

**Supporting information for****Stereoselective Synthesis of 1-Nitrobicyclo[3.1.0]hexanes and Fused Isoxazoline-N-oxides from Primary Nitro Compounds**

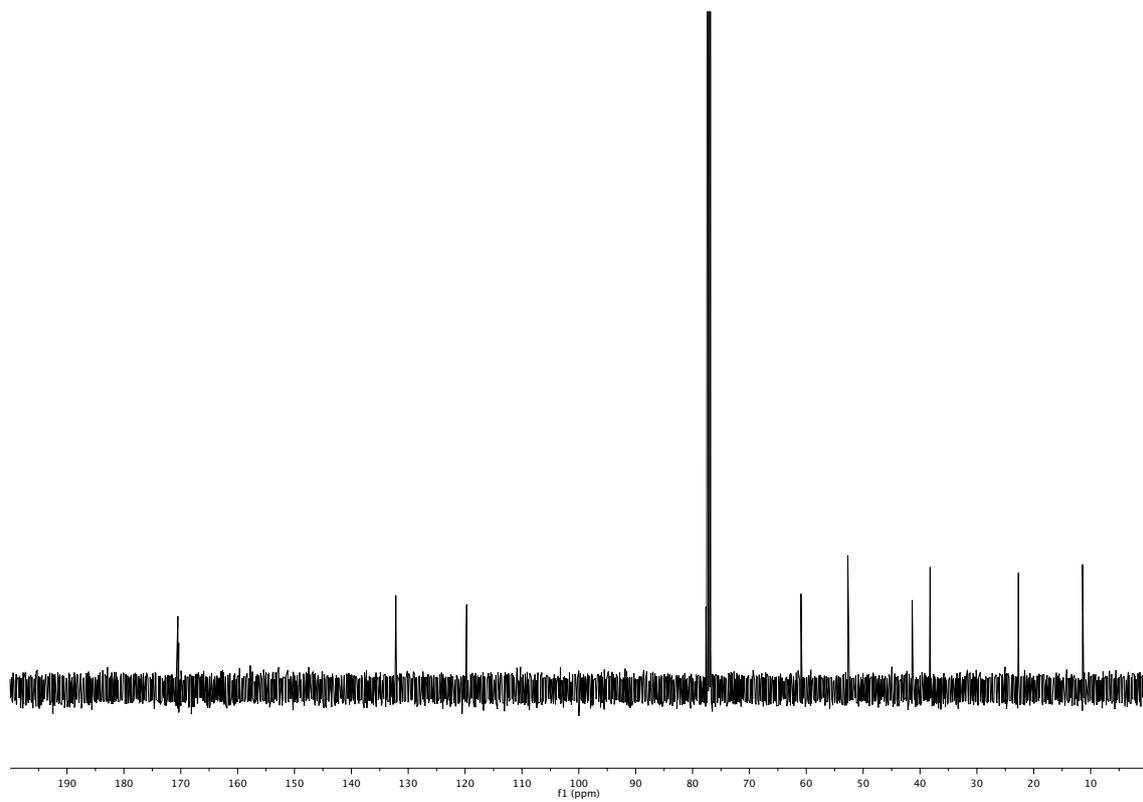
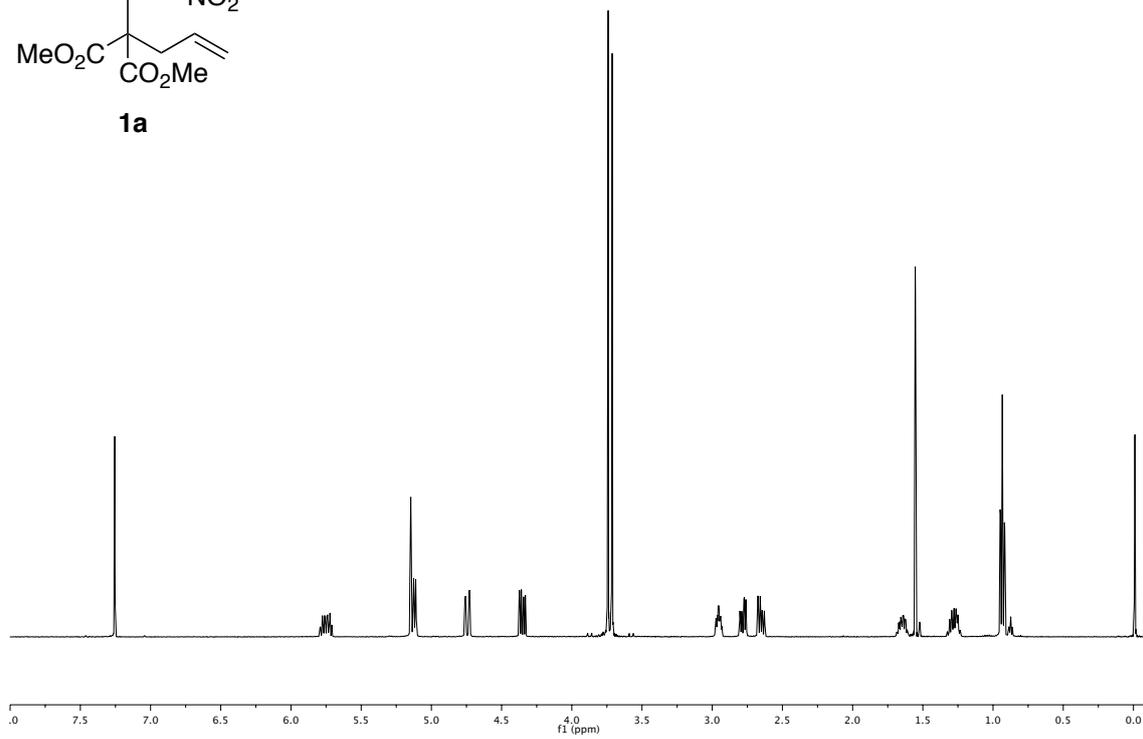
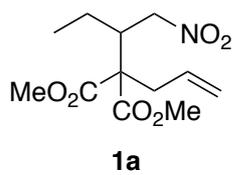
Akio Kamimura,<sup>\*,a</sup> Ryota Takeuchi,<sup>a</sup> Kosuke Ikeda,<sup>a</sup> Takaaki Moriyama,<sup>a</sup> and Michinori Sumimoto<sup>b</sup>

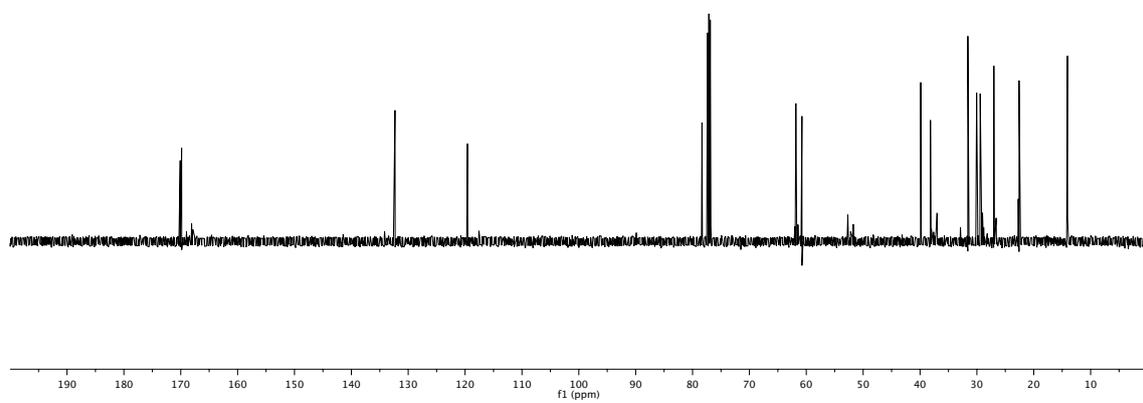
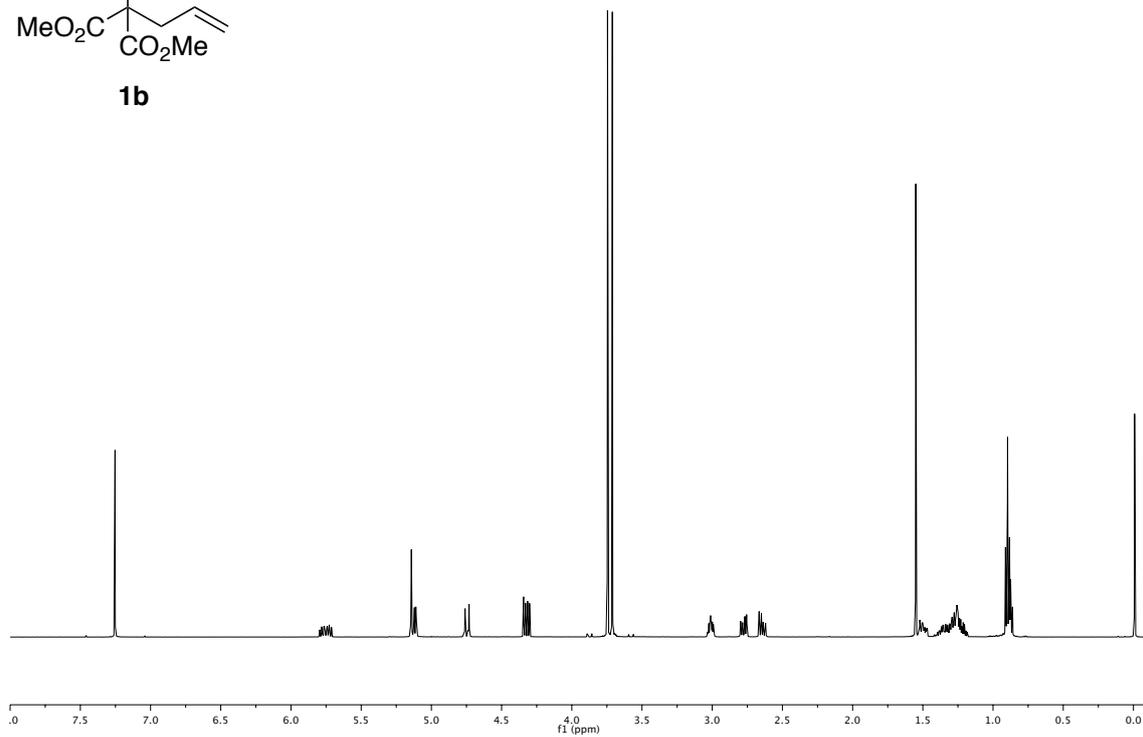
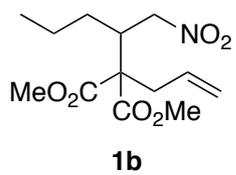
<sup>a</sup>*Department of Applied Molecular Bioscience, Graduate School of Medicine, Yamaguchi University, Ube 755-8611, Japan, and*

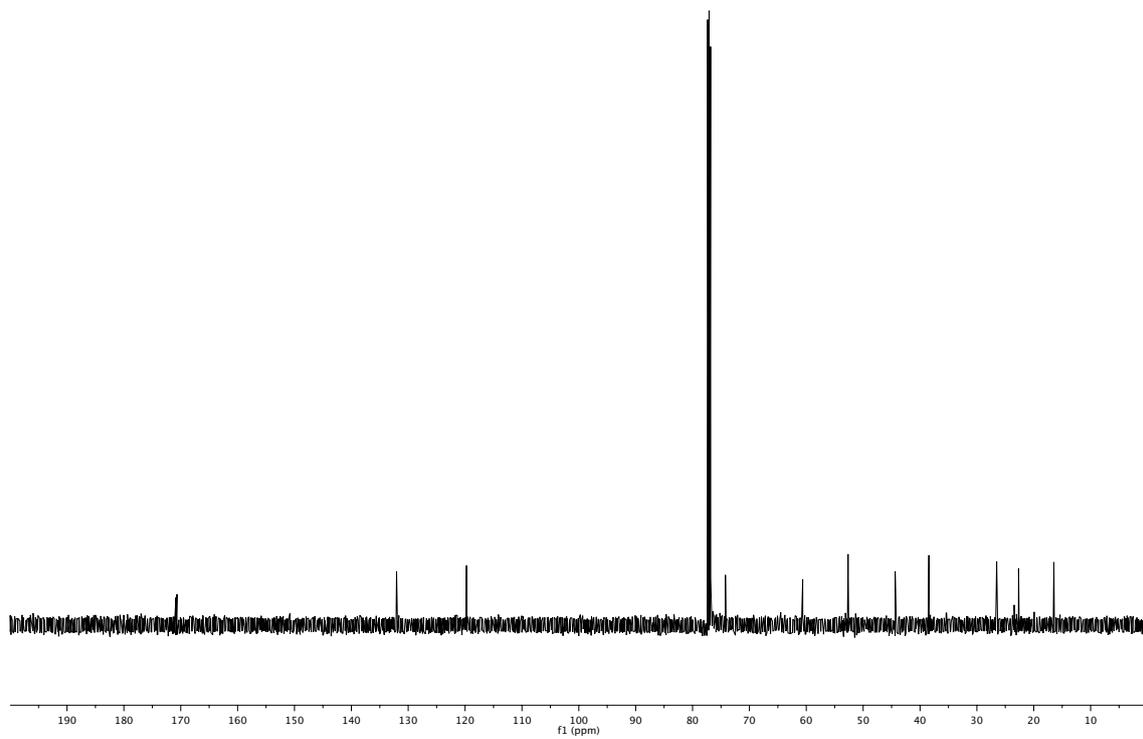
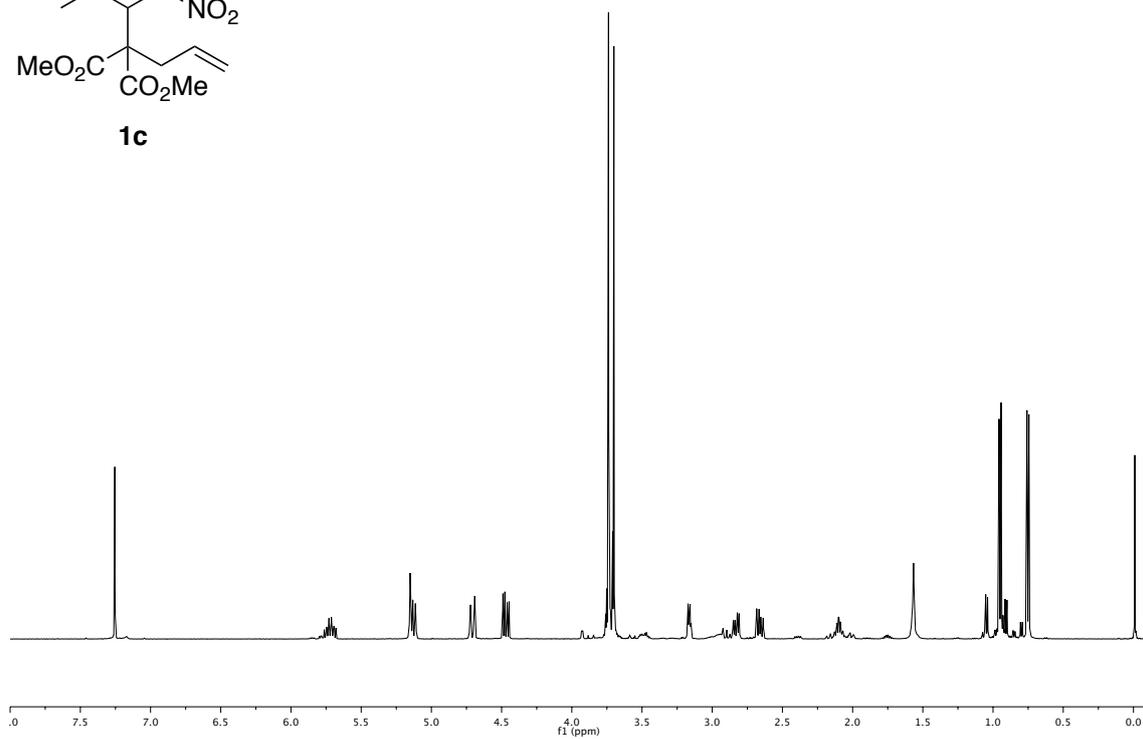
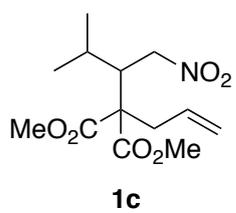
<sup>b</sup>*Department of Material Chemistry, Graduate School of Science and Engineering, Yamaguchi University, Ube 755-8611, Japan*

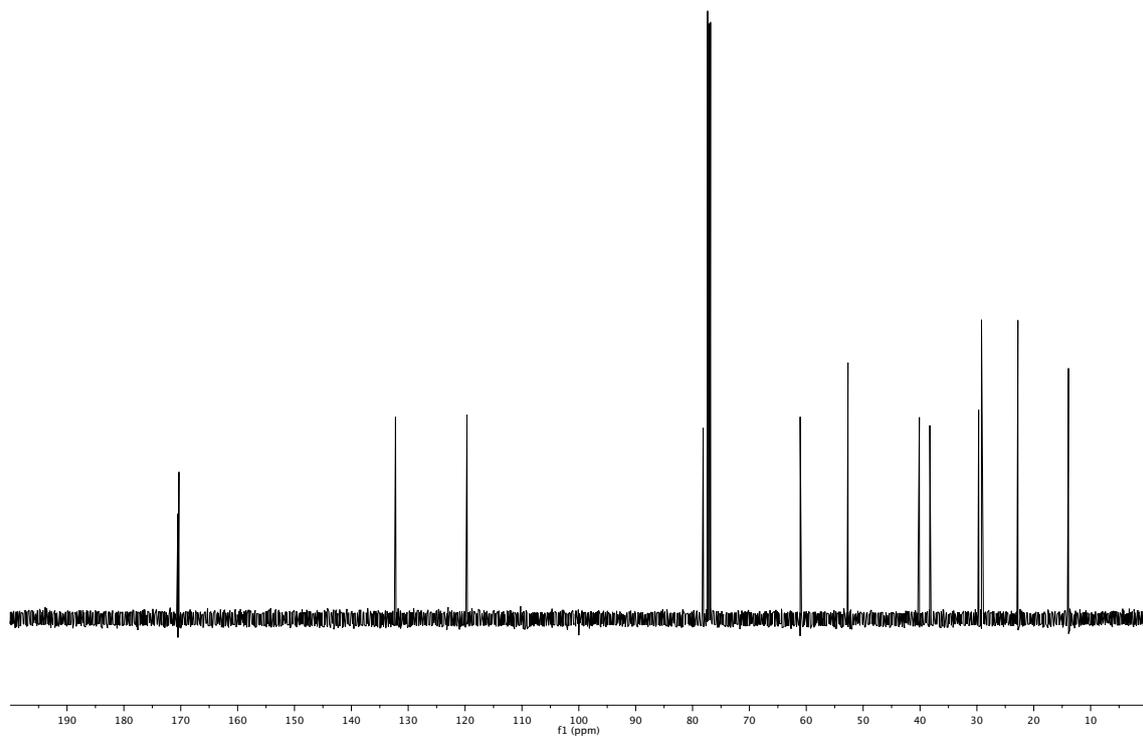
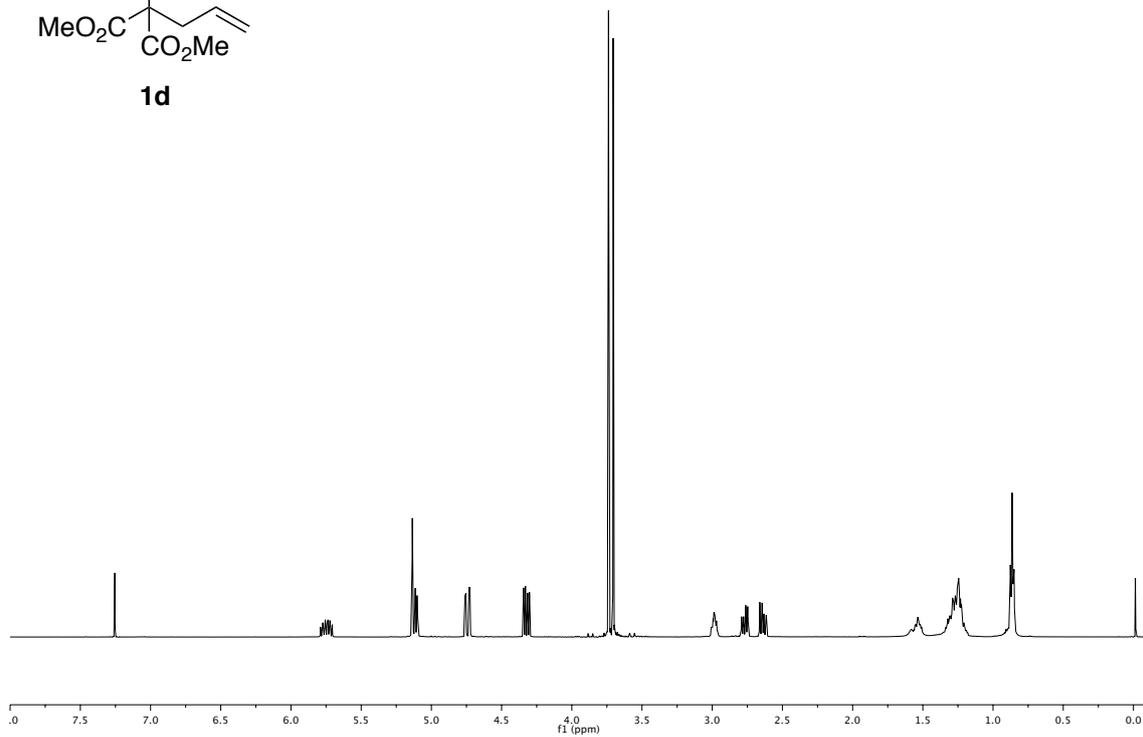
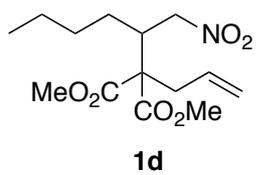
**Contents**

<sup>1</sup> H and <sup>13</sup> C NMR data for compounds <b>1</b> , <b>2</b> , <b>3</b> , <b>4</b> , <b>5</b> , <b>6</b> , <b>7</b> , and <b>8</b>	S2
Cartesian coordinates and total energy for <b>2a</b> , <b>2c</b> , <b>3a</b> , and <b>3c</b> calculated at the MP4(SDQ) level of theory	S58
ORTEP charts for <b>2d</b> , <b>2h</b> , <b>5</b> , <b>6aA</b> , <b>6eA</b> , <b>6eB</b> , and <b>7d</b>	S64

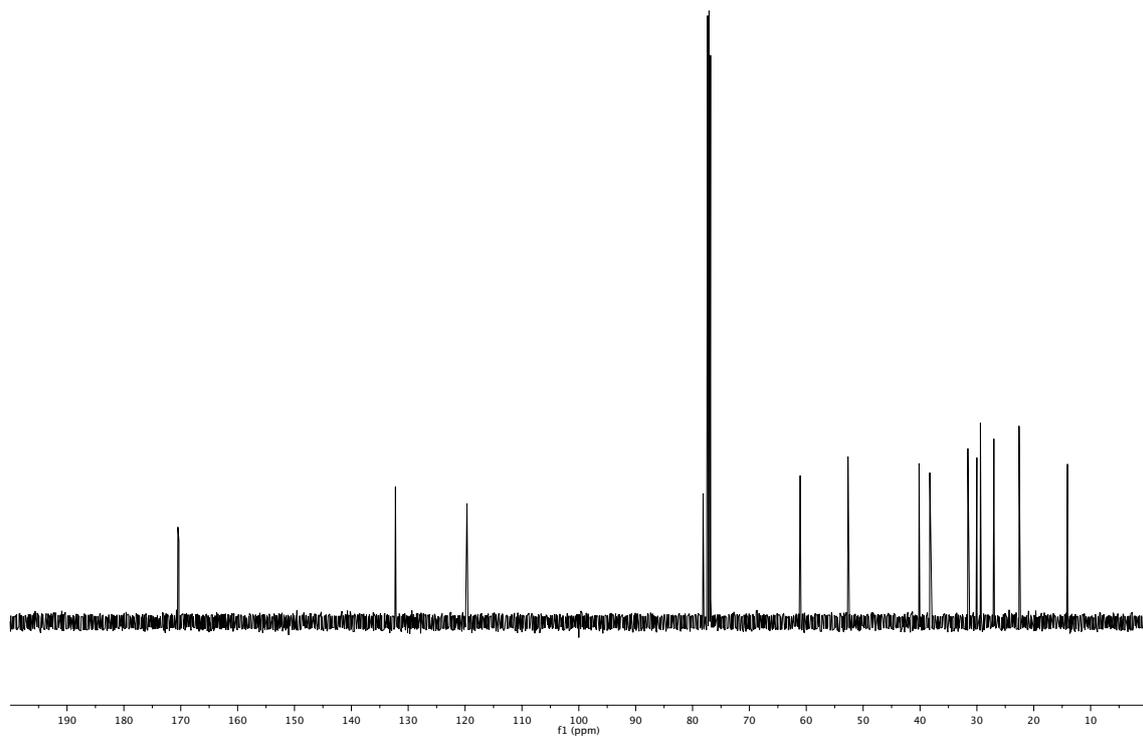
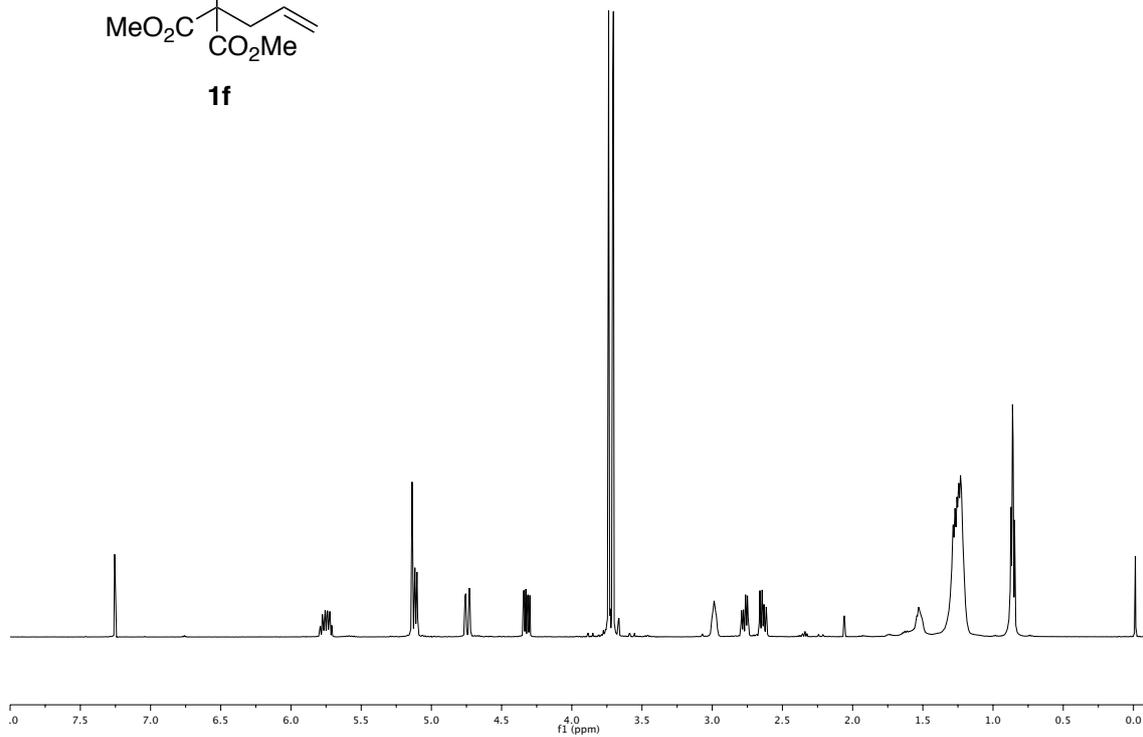
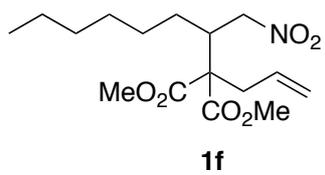


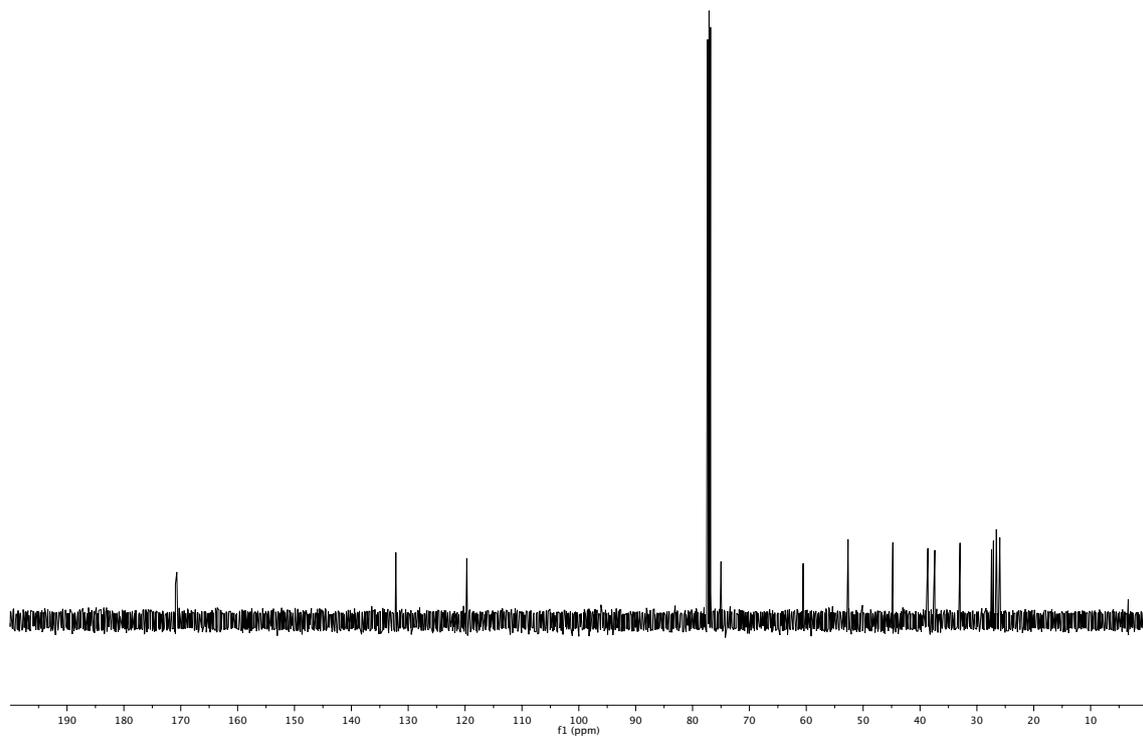
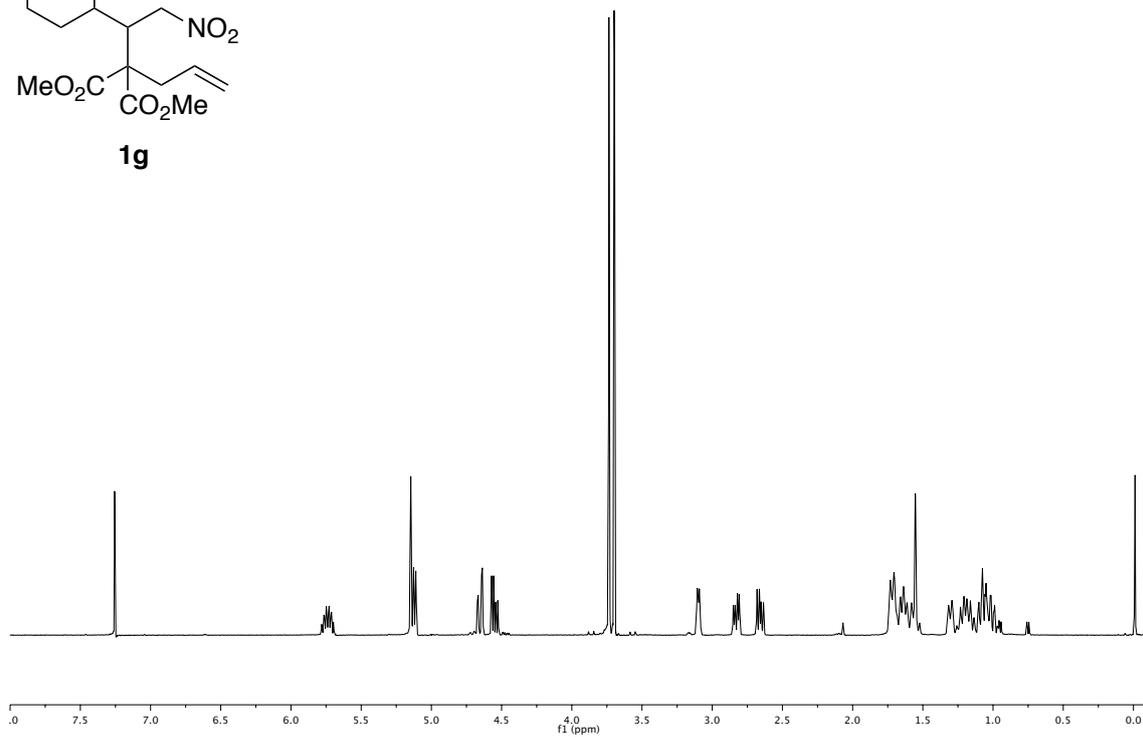
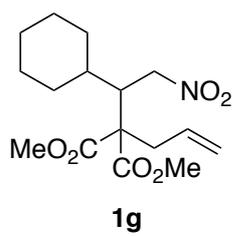


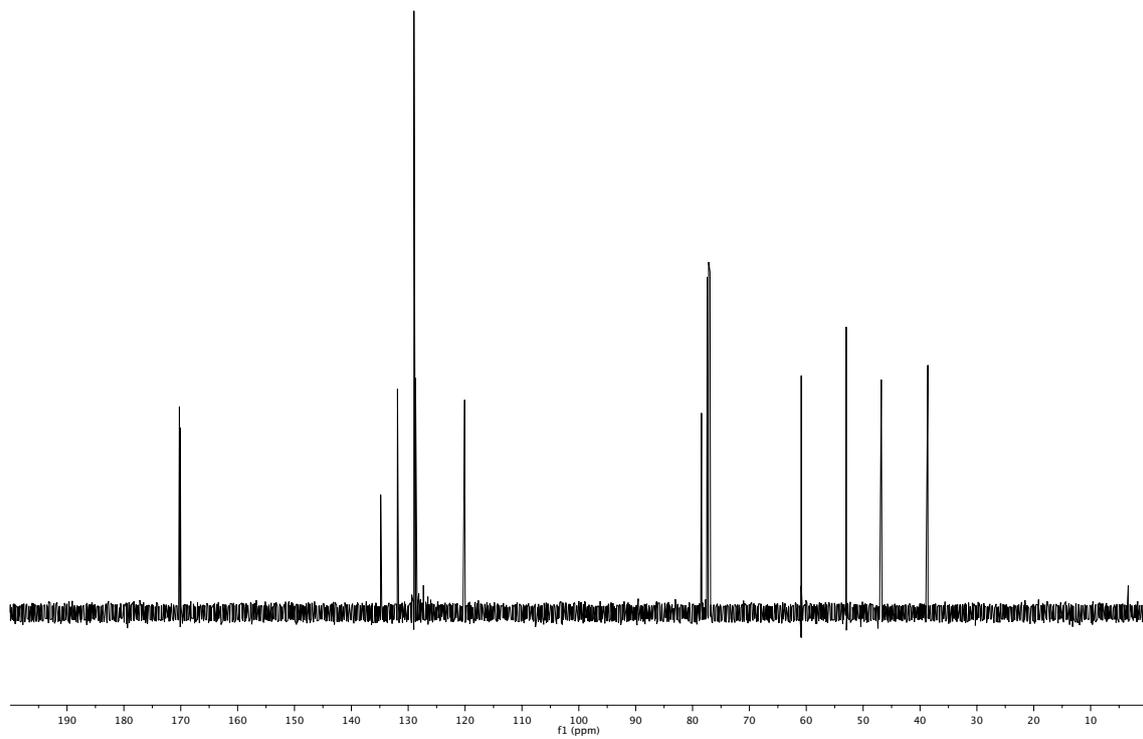
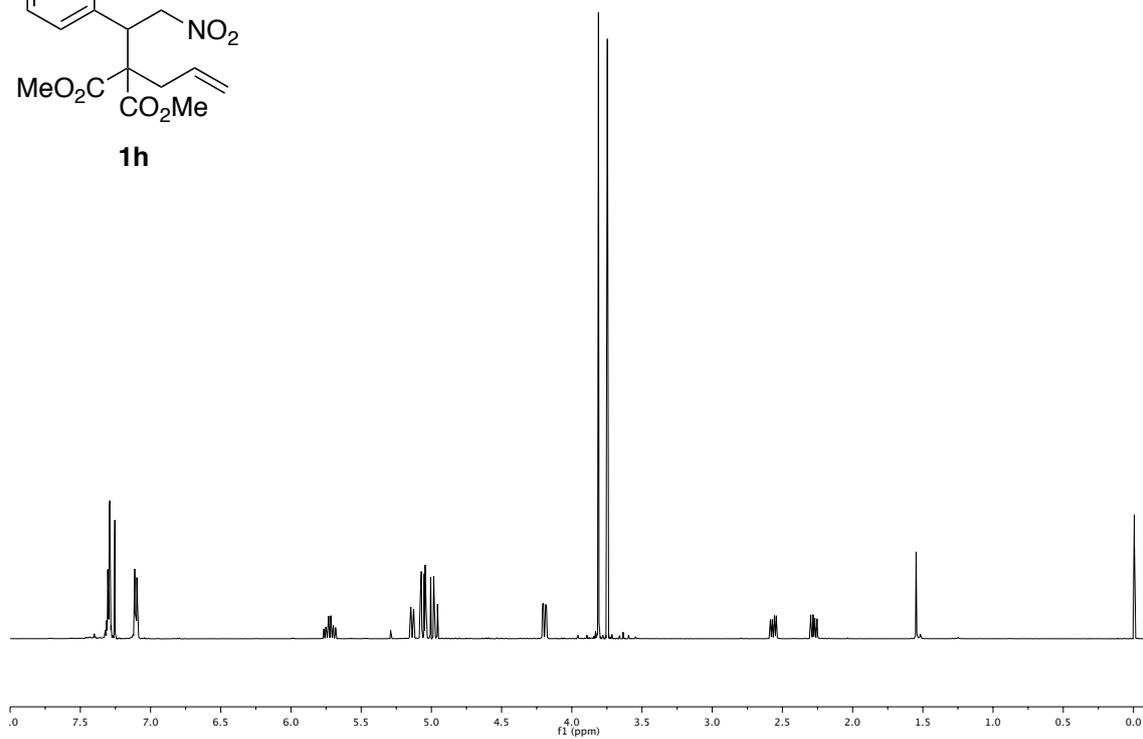
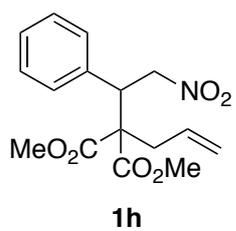


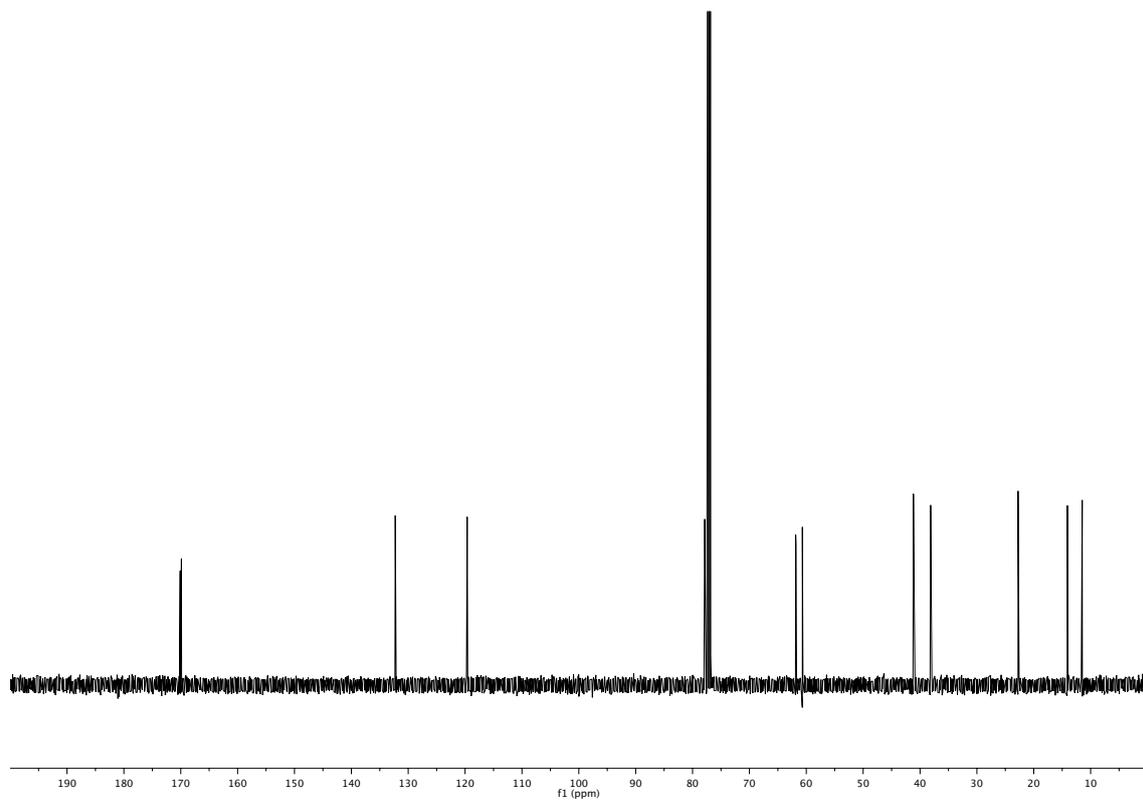
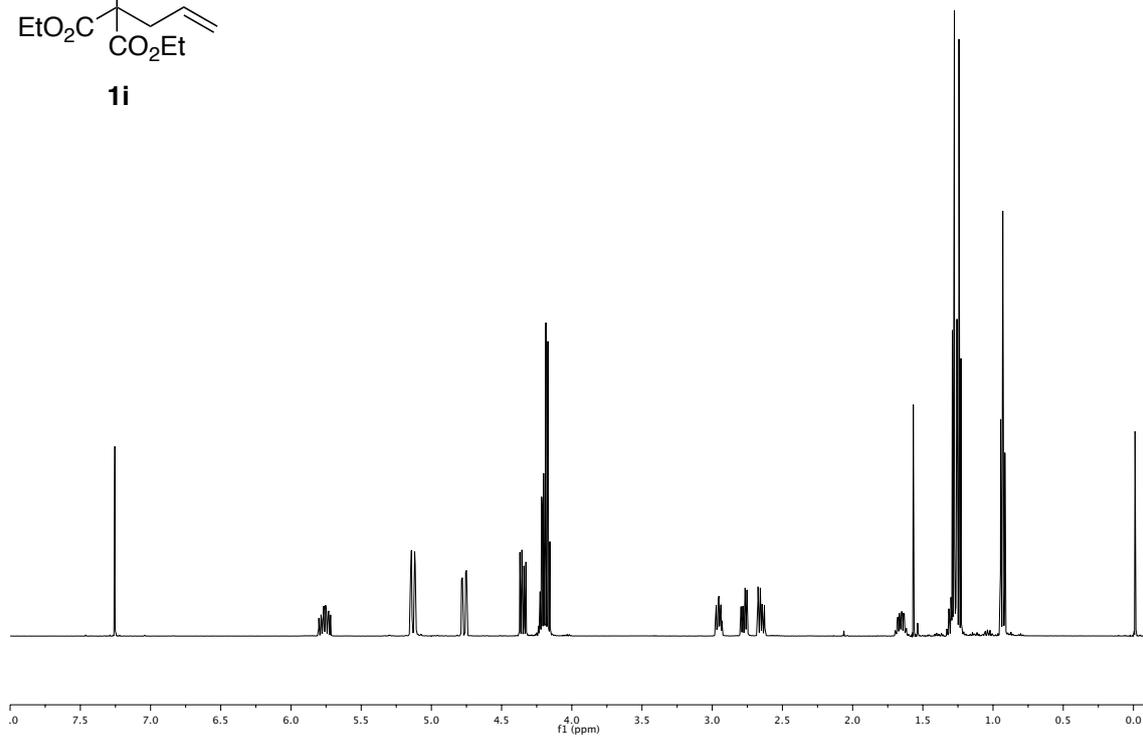
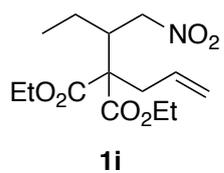




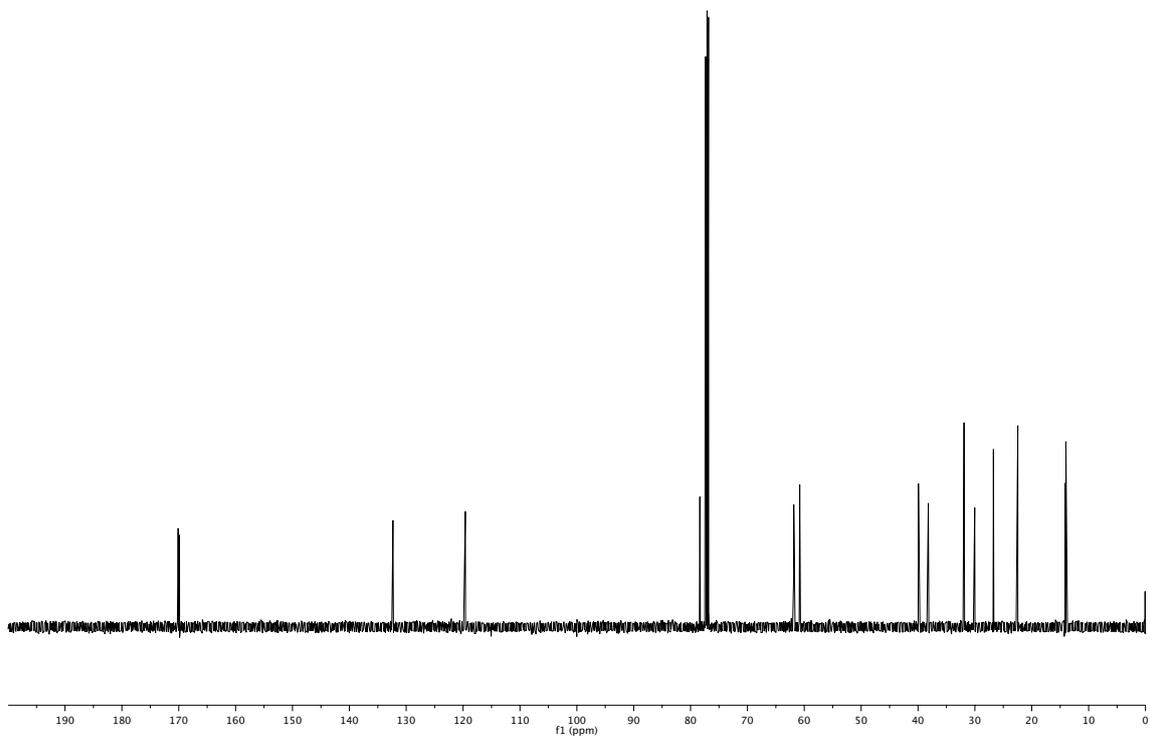
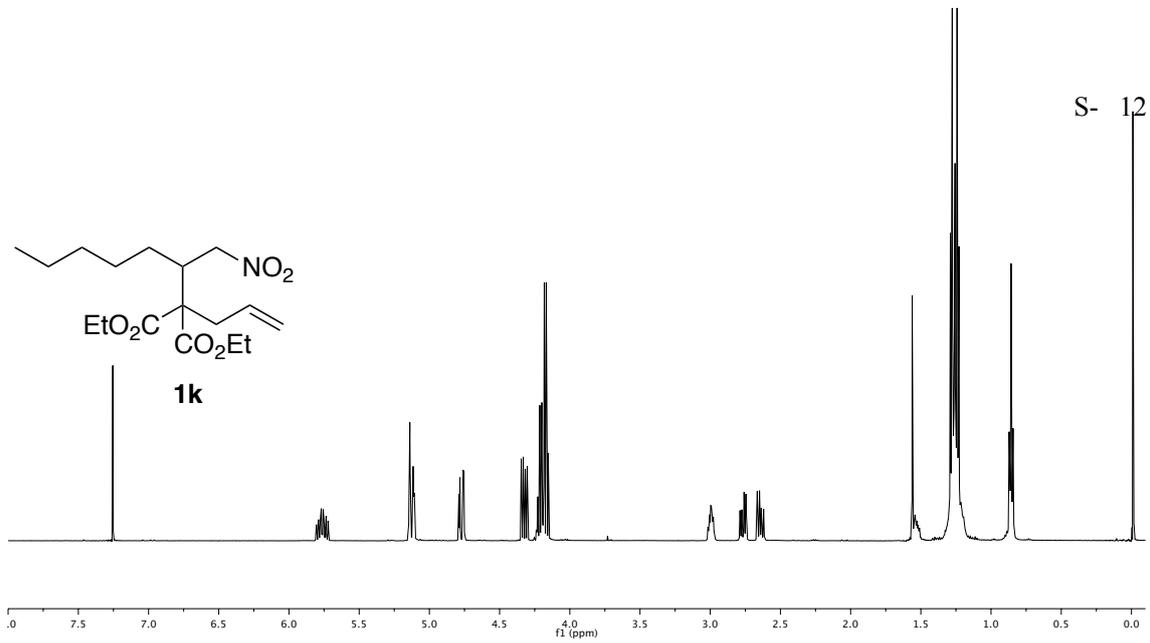


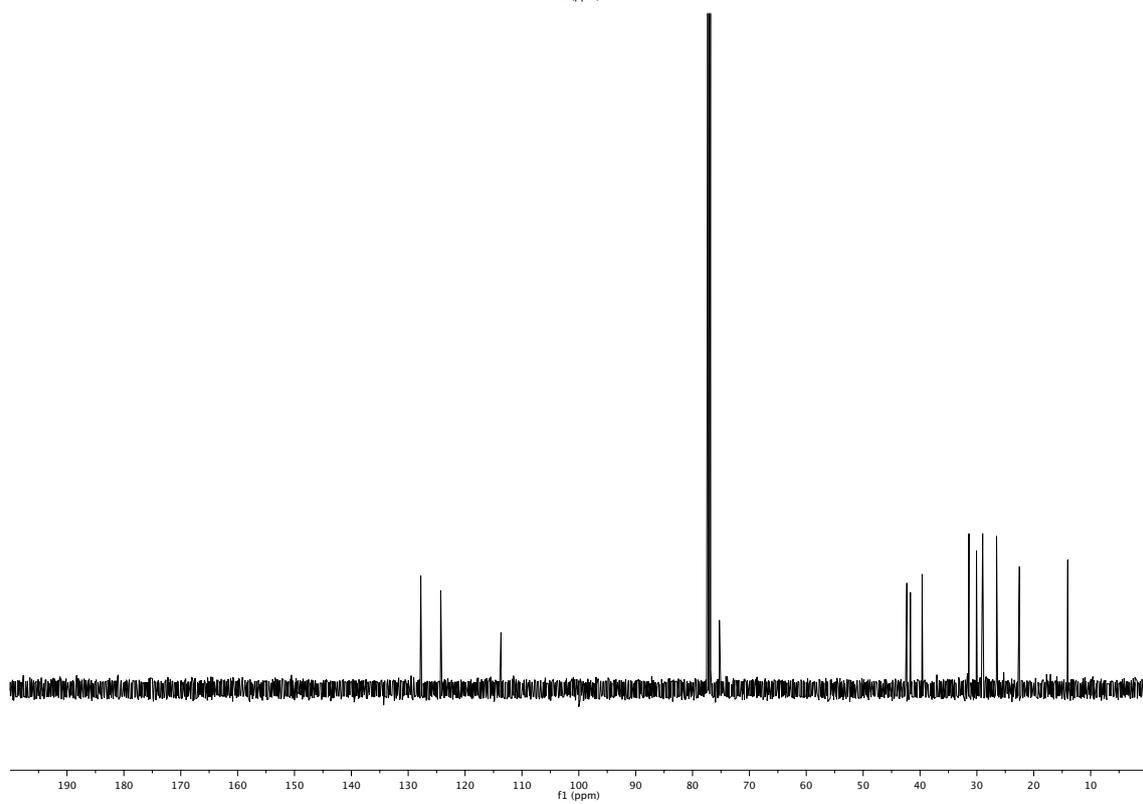
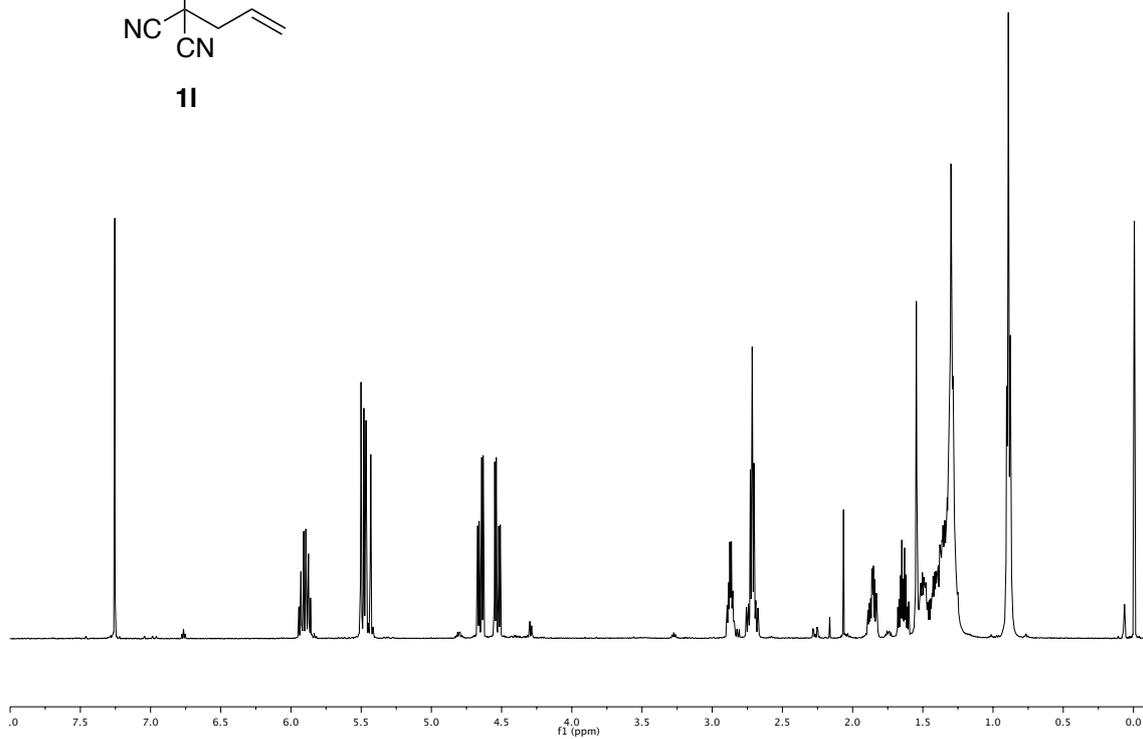
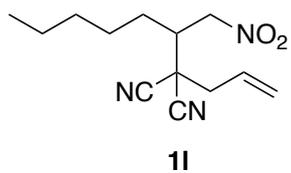


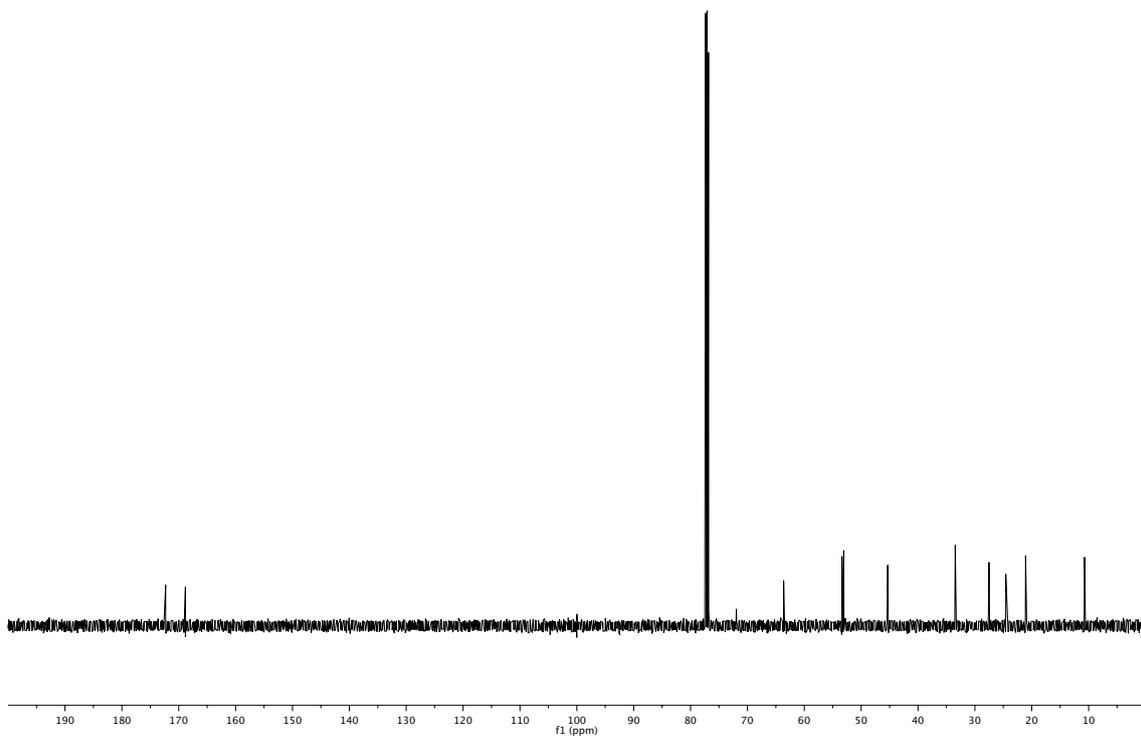
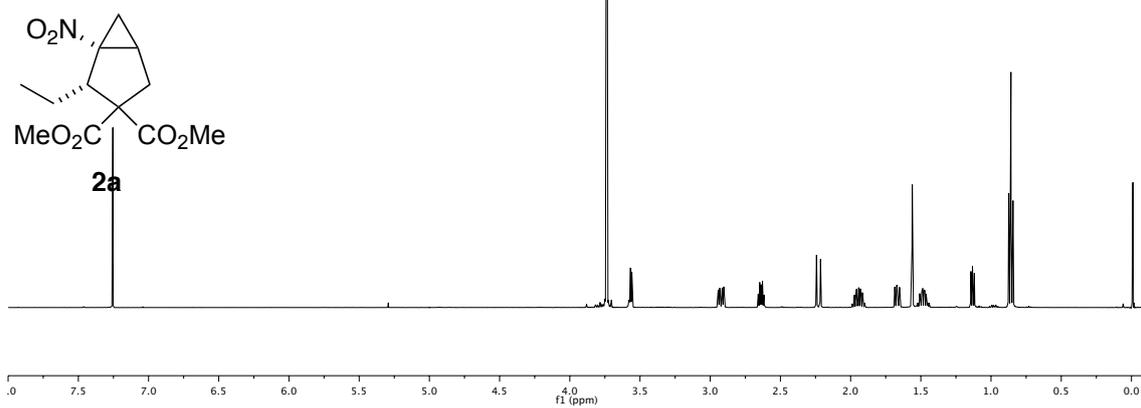


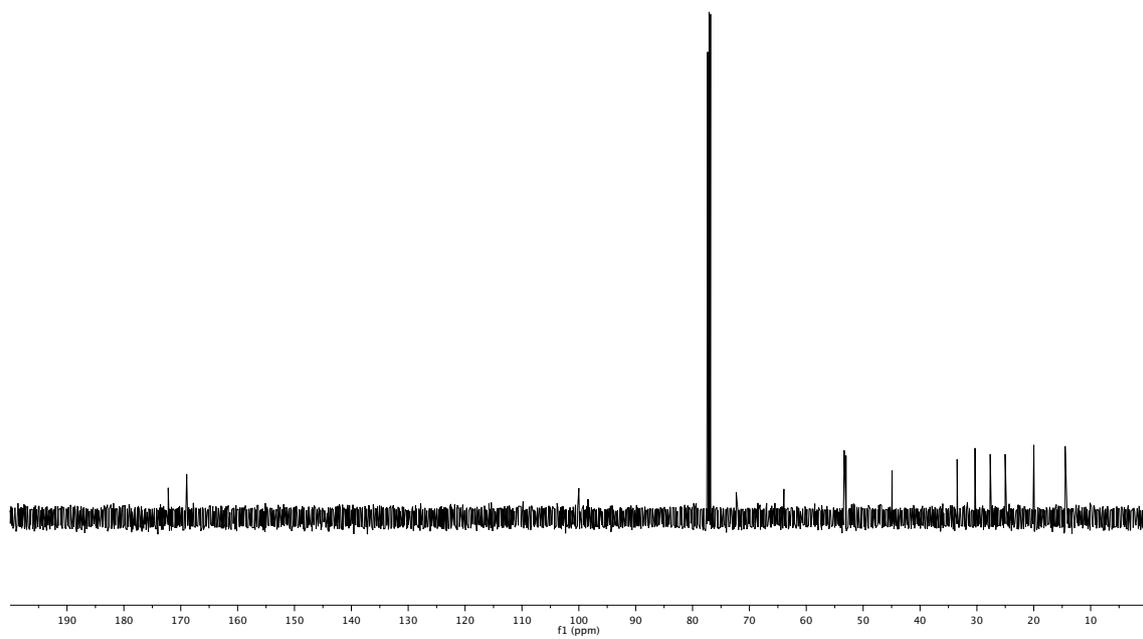
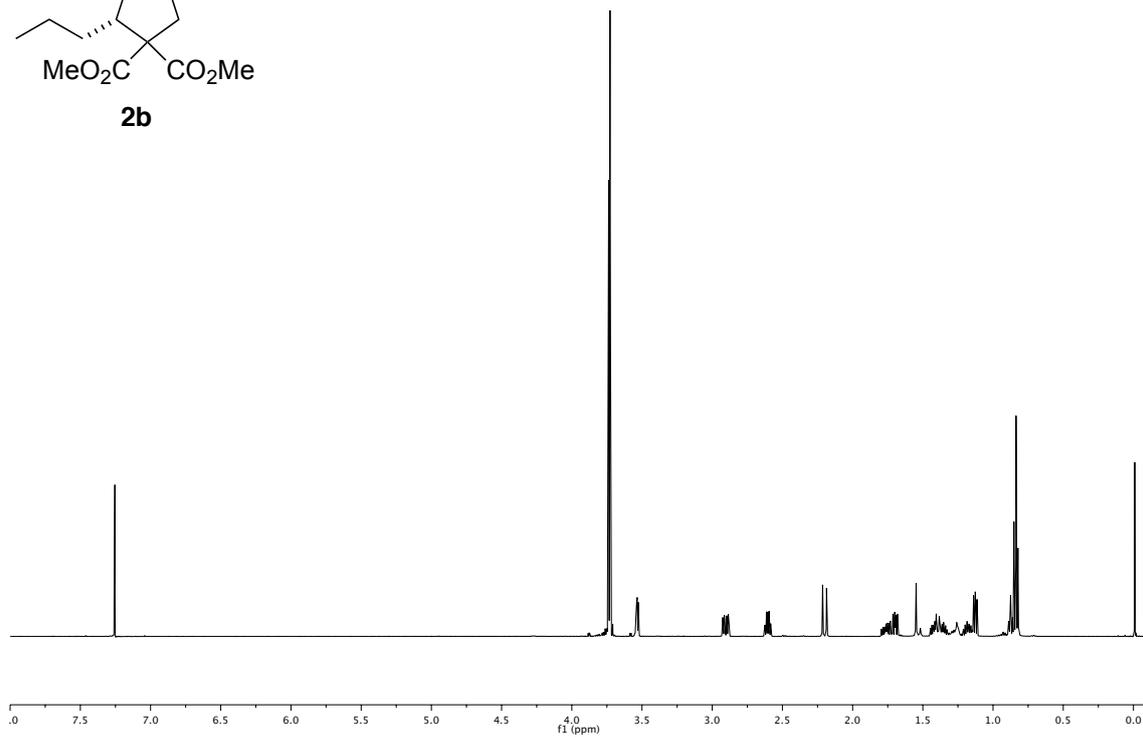
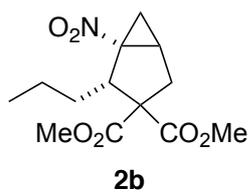


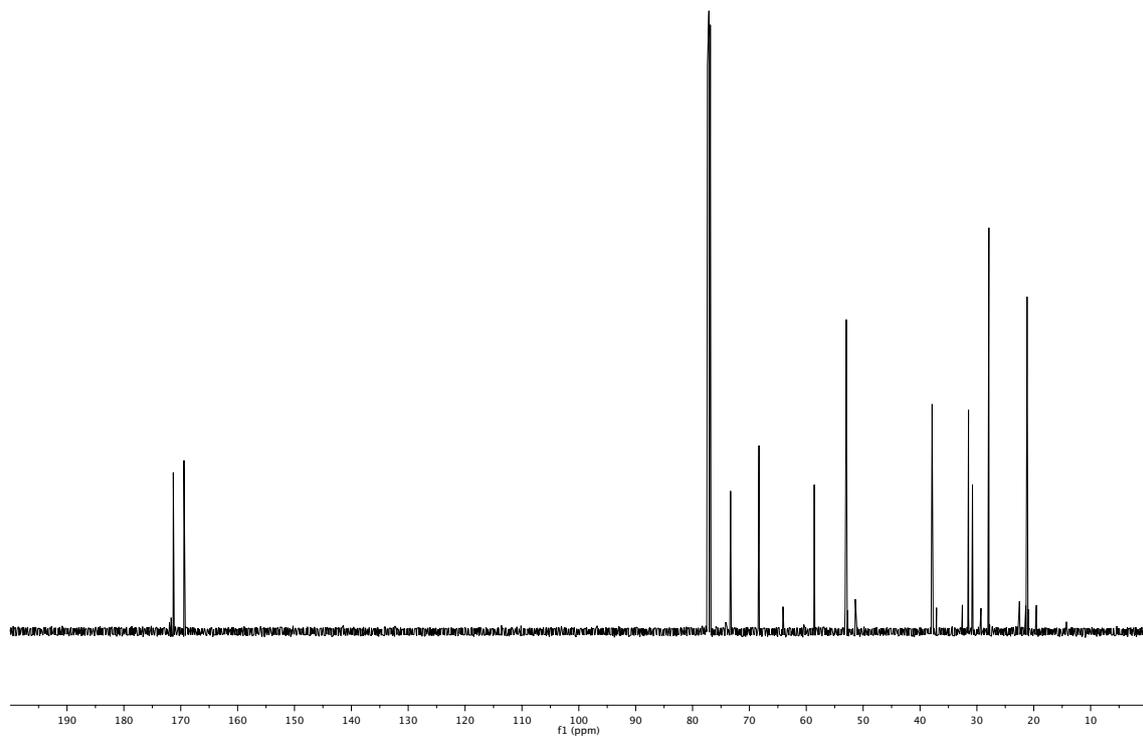
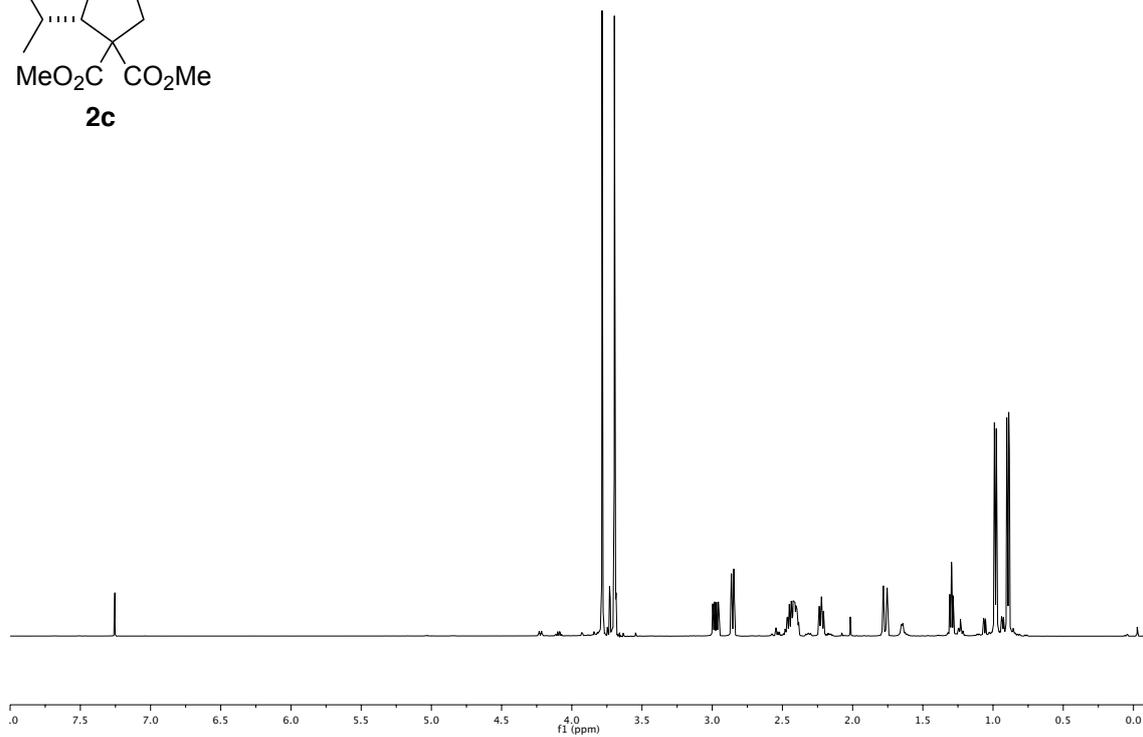
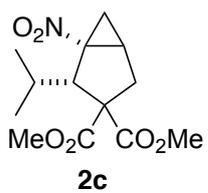


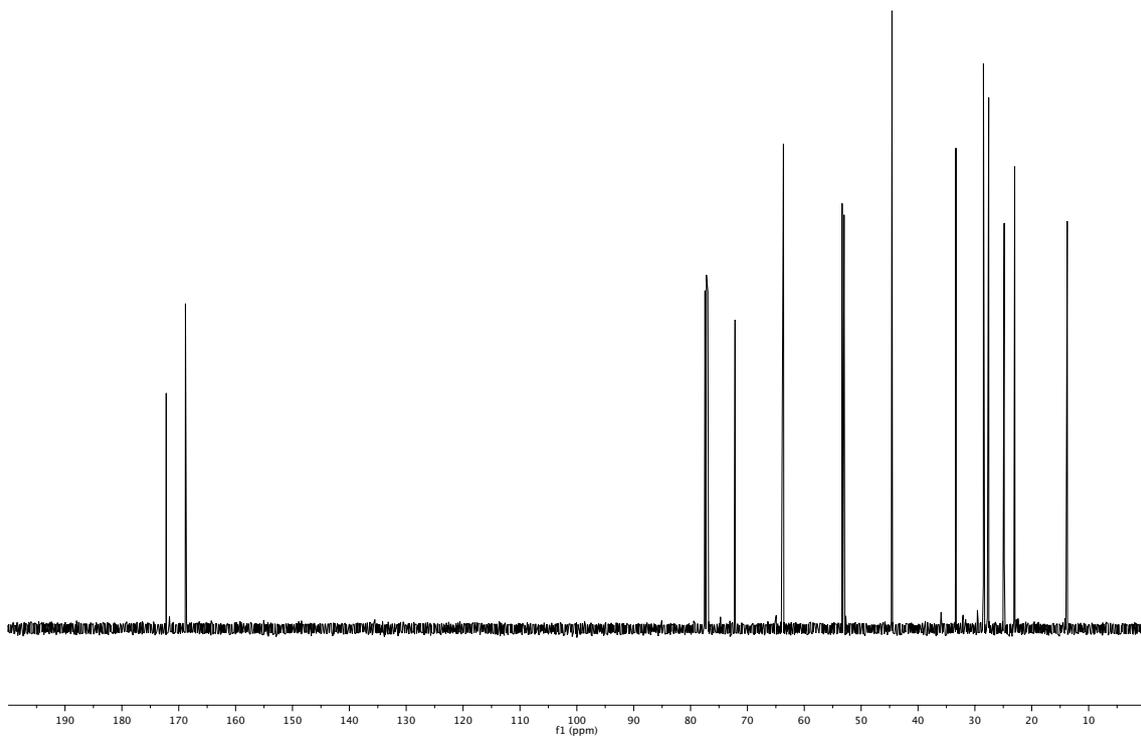
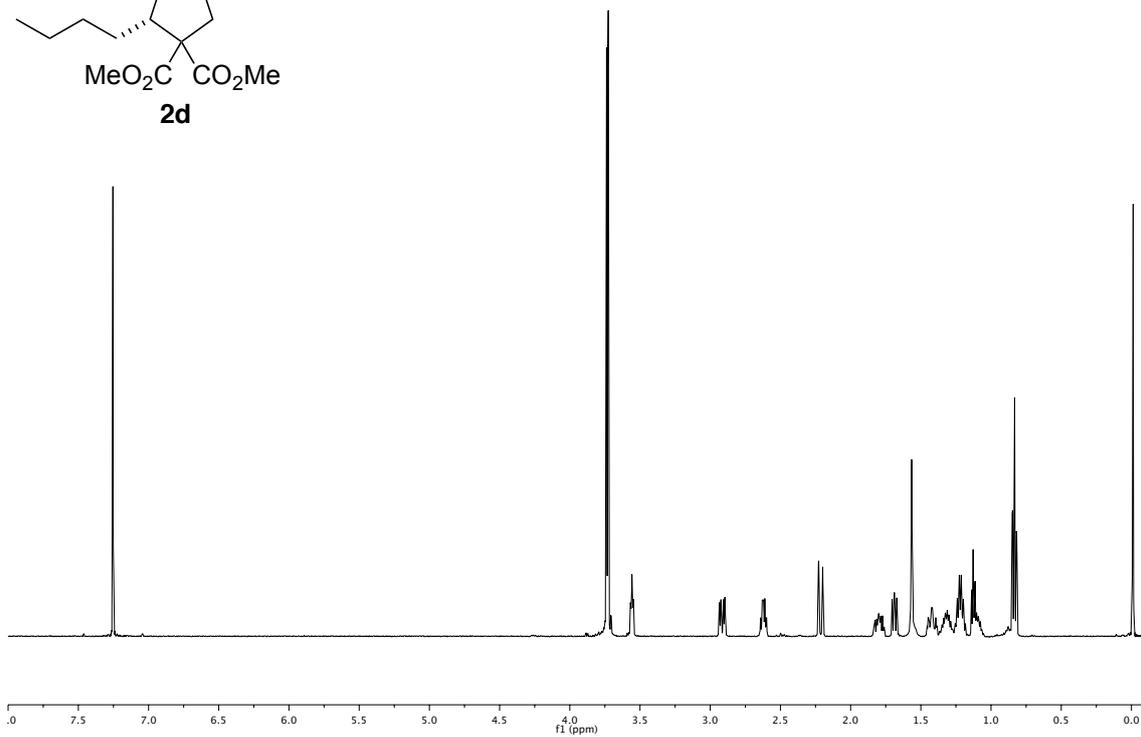
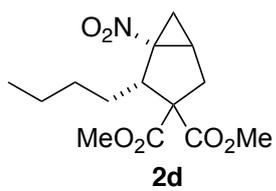


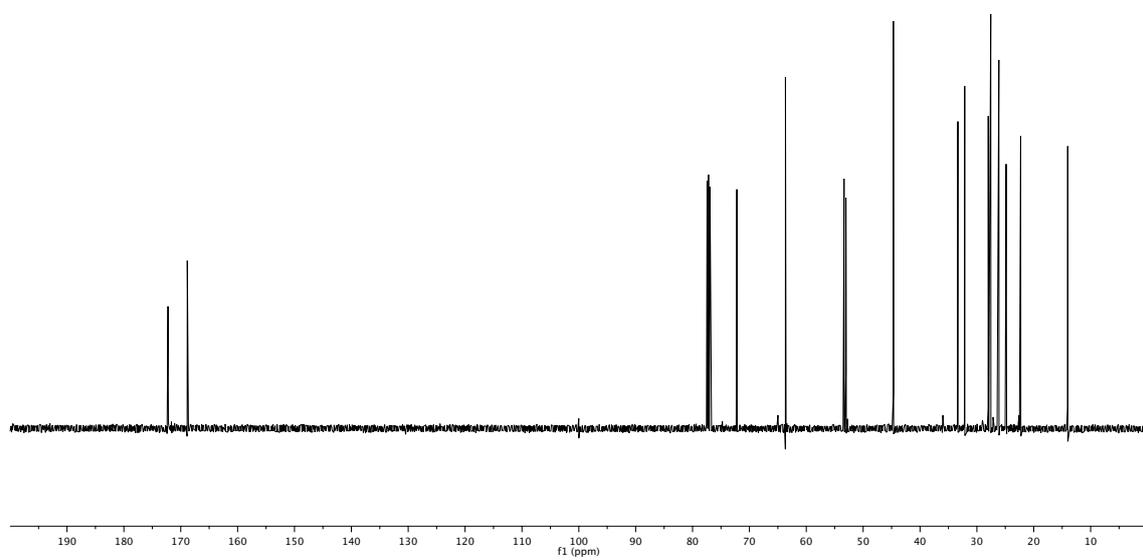
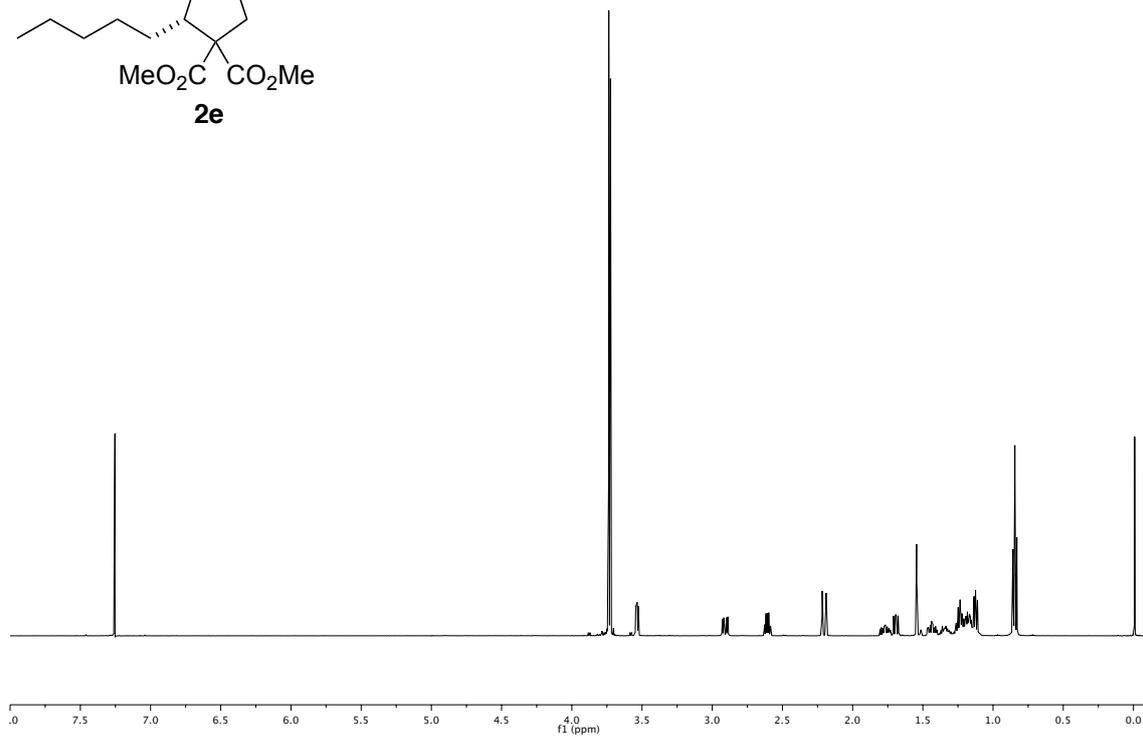
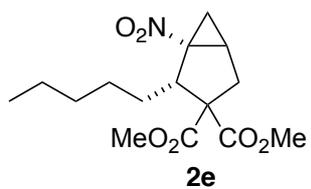


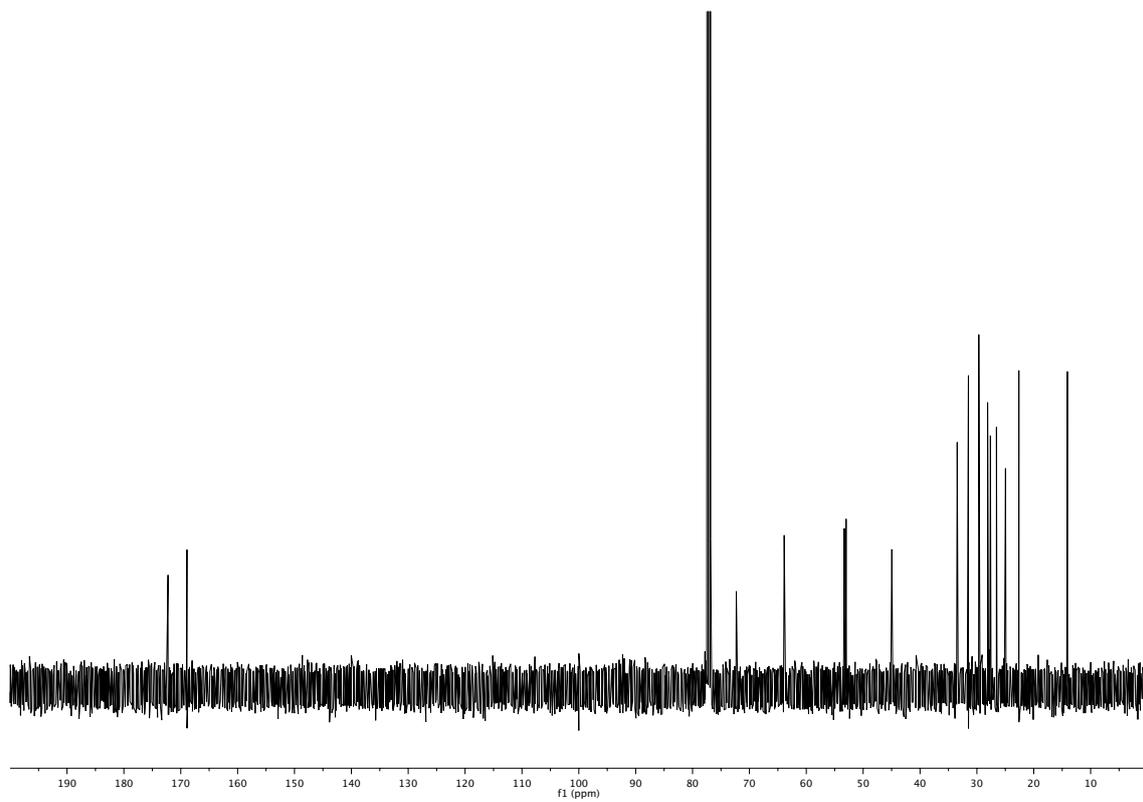
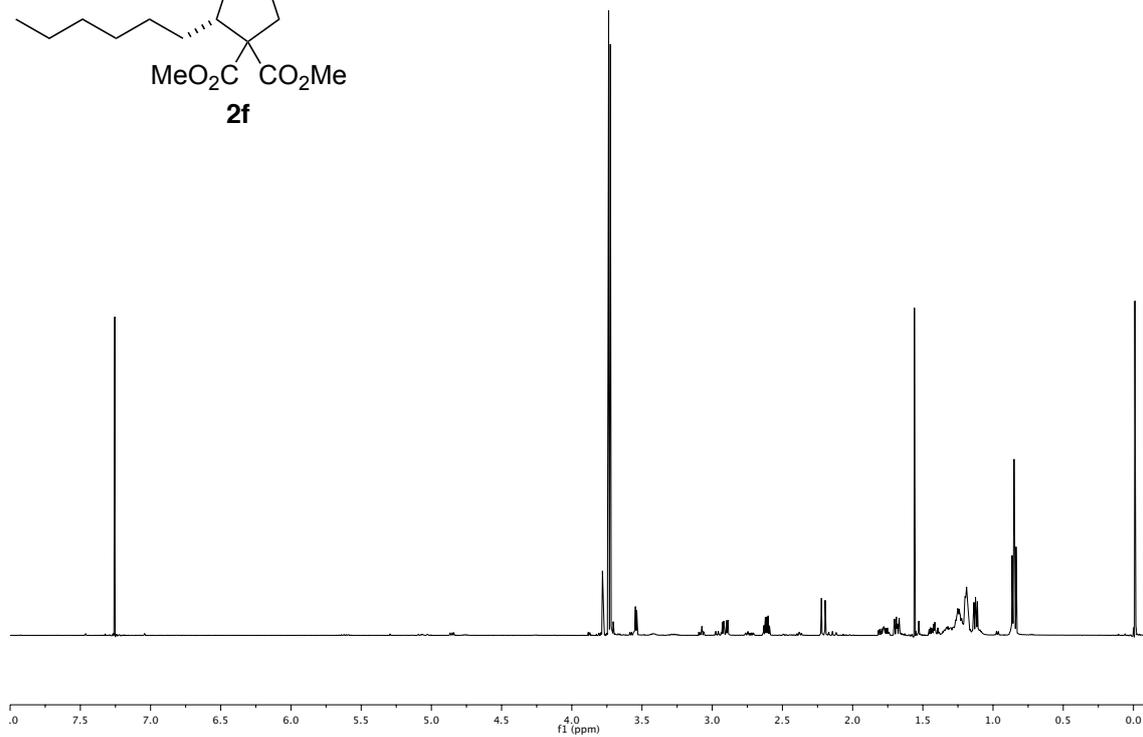
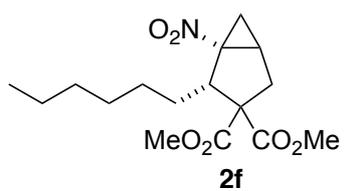


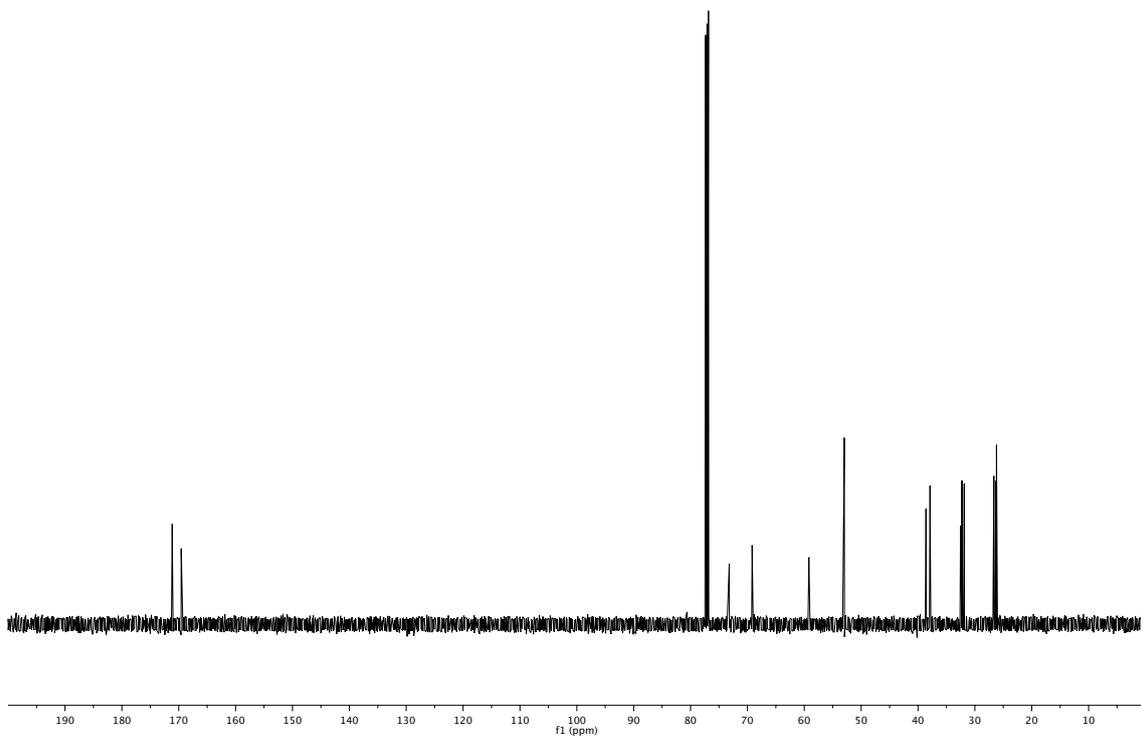
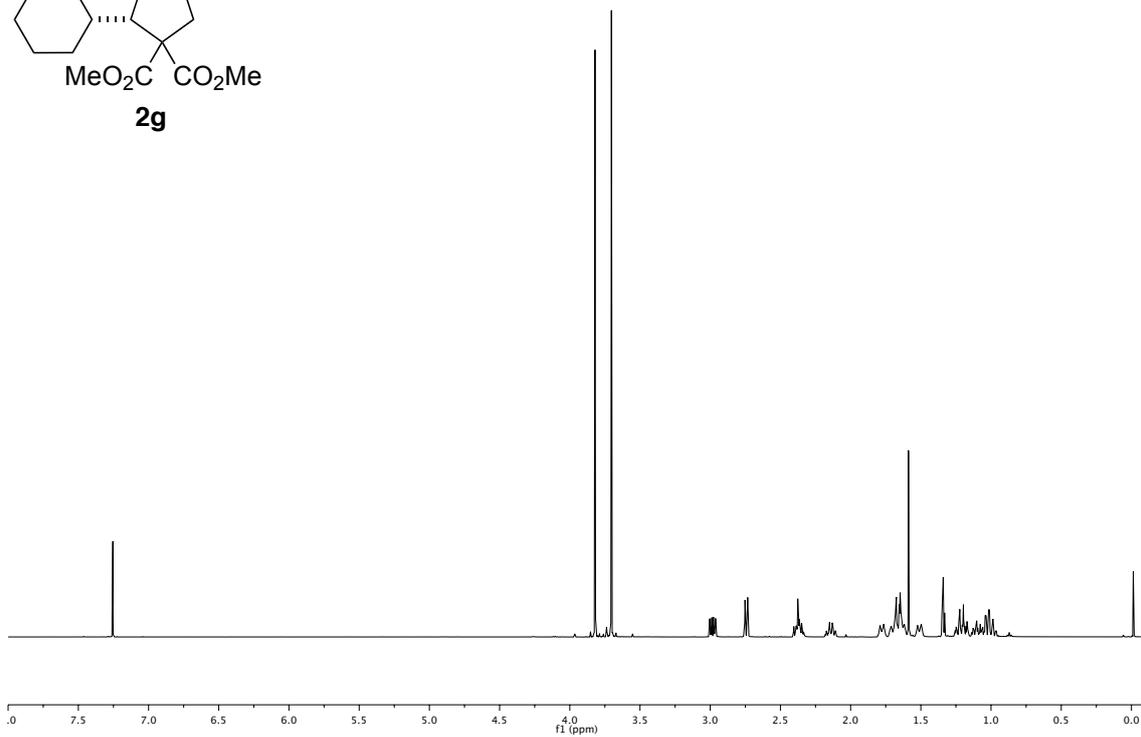
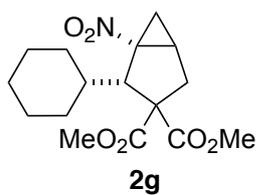


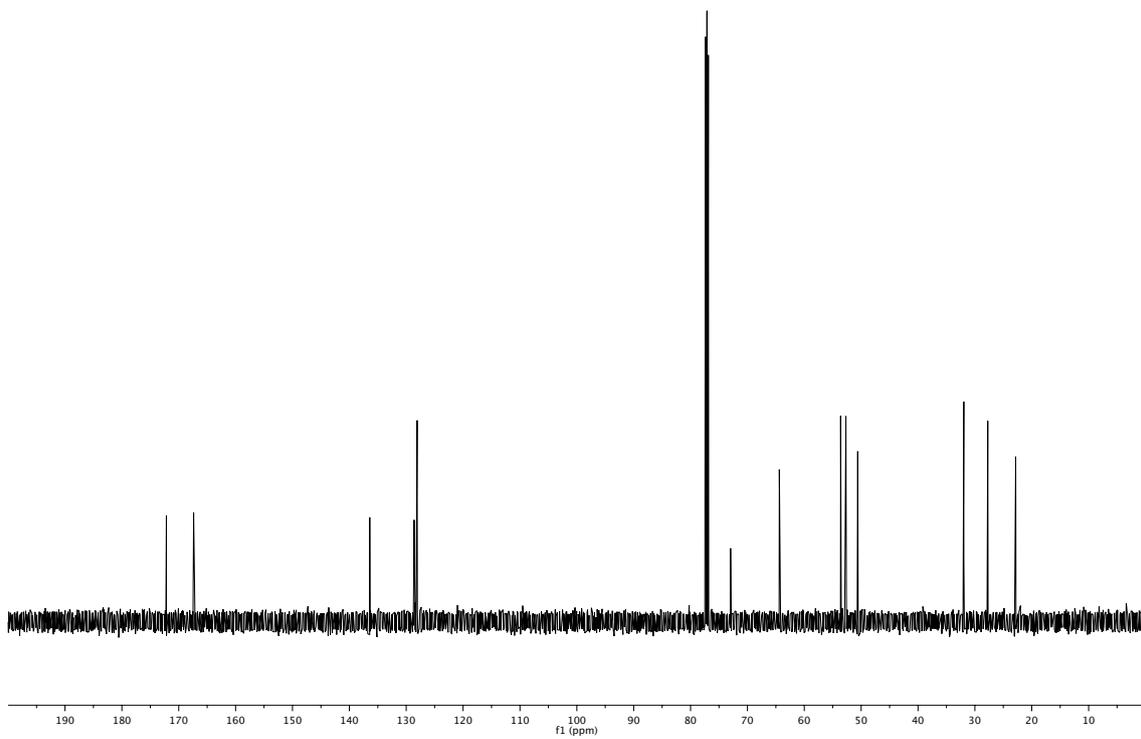
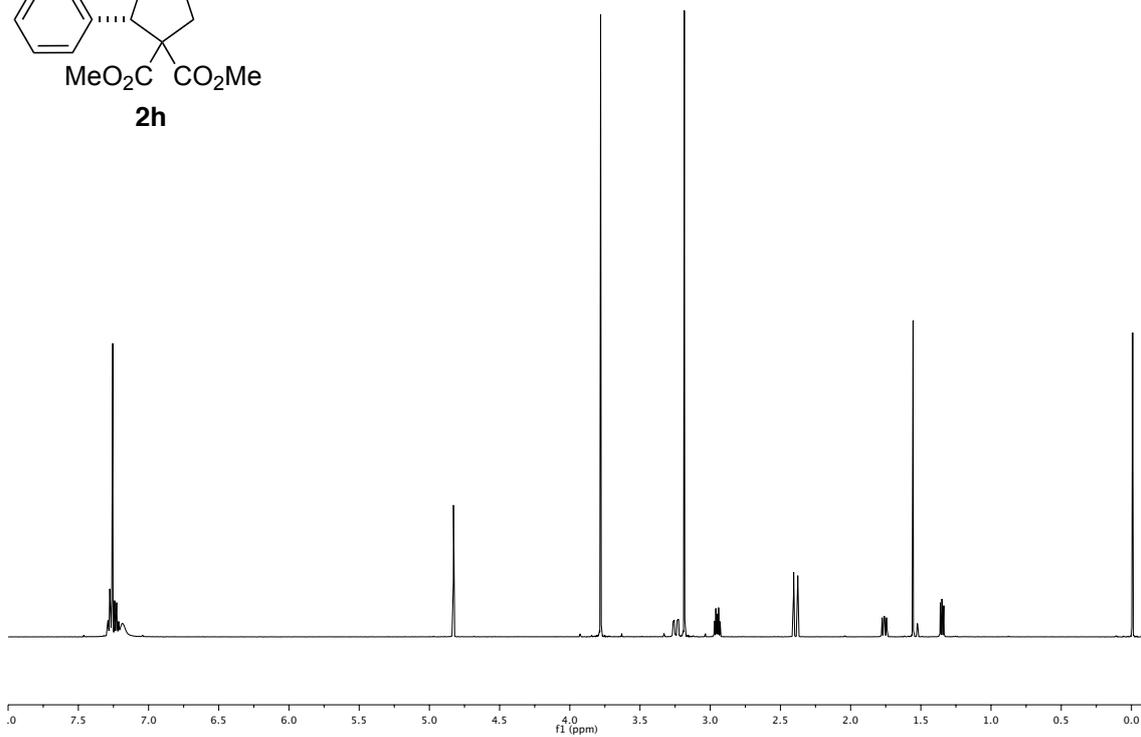
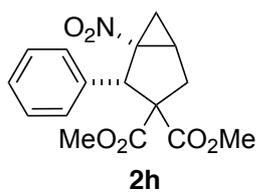


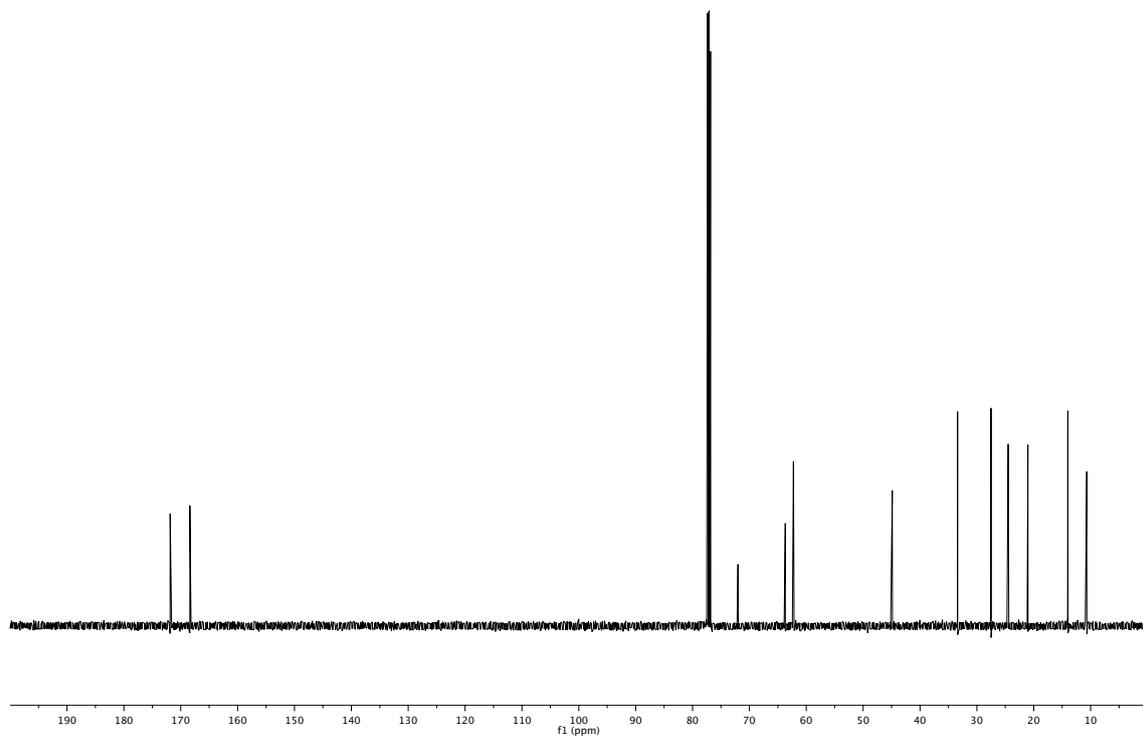
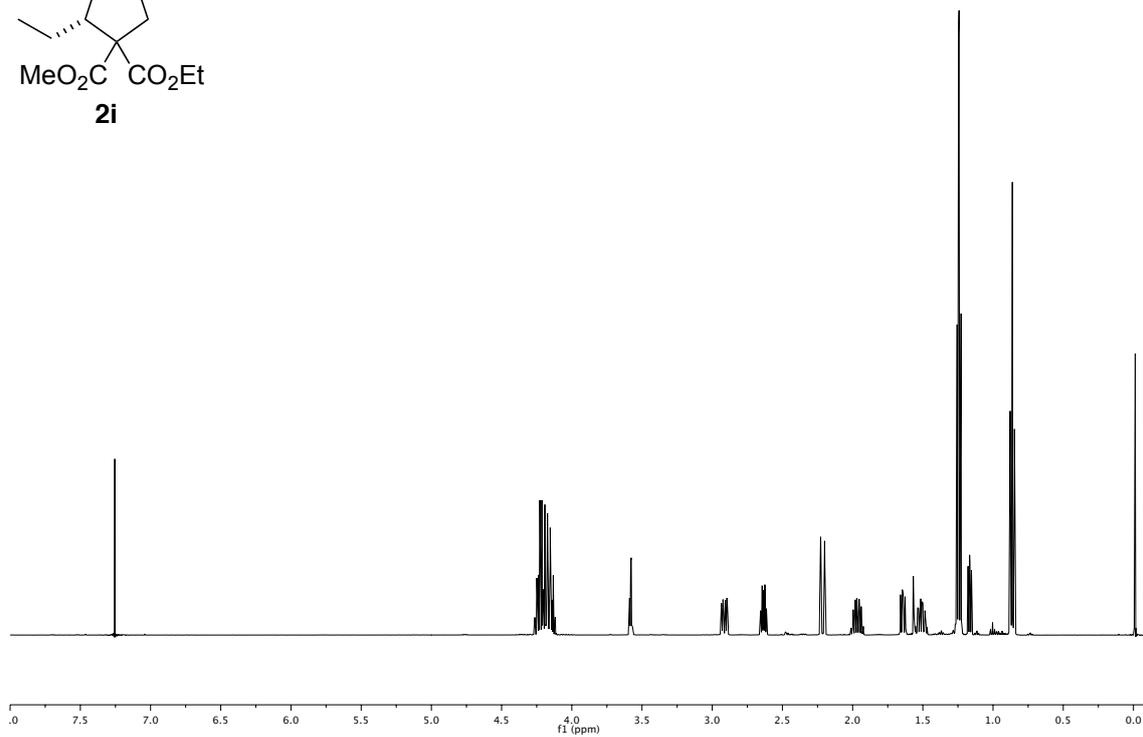
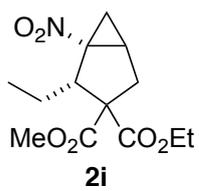


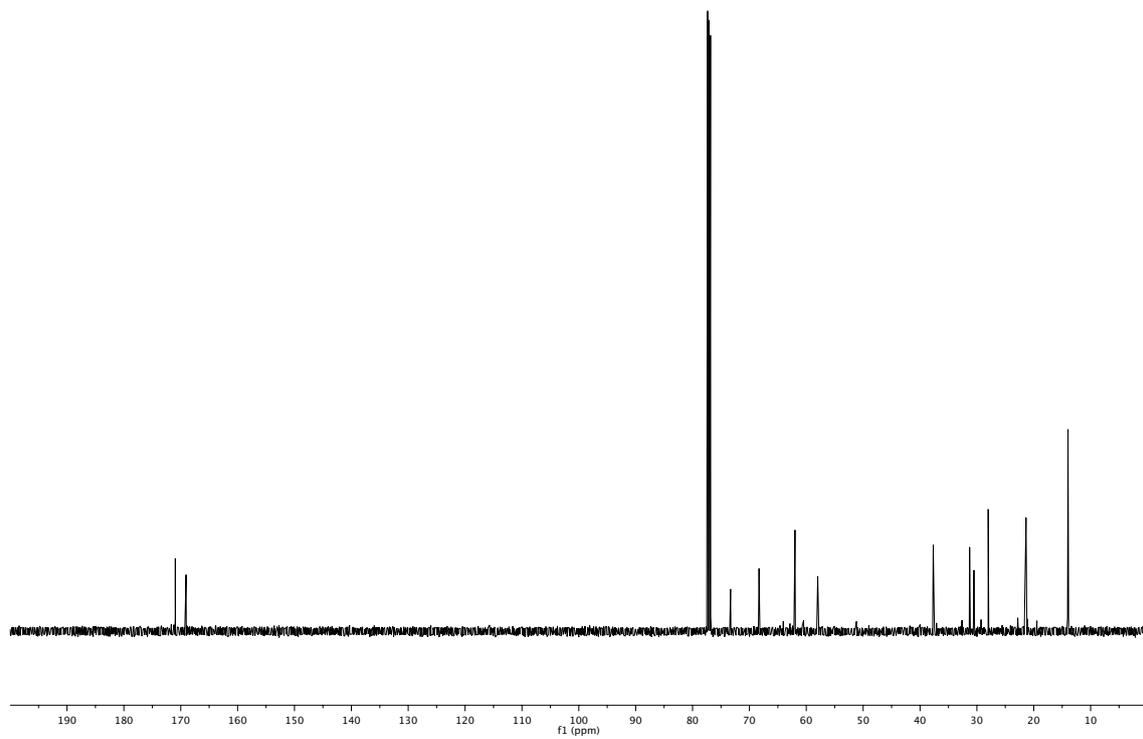
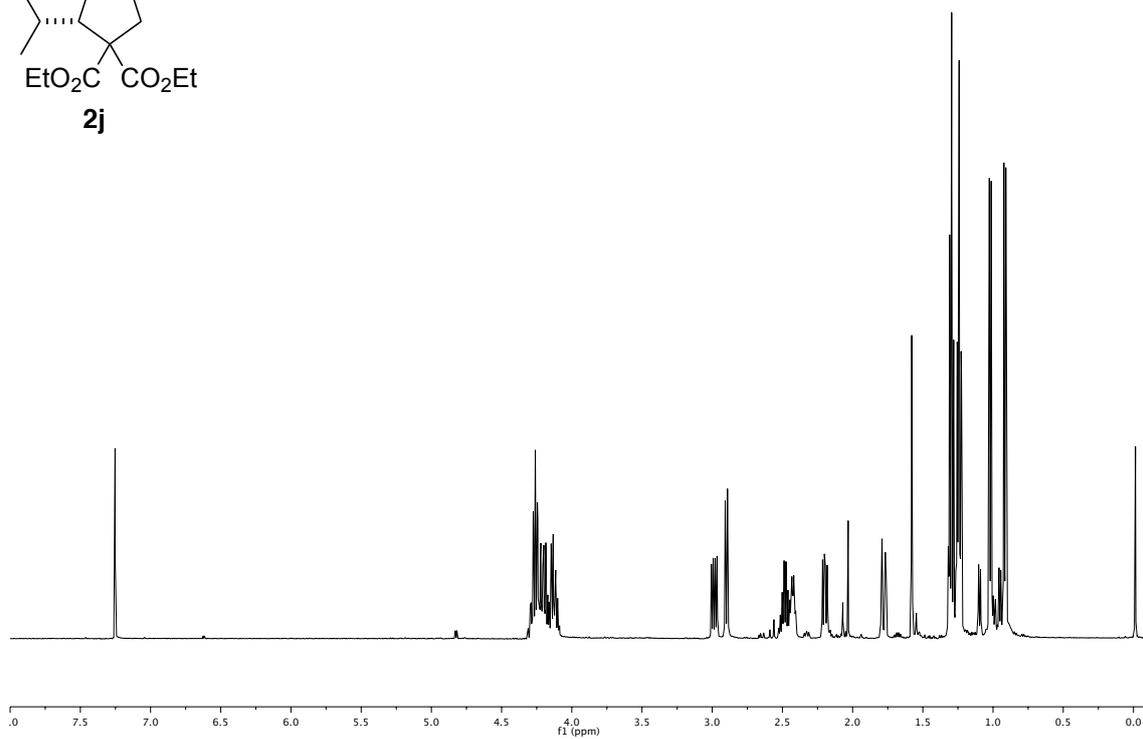
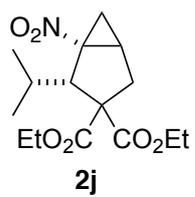


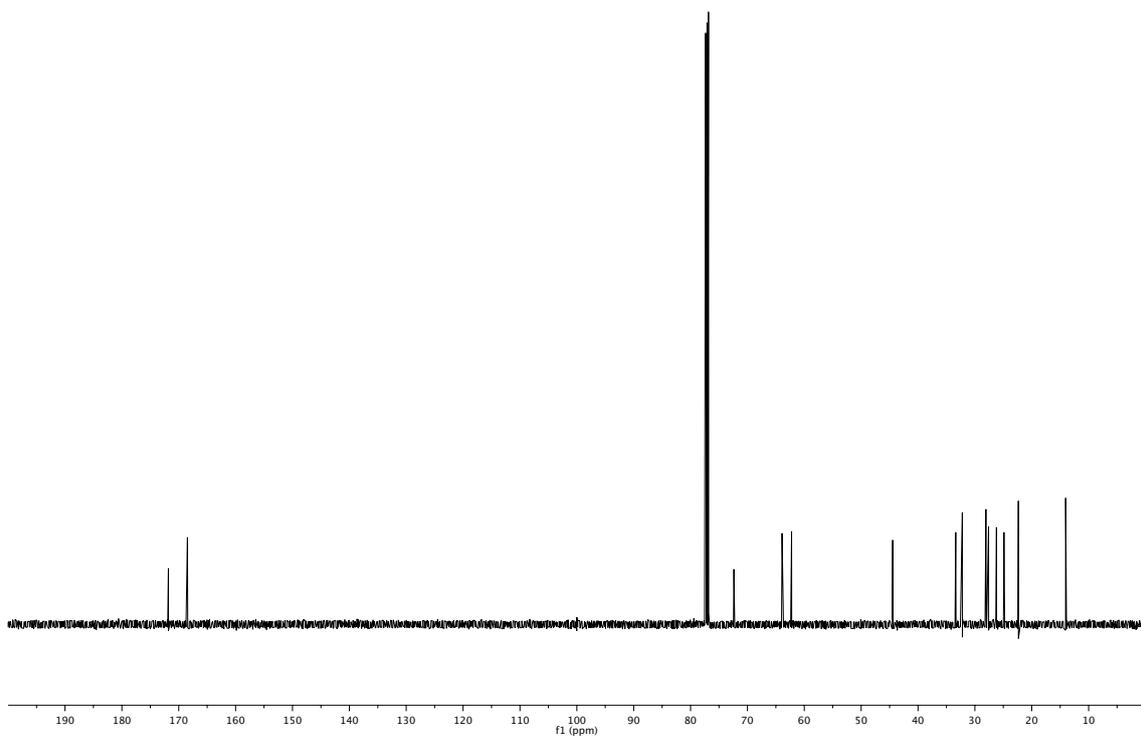
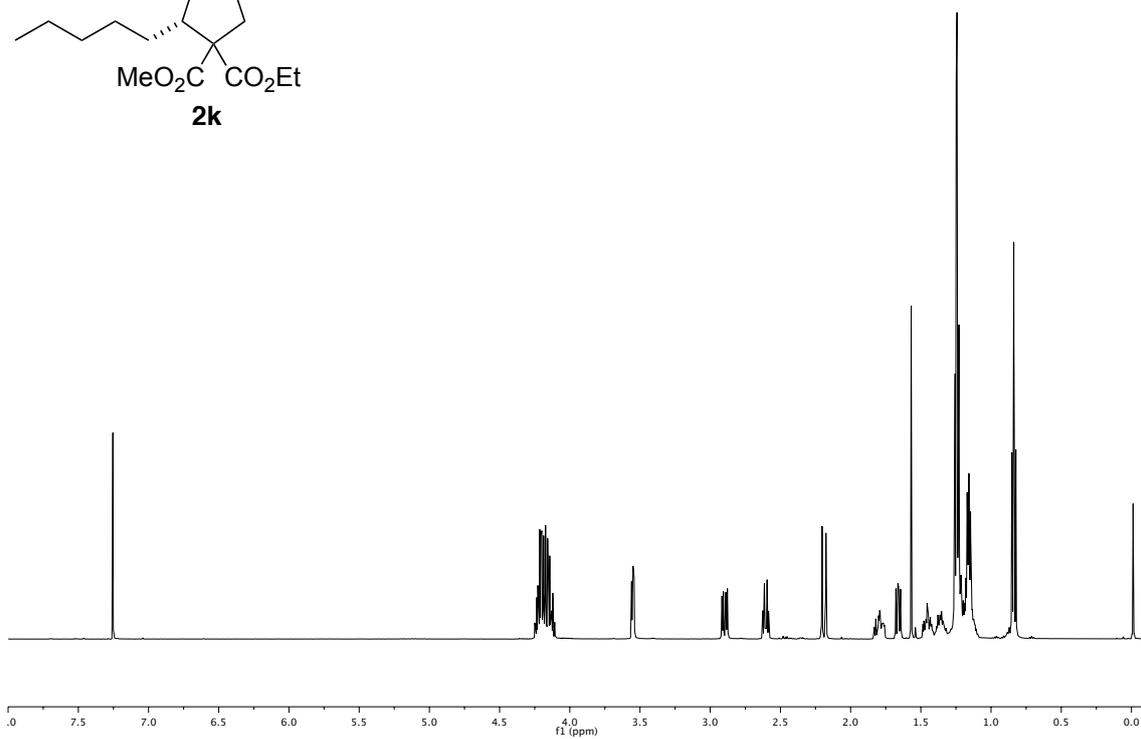
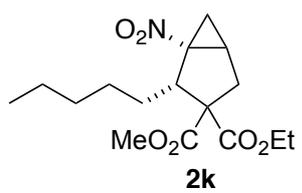


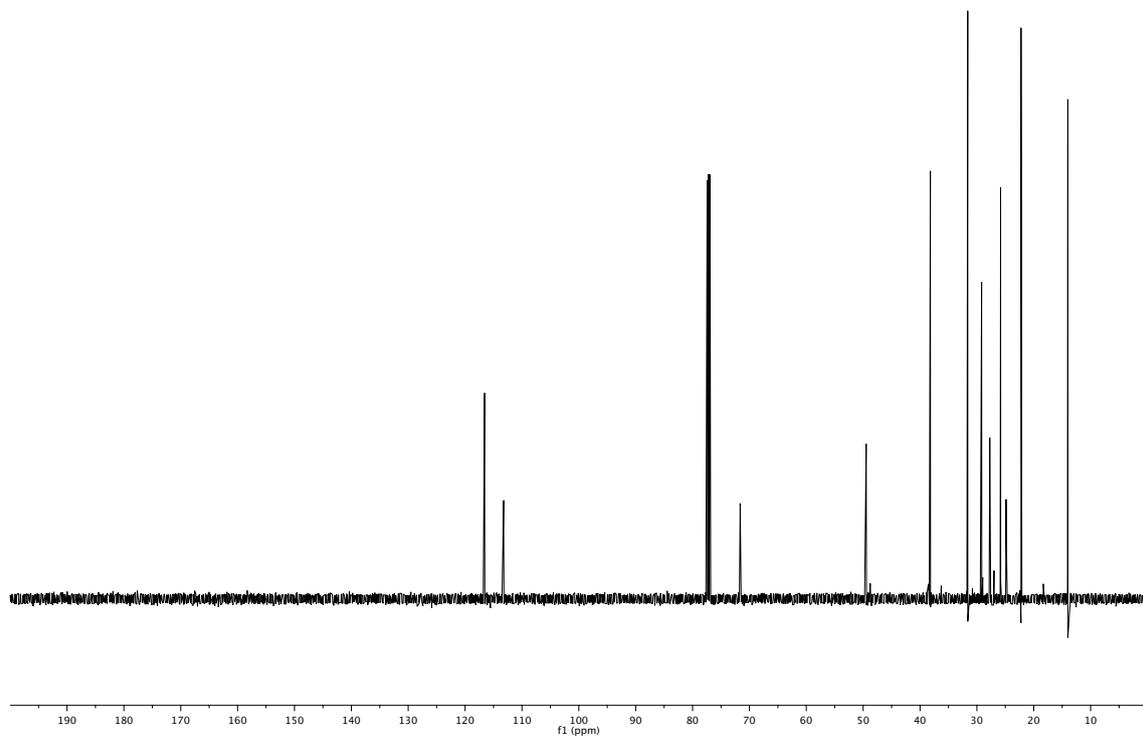
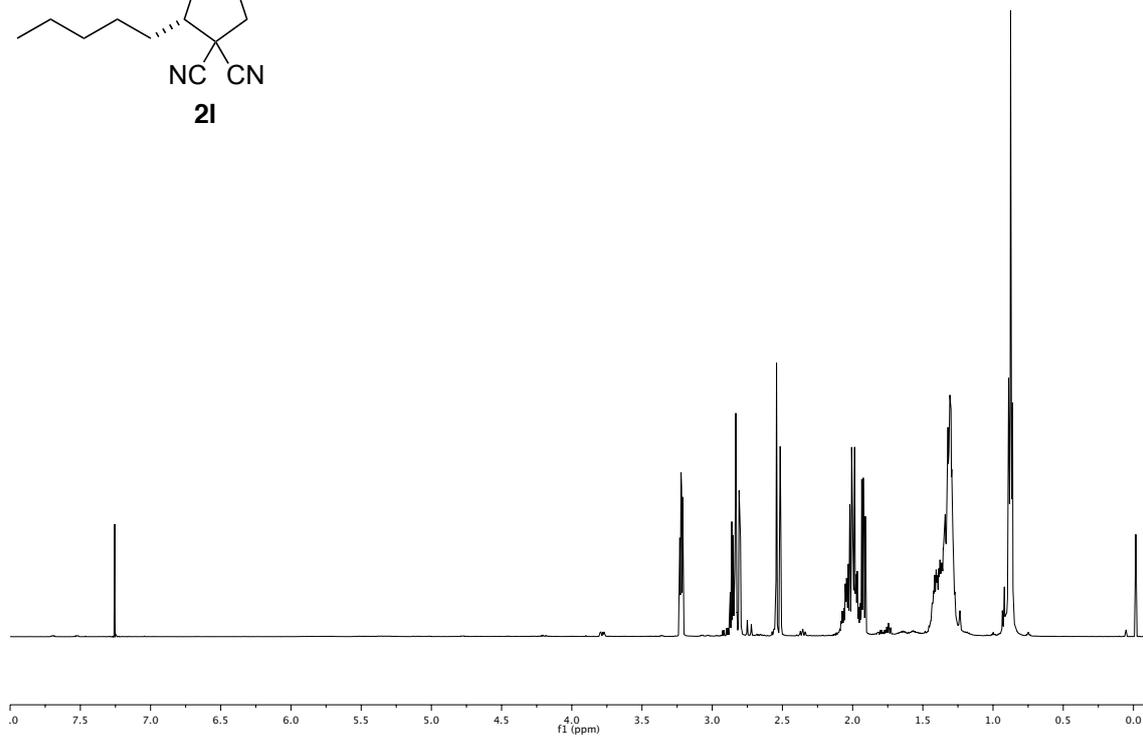
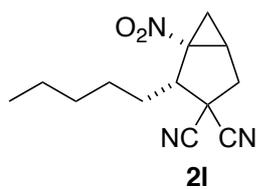


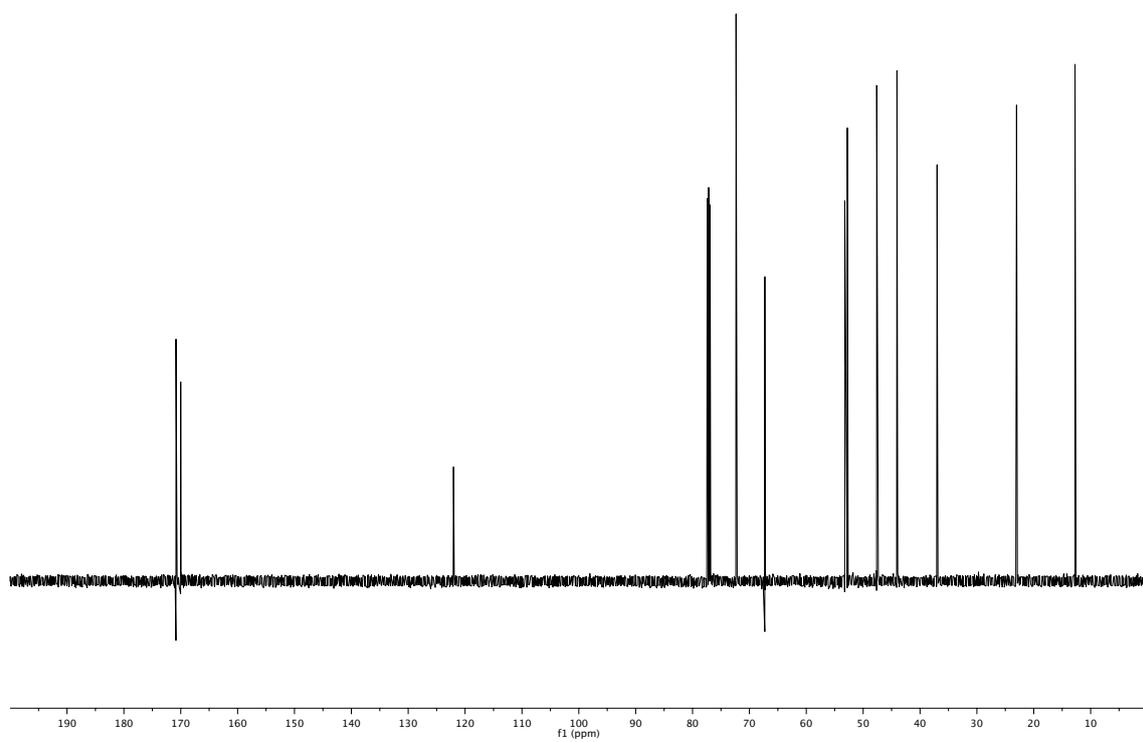
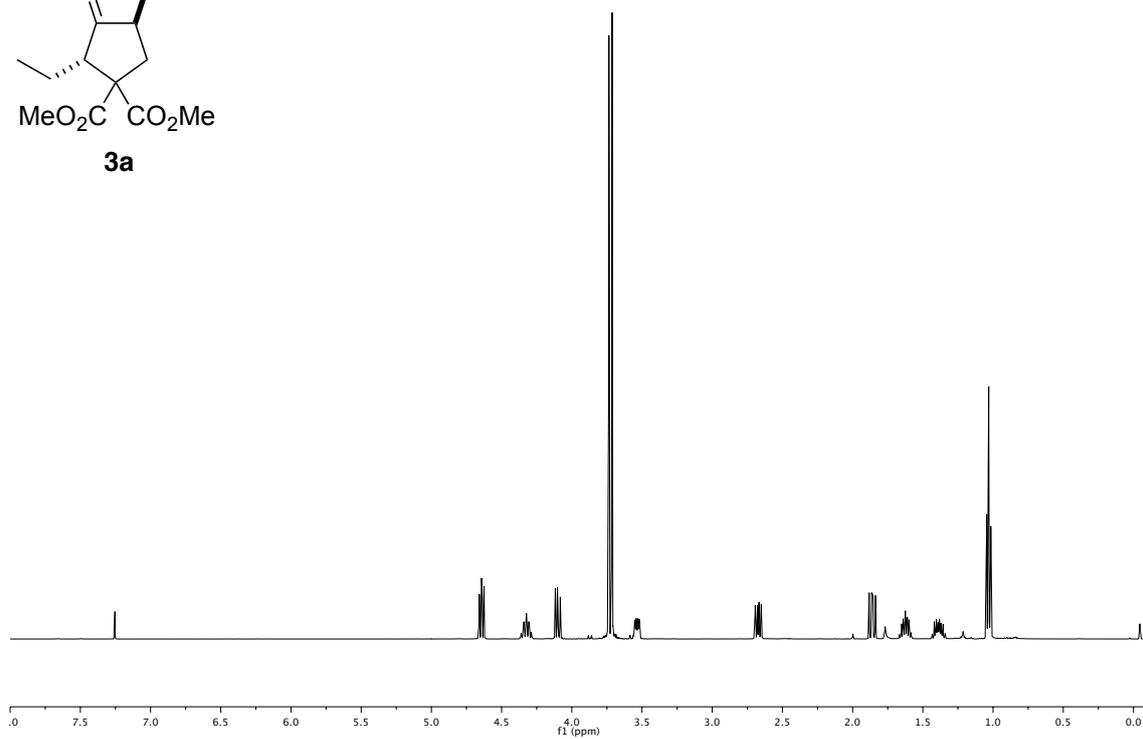
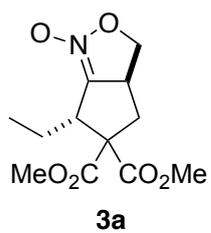


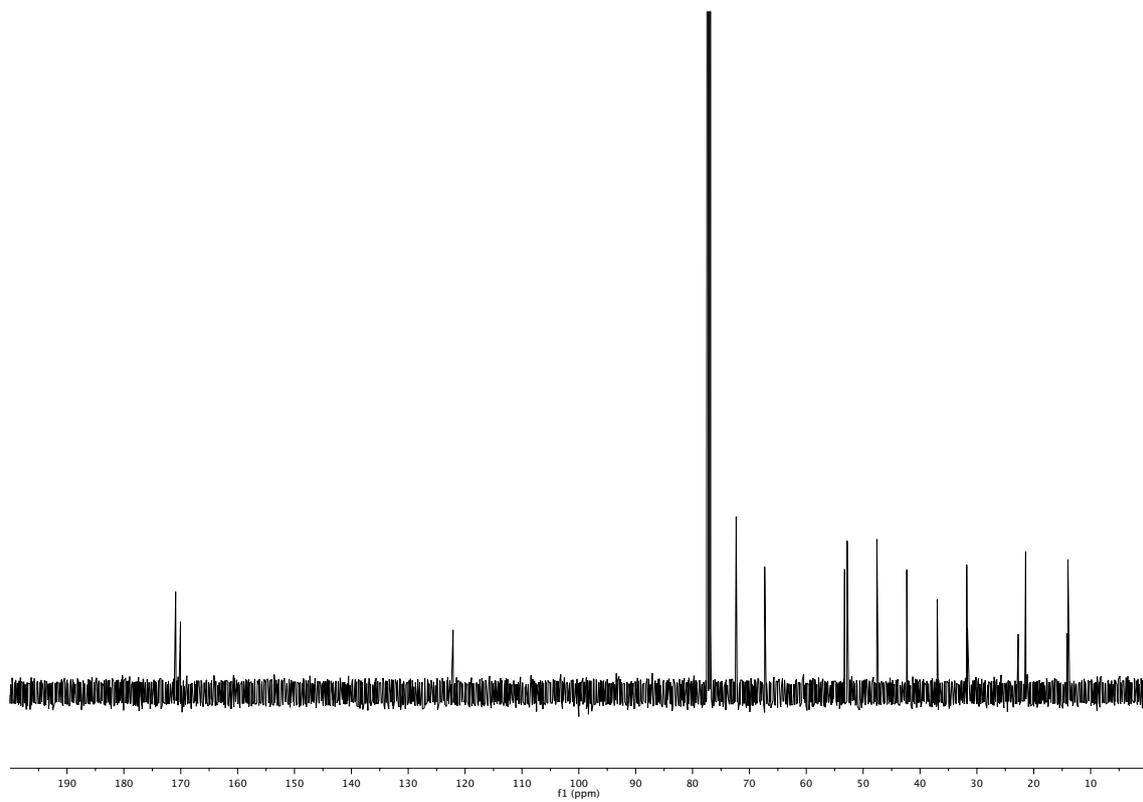
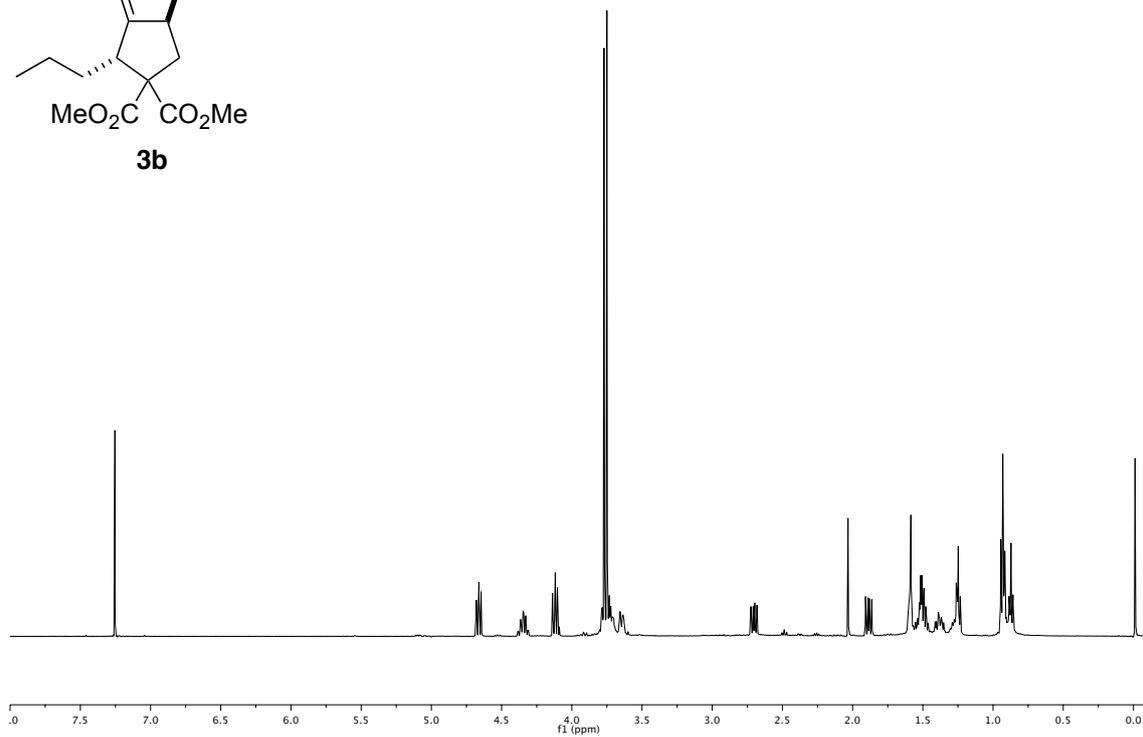
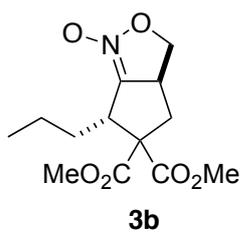


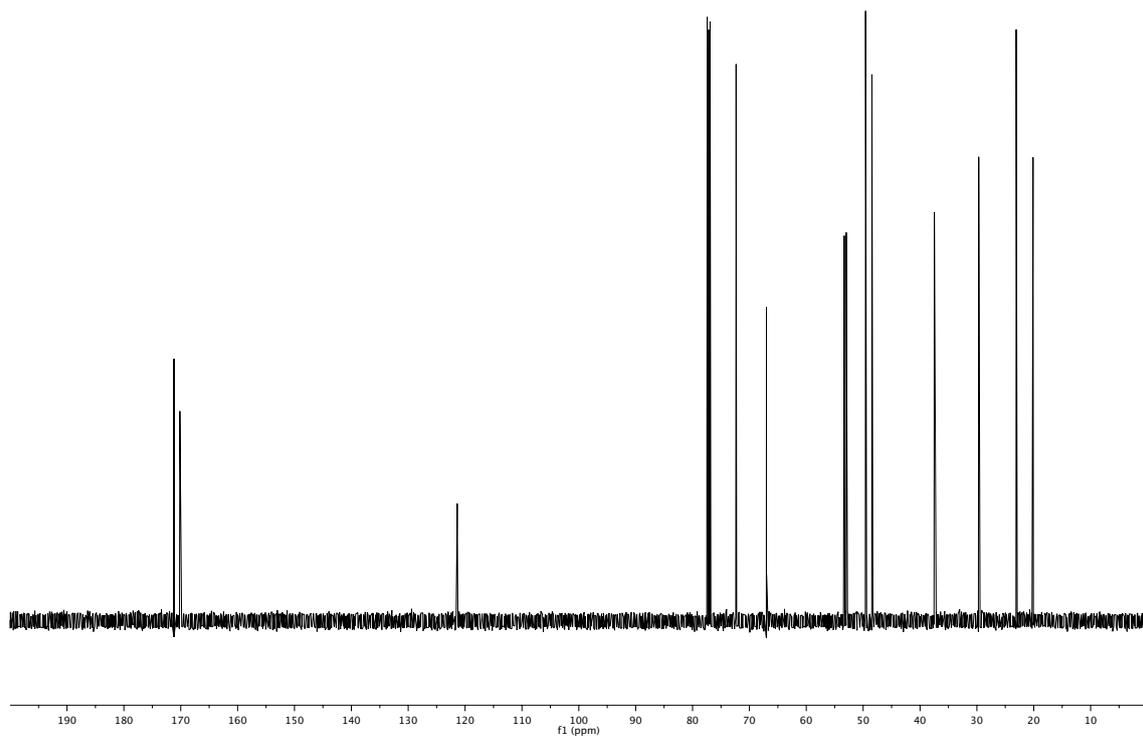
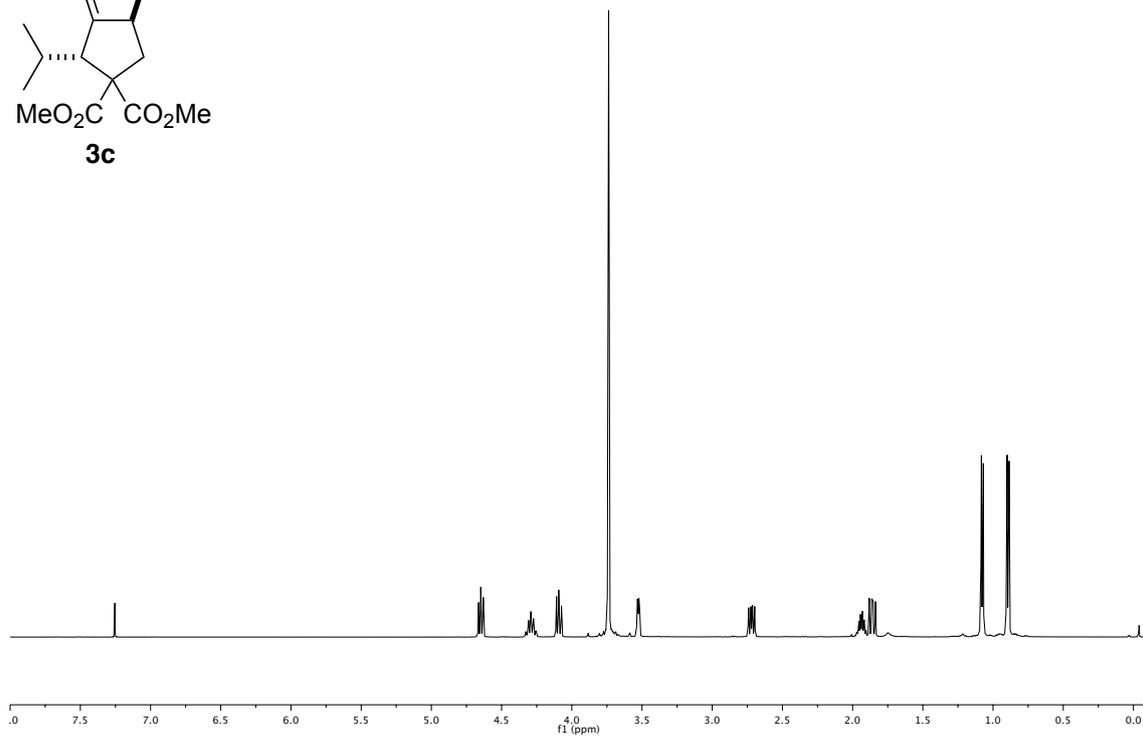
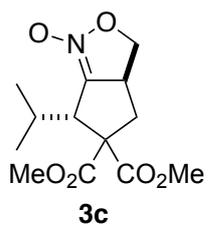


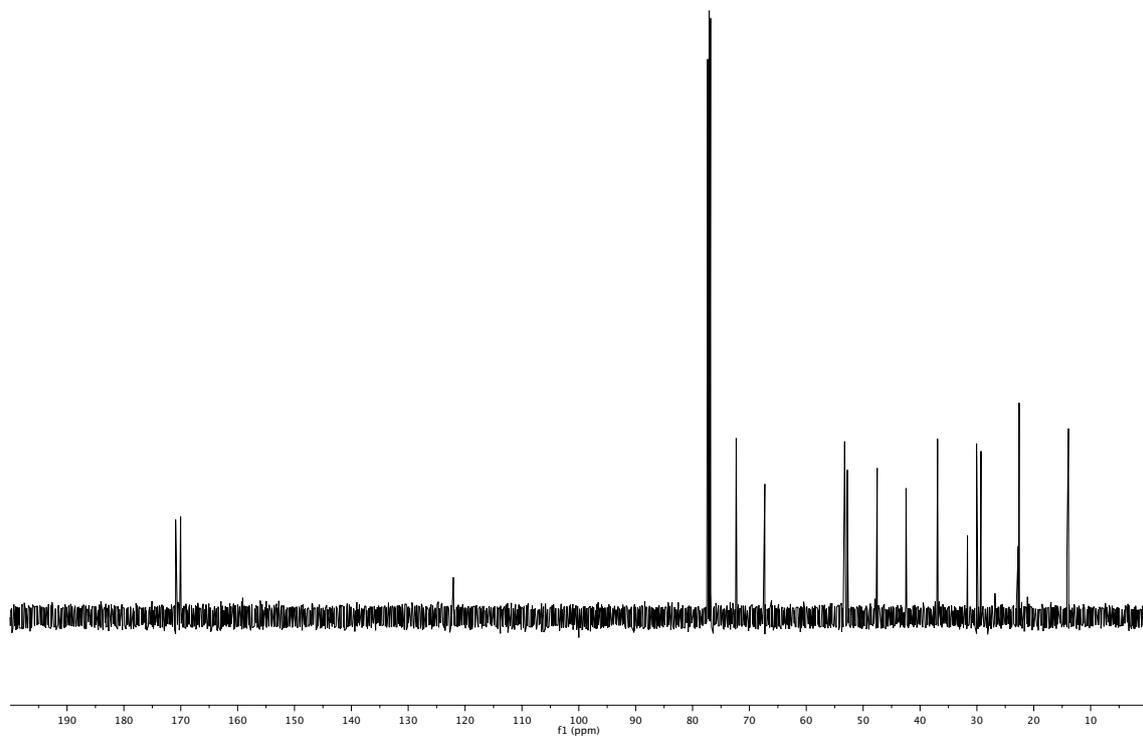
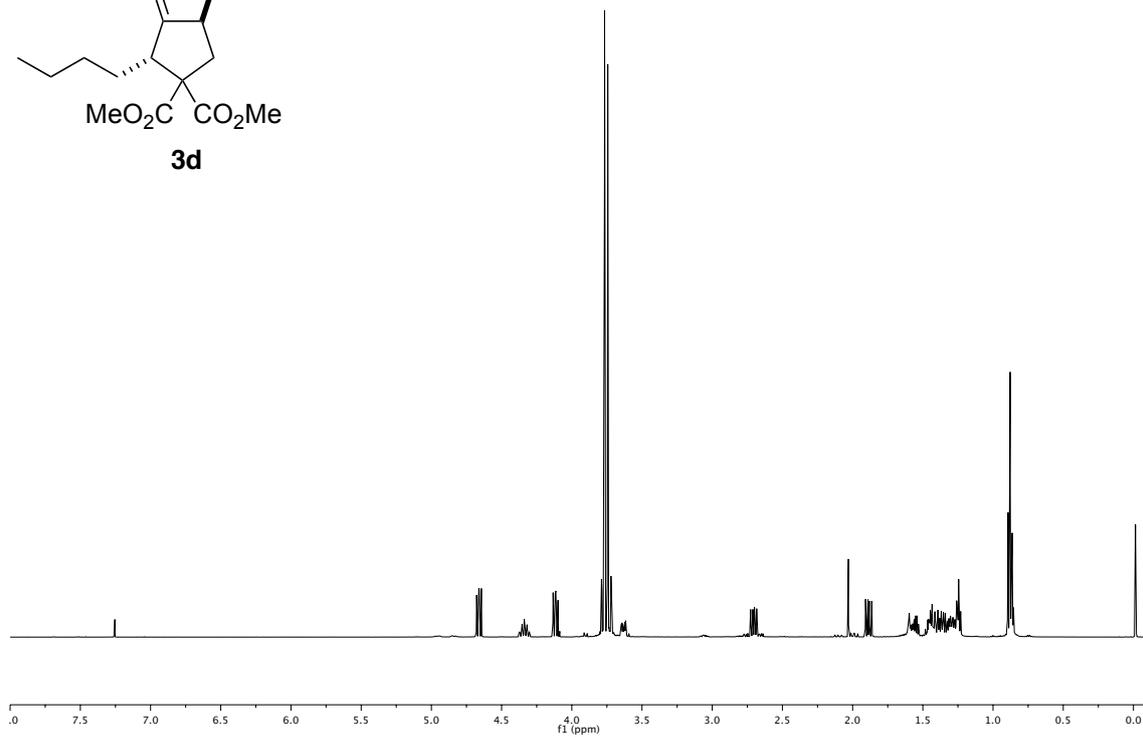
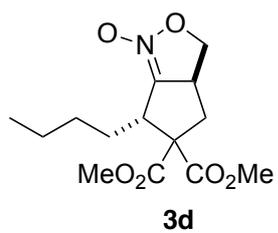


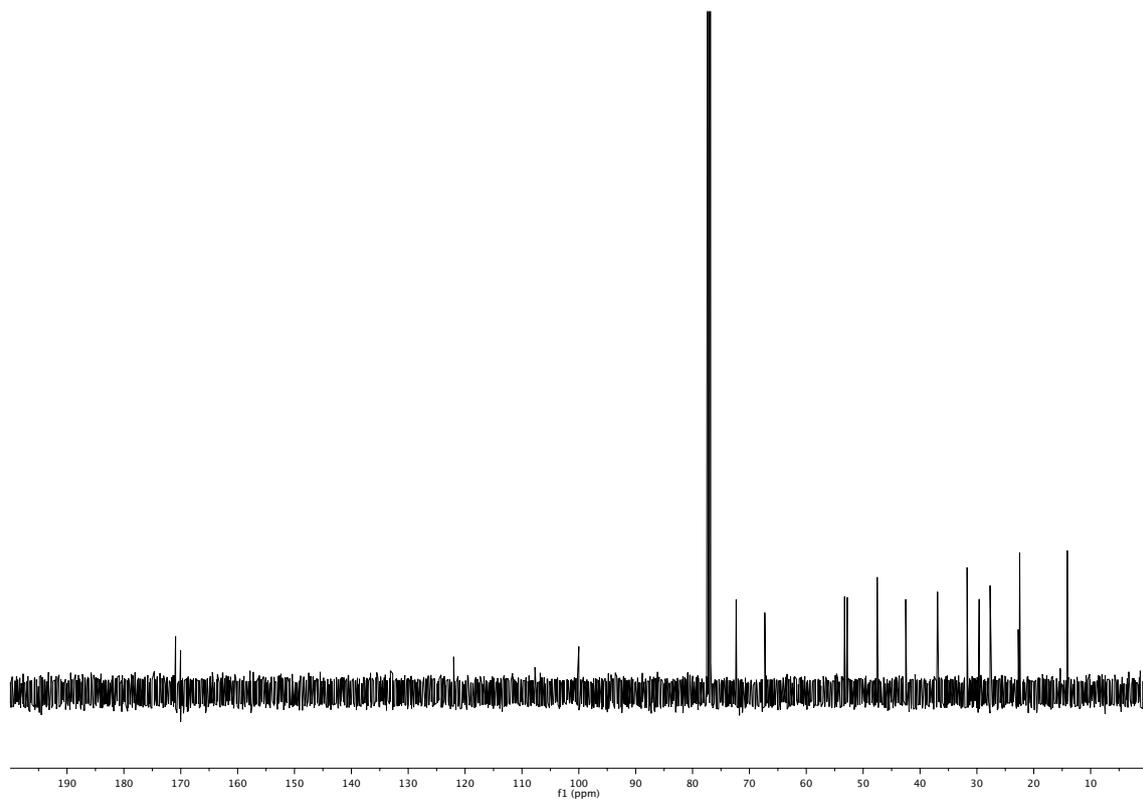
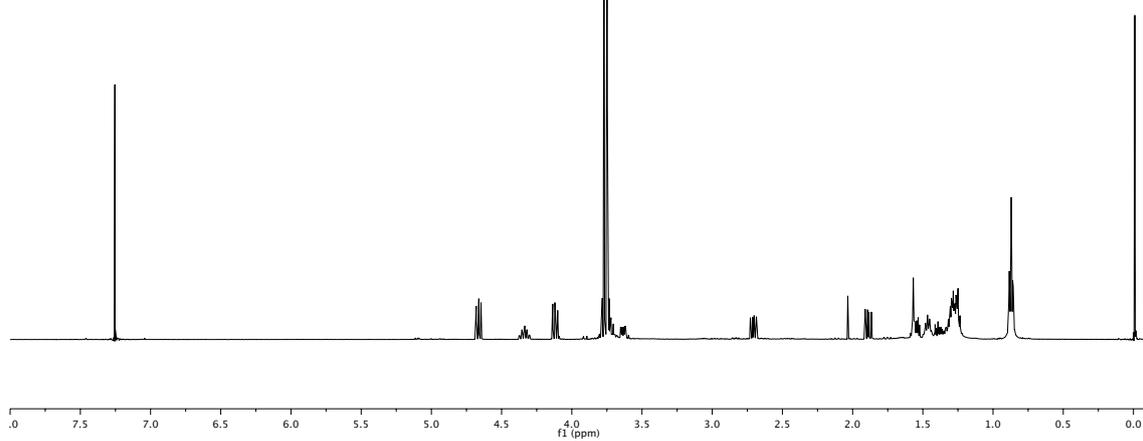
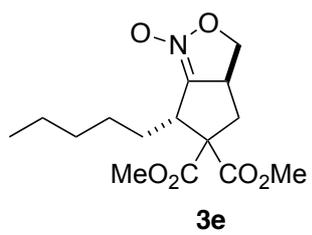


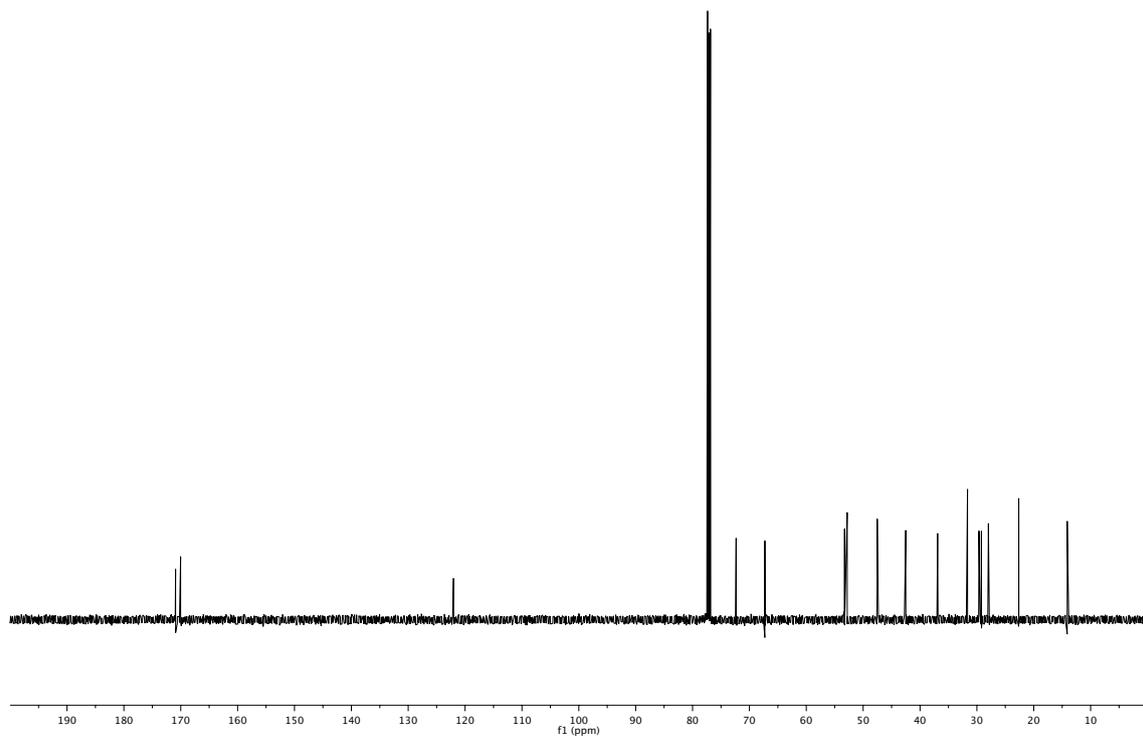
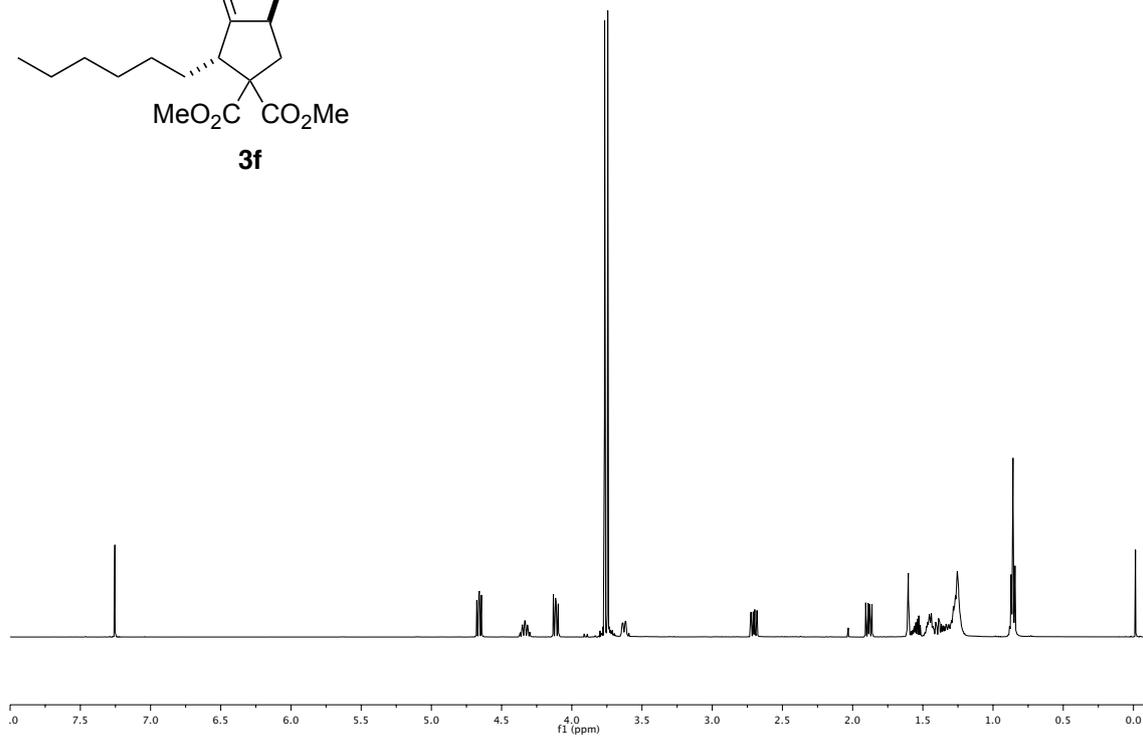
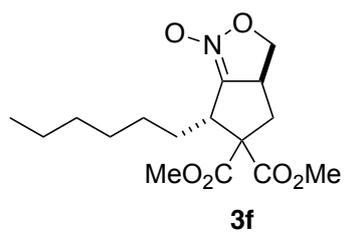


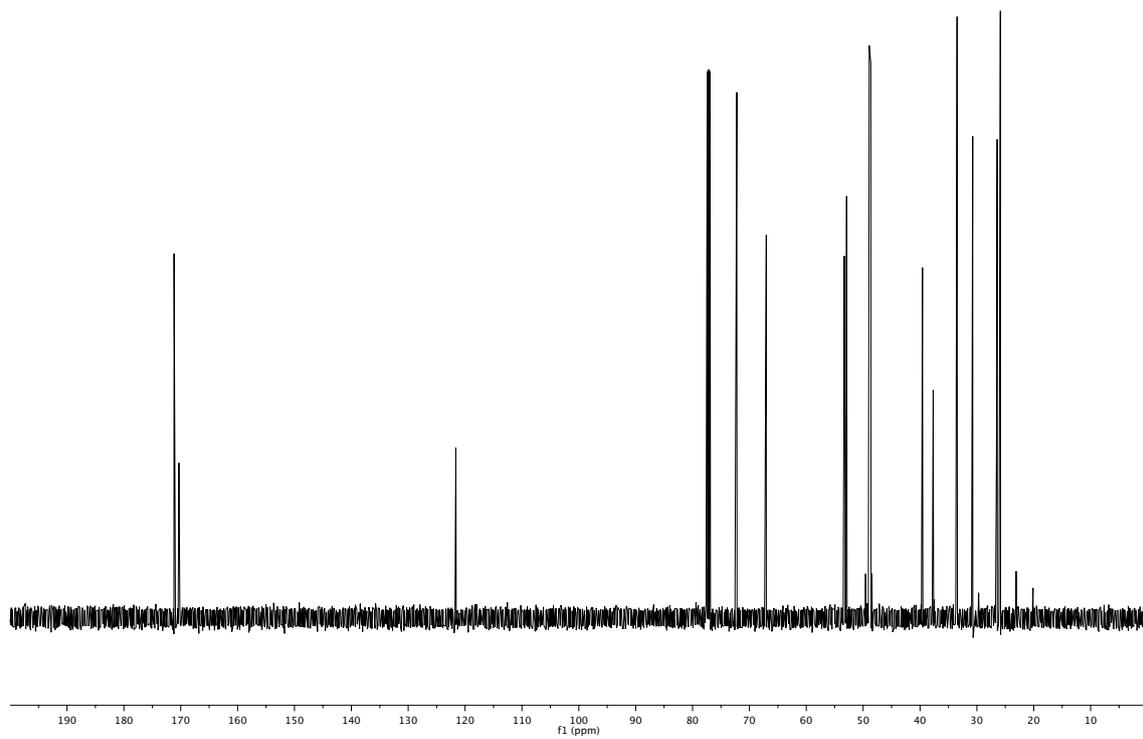
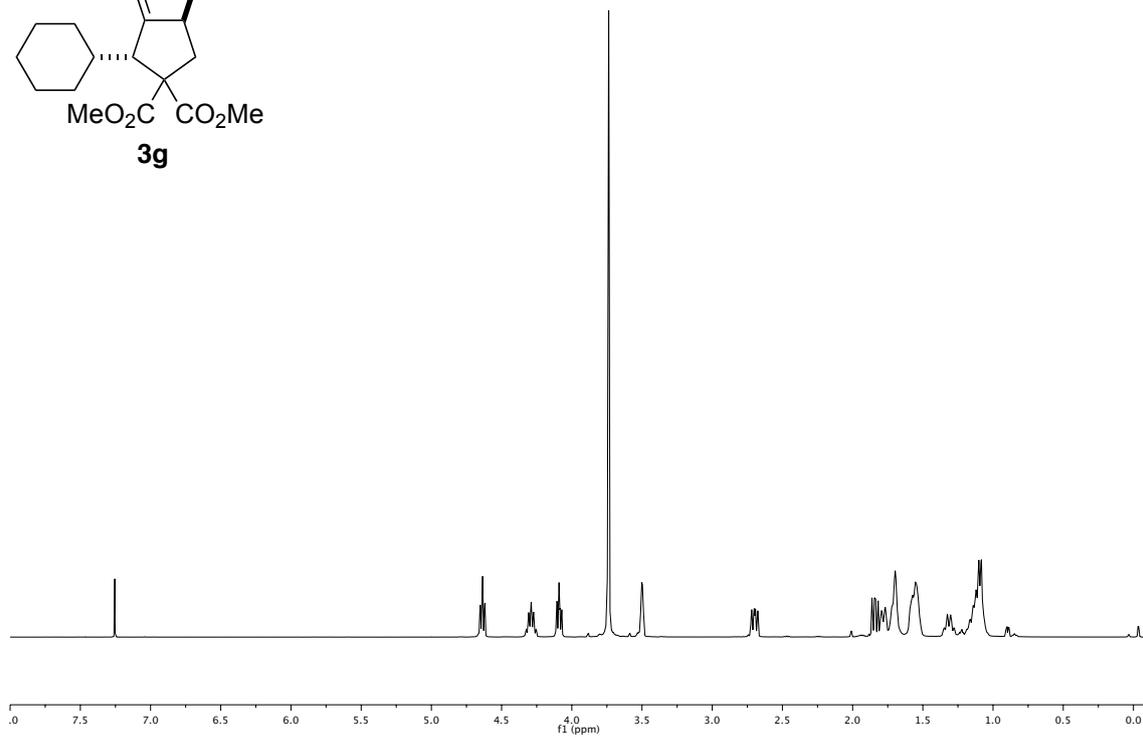
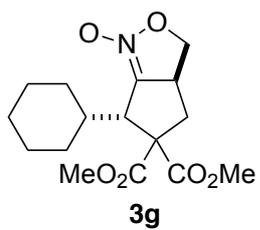


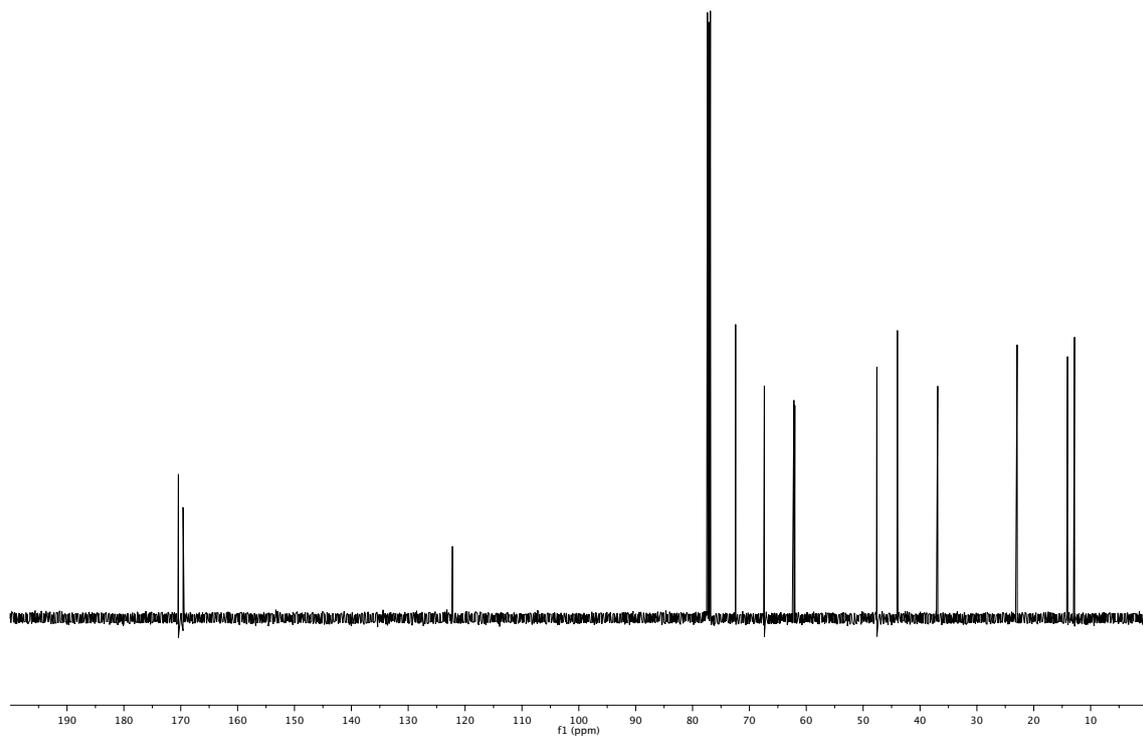
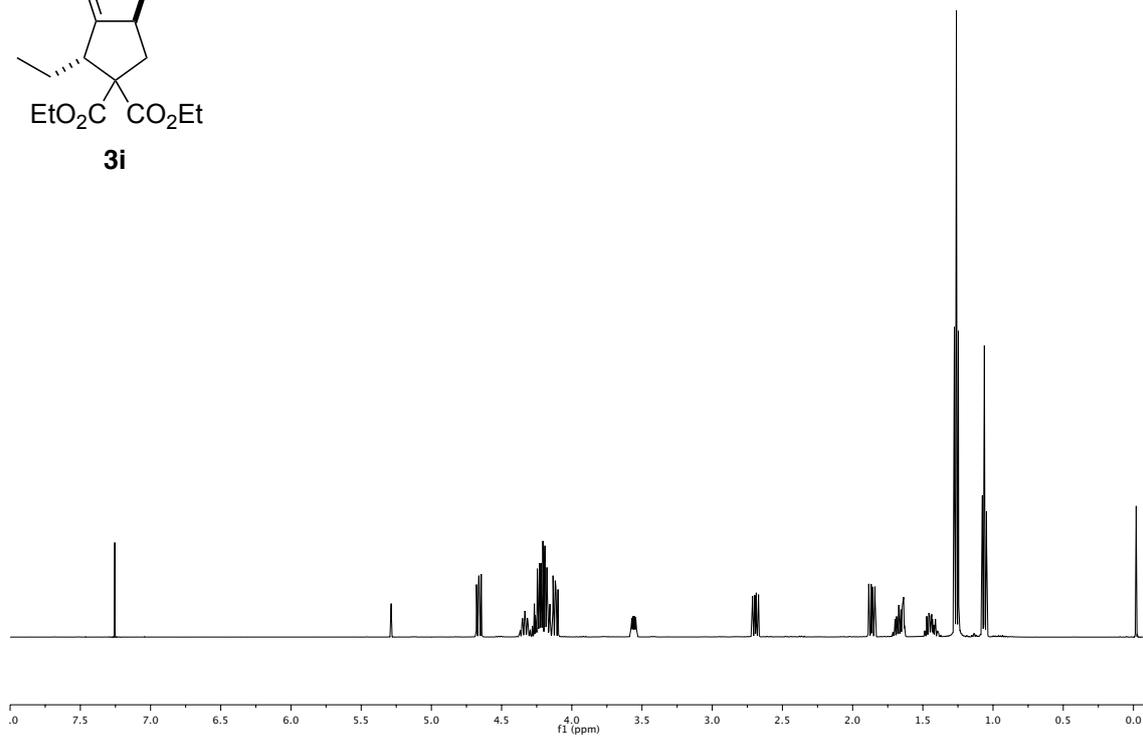
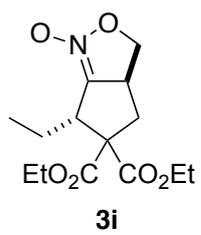


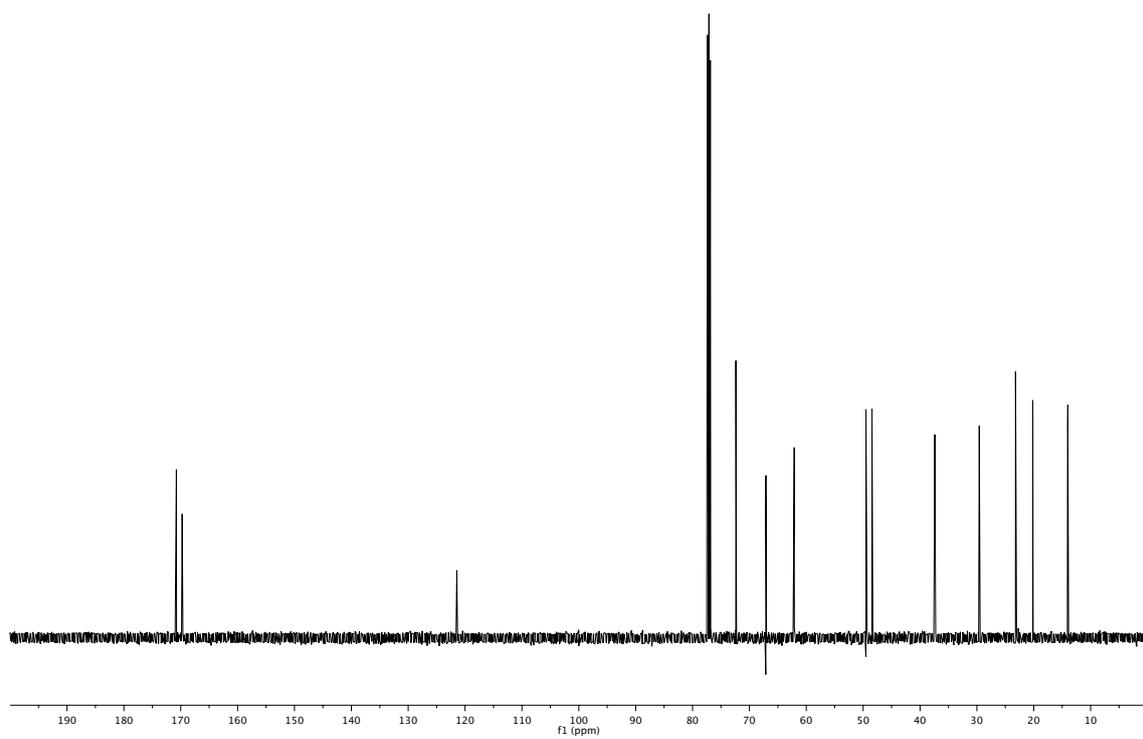
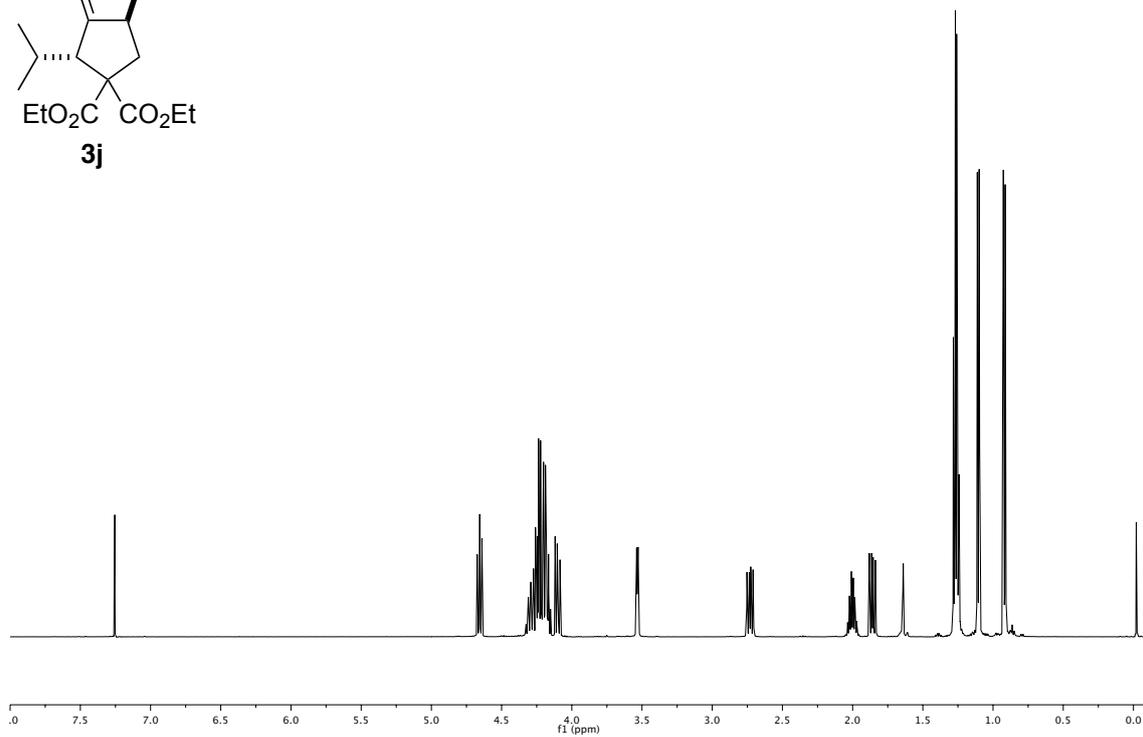
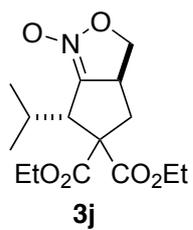


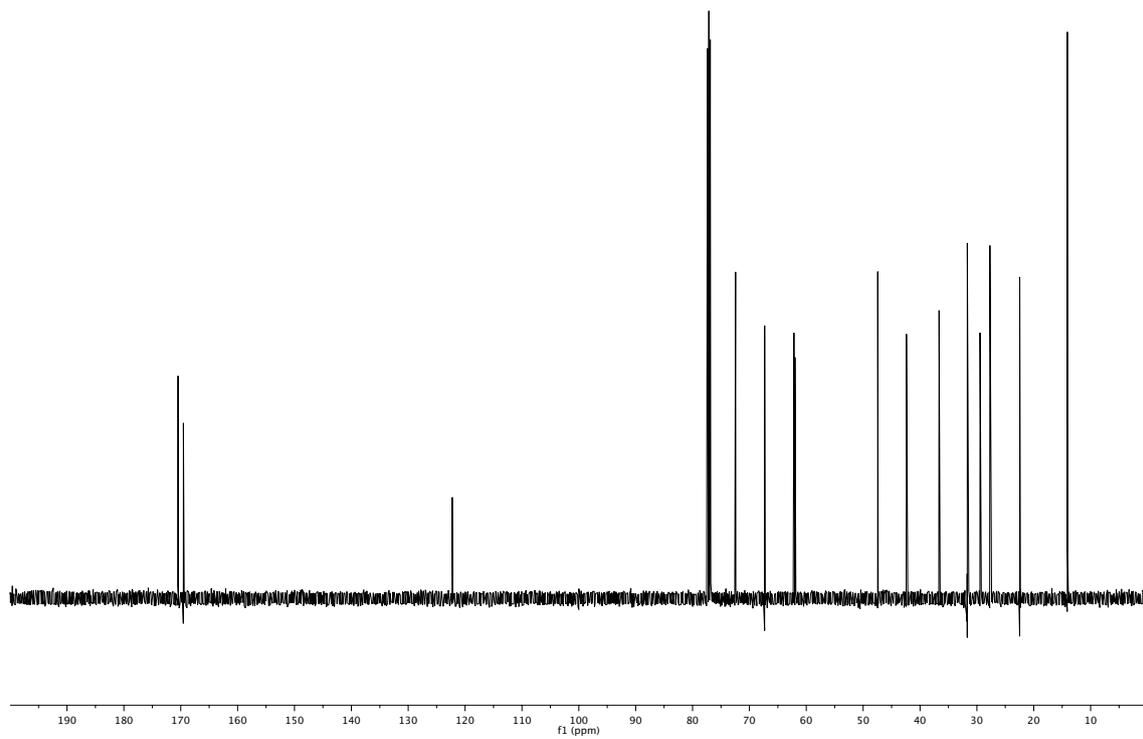
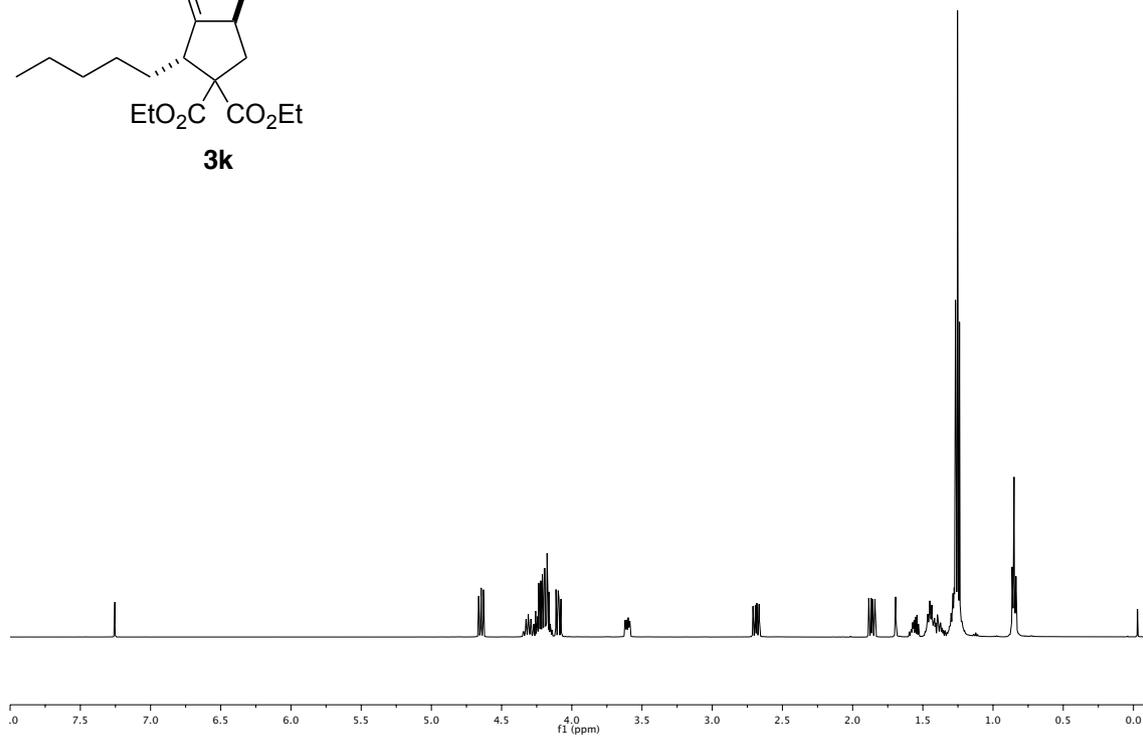
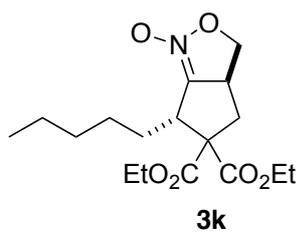


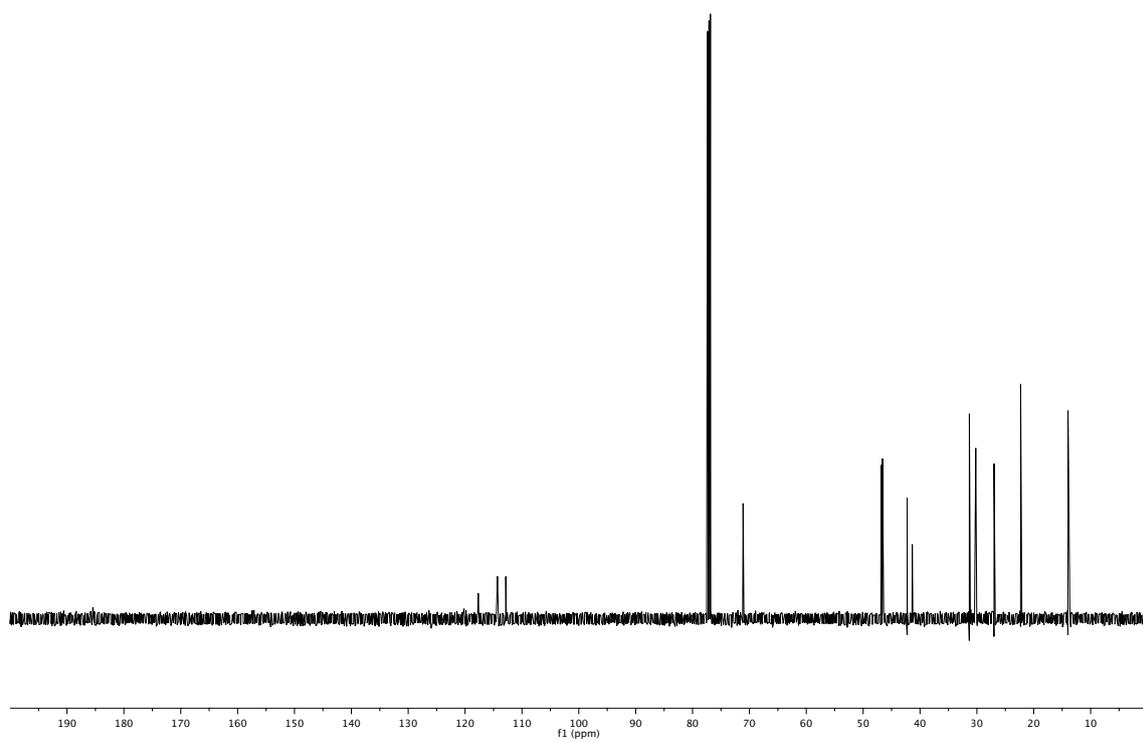
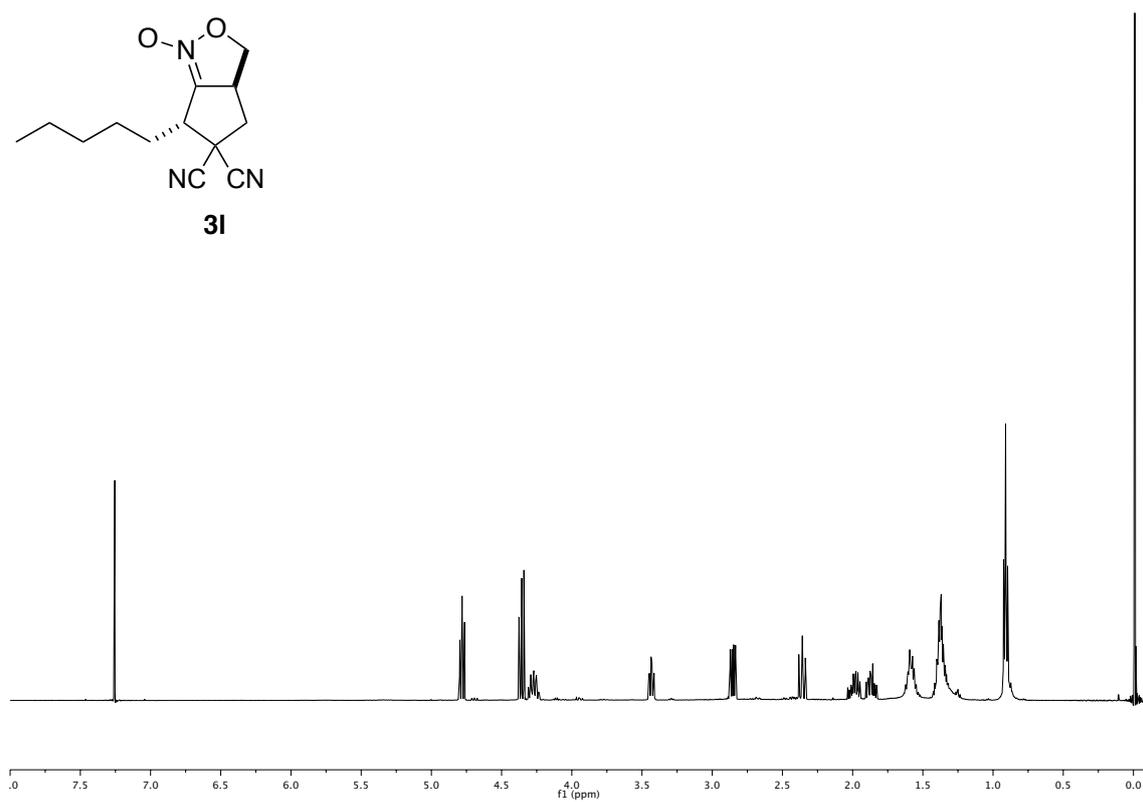
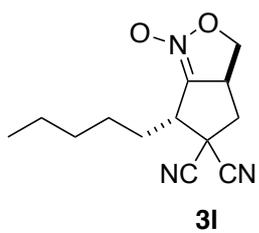


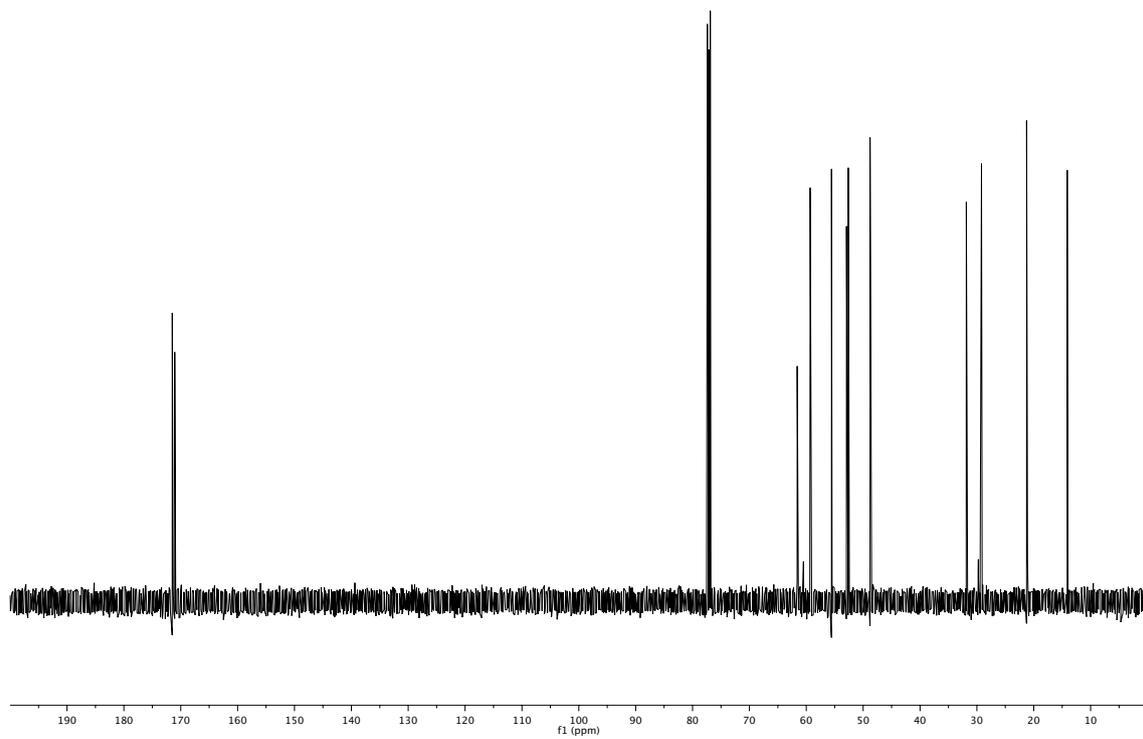
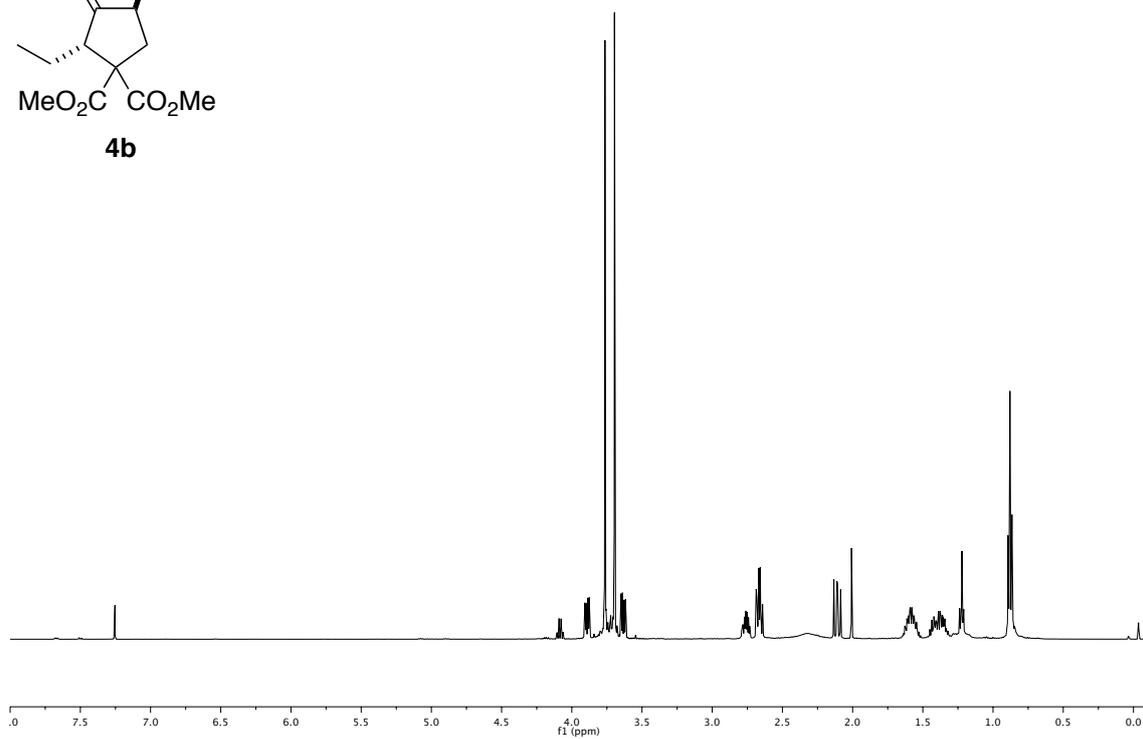
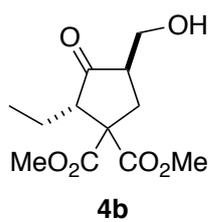


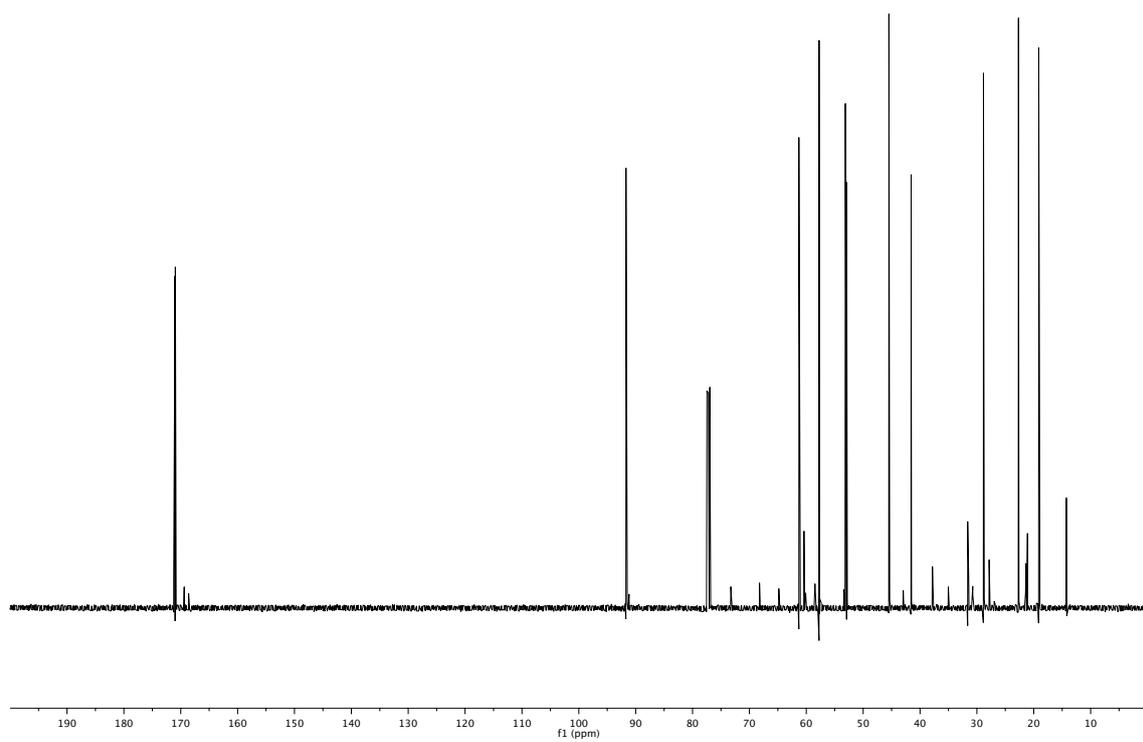
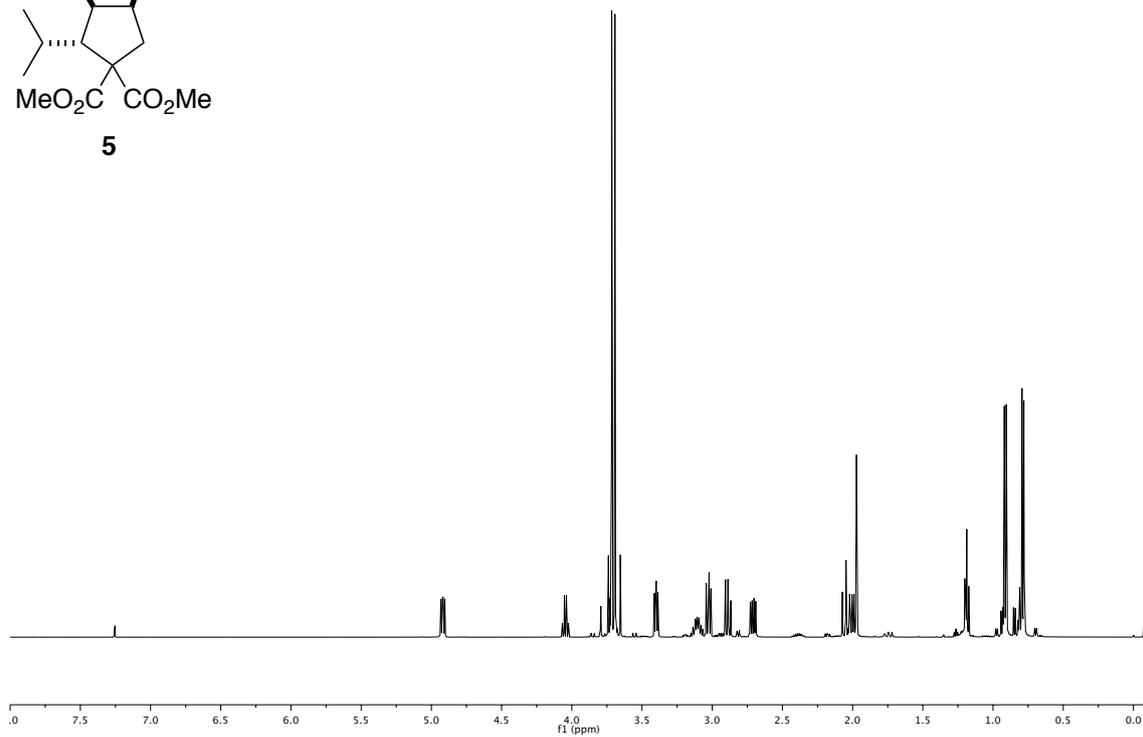
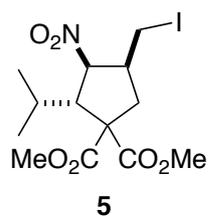


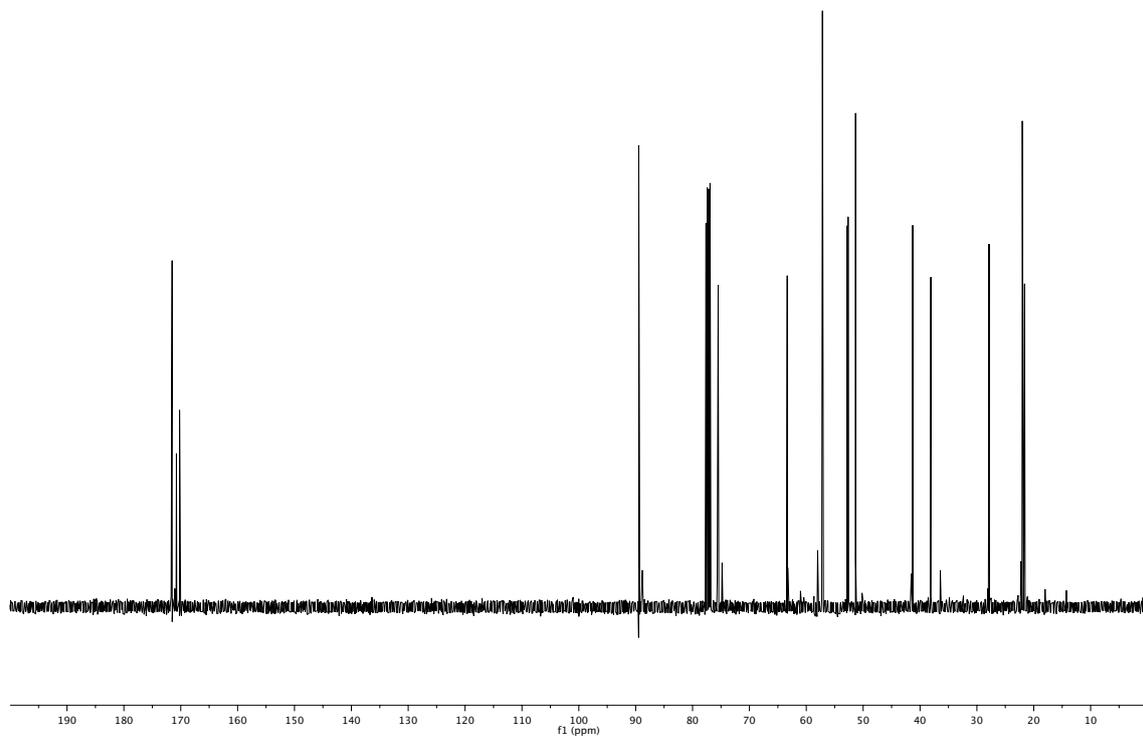
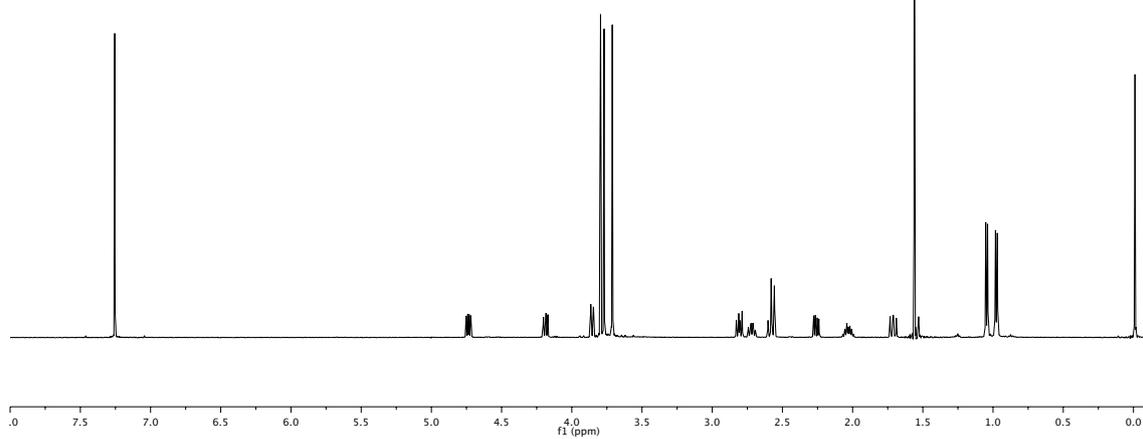
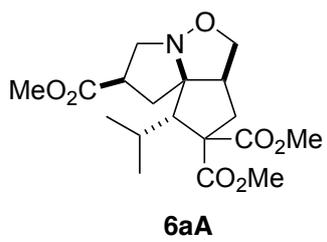


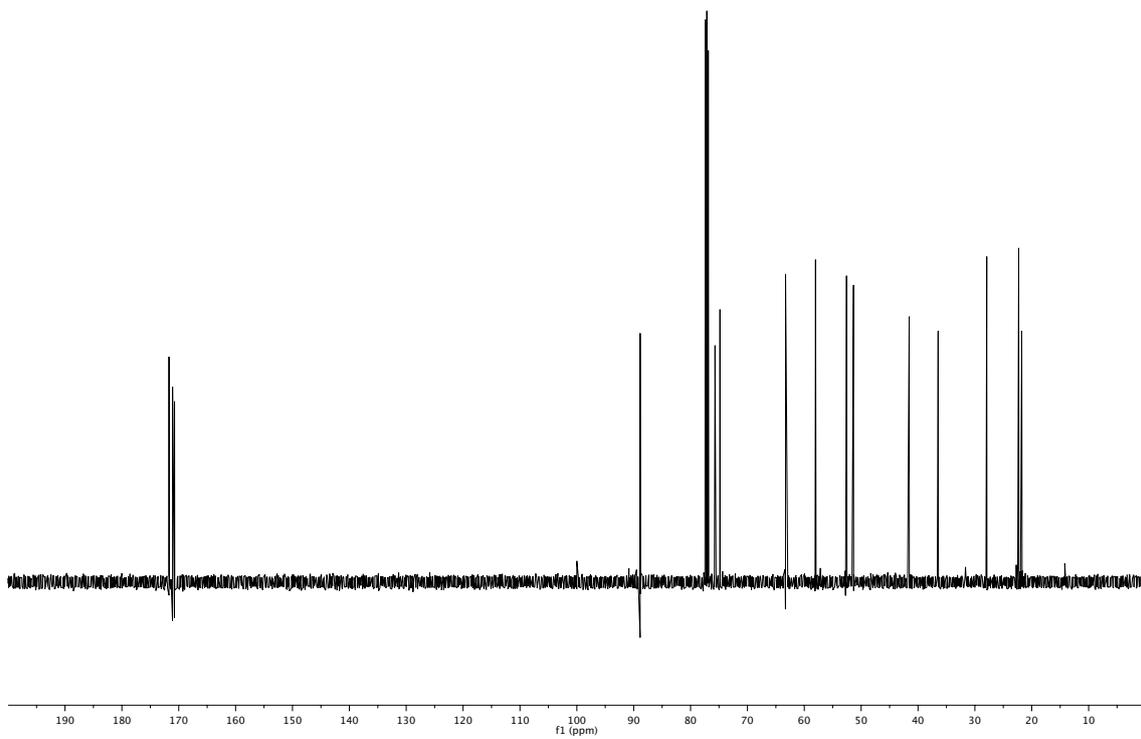
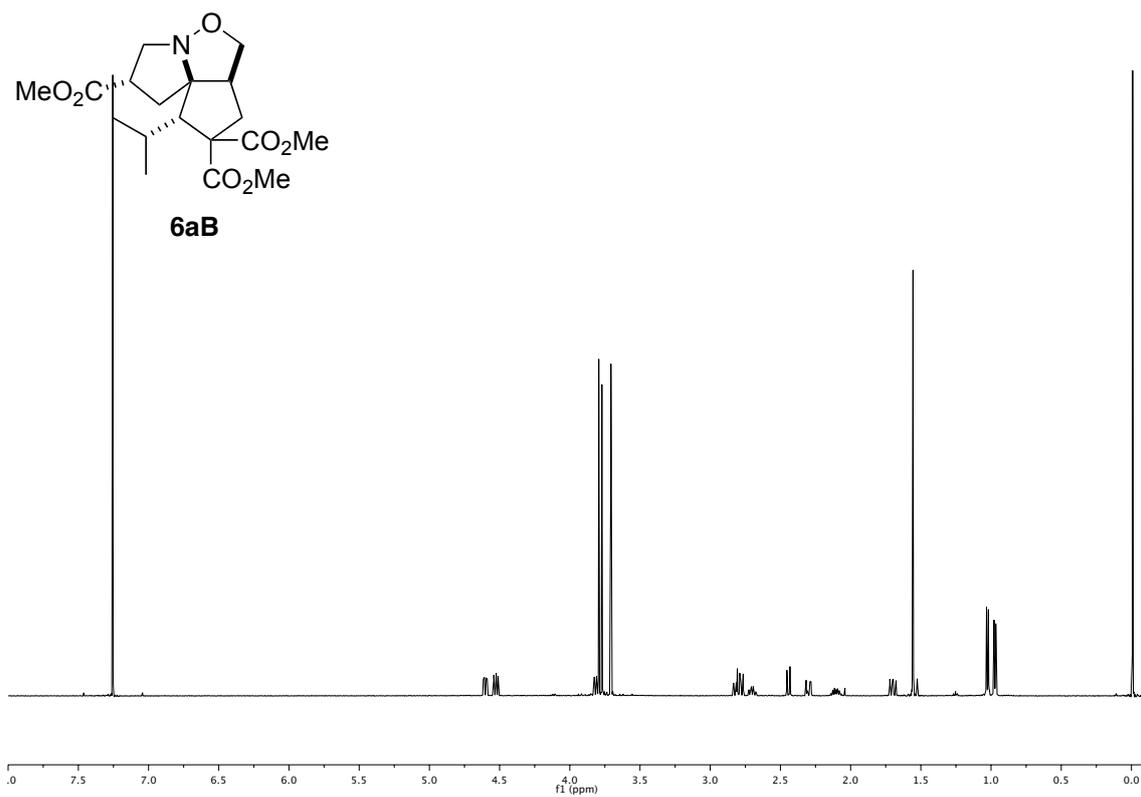


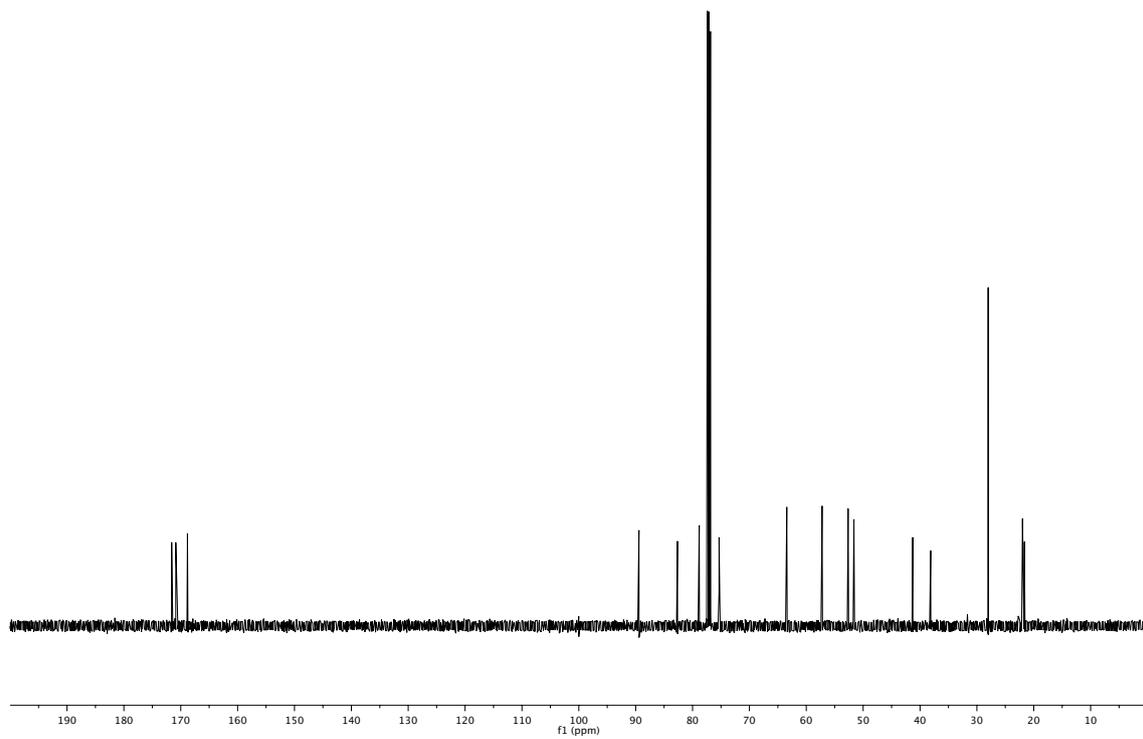
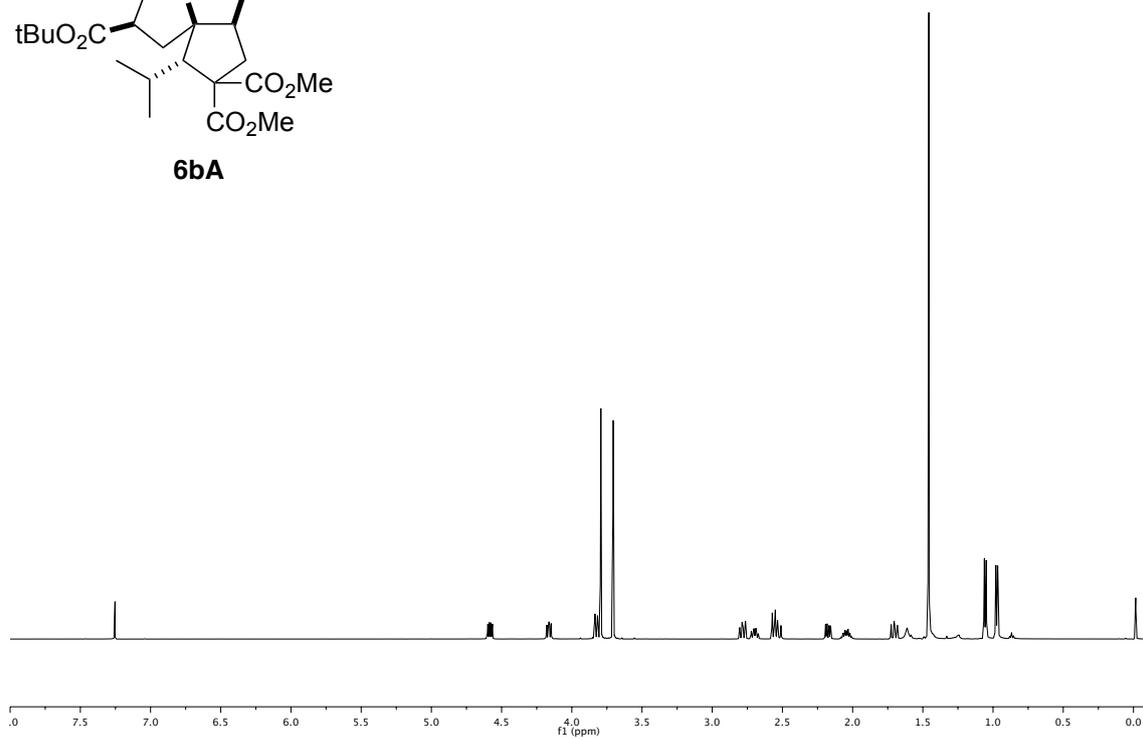
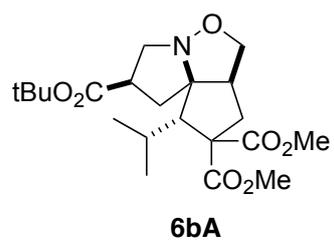


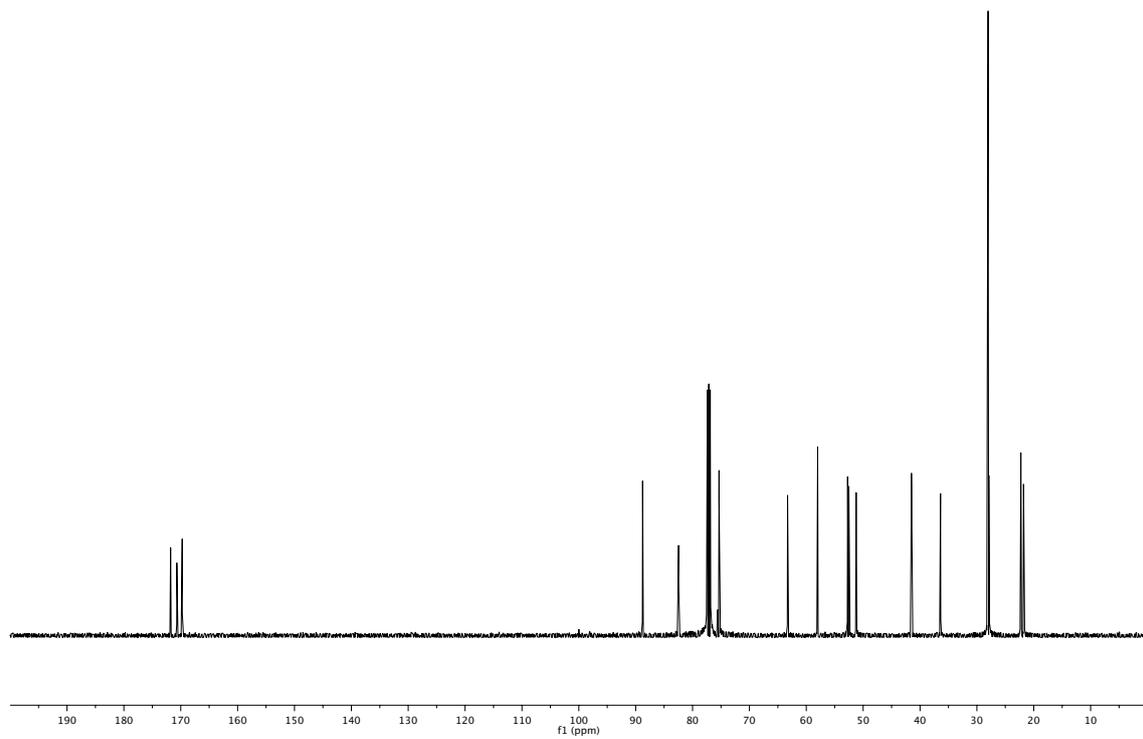
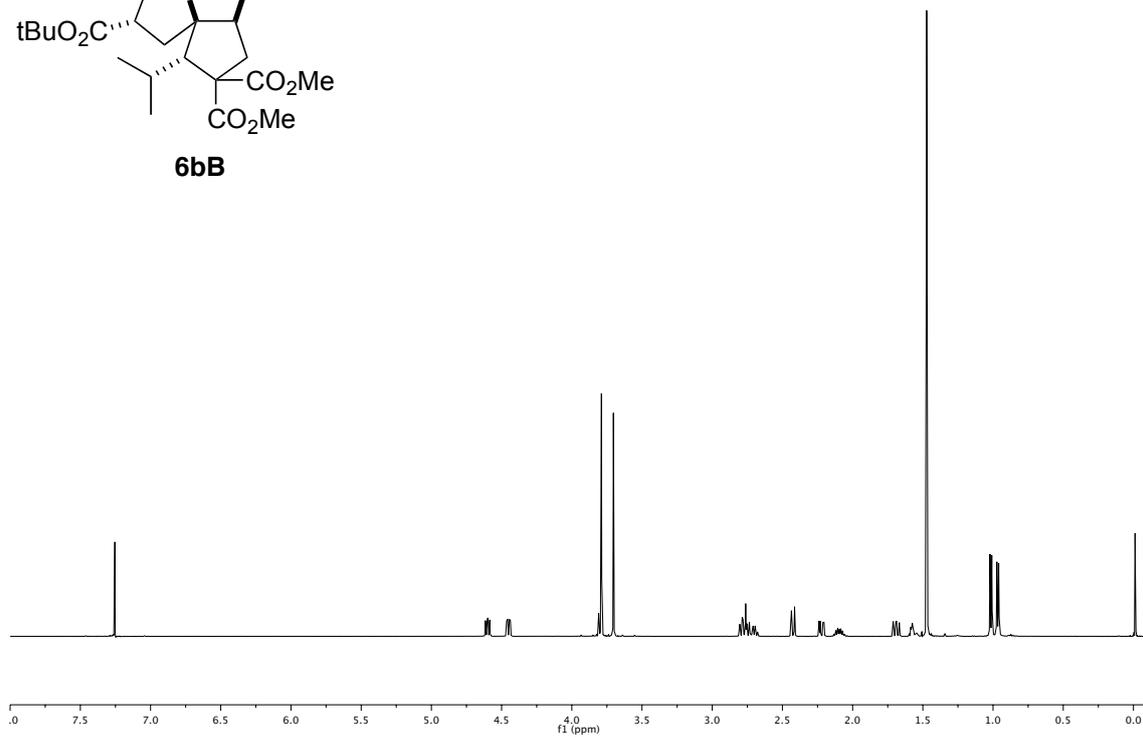
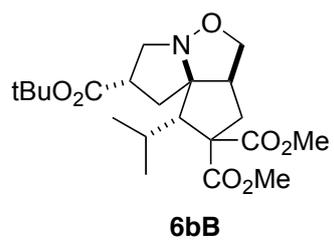


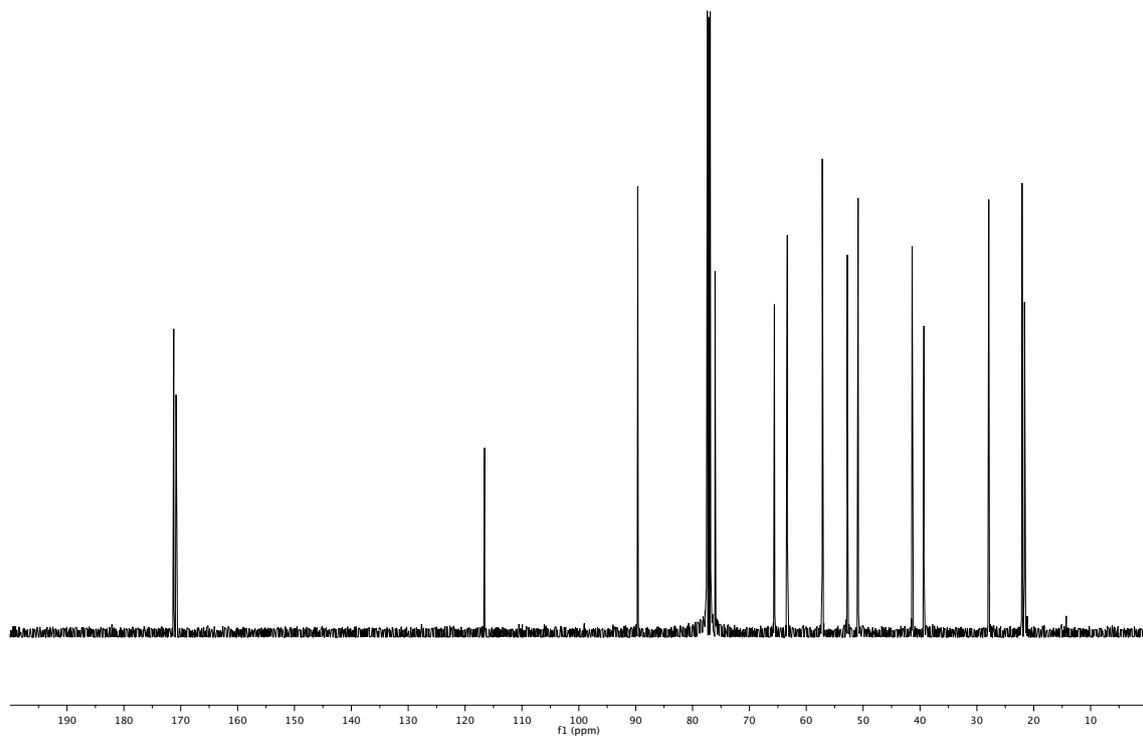
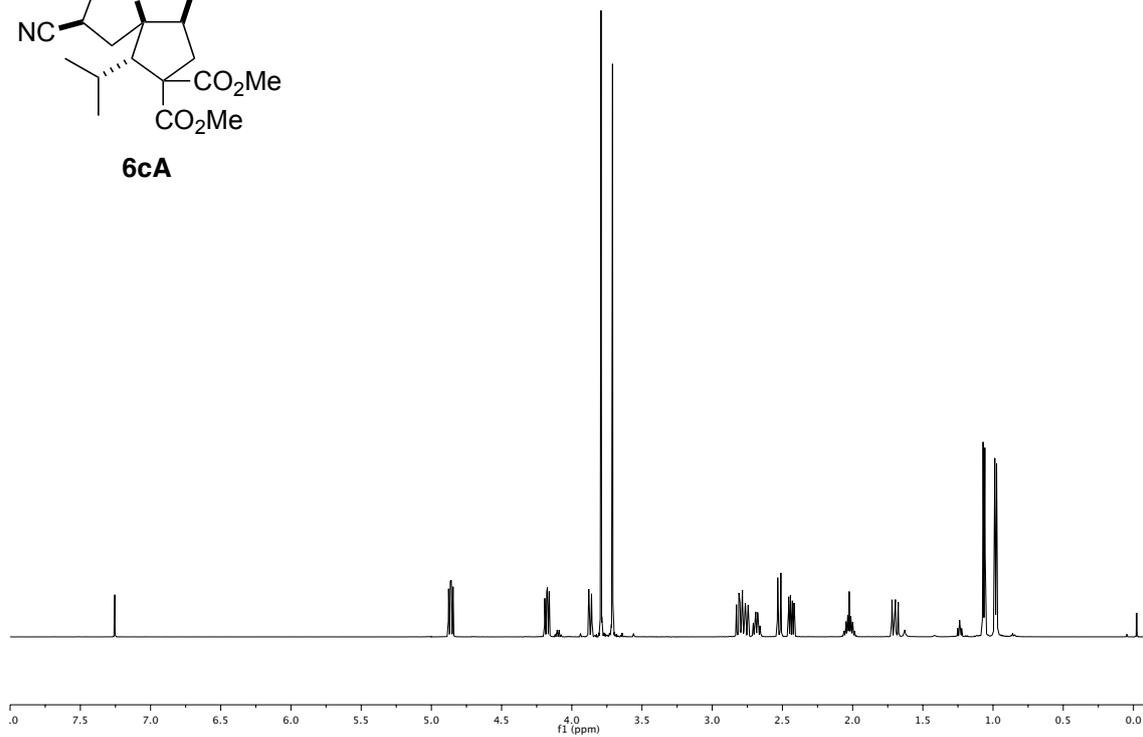
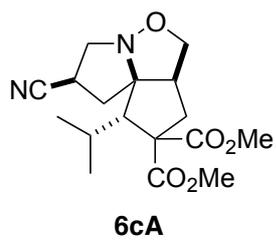


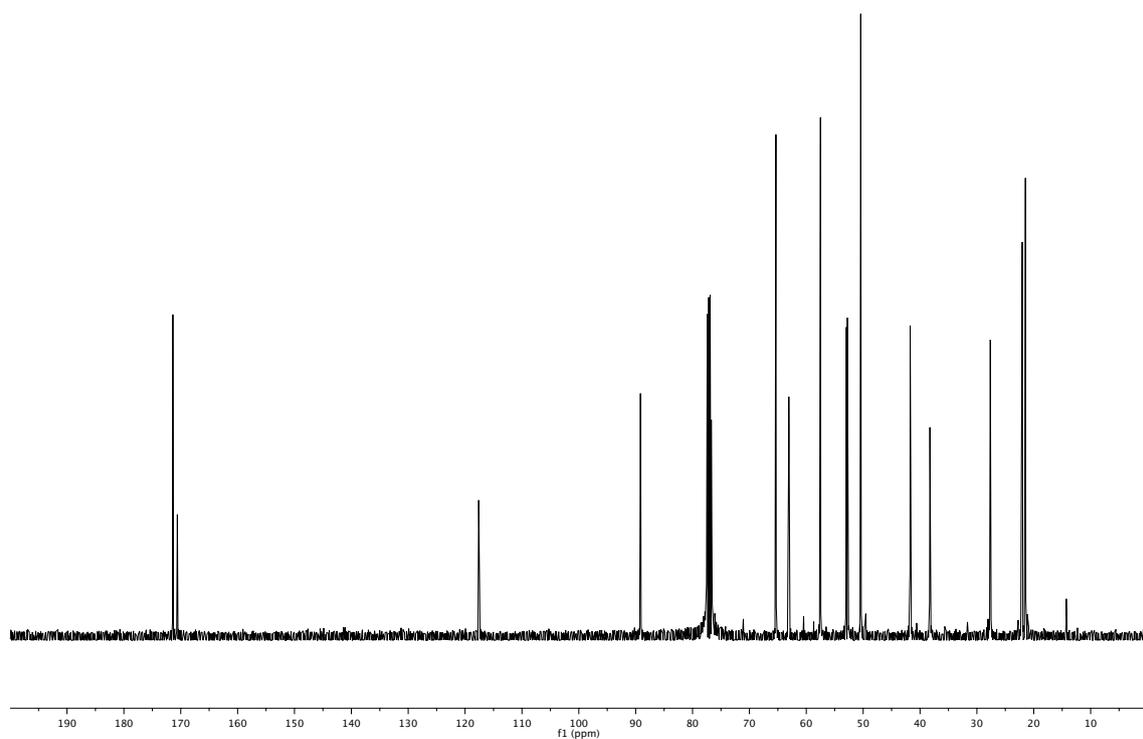
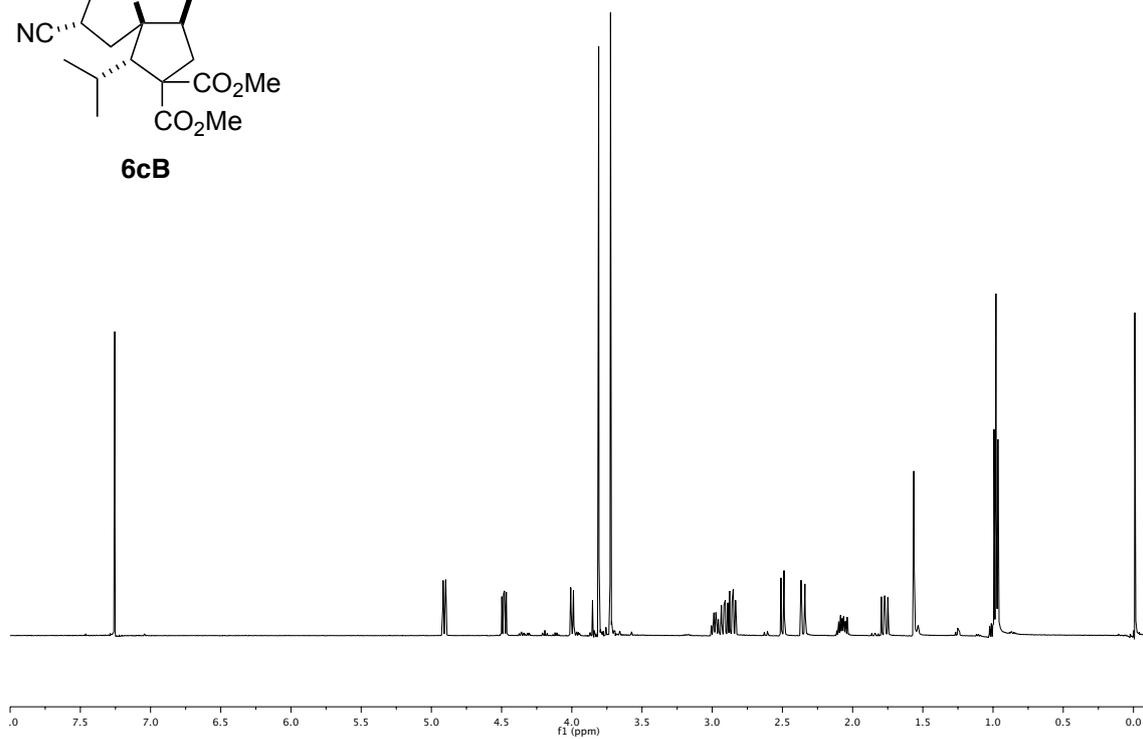
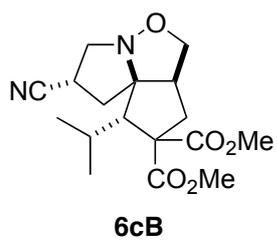


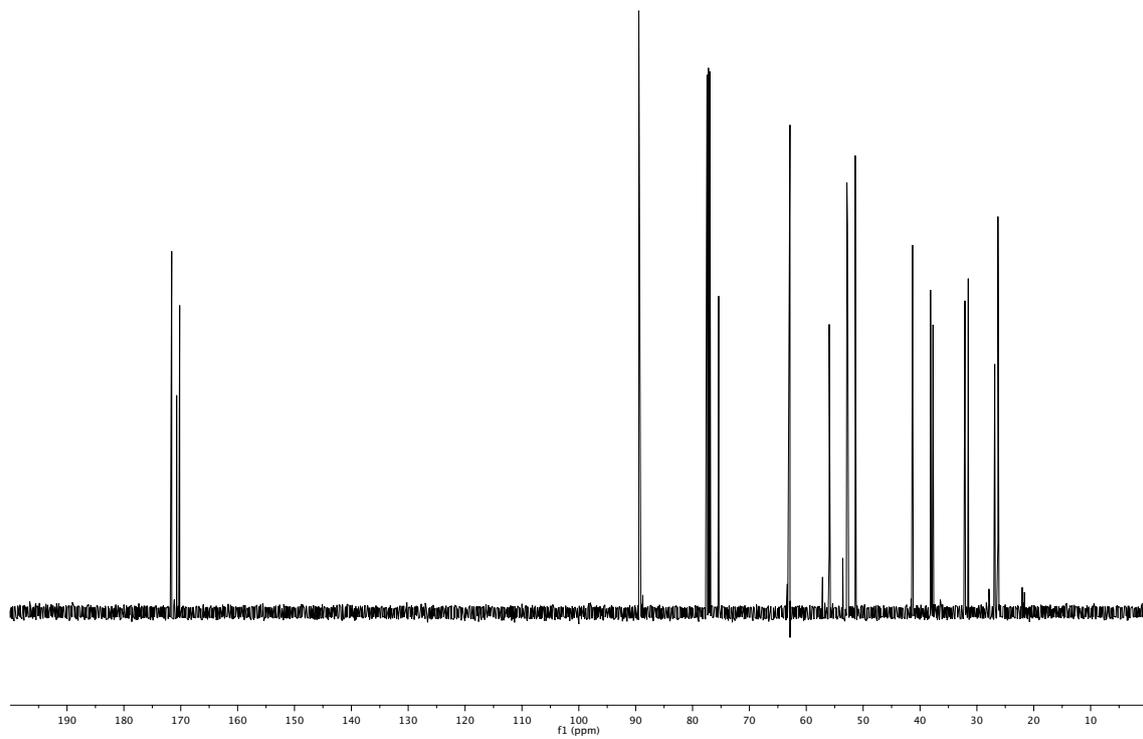
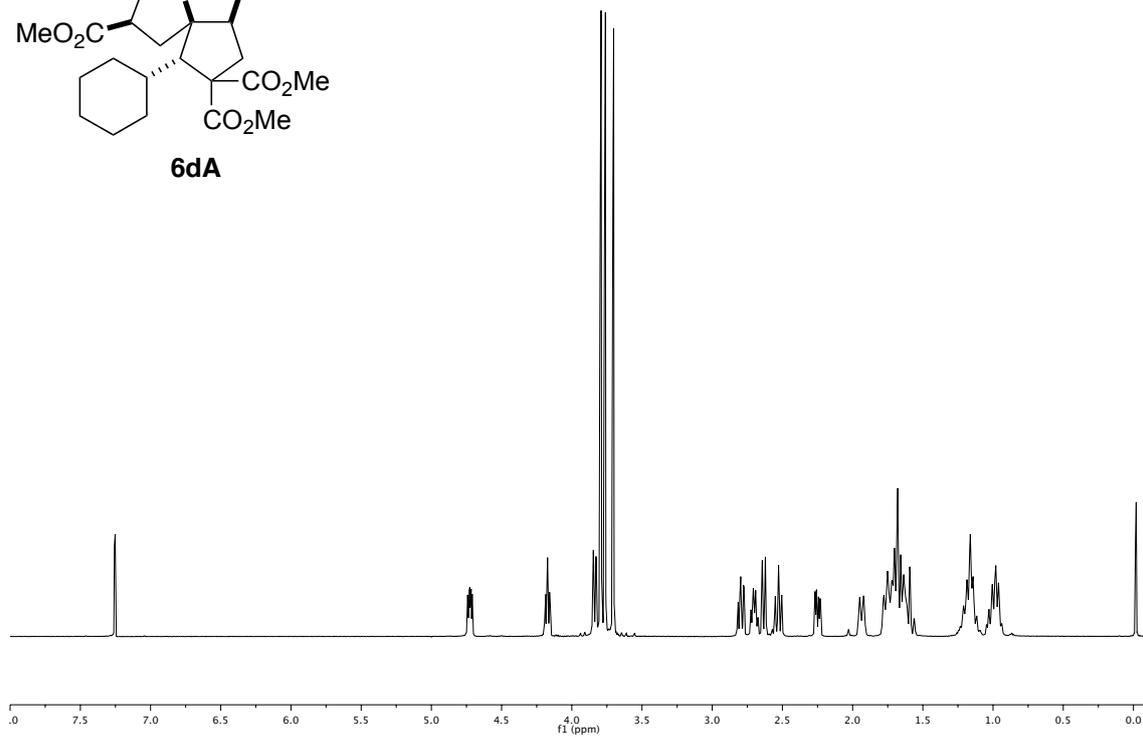
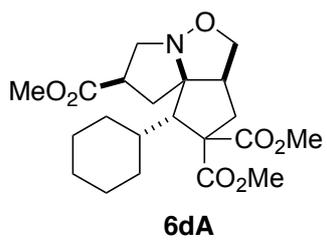


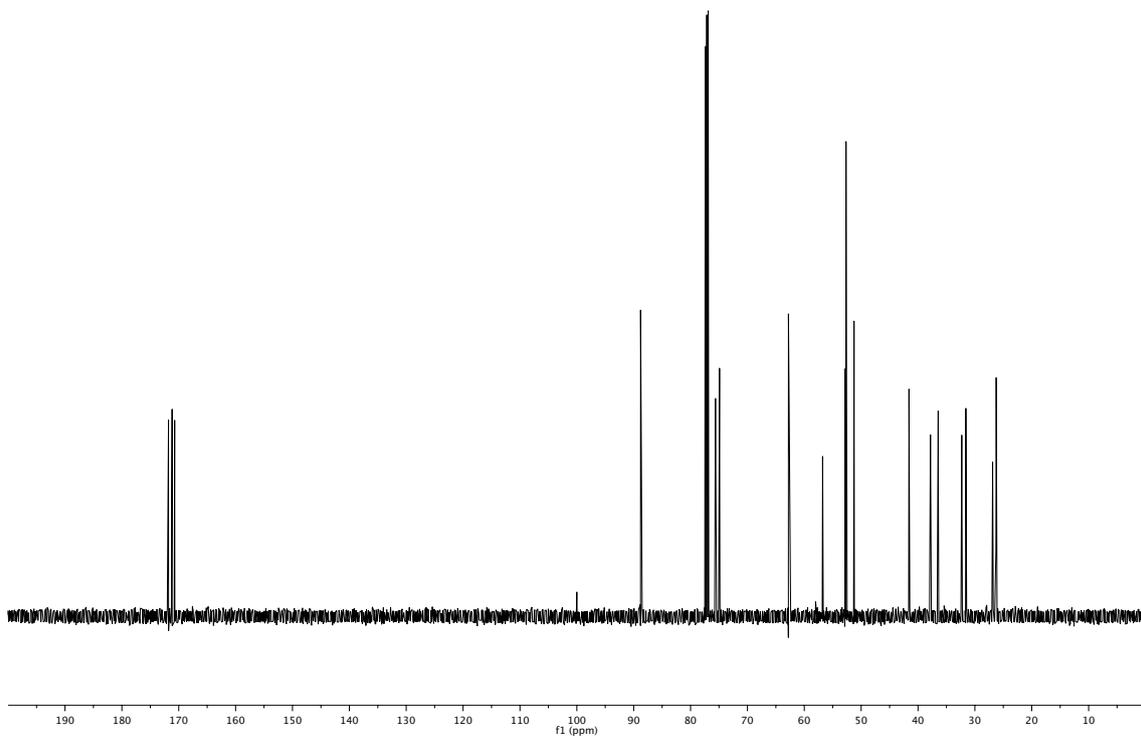
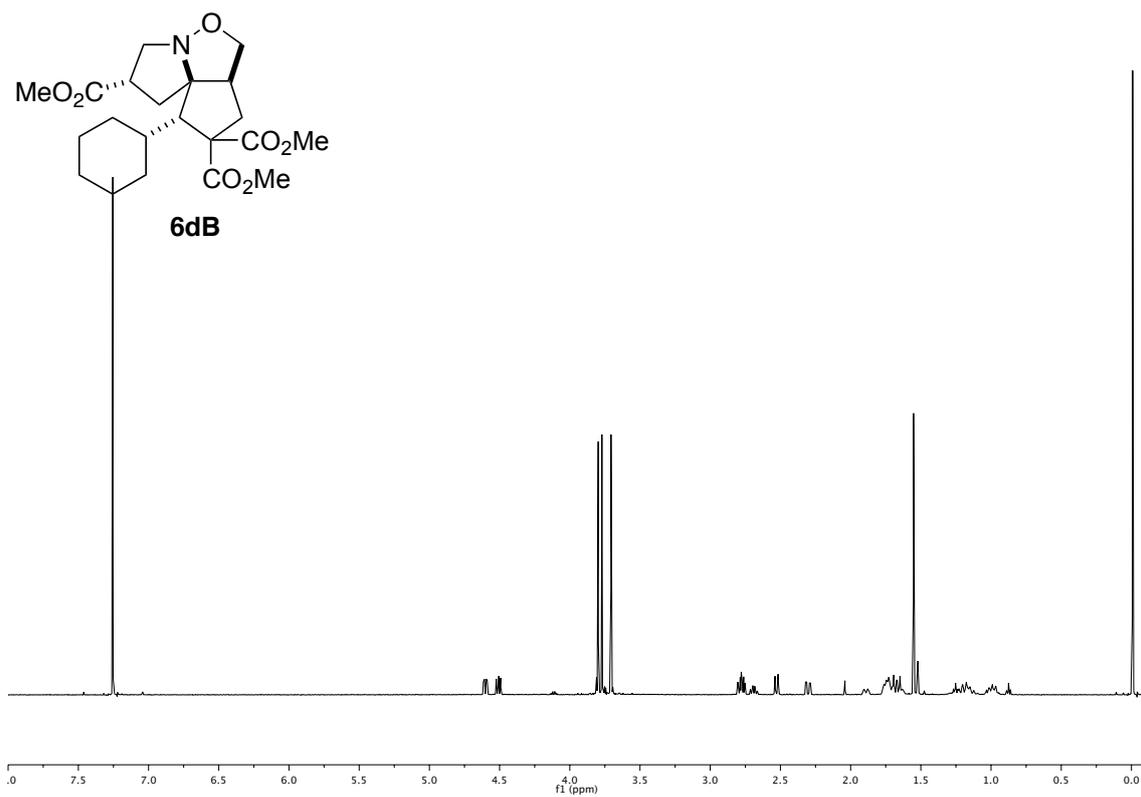


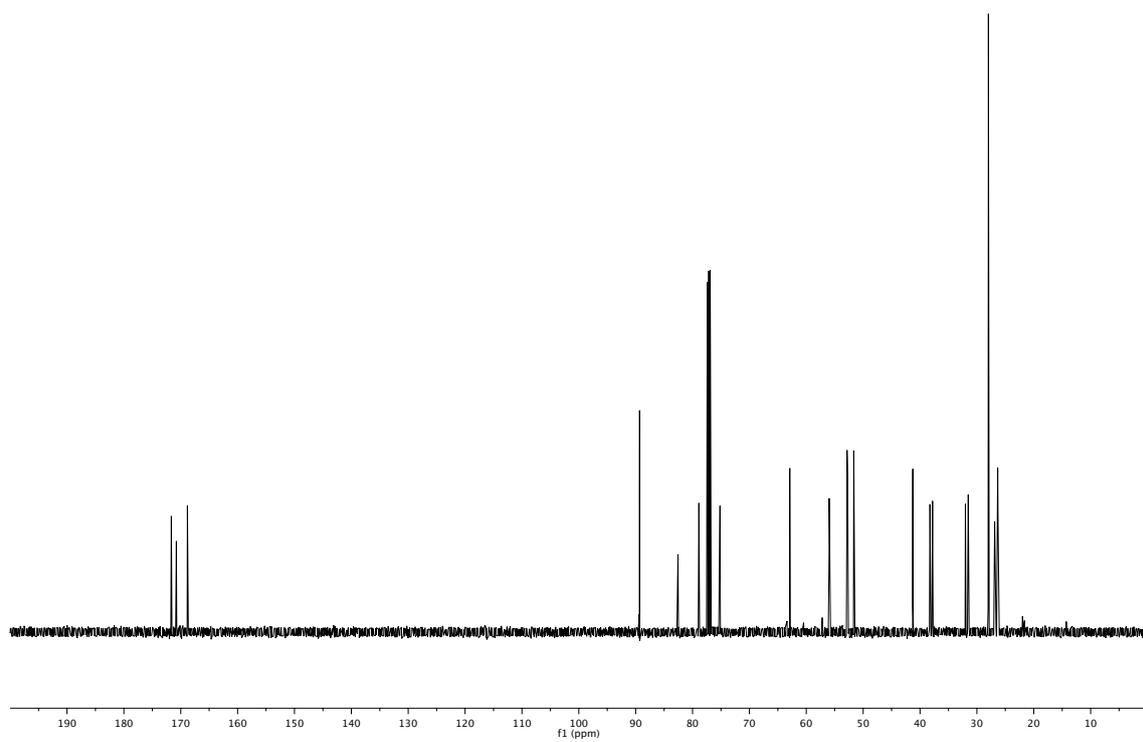
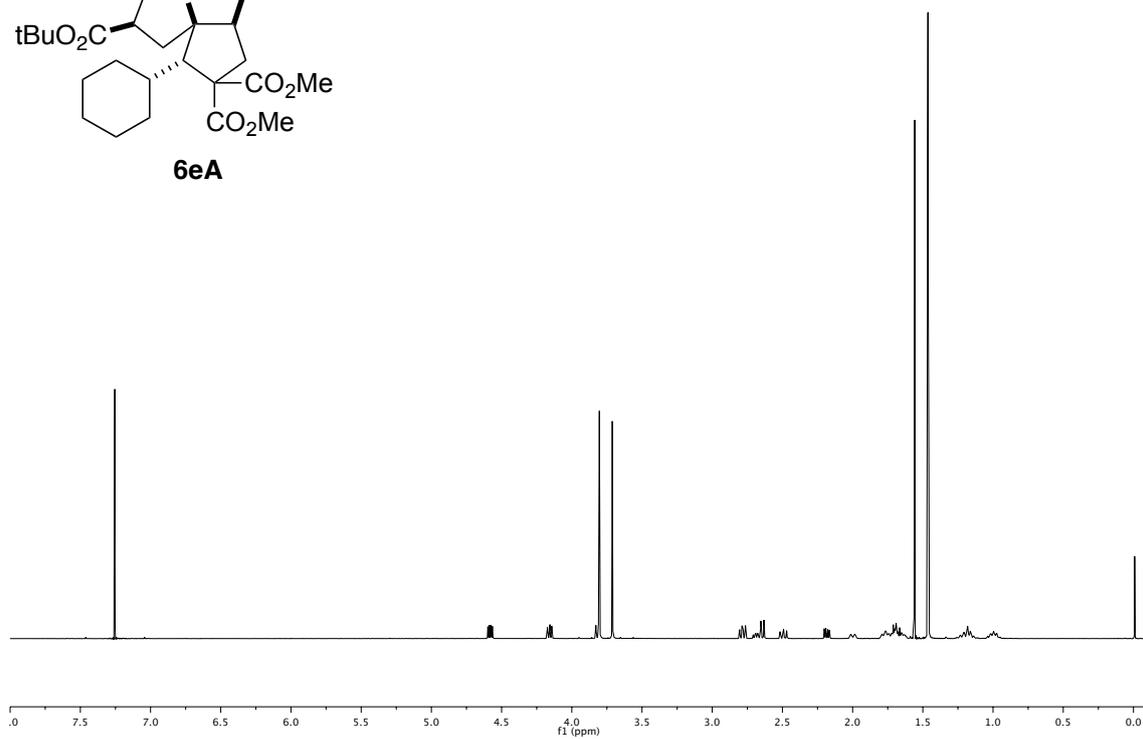
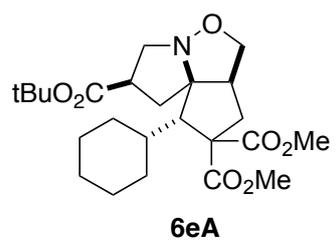


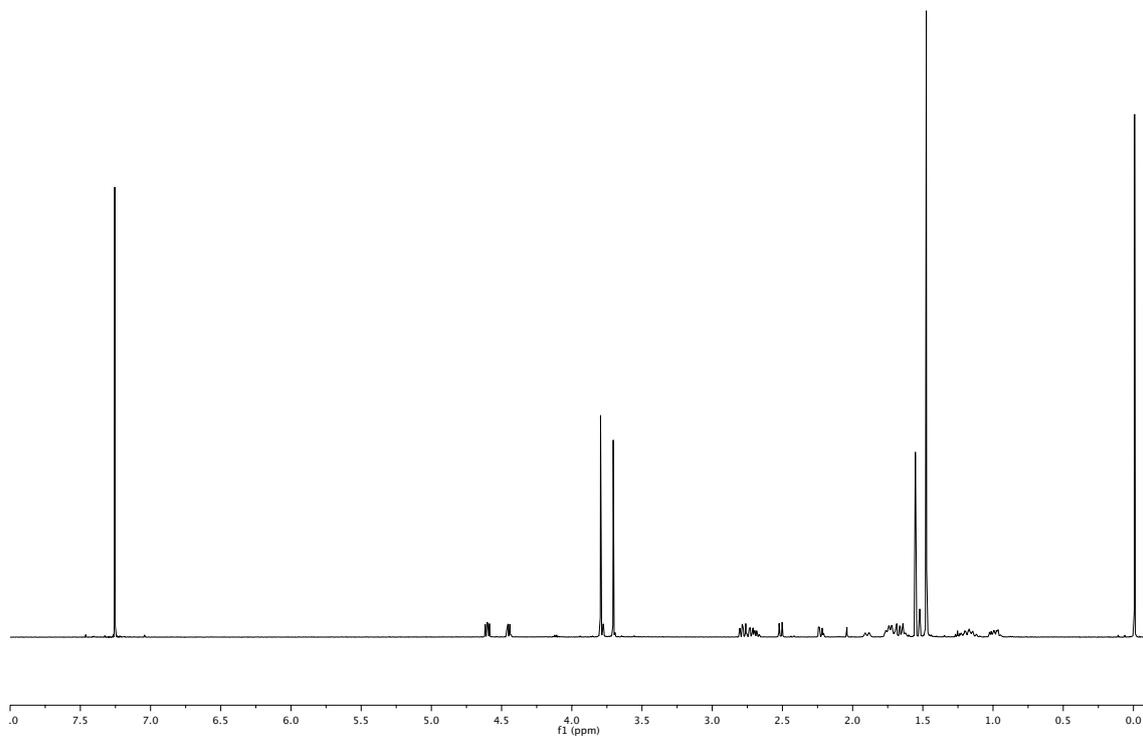
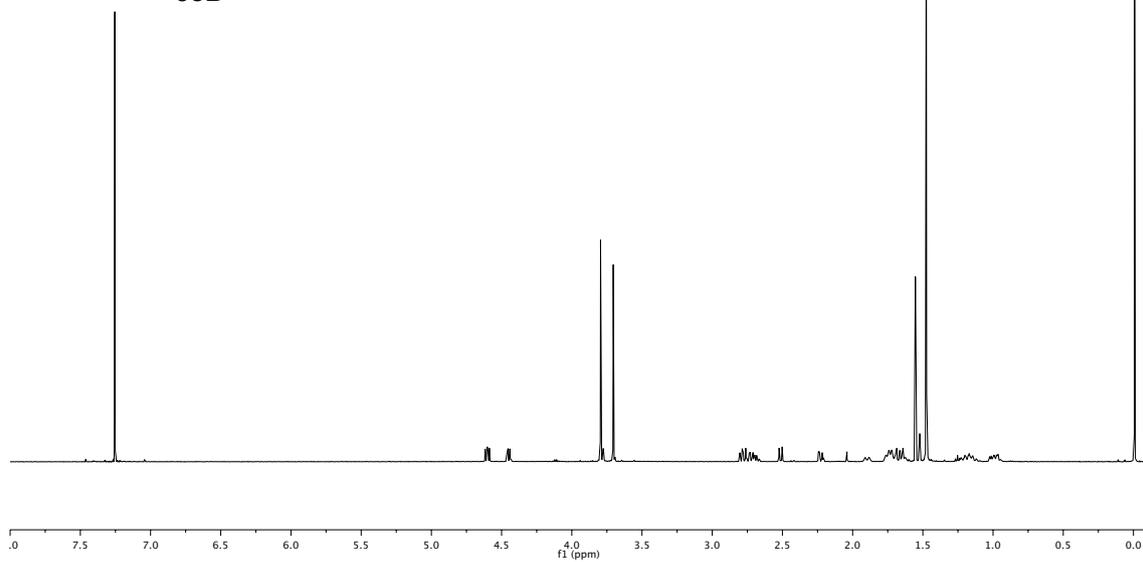
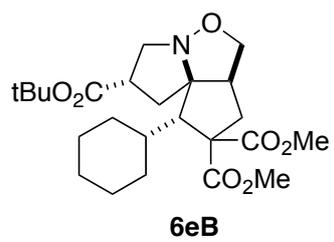


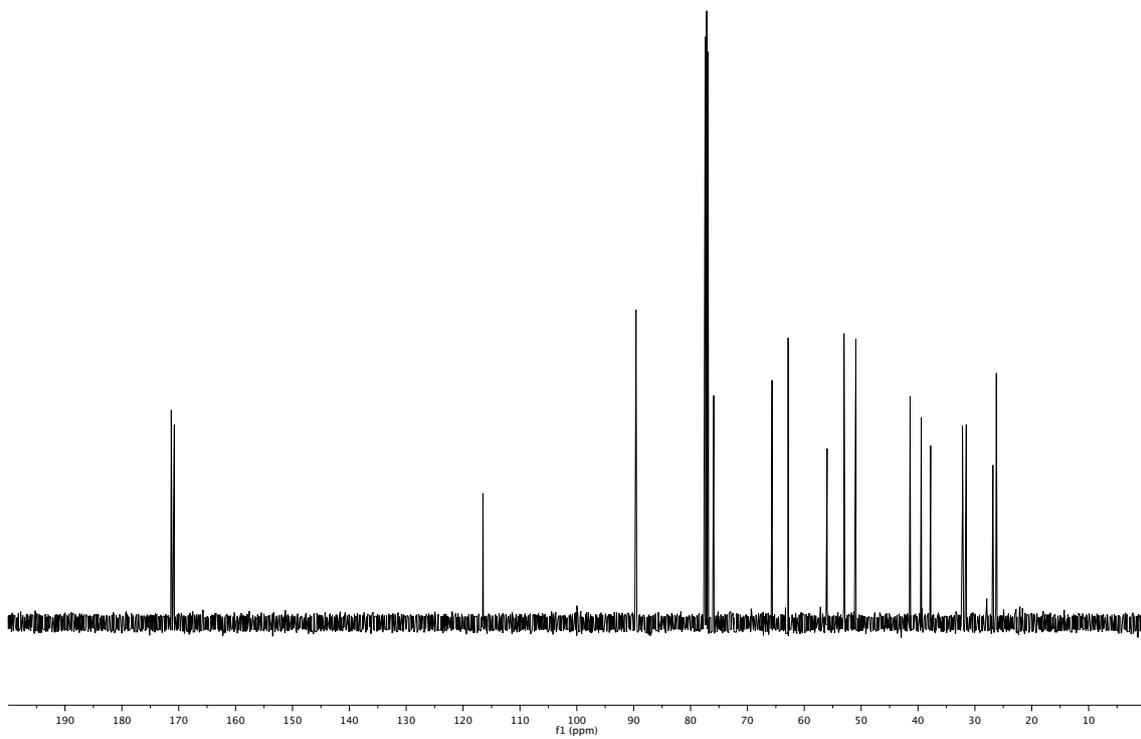
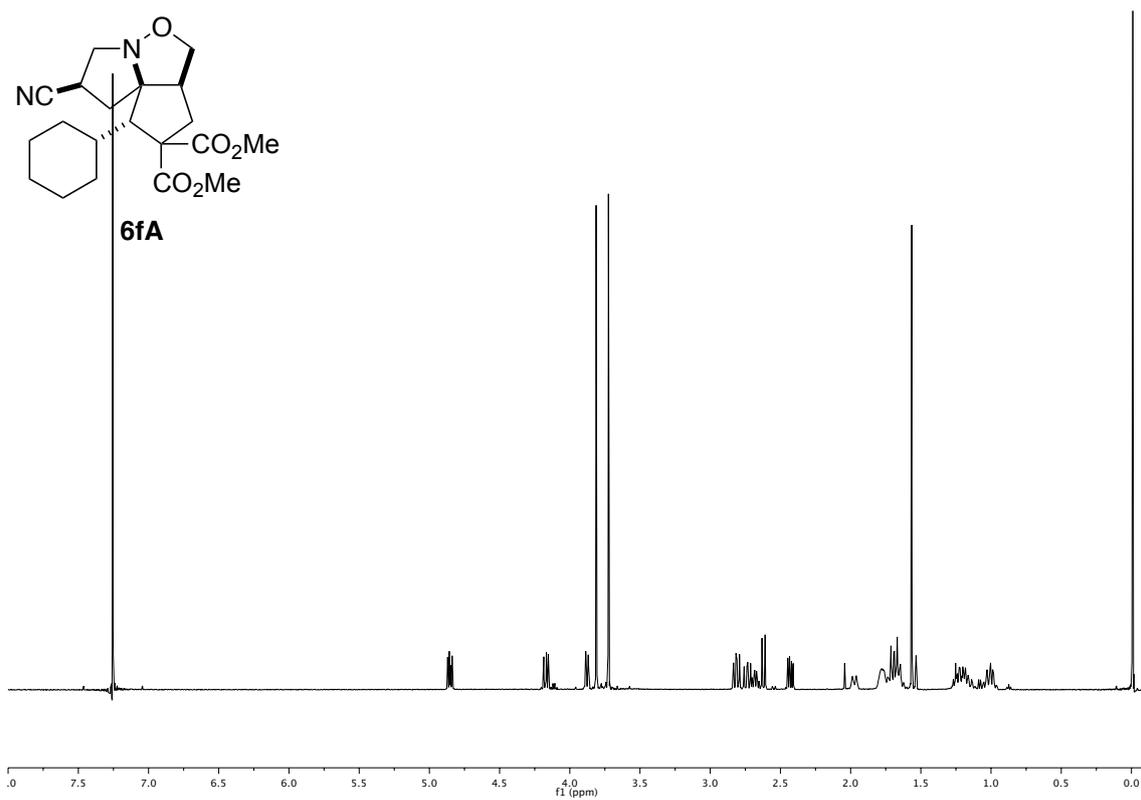


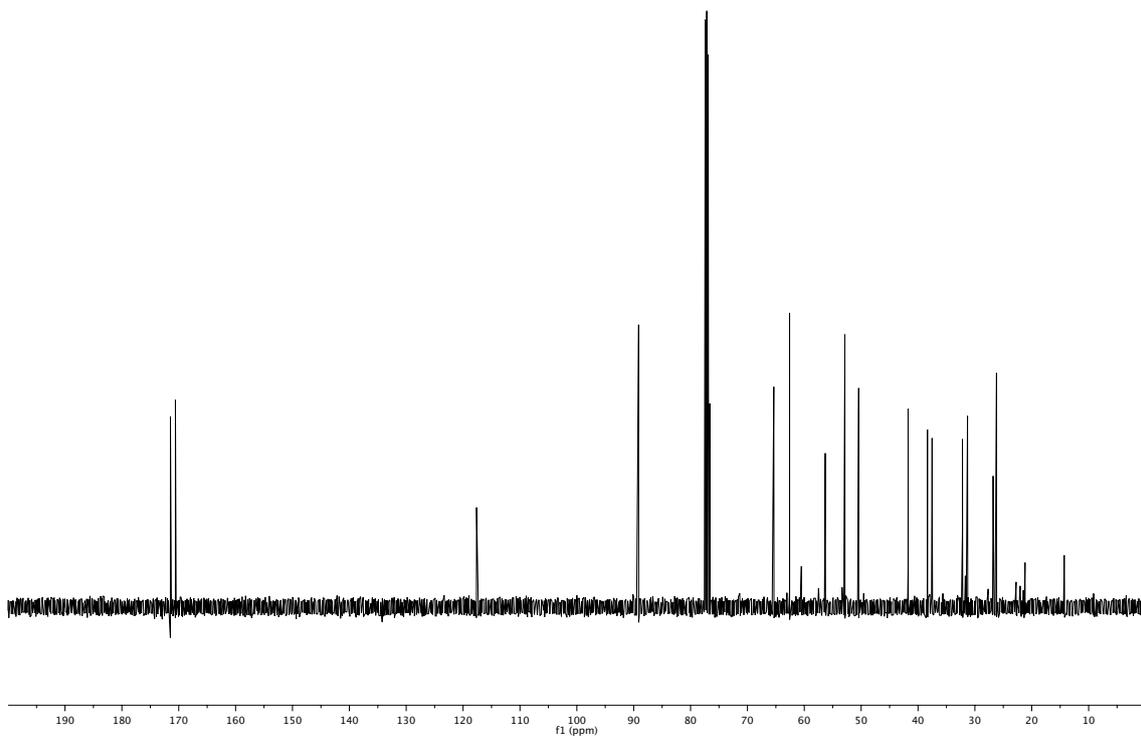
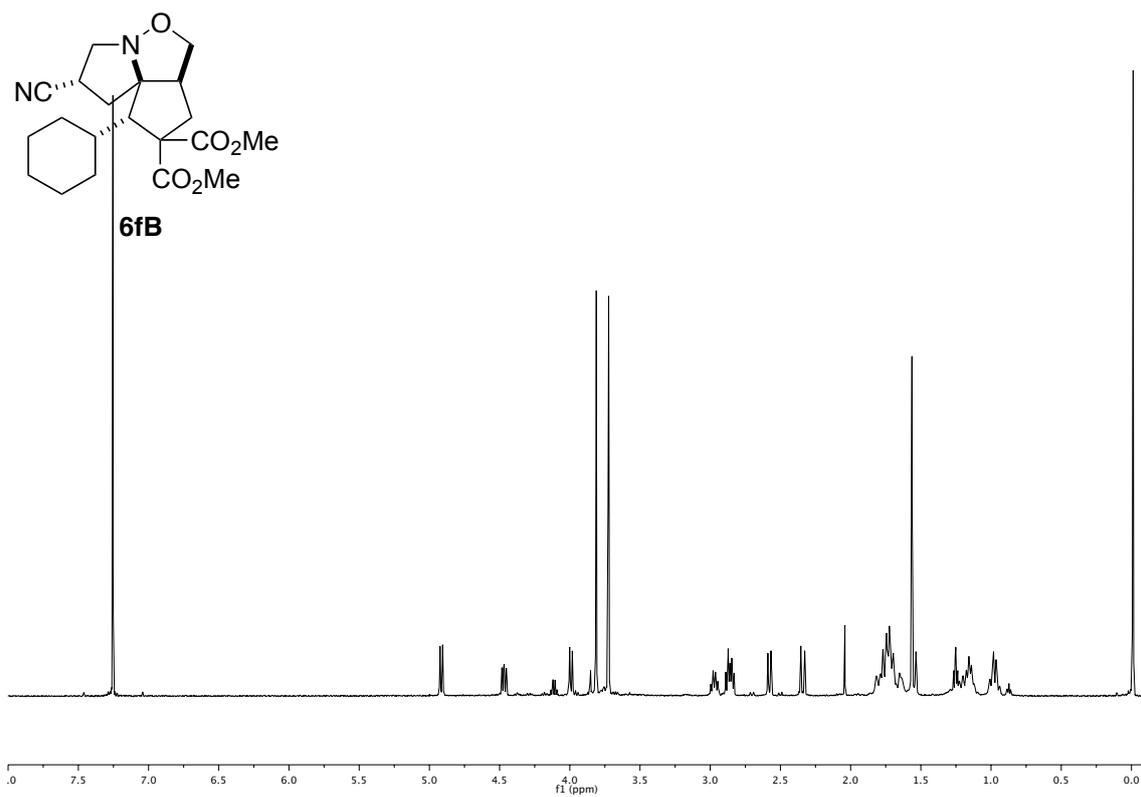


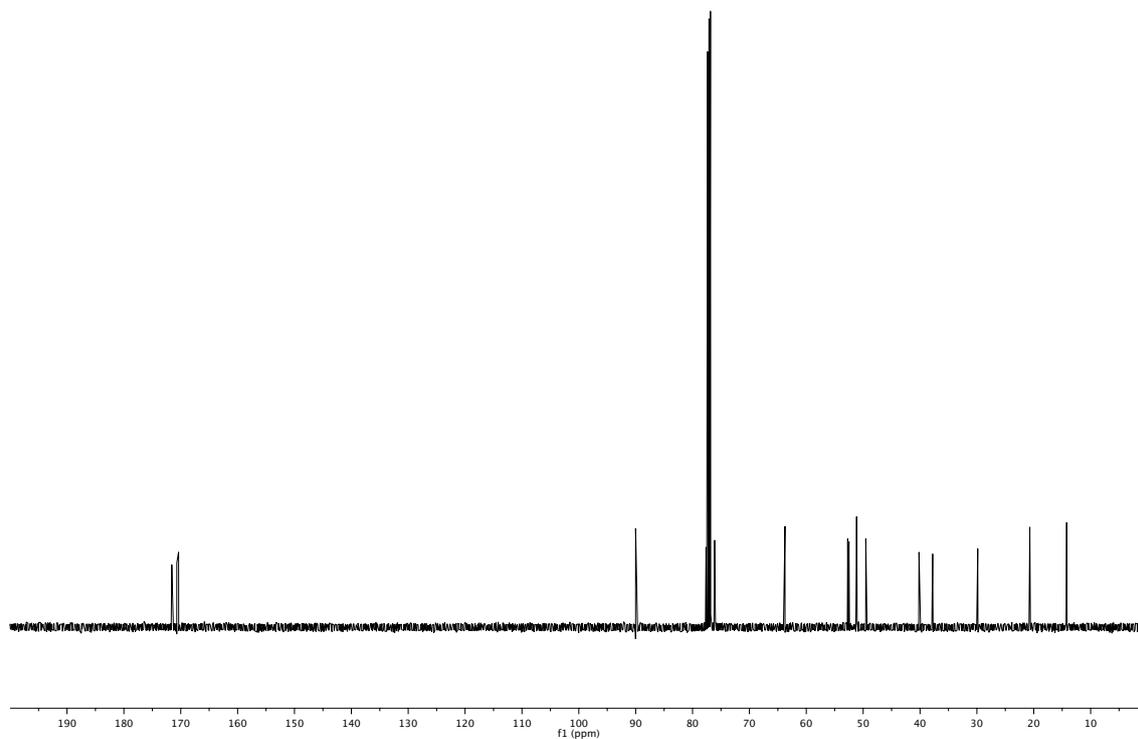
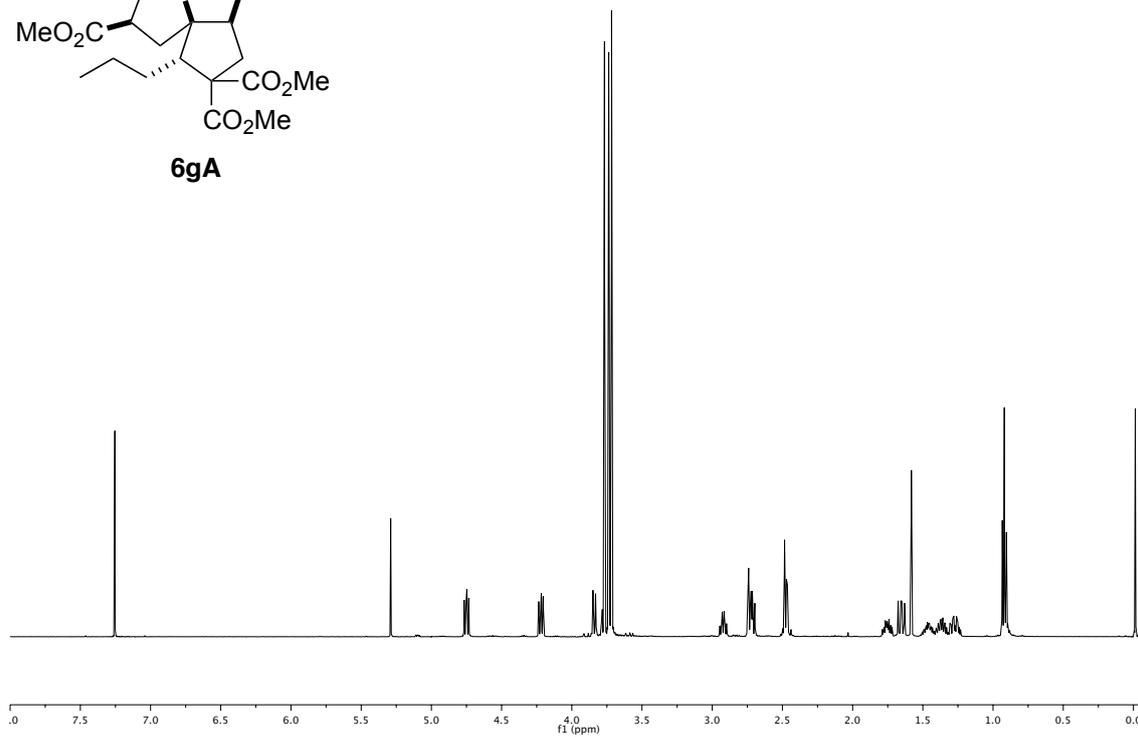
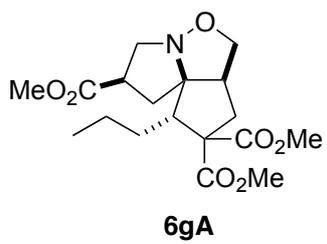


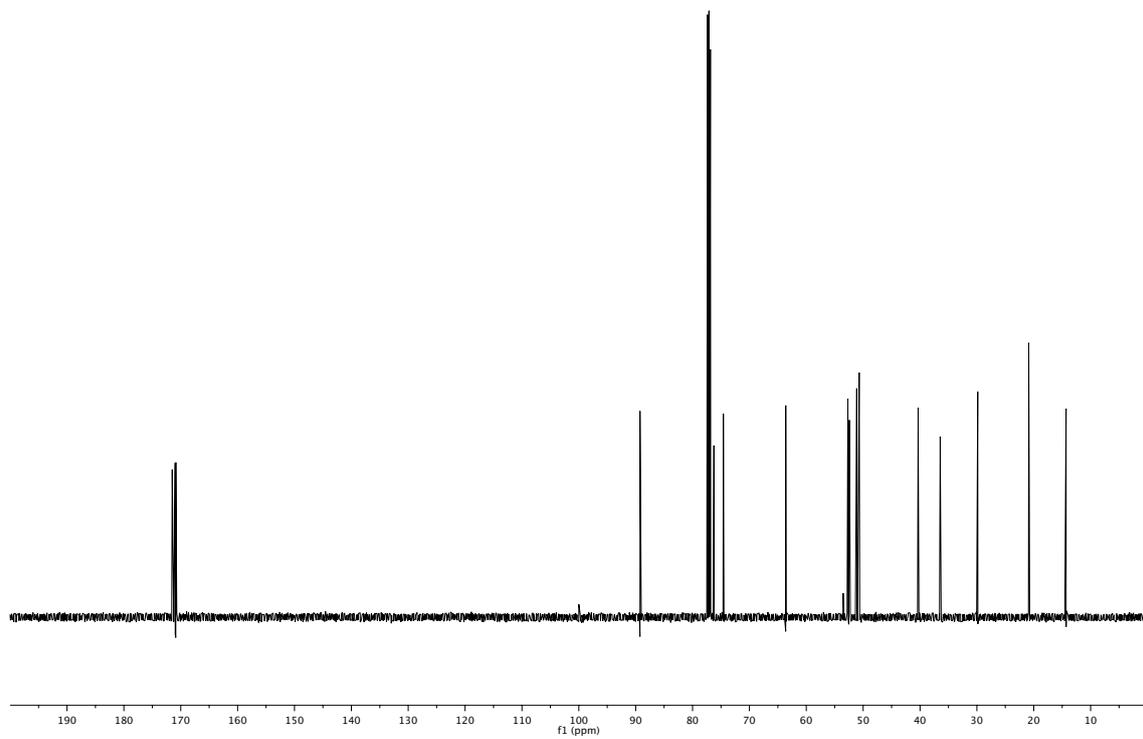
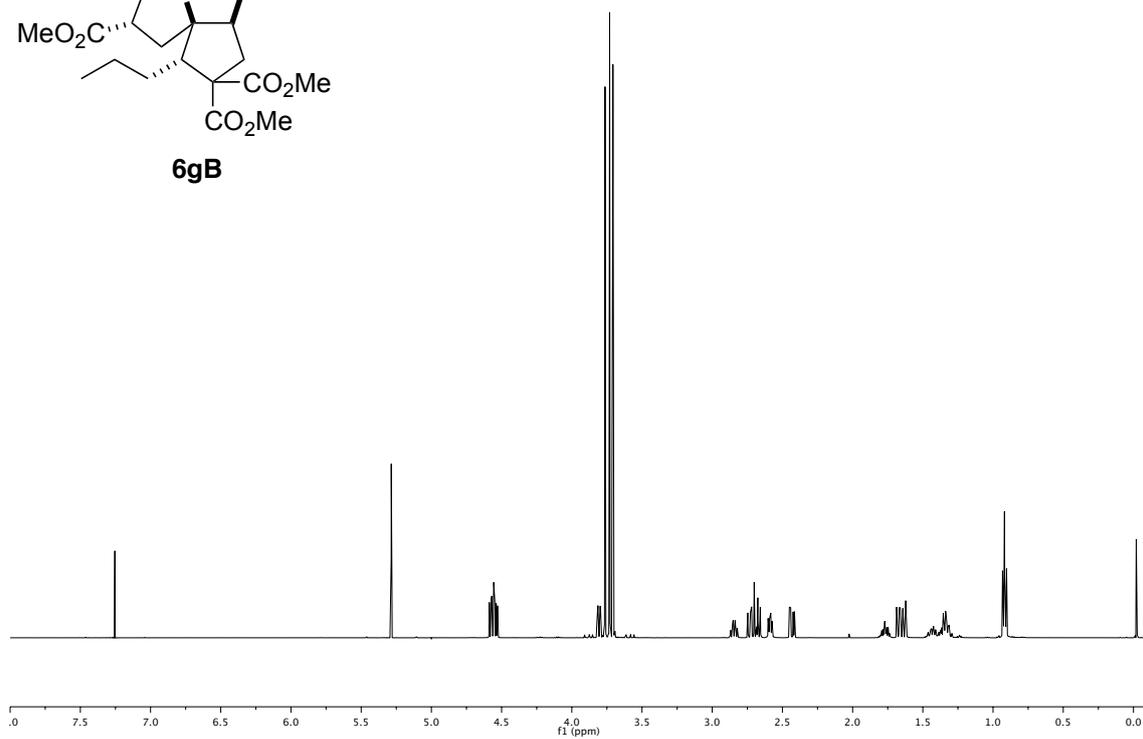
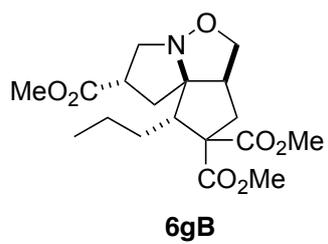


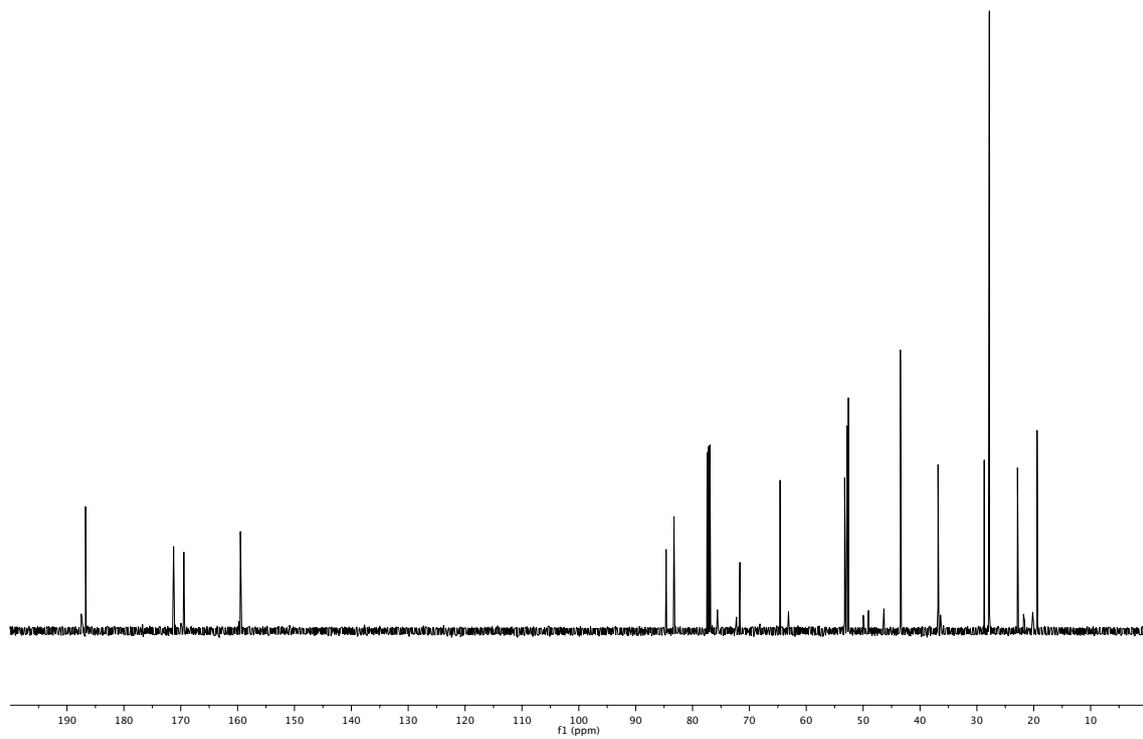
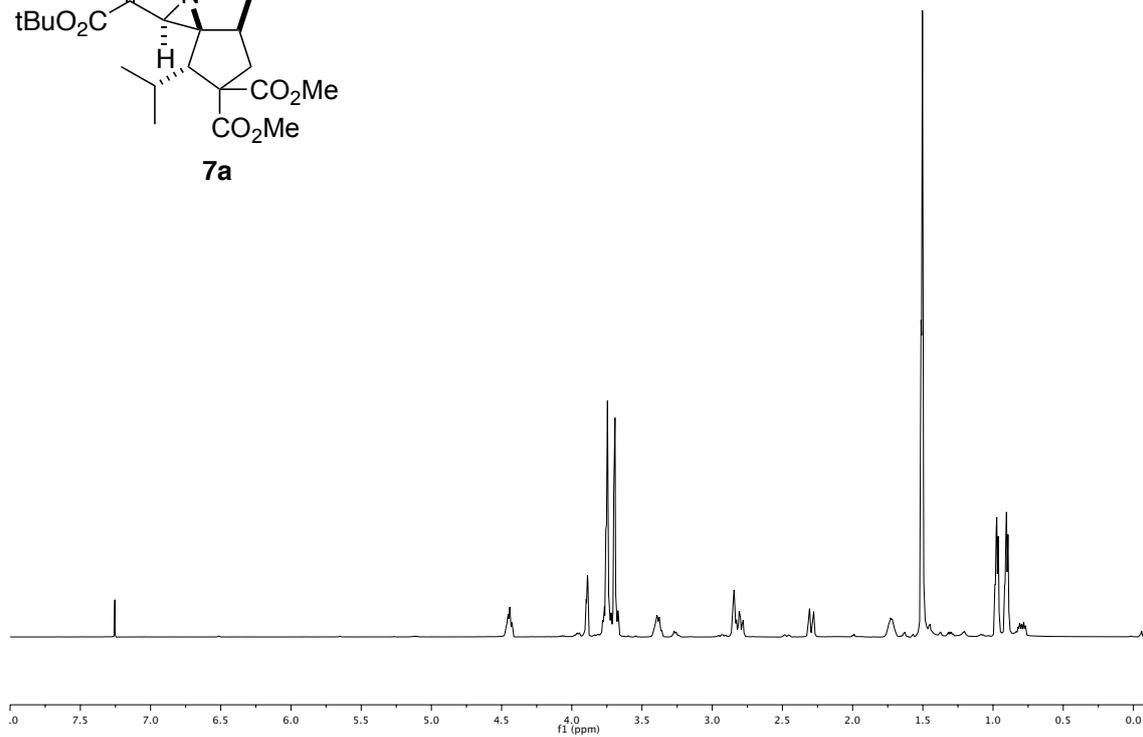
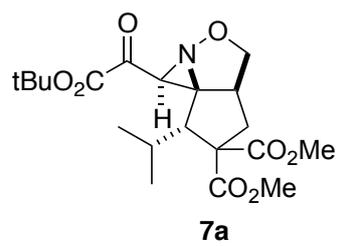


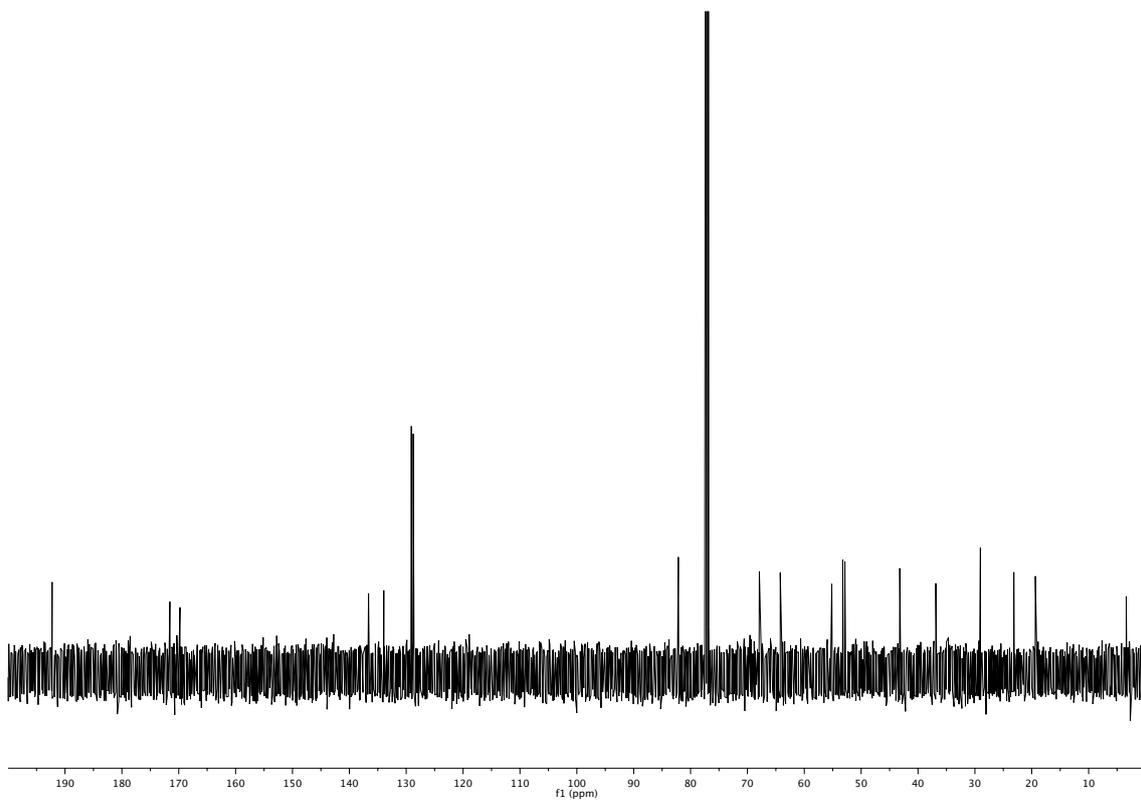
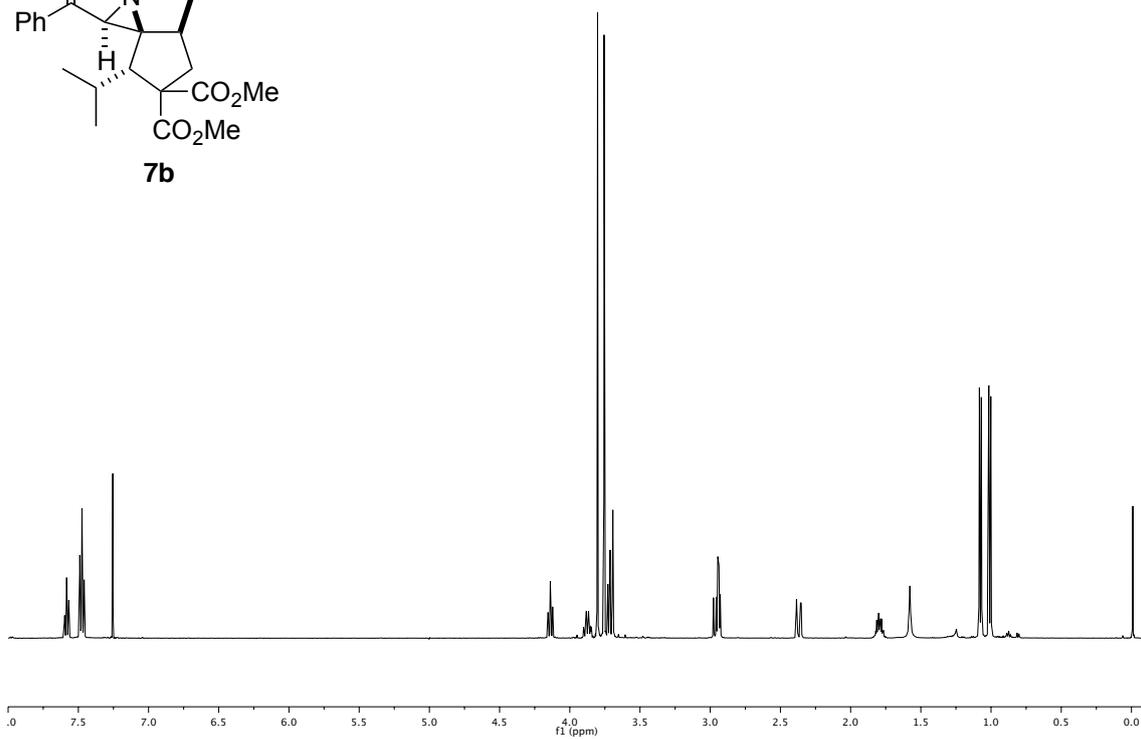
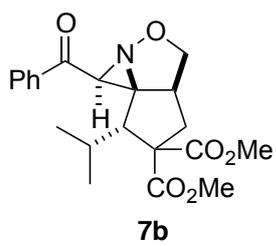


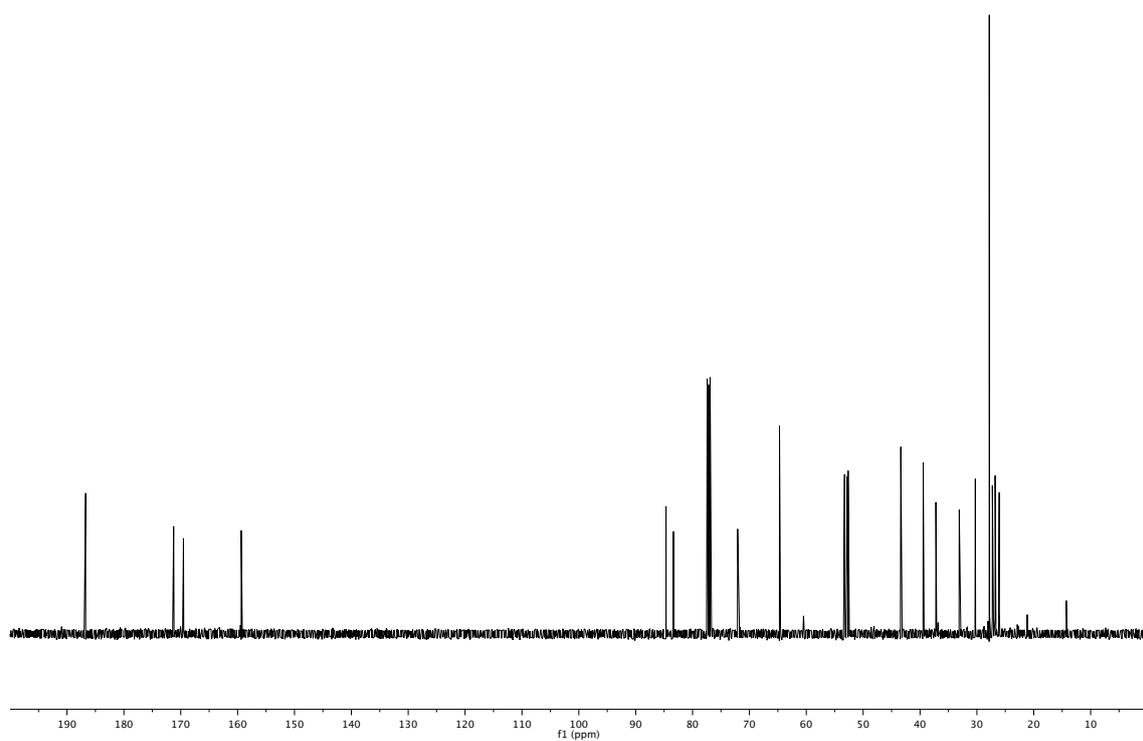
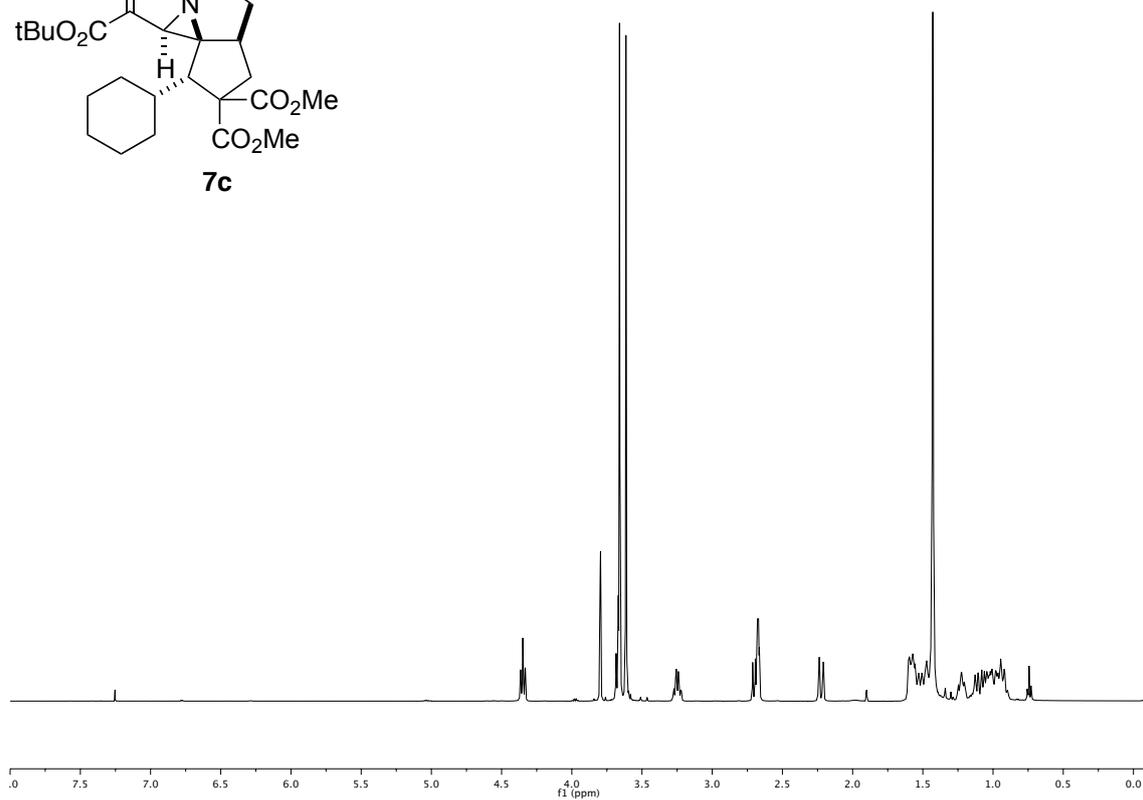
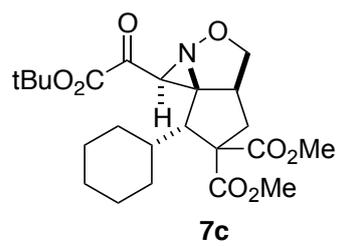


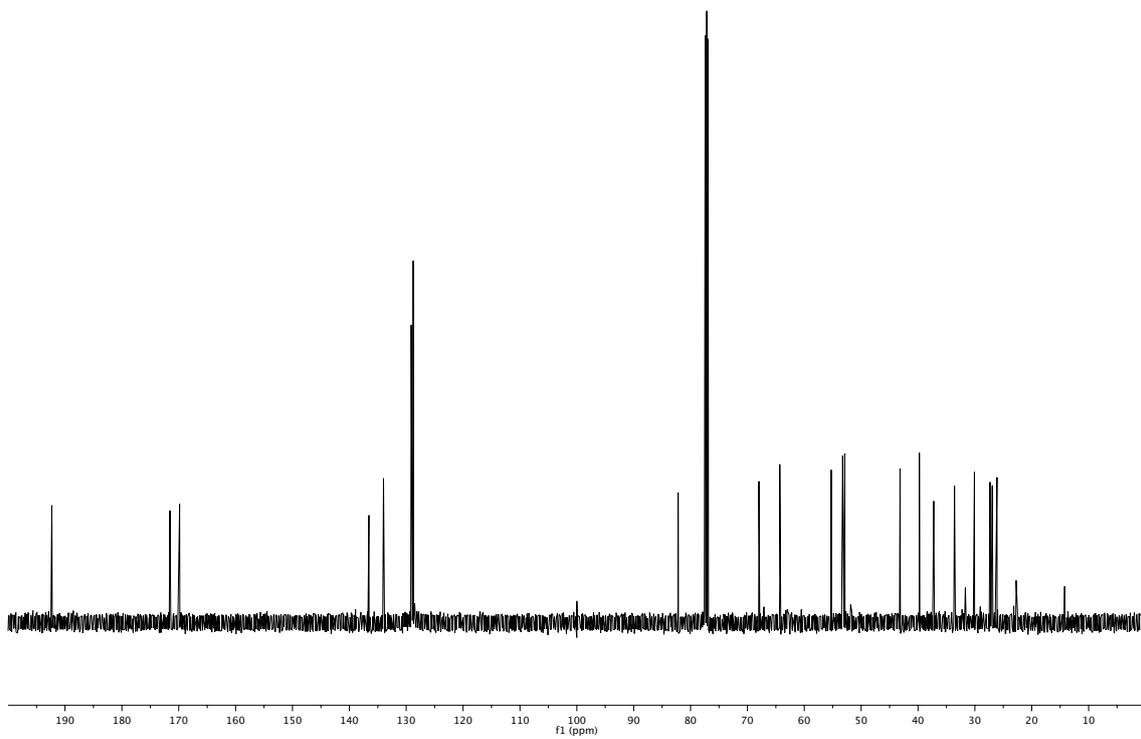
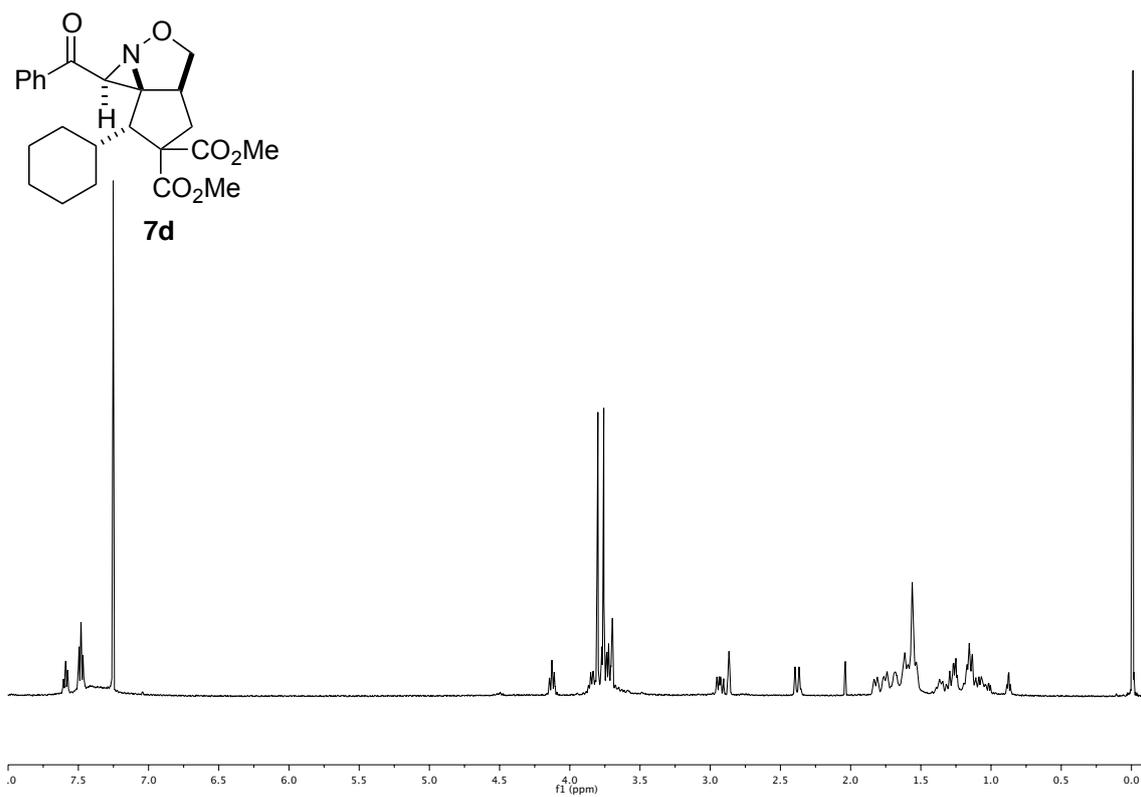


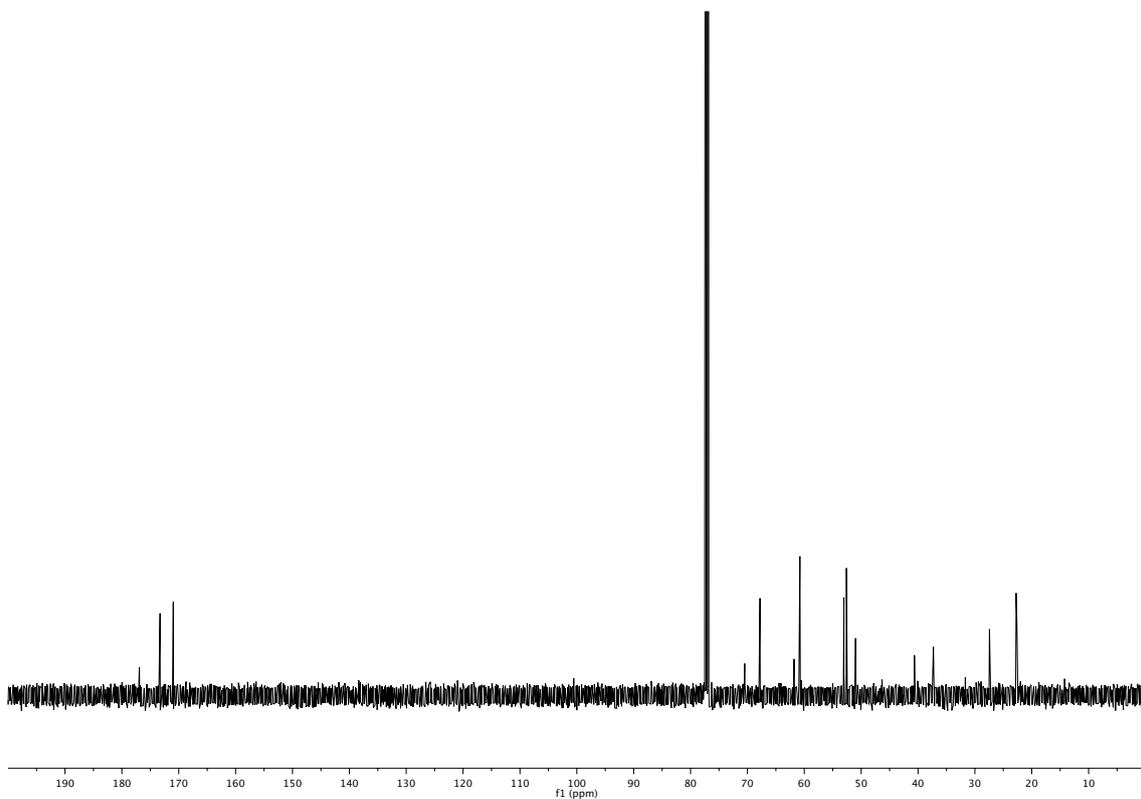
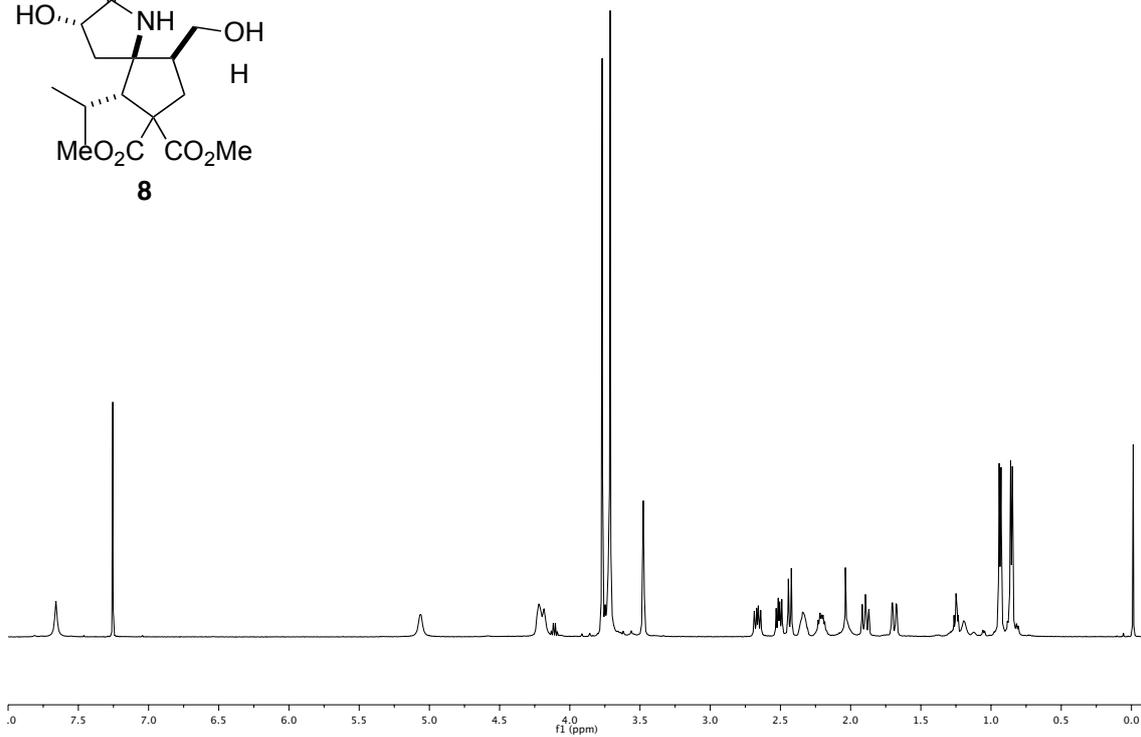
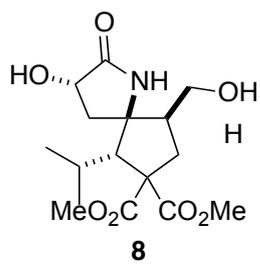












Cartesian coordinates calculated at the MP4(SDQ) level of theory.

**2a**

6	0	-0.877563	-0.011987	-0.163068
6	0	0.628690	-0.046211	-0.513813
6	0	1.163485	1.311217	-0.126910
6	0	-0.040034	2.206943	0.020914
6	0	-1.298971	1.470890	-0.388762
1	0	0.725466	-0.192501	-1.595956
1	0	1.138874	-0.878522	-0.016989
1	0	2.067249	1.700022	-0.588647
1	0	-2.151192	1.719346	0.255827
6	0	0.788756	1.830252	1.229615
1	0	1.407059	2.642167	1.605421
1	0	0.357532	1.189661	1.990841
7	0	0.040364	3.632839	-0.294450
8	0	1.156707	4.123086	-0.501147
8	0	-1.021247	4.267738	-0.283661
6	0	-1.632513	1.762816	-1.861699
1	0	-1.375898	2.800625	-2.097444
1	0	-1.008122	1.138476	-2.515539
6	0	-3.108713	1.569416	-2.185373
1	0	-3.304318	1.771642	-3.244416
1	0	-3.461585	0.556087	-1.973304
1	0	-3.722194	2.258935	-1.593262
6	0	-1.642052	-0.985969	-1.053704
6	0	-1.178102	-0.445928	1.268179
8	0	-1.269469	-1.388598	-2.133710
8	0	-2.809461	-1.341584	-0.482788
6	0	-3.592516	-2.270849	-1.257551
1	0	-3.030794	-3.194801	-1.414906
1	0	-4.488306	-2.454465	-0.665302
1	0	-3.849443	-1.835604	-2.226669
8	0	-1.871426	0.149452	2.062845
8	0	-0.583935	-1.628320	1.528569
6	0	-0.905056	-2.178177	2.821358
1	0	-1.983923	-2.330679	2.905920
1	0	-0.372074	-3.127109	2.871190
1	0	-0.572777	-1.504123	3.614547

MP4(SDQ) Energy = -971.34055608

**3a**

6	0	-0.295907	-0.882895	0.264073
6	0	1.217149	-0.700650	0.579441
6	0	1.692761	0.338119	-0.438948
6	0	0.474571	1.173671	-0.562021
6	0	-0.806932	0.544364	-0.135048
1	0	1.751578	-1.655002	0.538800
1	0	1.309869	-0.286082	1.594770
1	0	1.960437	-0.145917	-1.388314
1	0	-1.156809	1.032532	0.792301
7	0	0.739603	2.462877	-0.569653
8	0	0.069038	3.475050	-0.572739
8	0	2.224142	2.629535	-0.613499
6	0	2.710794	1.398284	-0.031648
1	0	2.751382	1.517414	1.061881
1	0	3.714686	1.245471	-0.435693
6	0	-1.932665	0.649705	-1.166023
1	0	-1.938288	1.691819	-1.516803
1	0	-1.689845	0.039744	-2.048886
6	0	-3.310219	0.304117	-0.616613
1	0	-4.075745	0.432342	-1.390996
1	0	-3.366536	-0.724999	-0.252779
1	0	-3.569407	0.963487	0.219864
6	0	-0.451659	-1.842872	-0.903575
6	0	-1.010878	-1.436141	1.479917
8	0	-1.851125	-0.862423	2.137799
8	0	0.393980	-2.057791	-1.746713
8	0	-0.529005	-2.661081	1.773316
8	0	-1.675147	-2.400335	-0.912305
6	0	-1.929091	-3.269695	-2.033349
1	0	-2.952090	-3.619784	-1.899230
1	0	-1.827428	-2.716962	-2.970675
1	0	-1.226722	-4.106553	-2.028302
6	0	-1.144681	-3.282762	2.918161
1	0	-2.218004	-3.399728	2.749601
1	0	-0.659334	-4.253273	3.015117
1	0	-0.983179	-2.676441	3.812534

MP4(SDQ) Energy = -971.33979256

**2c**

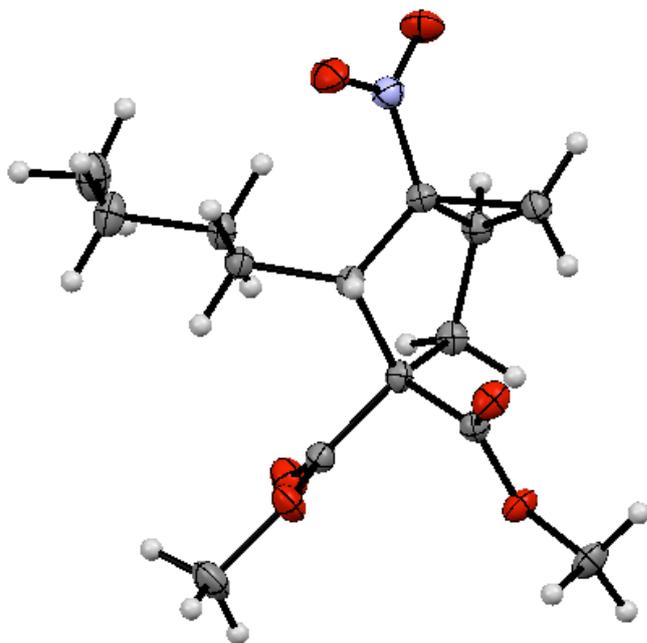
6	0	-0.823346	-0.000640	-0.135929
6	0	0.685562	0.207082	-0.411027
6	0	0.969337	1.635754	-0.017901
6	0	-0.358472	2.315791	0.141758
6	0	-1.499349	1.401767	-0.264222
1	0	0.879551	0.051372	-1.476270
1	0	1.294594	-0.518173	0.140580
1	0	1.808787	2.168778	-0.456370
1	0	-2.328061	1.454416	0.454221
6	0	0.498441	2.043722	1.353701
1	0	0.971956	2.929163	1.773306
1	0	0.174409	1.311600	2.085858
7	0	-0.509555	3.755725	-0.095316
8	0	0.369866	4.355254	-0.727630
8	0	-1.505126	4.286310	0.409008
6	0	-2.056526	1.681343	-1.680737
1	0	-2.666325	0.798320	-1.928232
6	0	-3.027842	2.862978	-1.725447
1	0	-3.612058	2.814214	-2.652824
1	0	-3.728947	2.850400	-0.883113
1	0	-2.518909	3.831389	-1.720224
6	0	-1.420104	-1.016560	-1.102059
6	0	-1.085512	-0.591898	1.249229
8	0	-0.889876	-1.450370	-2.099948
8	0	-2.653478	-1.371703	-0.688226
6	0	-3.317132	-2.324499	-1.541968
1	0	-2.731739	-3.244831	-1.606034
1	0	-4.282335	-2.508224	-1.071335
1	0	-3.446480	-1.907790	-2.544133
8	0	-1.793669	-0.122459	2.112001
8	0	-0.424950	-1.760937	1.375510
6	0	-0.674524	-2.452452	2.615251
1	0	-1.740896	-2.668758	2.716044
1	0	-0.094423	-3.372522	2.553018
1	0	-0.347885	-1.843975	3.461863
6	0	-0.992296	1.833721	-2.766157
1	0	-0.317505	2.672981	-2.559026
1	0	-0.390038	0.931056	-2.900244
1	0	-1.477320	2.040535	-3.728511

MP4(SDQ) Energy = - 1010.5364867

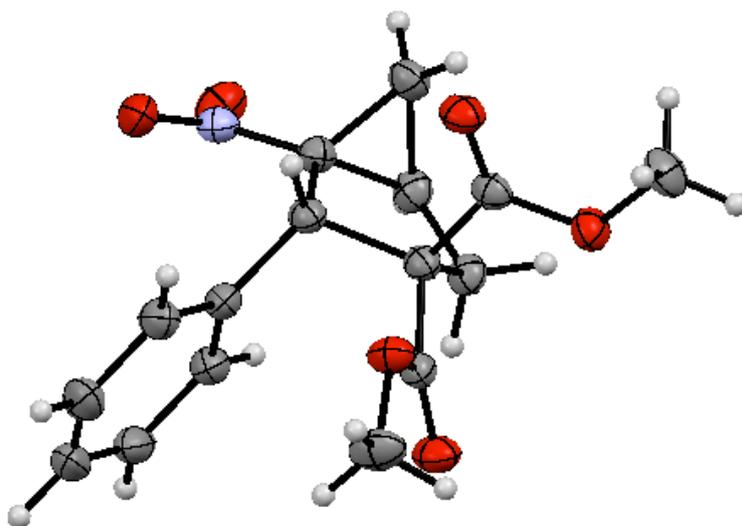
**3c**

6	0	-0.314790	-0.850735	0.238066
6	0	1.210390	-0.712741	0.506793
6	0	1.679635	0.365357	-0.473976
6	0	0.485459	1.247059	-0.487259
6	0	-0.812299	0.595236	-0.136655
1	0	1.723672	-1.674710	0.407324
1	0	1.348508	-0.344522	1.534550
1	0	1.891640	-0.073241	-1.457797
1	0	-1.208112	1.063737	0.782796
7	0	0.795074	2.507183	-0.236489
8	0	0.156810	3.514595	-0.011647
8	0	2.270845	2.658119	-0.302978
6	0	2.768688	1.334284	-0.012059
1	0	2.943827	1.257548	1.071021
1	0	3.713026	1.234072	-0.552553
6	0	-1.916811	0.684929	-1.206175
1	0	-1.654347	0.008840	-2.037058
6	0	-3.272966	0.285946	-0.632701
1	0	-4.039376	0.306504	-1.417896
1	0	-3.274200	-0.710431	-0.184876
1	0	-3.575187	0.999326	0.145275
6	0	-0.511261	-1.804298	-0.930252
6	0	-1.000479	-1.399104	1.473545
8	0	-1.837602	-0.831461	2.140584
8	0	0.292575	-1.975164	-1.823466
8	0	-0.495475	-2.613708	1.772587
8	0	-1.706069	-2.416579	-0.874771
6	0	-1.989595	-3.278079	-1.994652
1	0	-2.984920	-3.678266	-1.804164
1	0	-1.972880	-2.704616	-2.924955
1	0	-1.250487	-4.080731	-2.050363
6	0	-1.084653	-3.231413	2.933224
1	0	-2.158439	-3.366750	2.782034
1	0	-0.583166	-4.193326	3.034005
1	0	-0.919648	-2.612630	3.818391
6	0	-1.996370	2.095110	-1.780524
1	0	-2.232278	2.827432	-0.999141
1	0	-1.054095	2.404018	-2.247494
1	0	-2.783529	2.147070	-2.542844

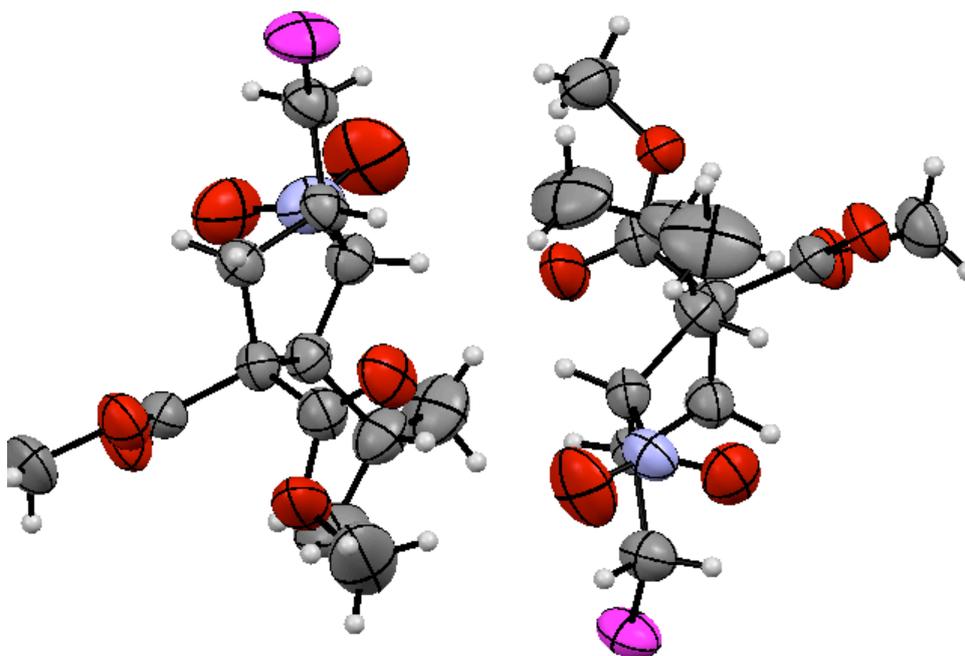
MP4(SDQ) Energy = -1010.5385619



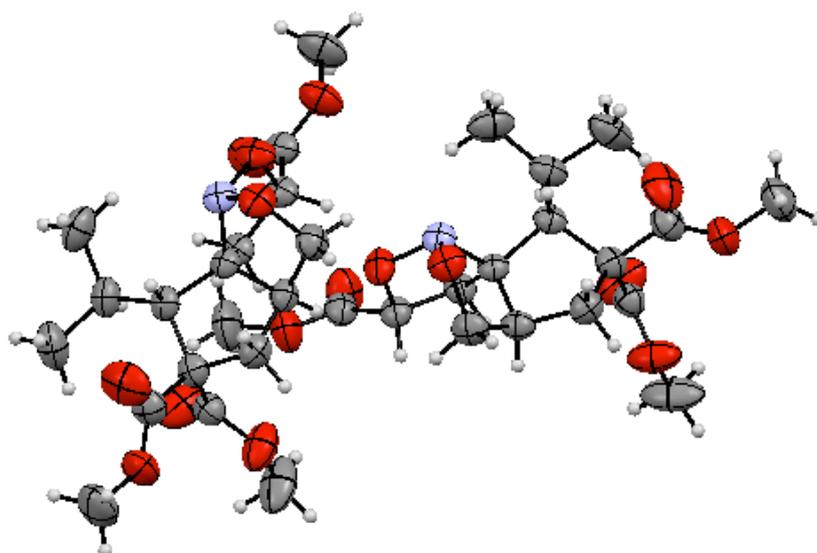
**Chart 1.** ORTEP chart for compound 2d



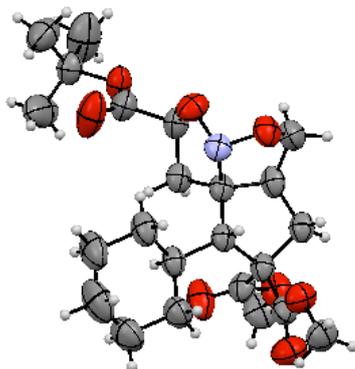
**Chart 2.** ORTEP chart for compound 2h



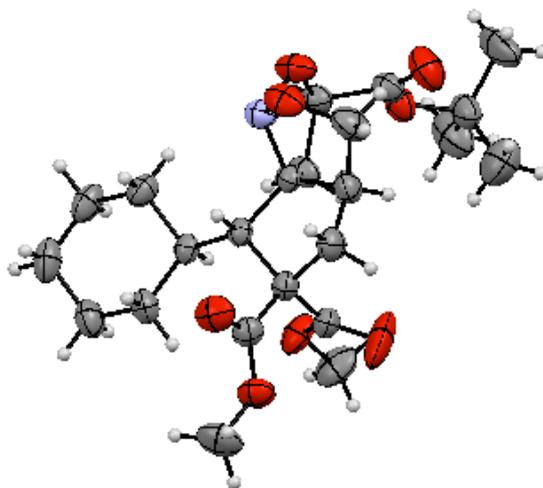
**Chart 3. ORTEP chart for compound 5**



**Chart 4. ORTEP chart for compound 6aA**



**Chart 5. ORTEP chart for compound 6eA**



**Chart 6. ORTEP chart for compound 6eB**

