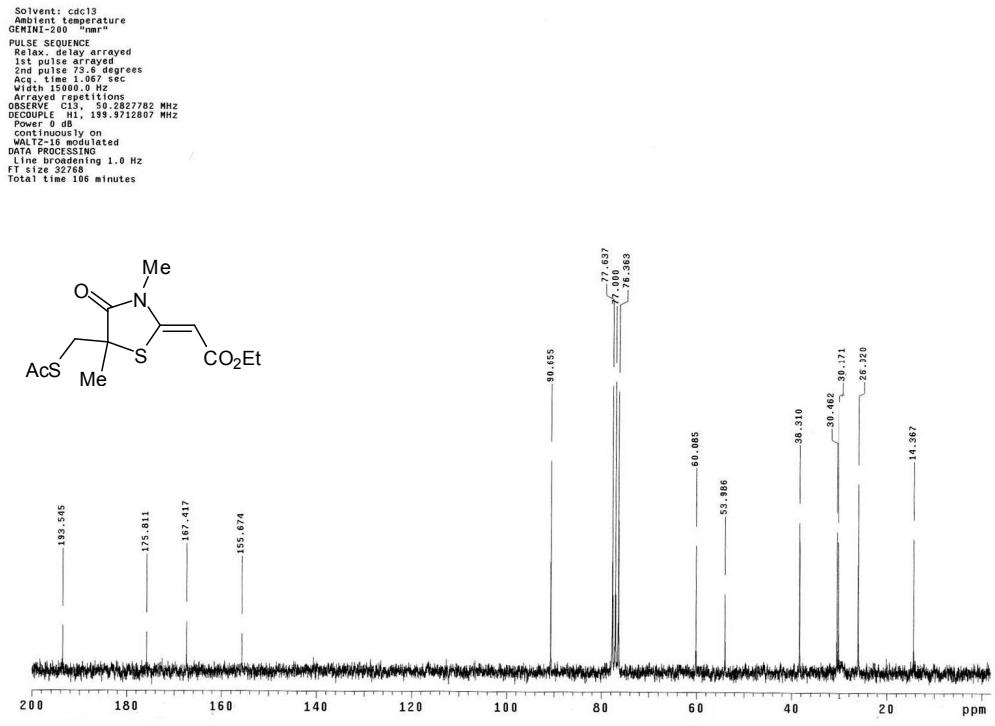
^{1}H NMR spectrum for **43** (200 MHz, $CDCl_3$)



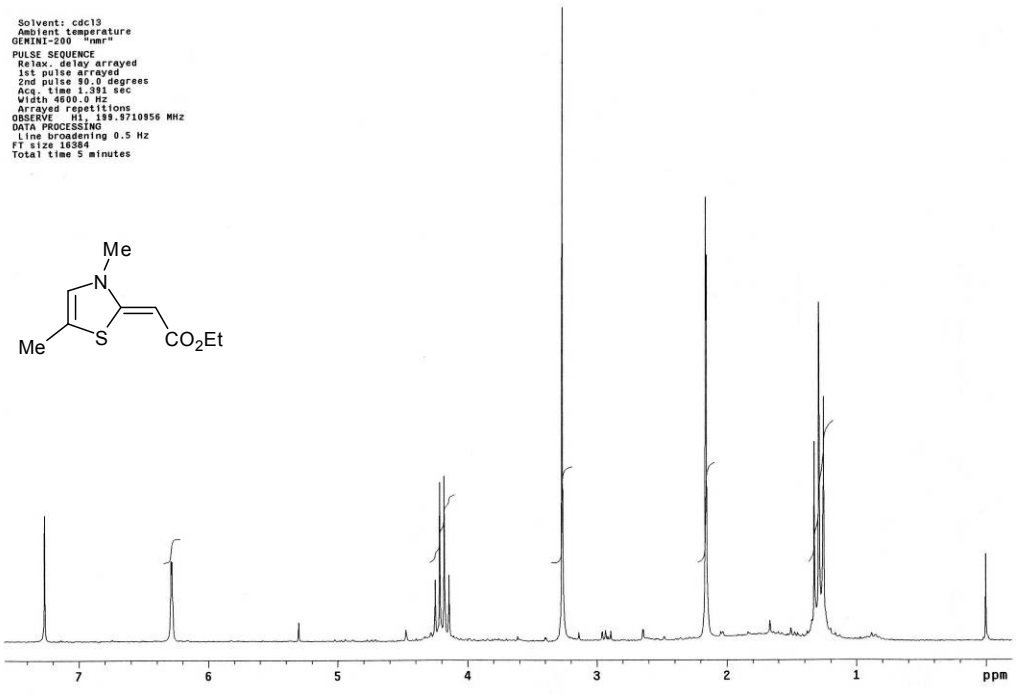
^{13}C NMR spectrum for **43** (50 MHz, $CDCl_3$)



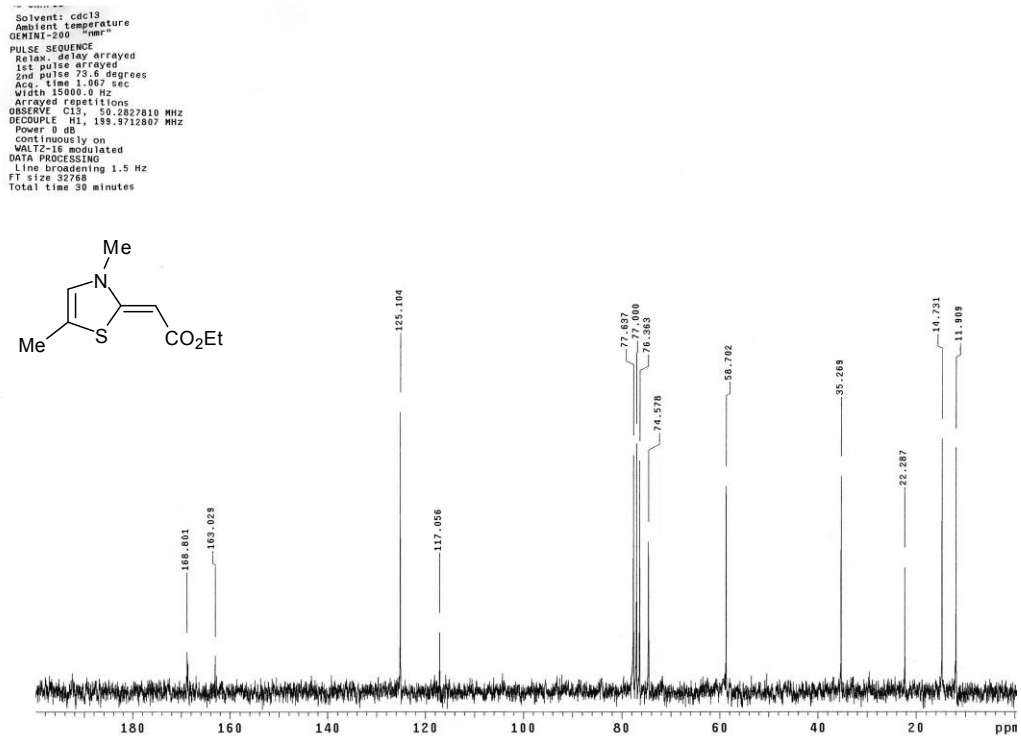
^{1}H NMR spectrum for **44** (200 MHz, $CDCl_3$)



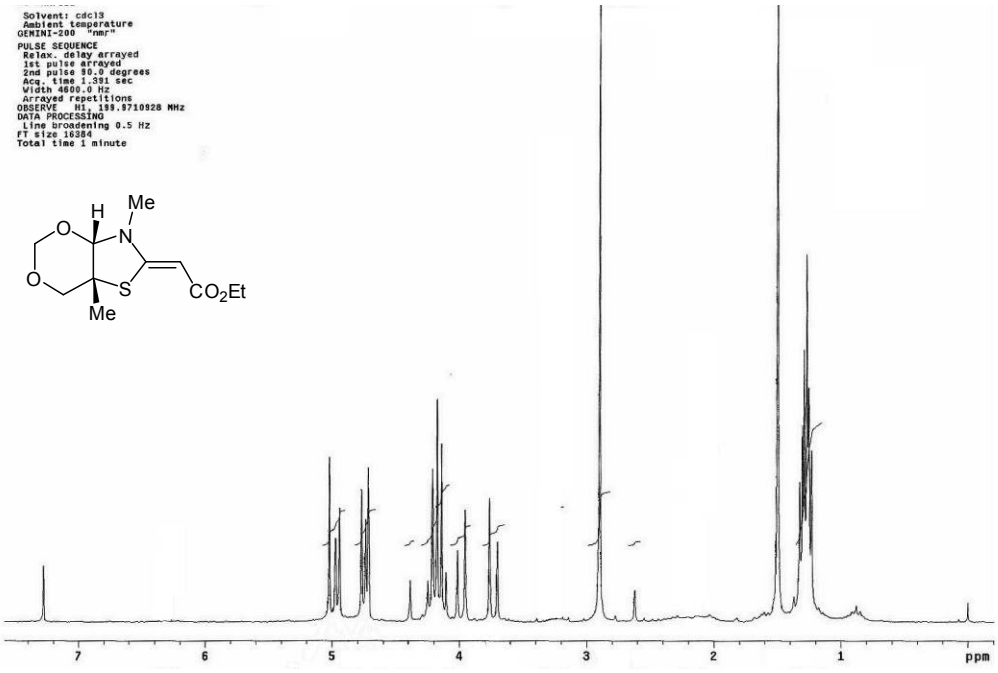
^{13}C NMR spectrum for **44** (50 MHz, $CDCl_3$)



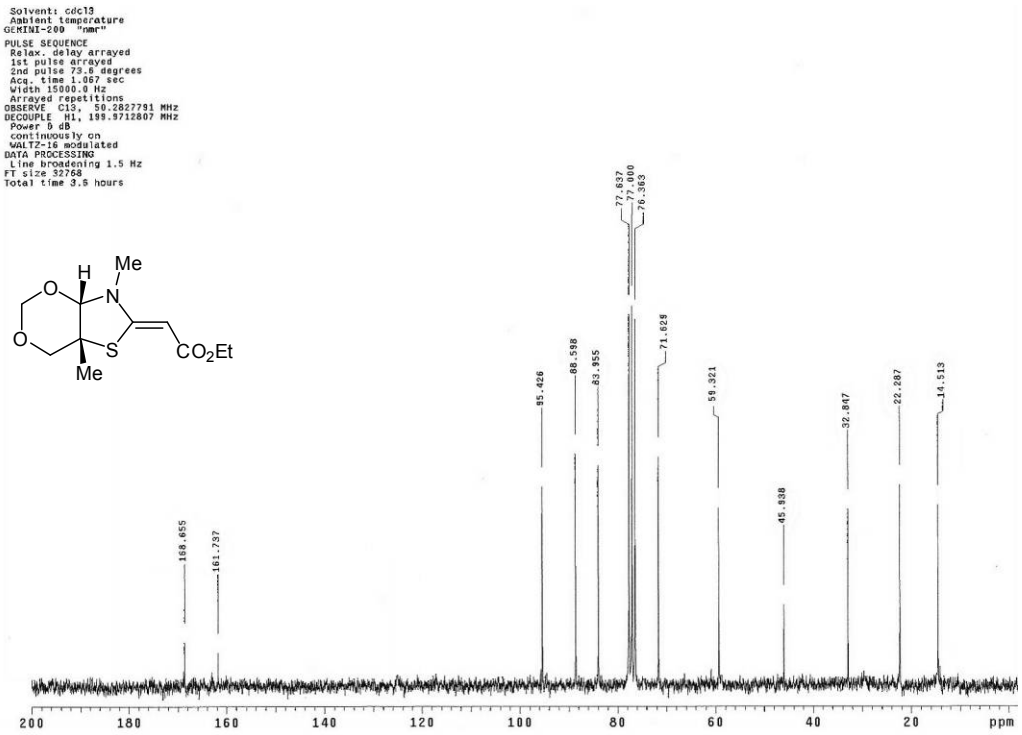
^{1}H NMR spectrum for **47** (200 MHz, $CDCl_3$)



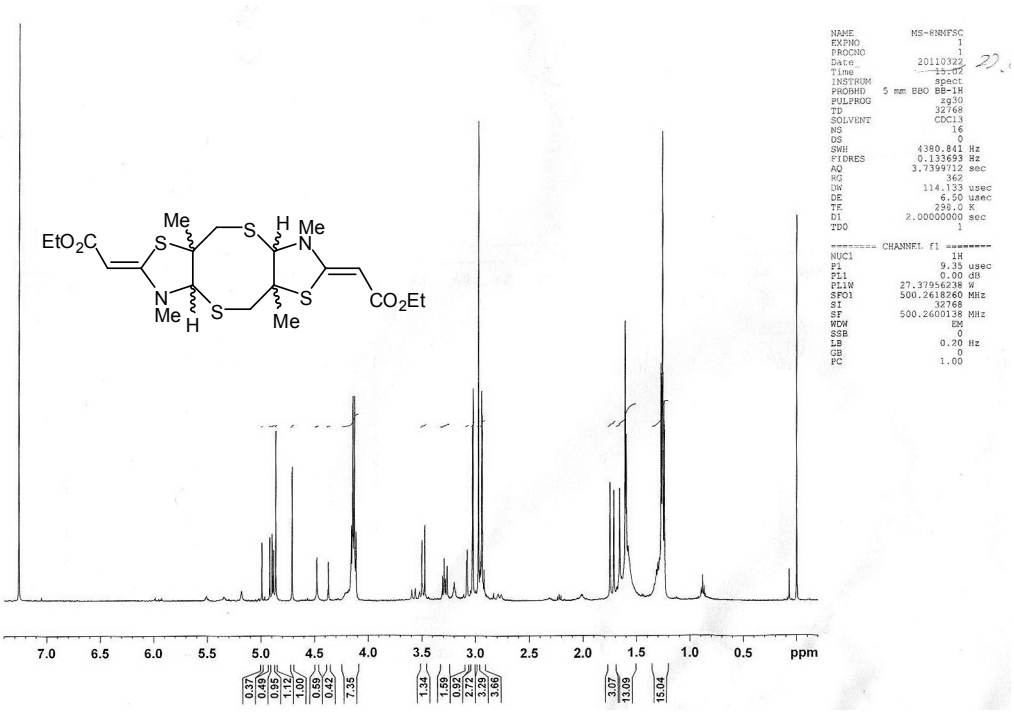
^{13}C NMR spectrum for **47** (50 MHz, $CDCl_3$)



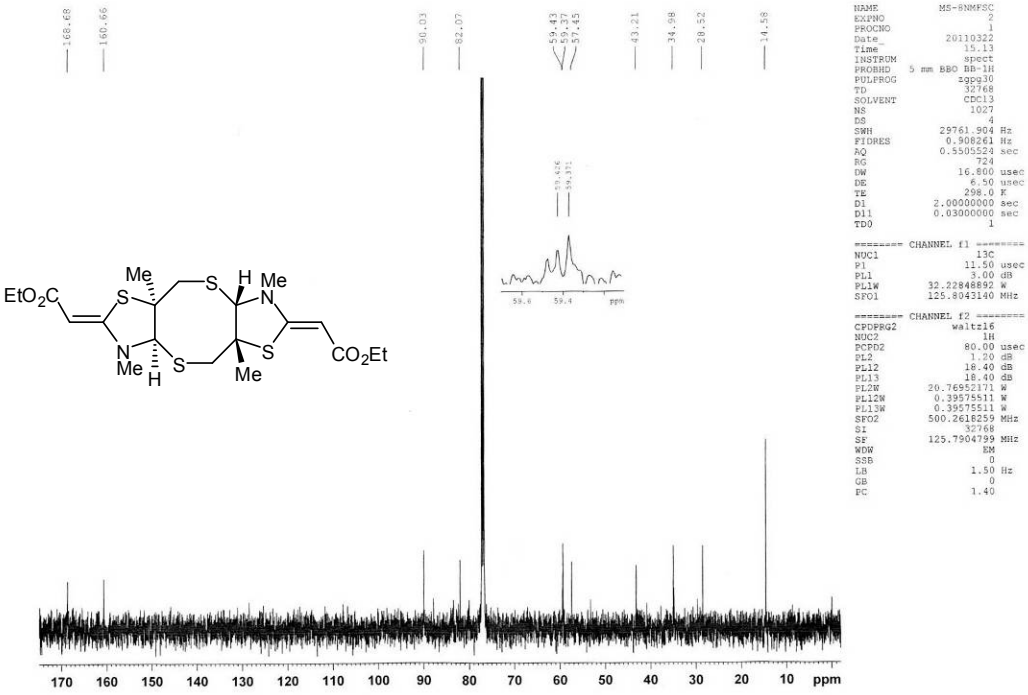
^{1}H NMR spectrum for **48** (200 MHz, $CDCl_3$)



^{13}C NMR spectrum for **48** (50 MHz, $CDCl_3$)



^{1}H NMR spectrum for mixure of **51** (500 MHz, $CDCl_3$)



^{13}C NMR spectrum for **51** (125 MHz, $CDCl_3$)