

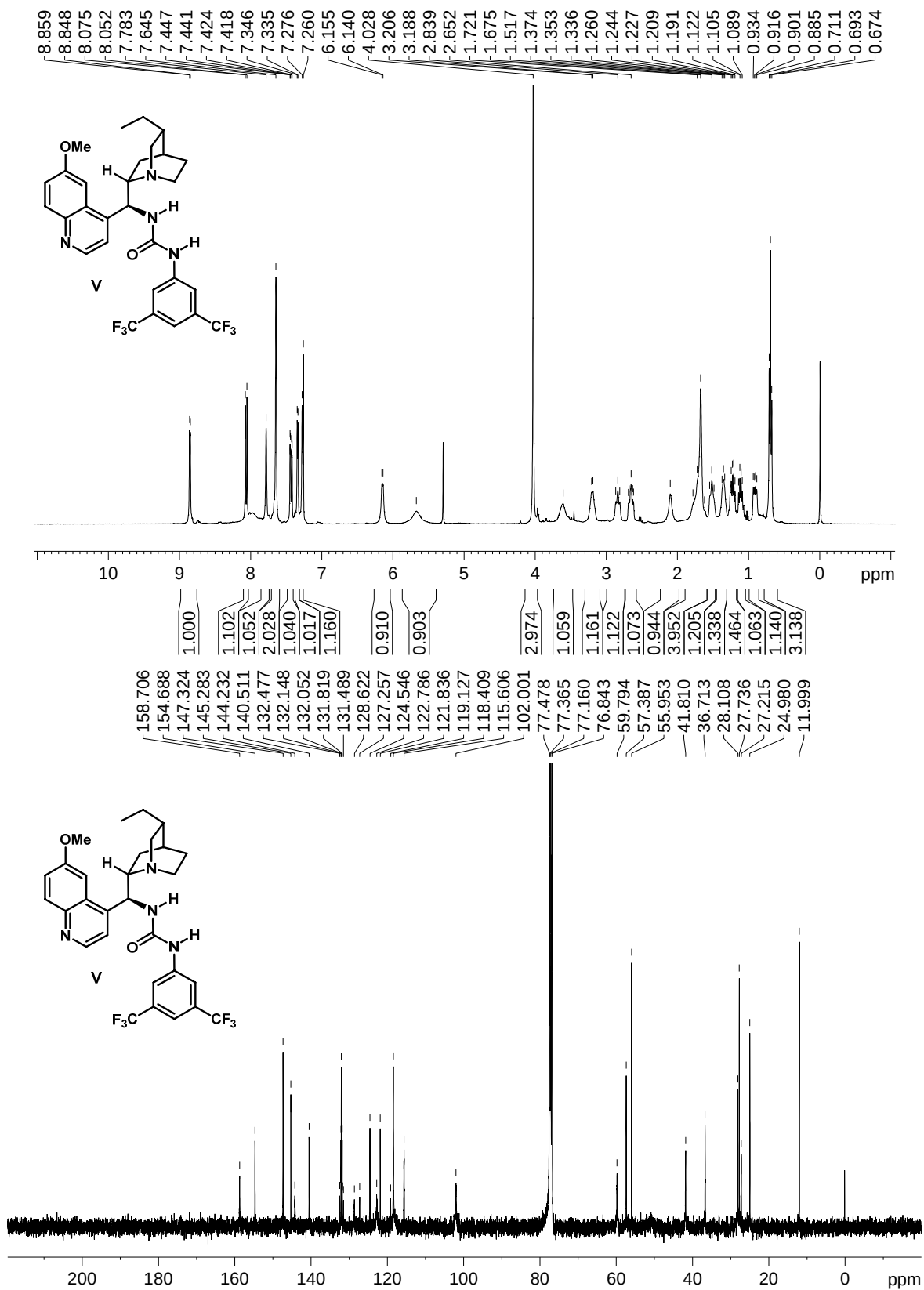
Organocatalytic Enantioselective Formal C(sp²)-H Alkylation

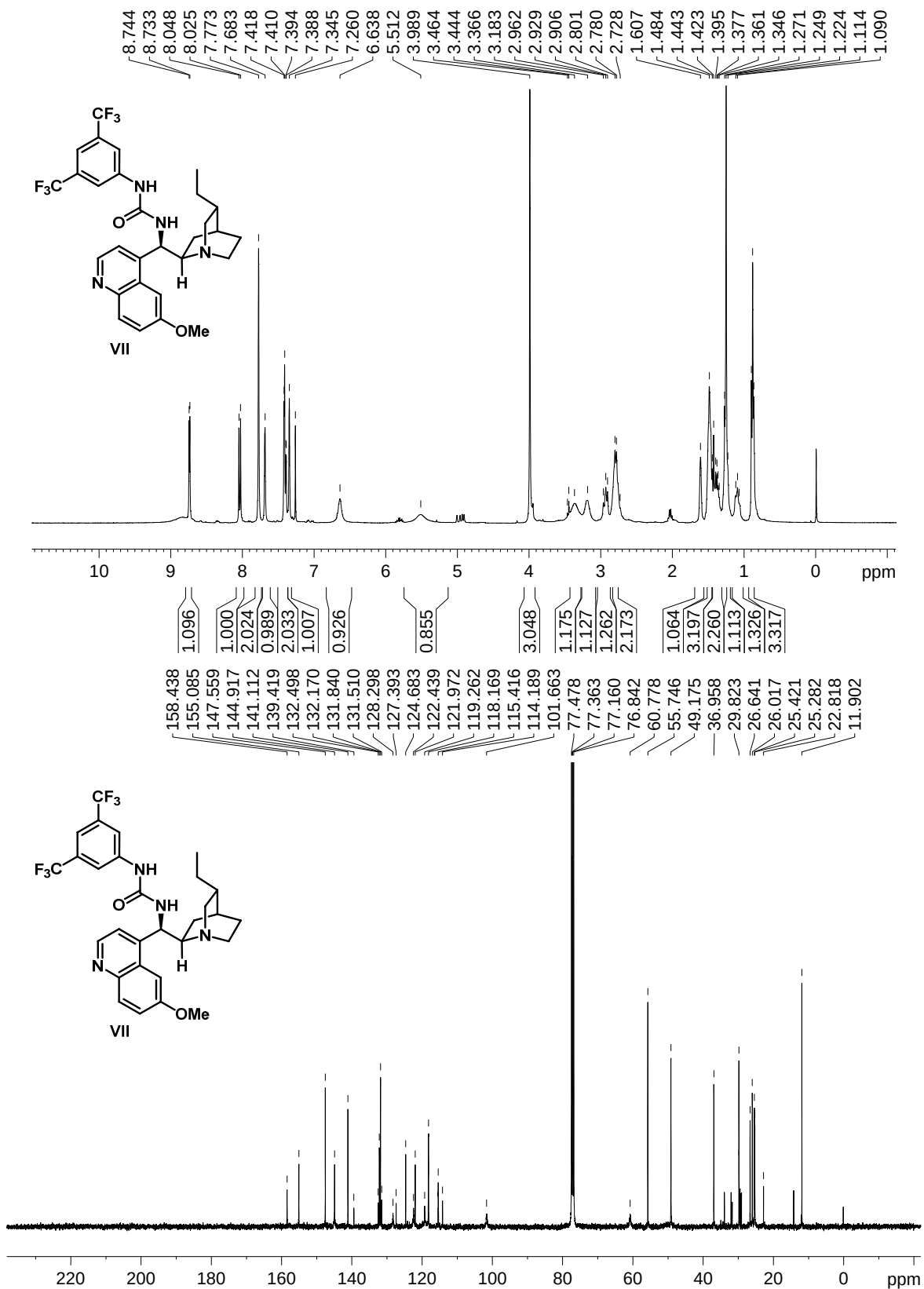
Madhu Sudan Manna and Santanu Mukherjee*

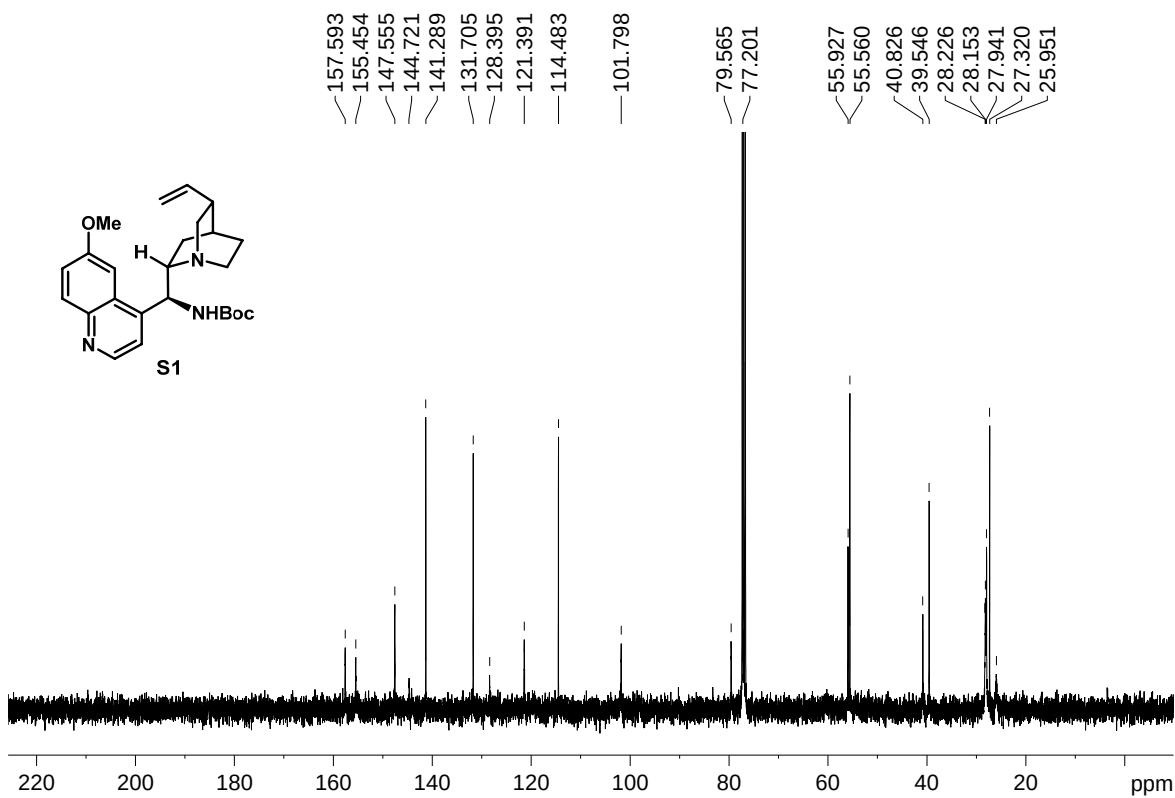
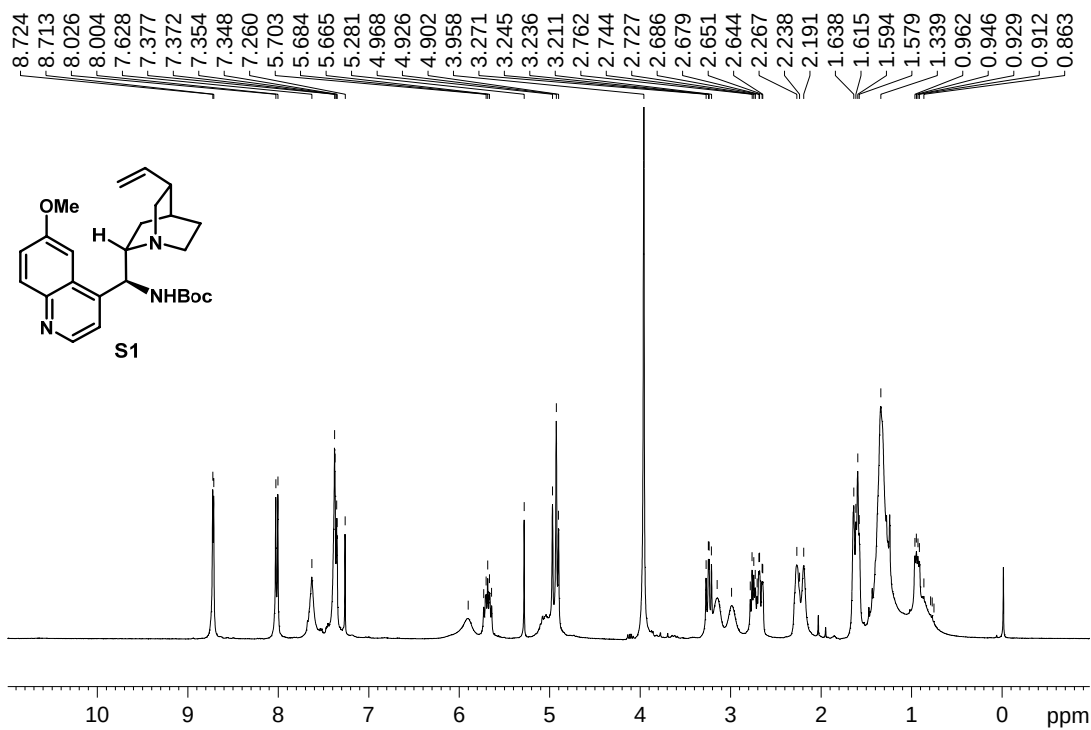
Department of Organic Chemistry, Indian Institute of Science, Bangalore 560 012, INDIA

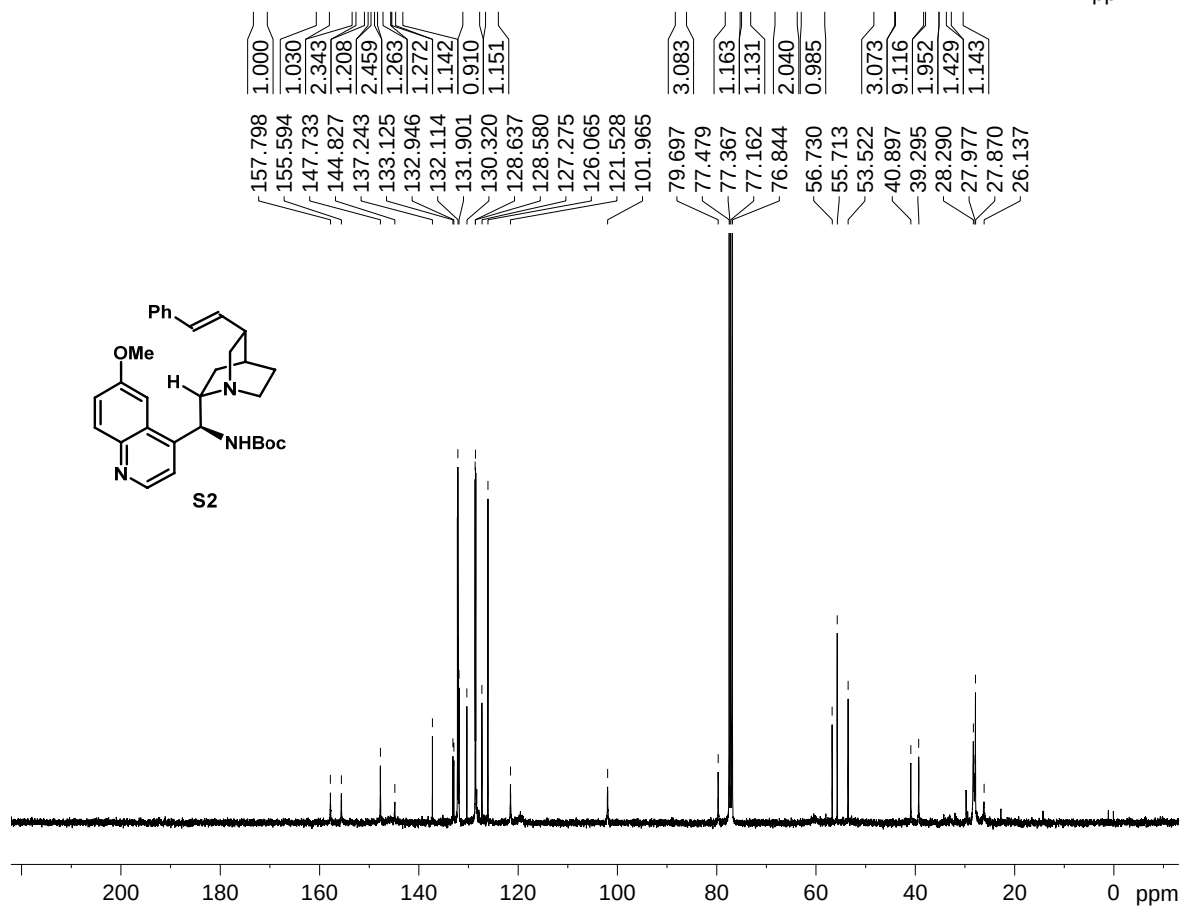
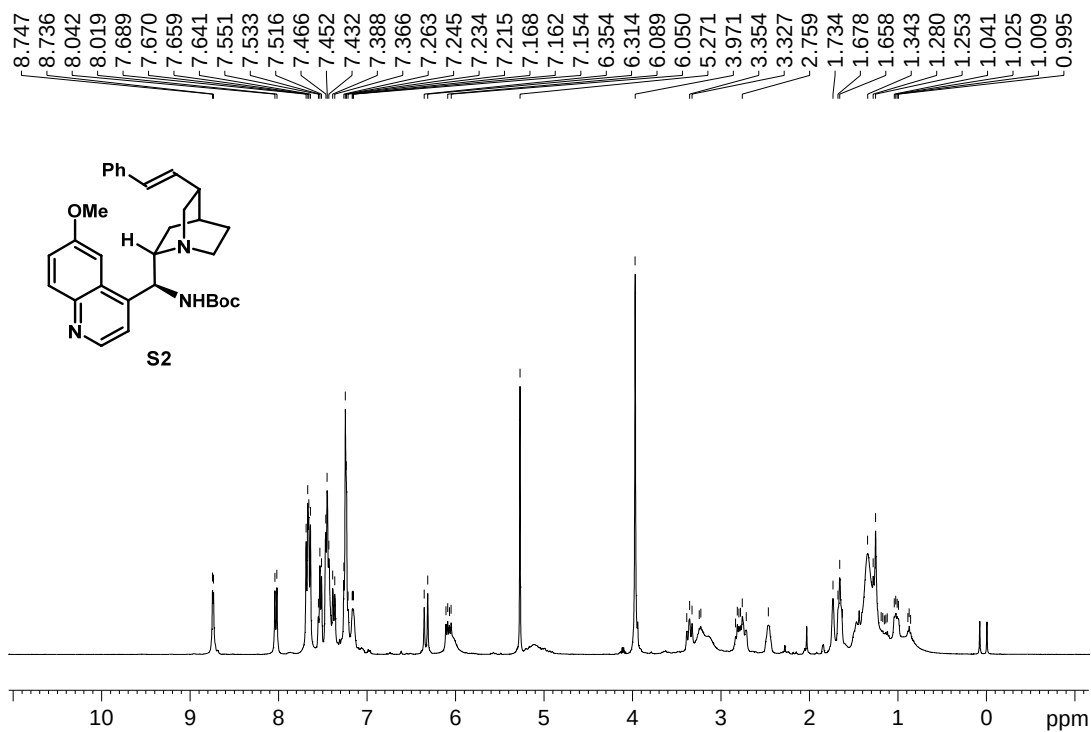
sm@orgchem.iisc.ernet.in

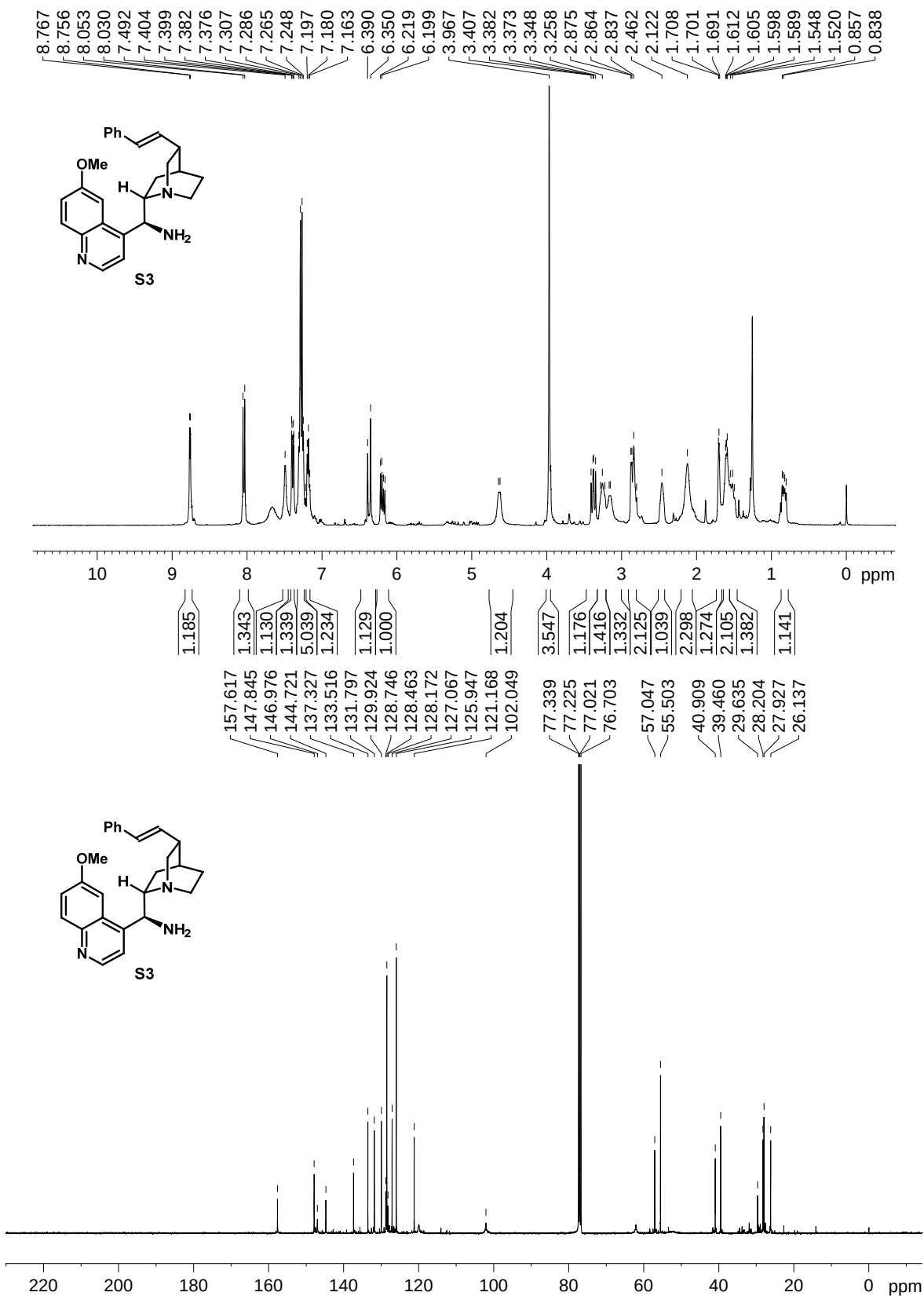
SUPPORTING INFORMATION: PART B

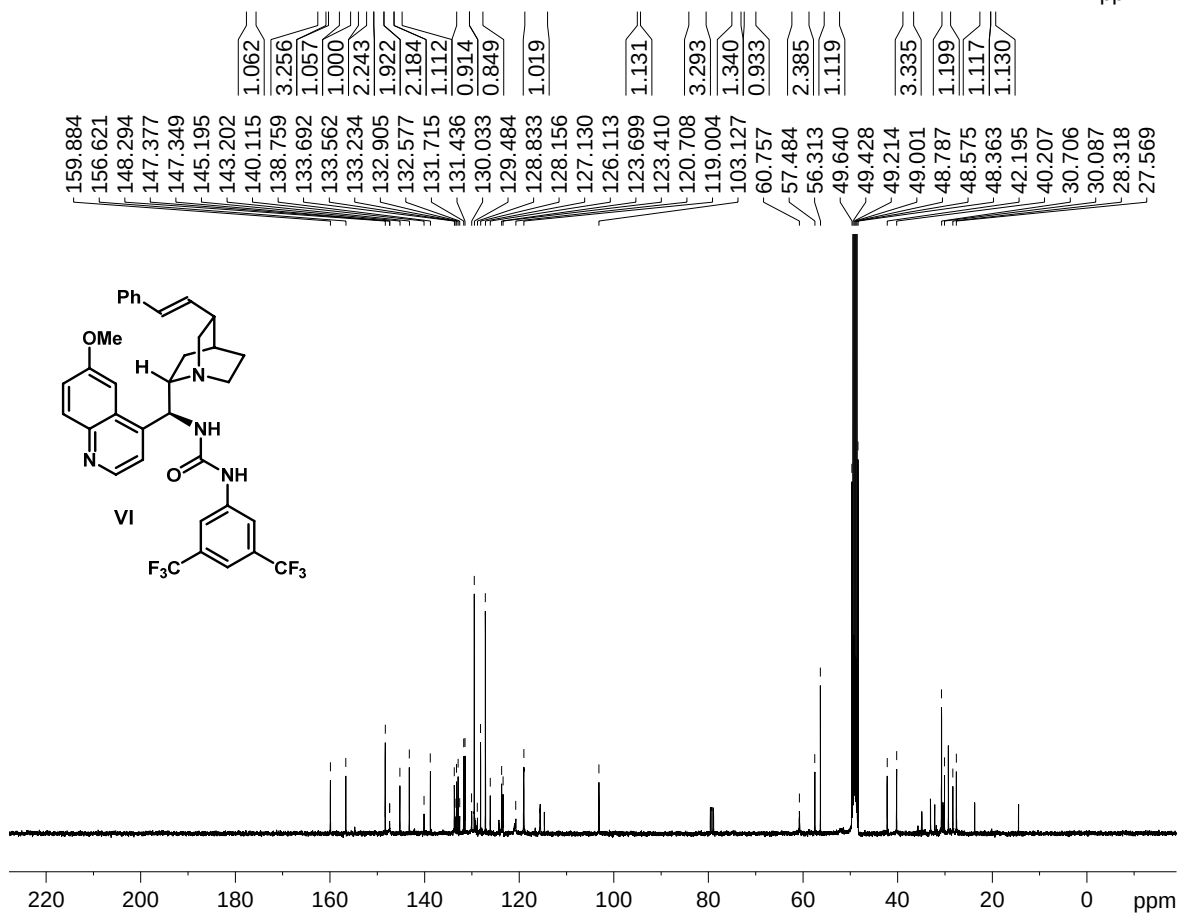
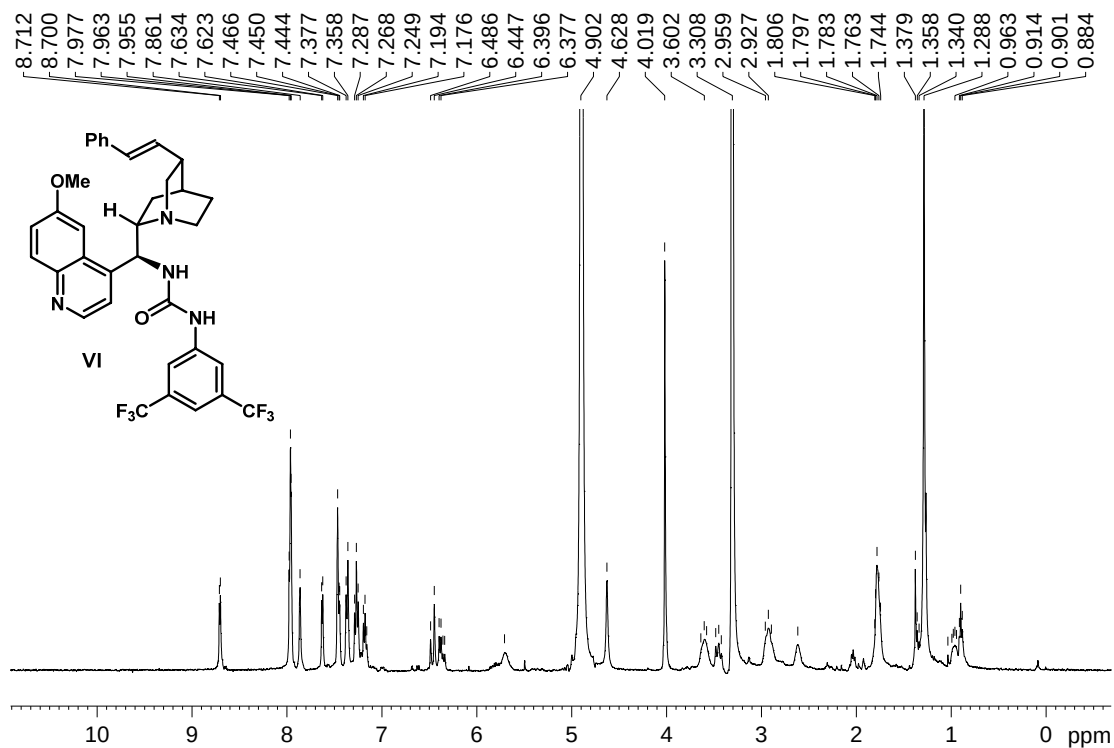


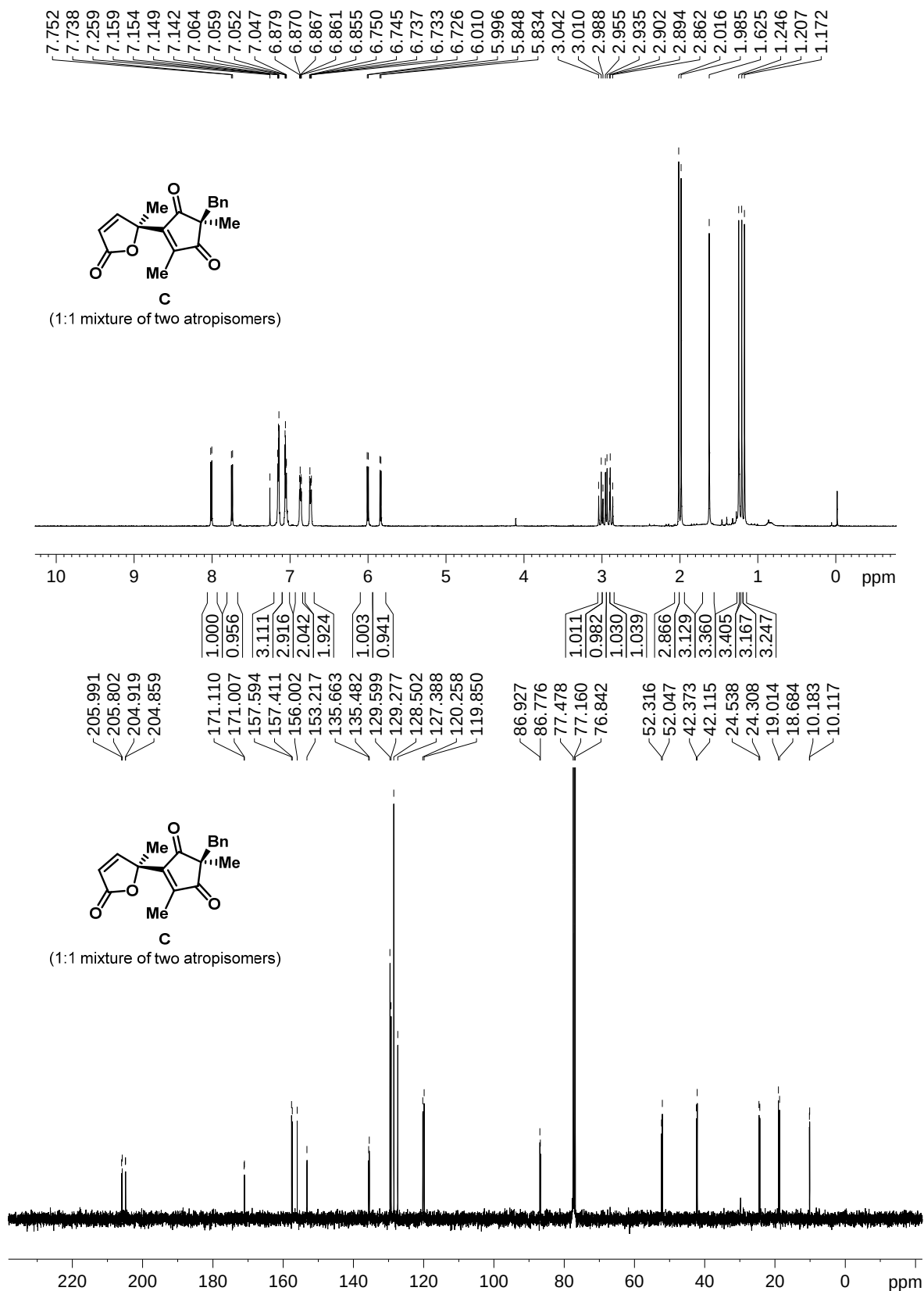




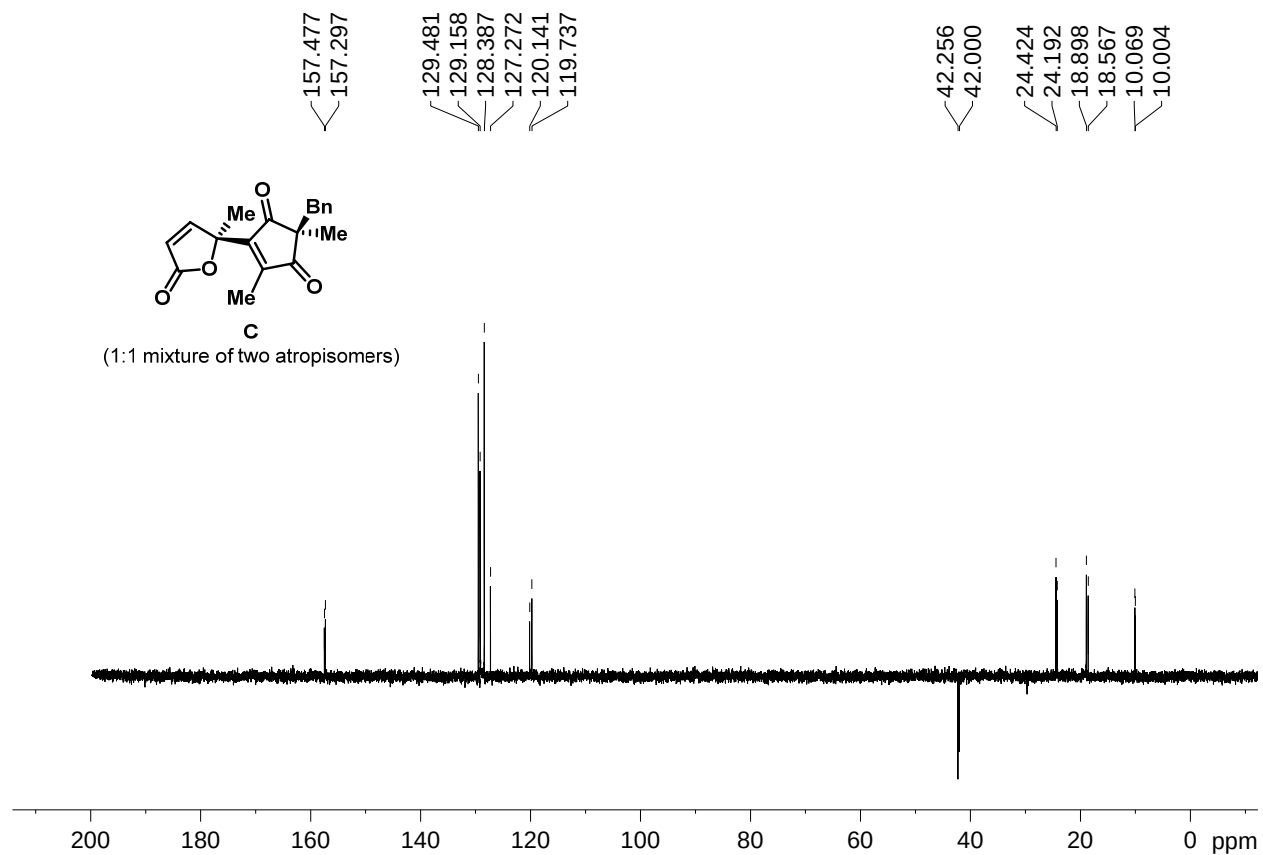


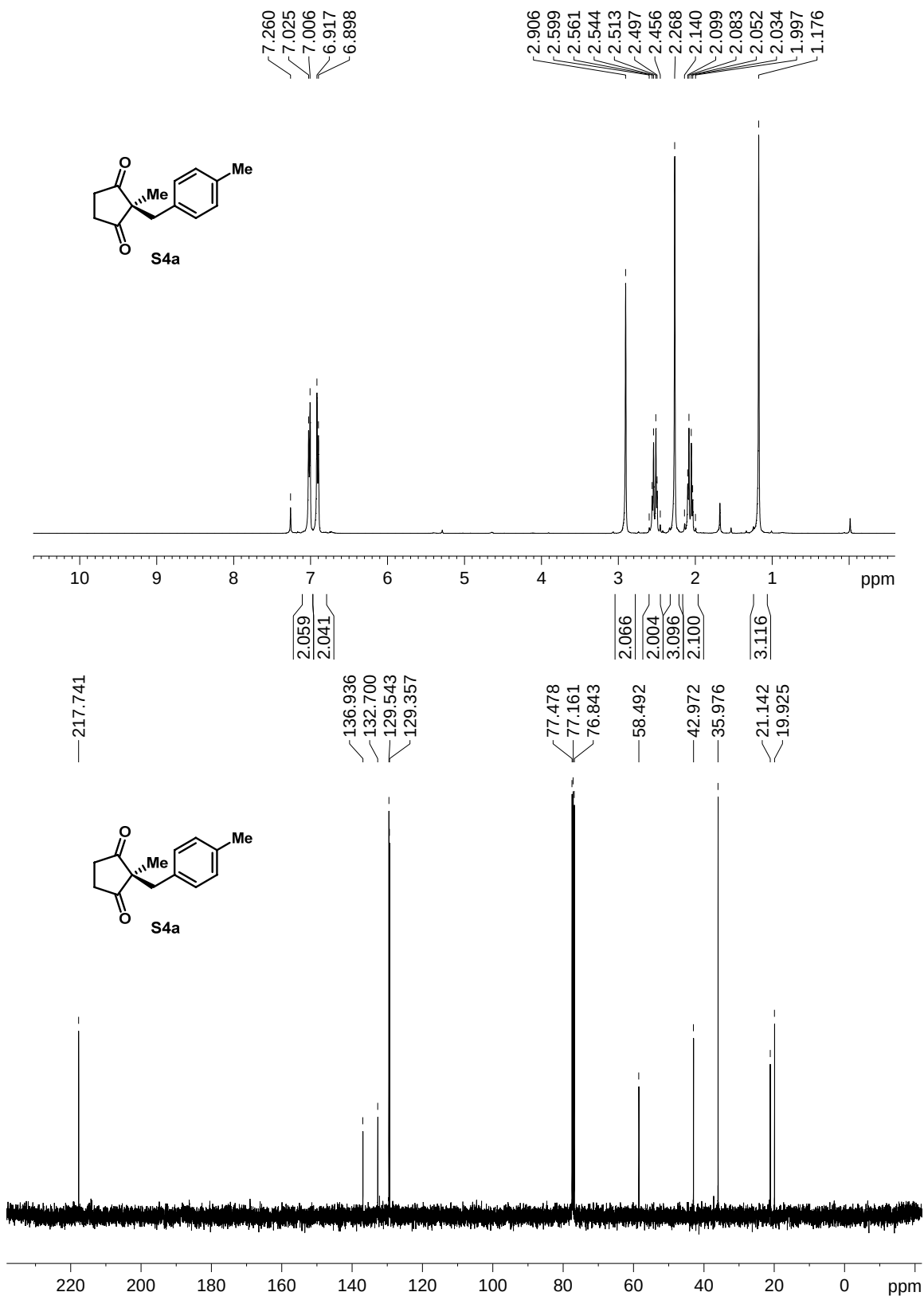


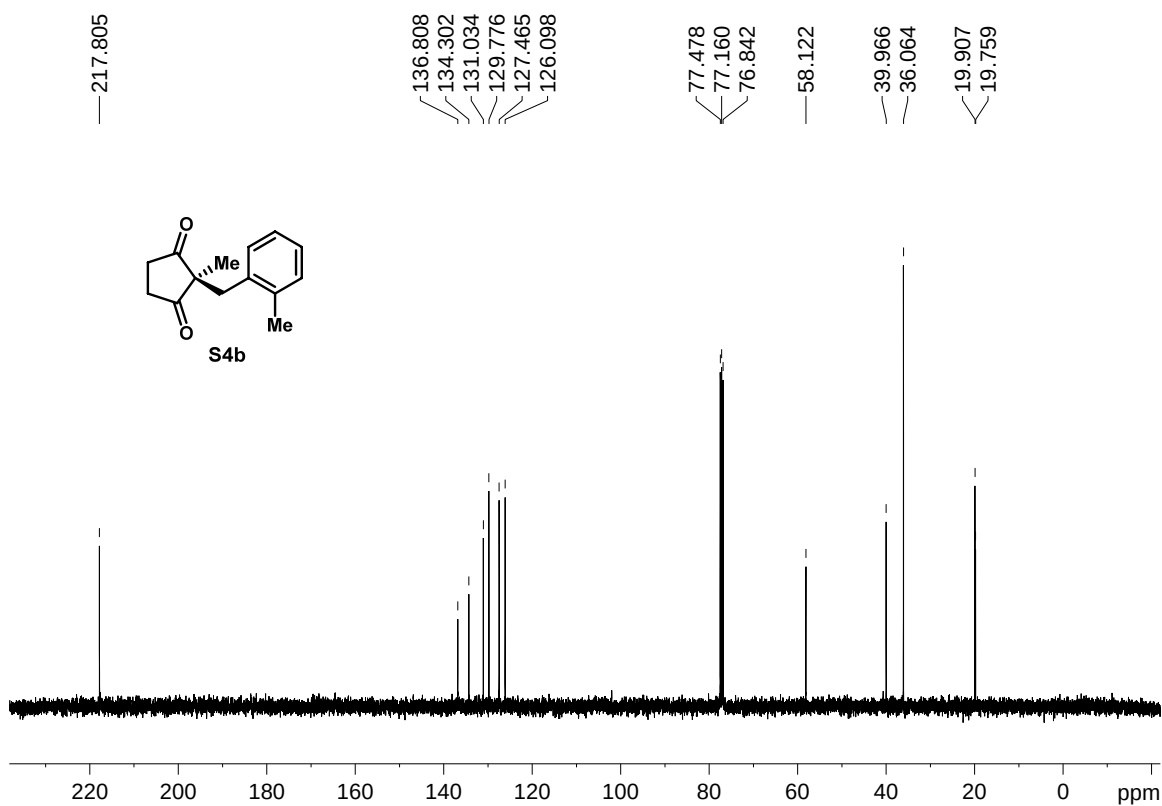
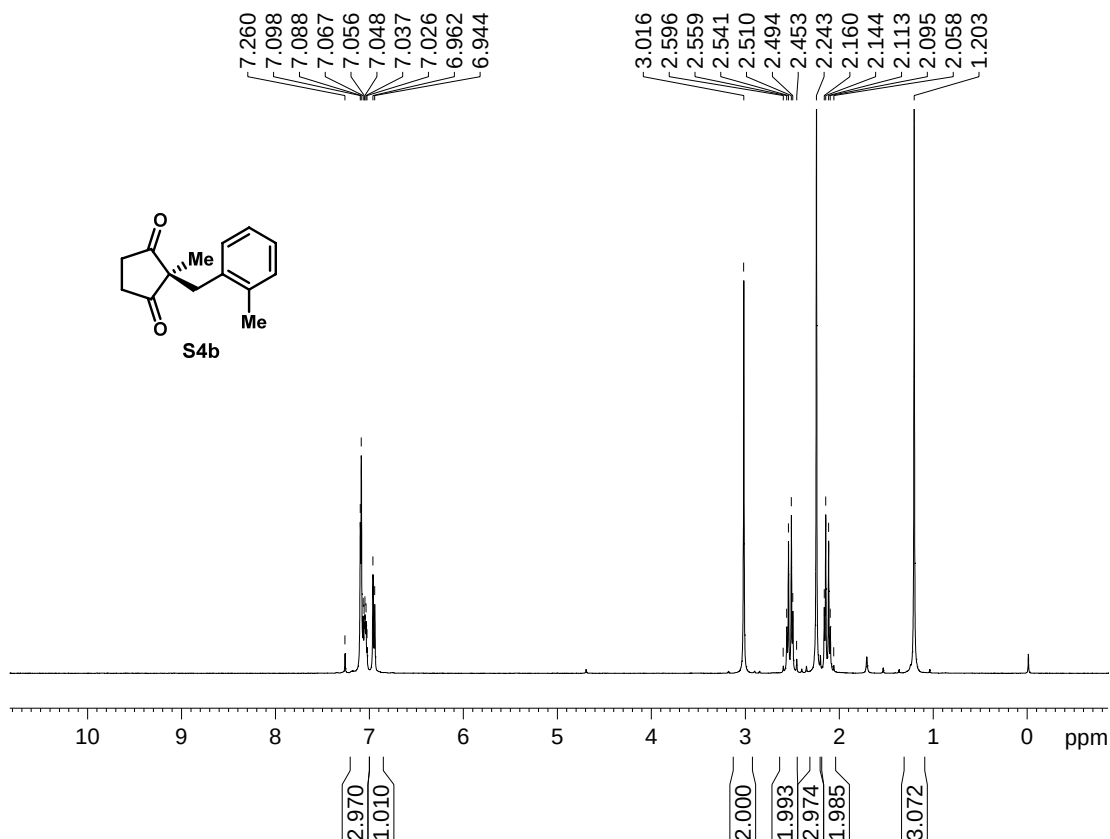


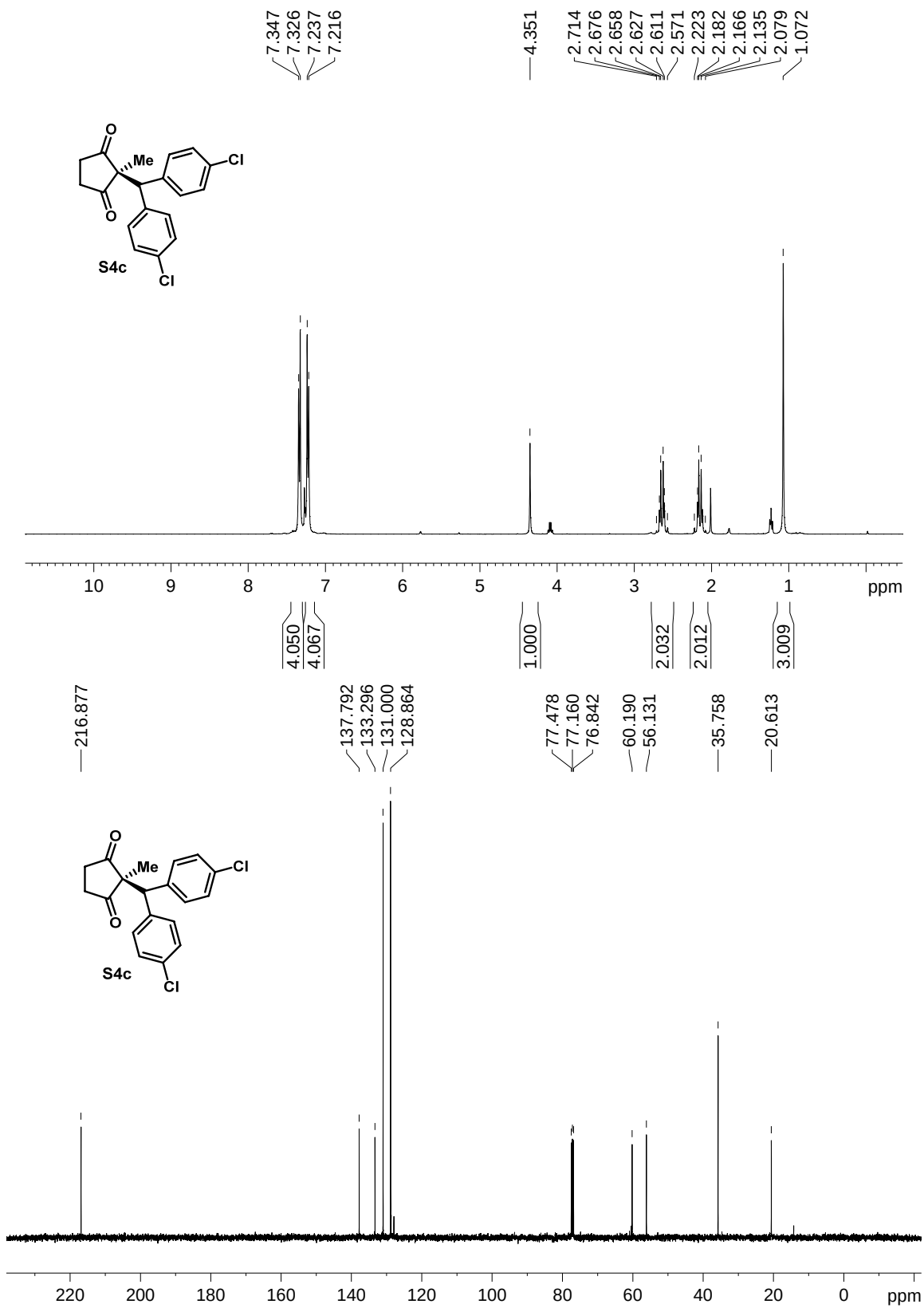


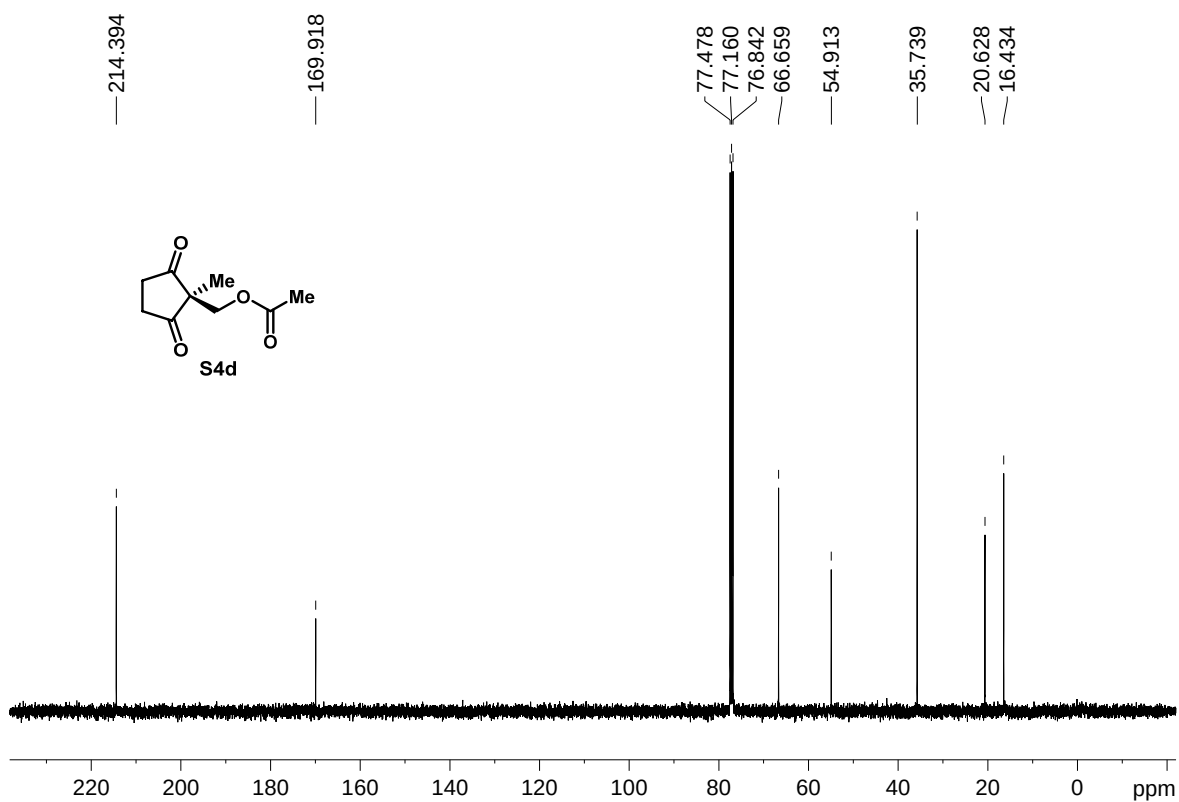
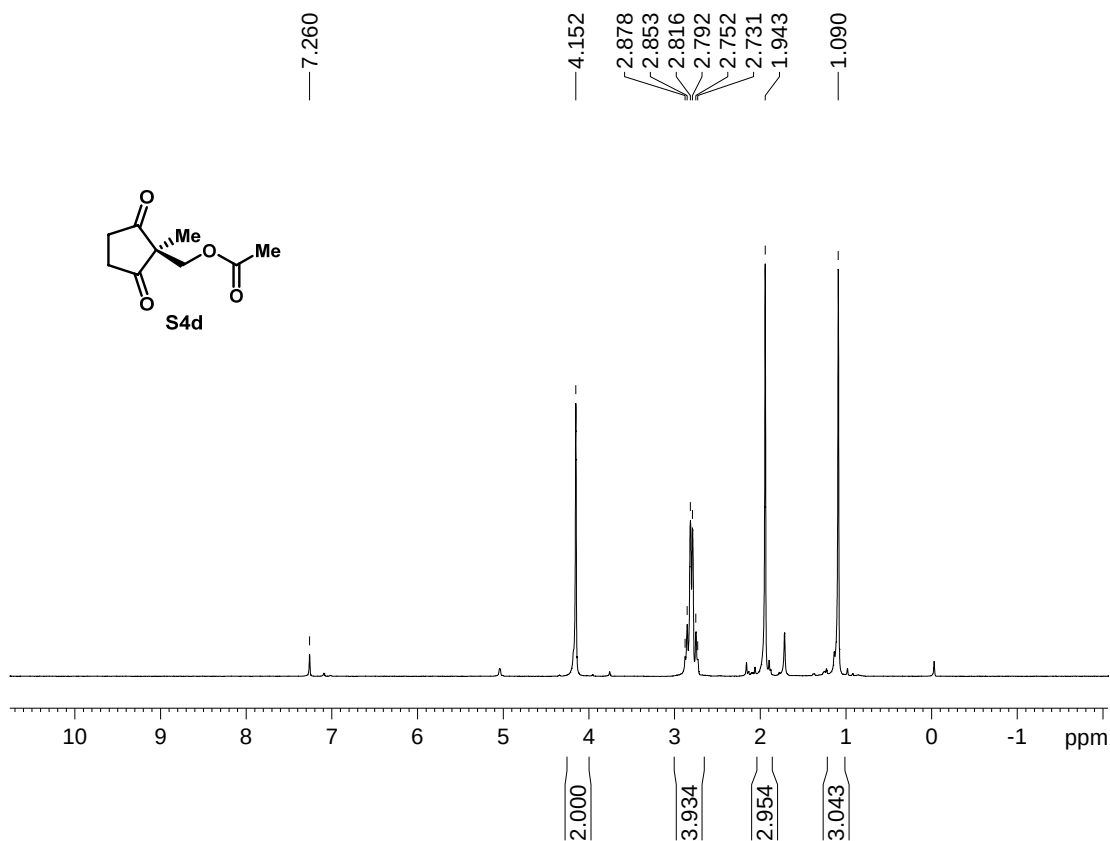
DEPT NMR Spectrum of **C**:

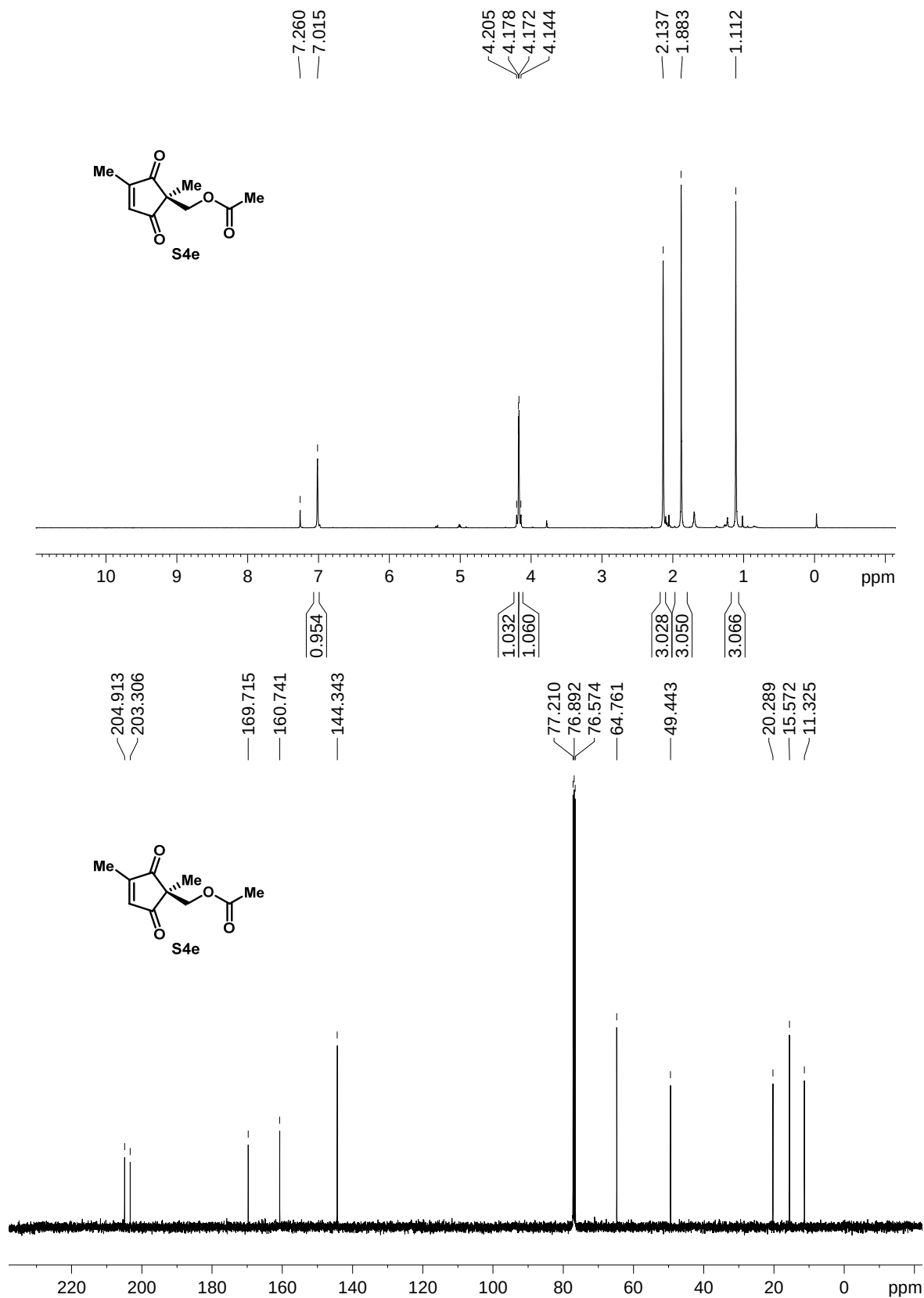


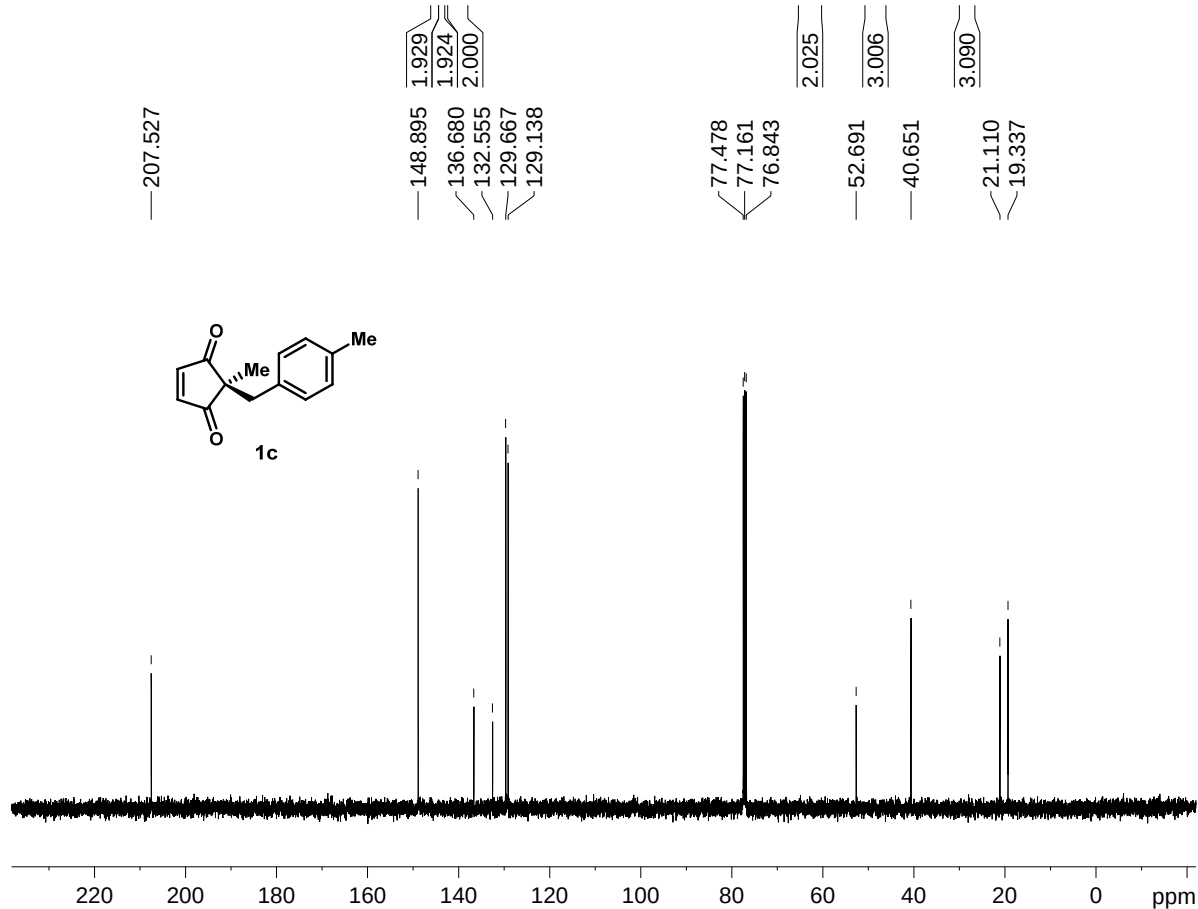
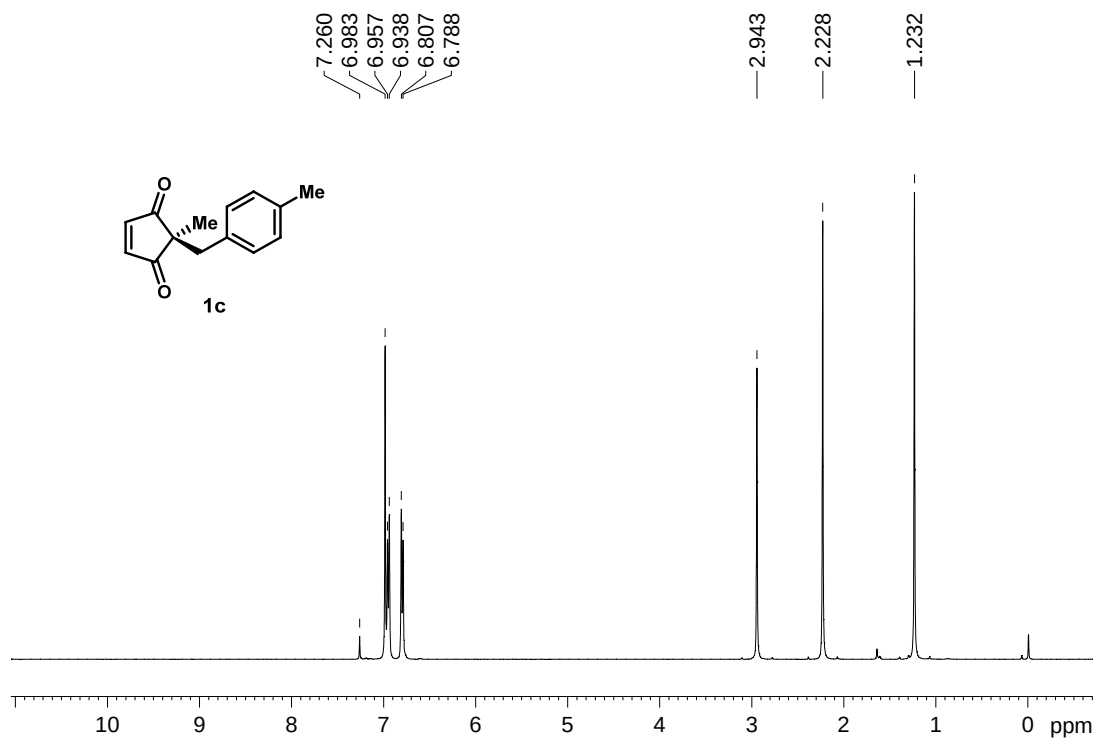


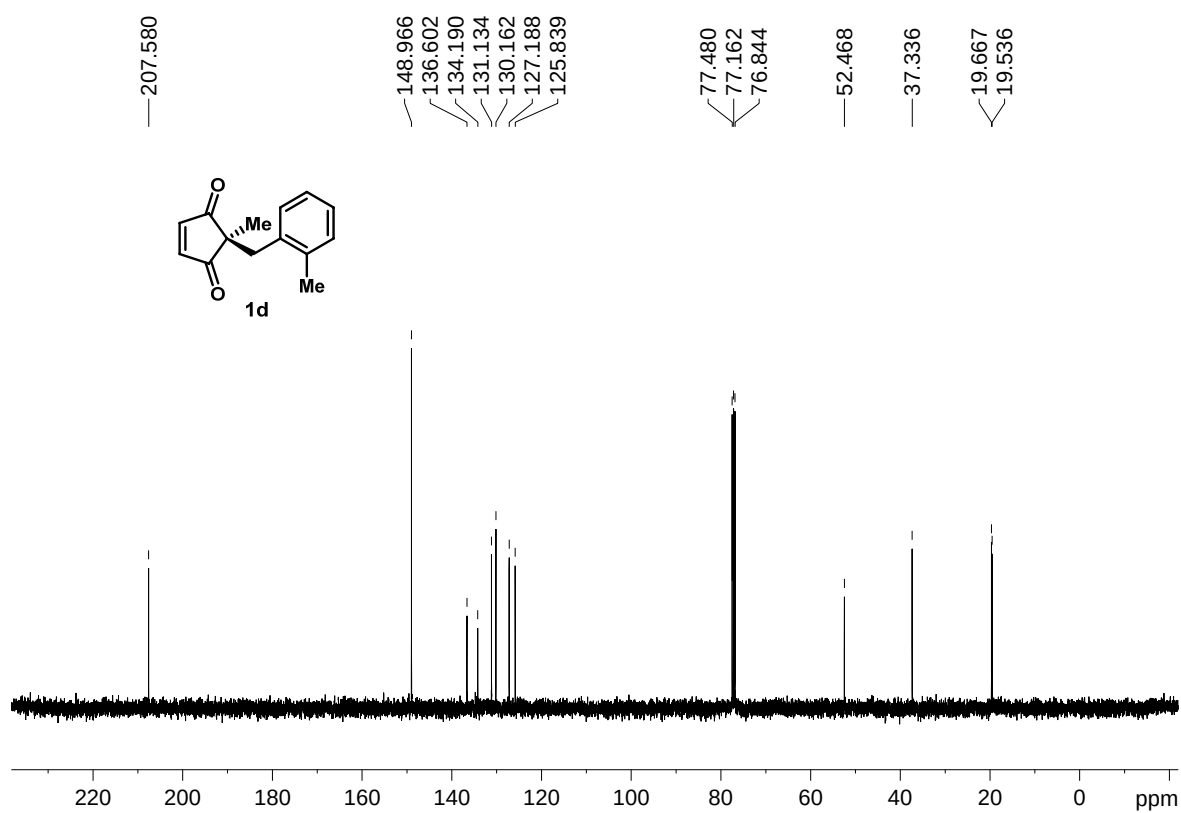
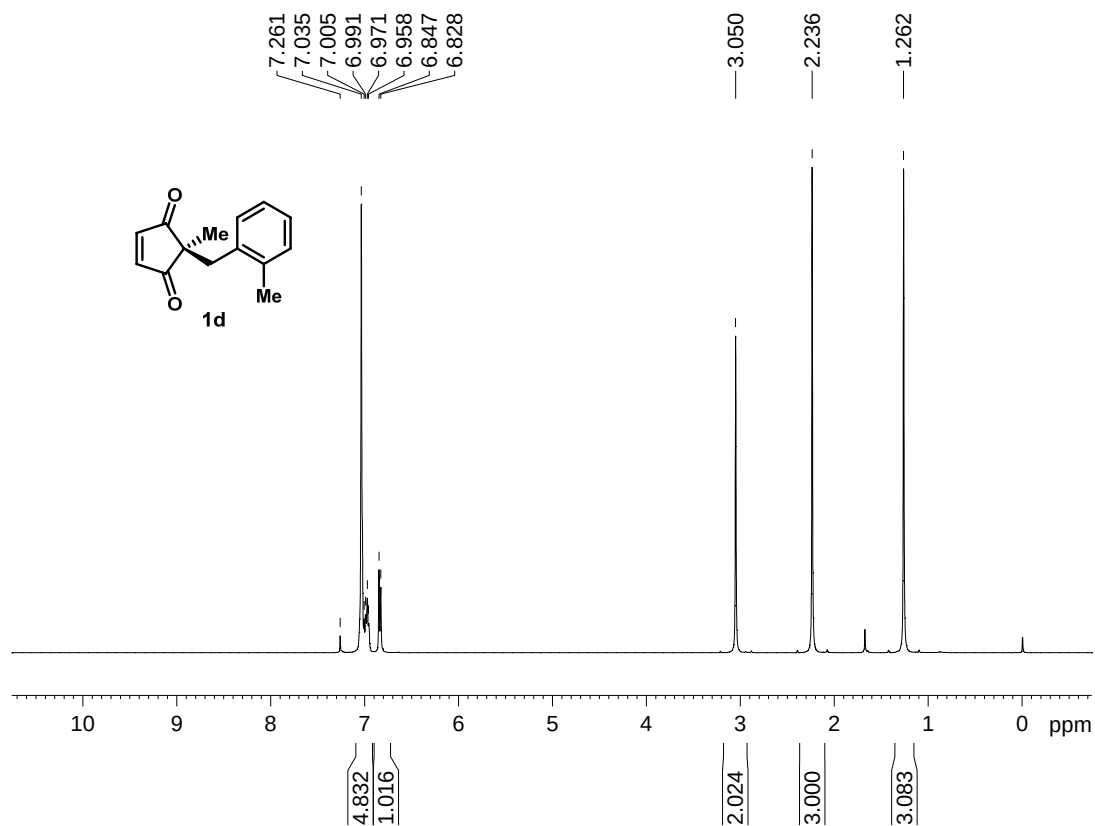


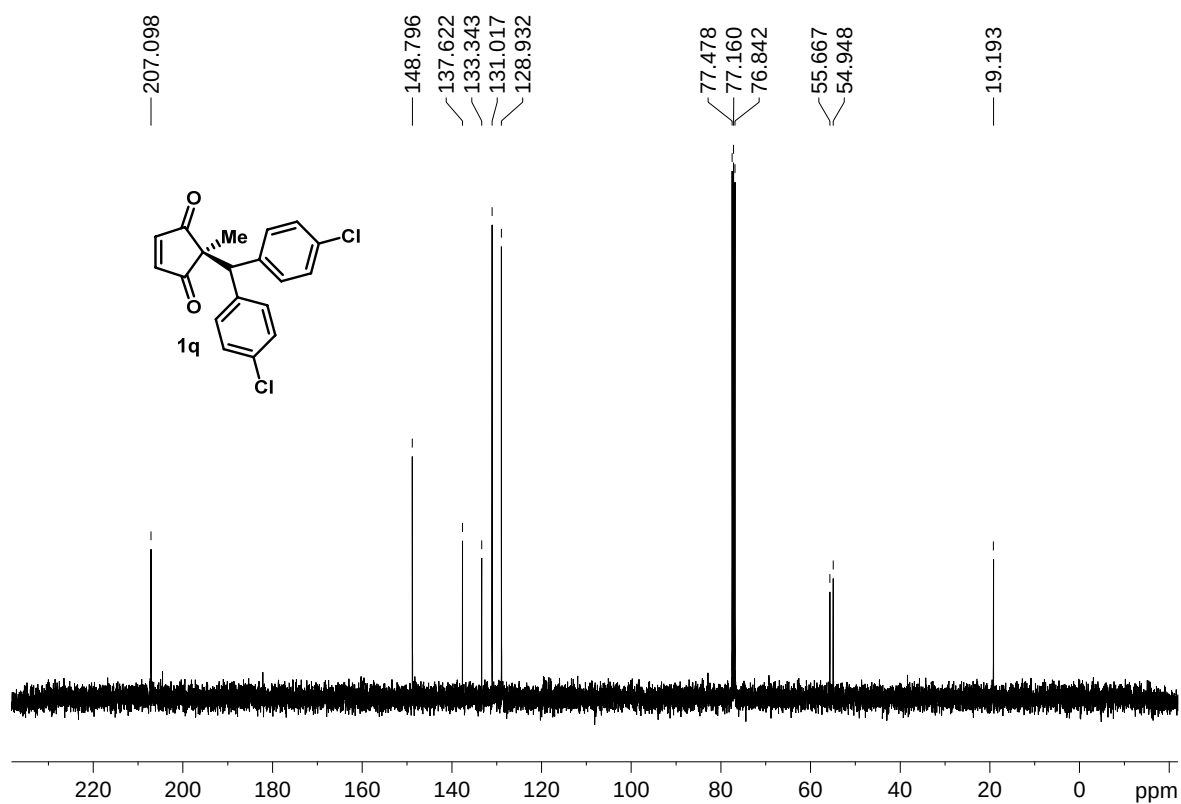
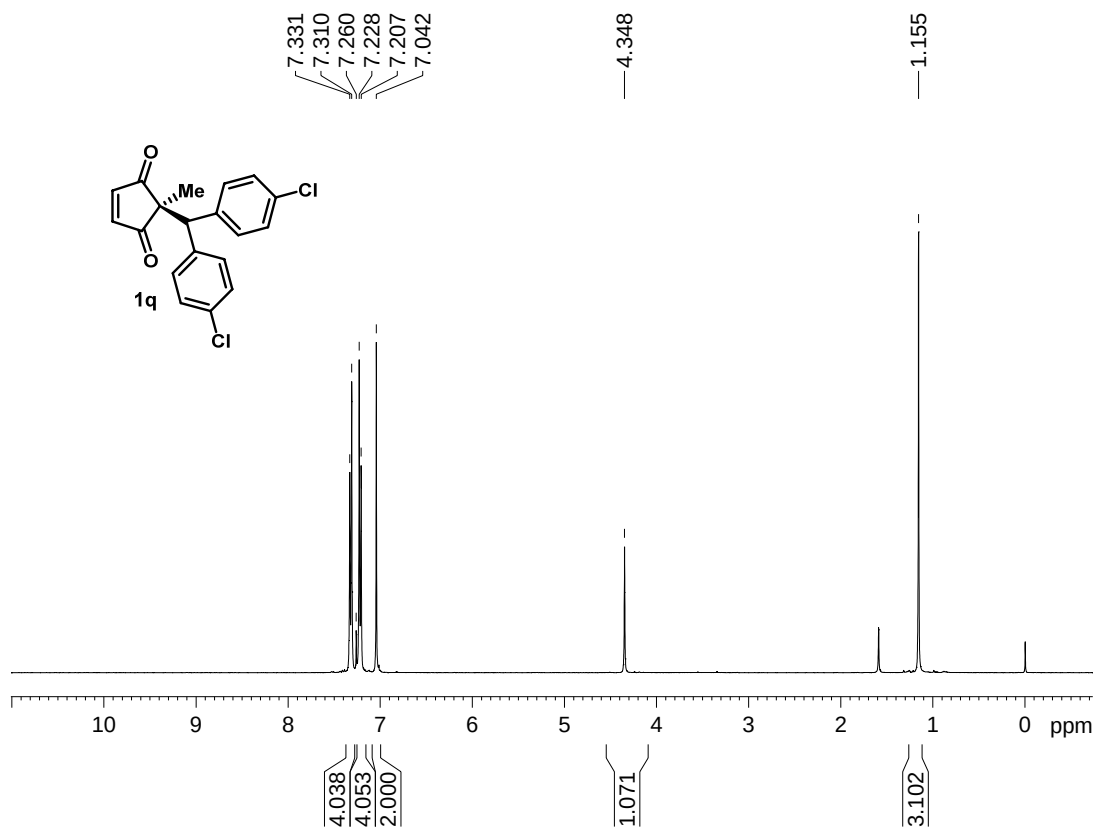


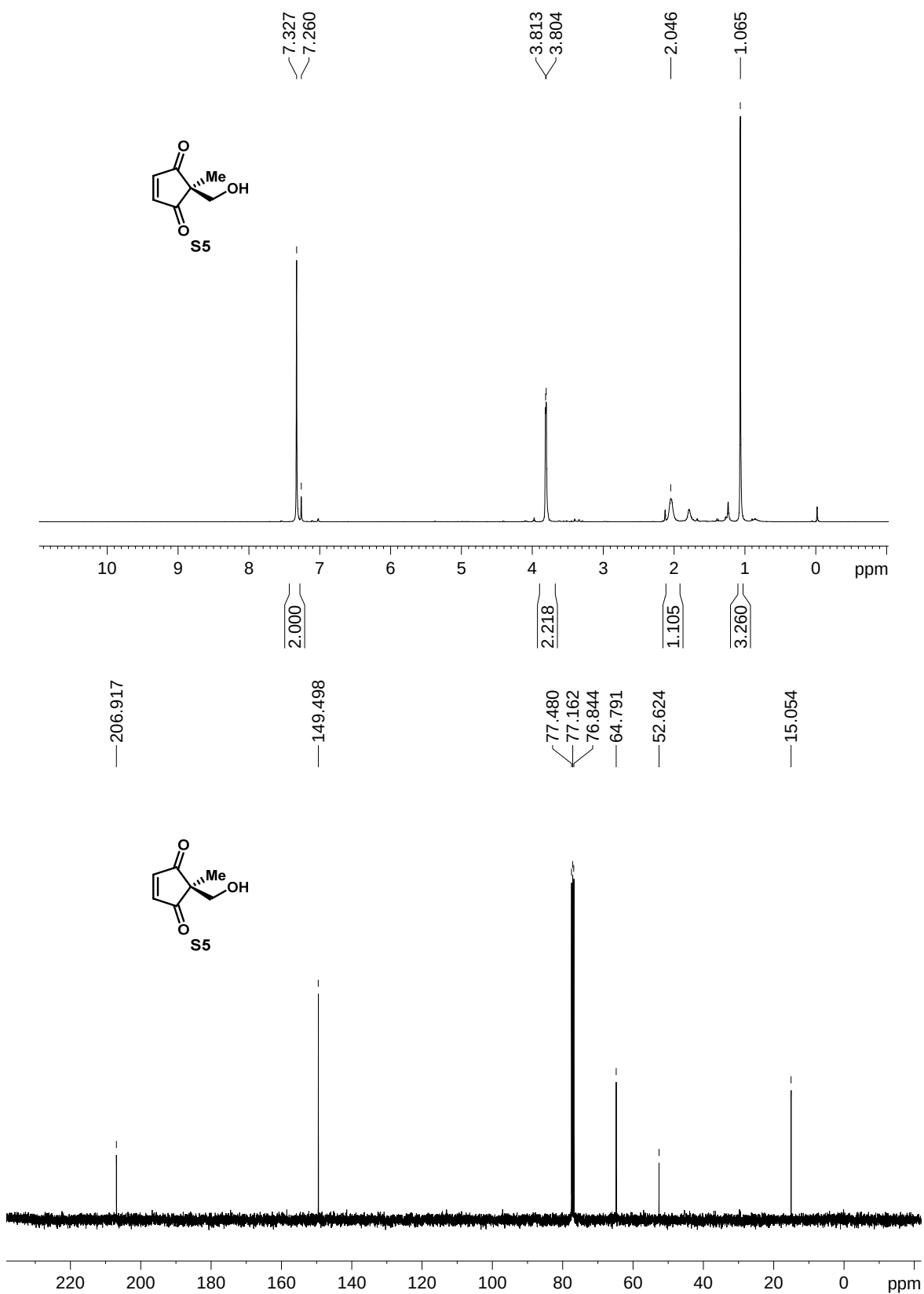


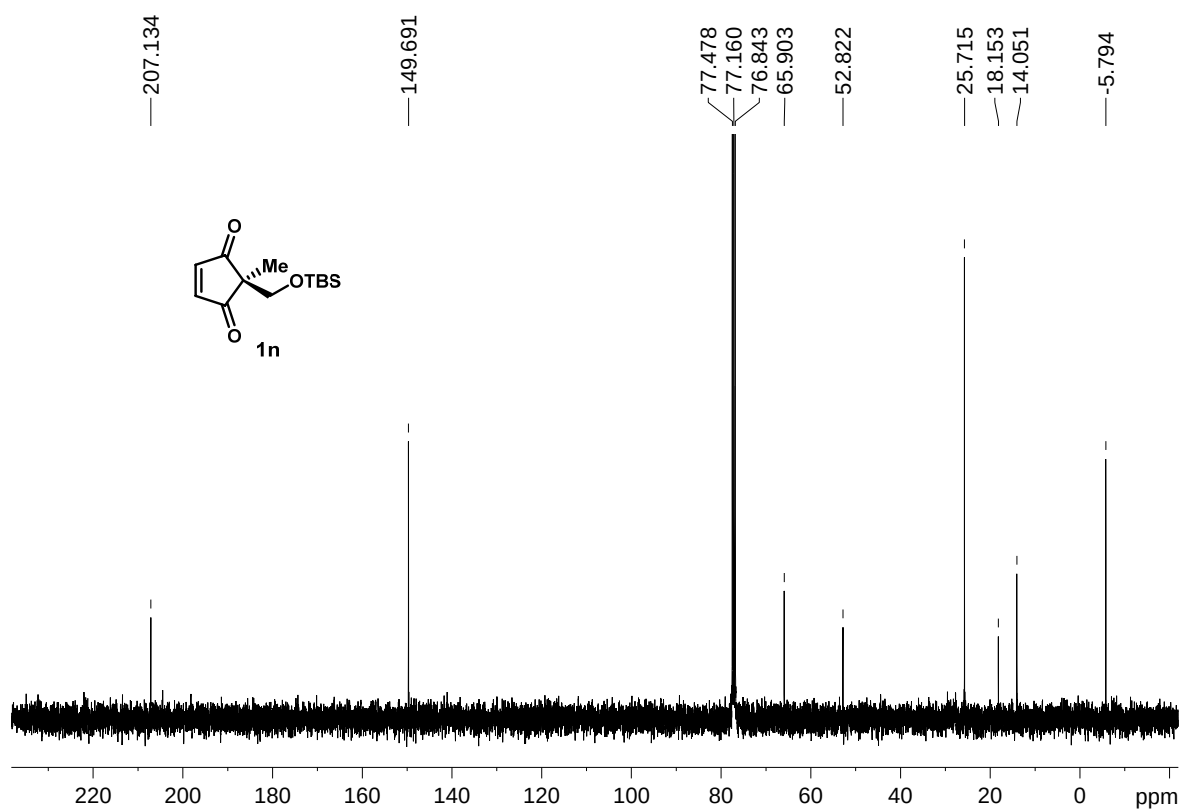
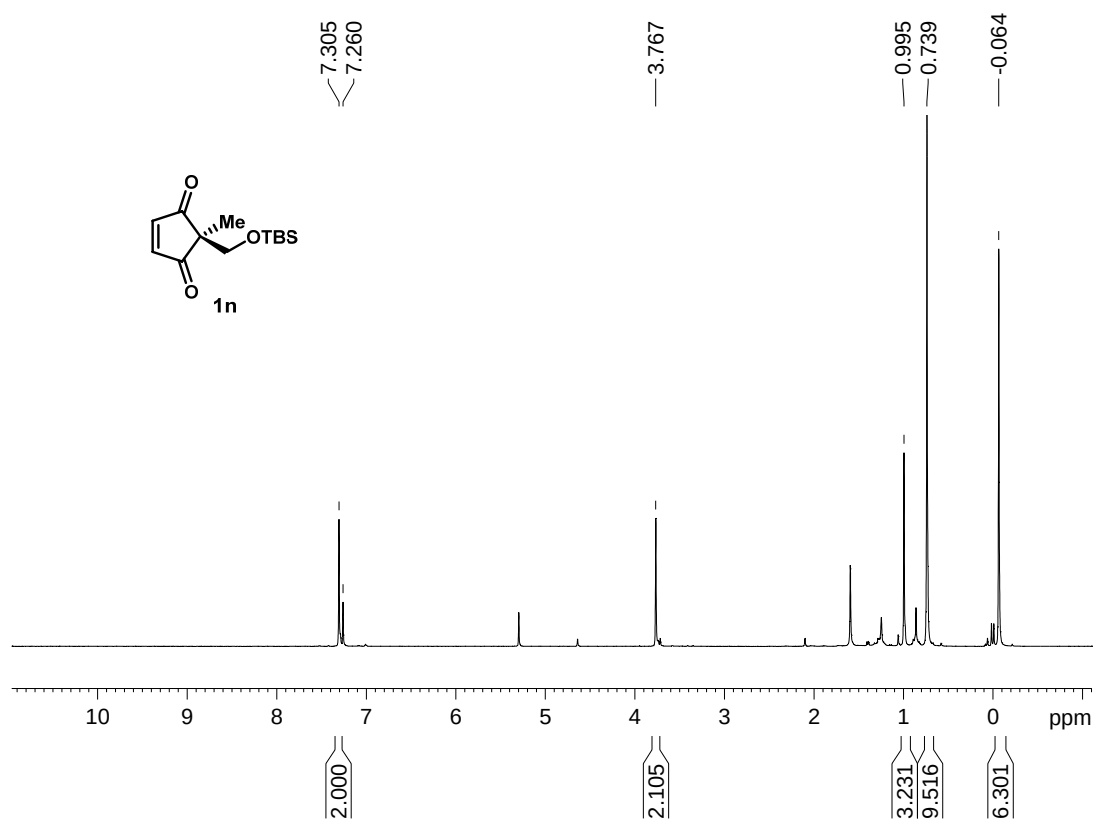


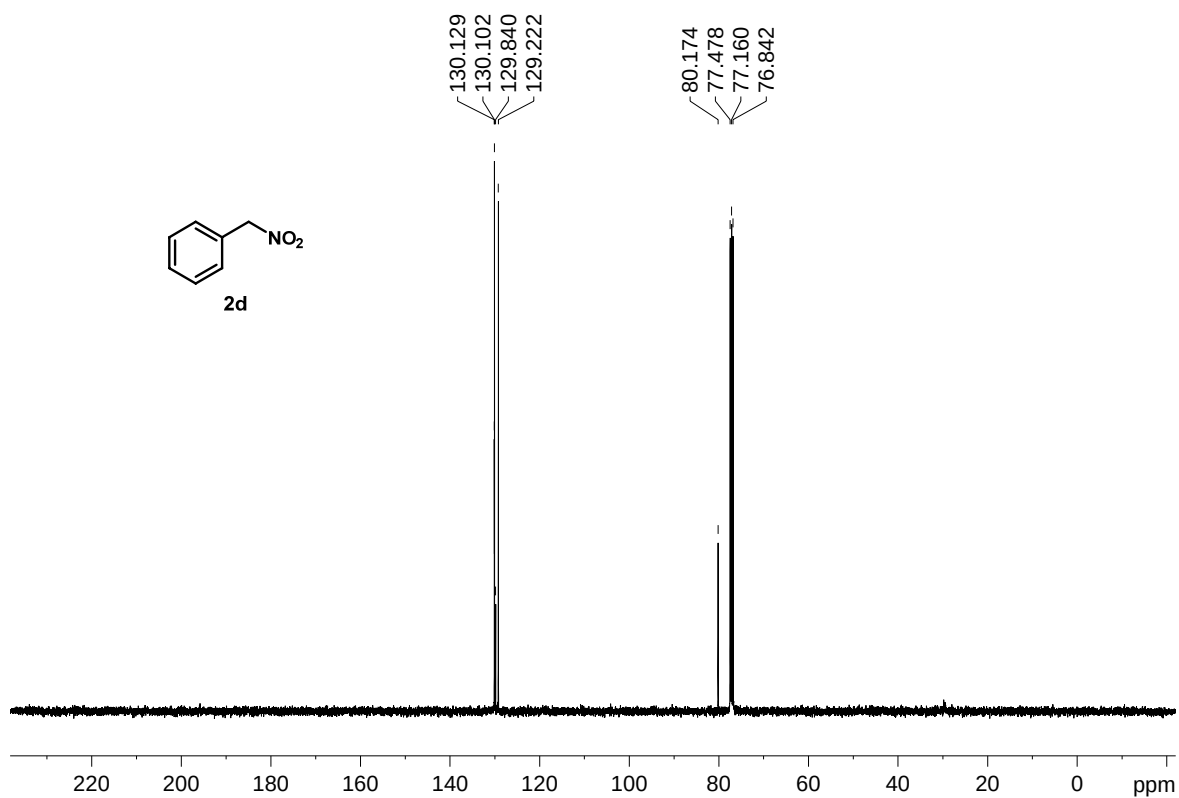
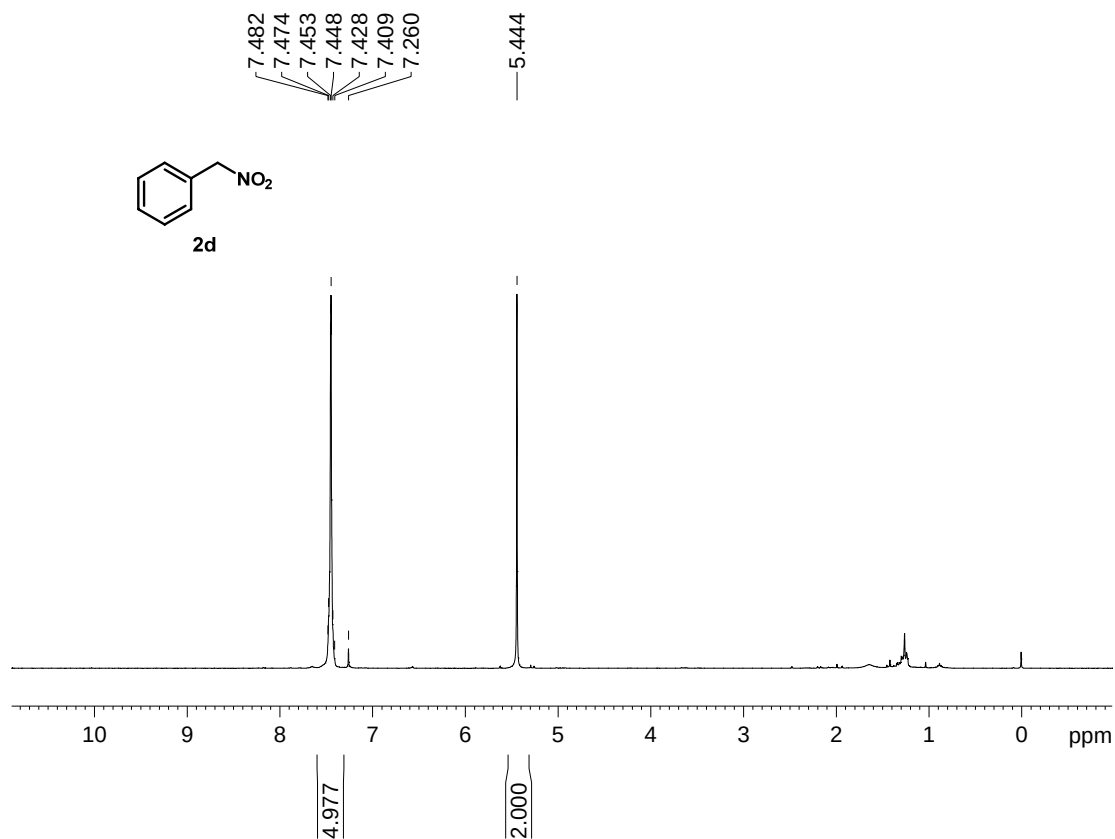


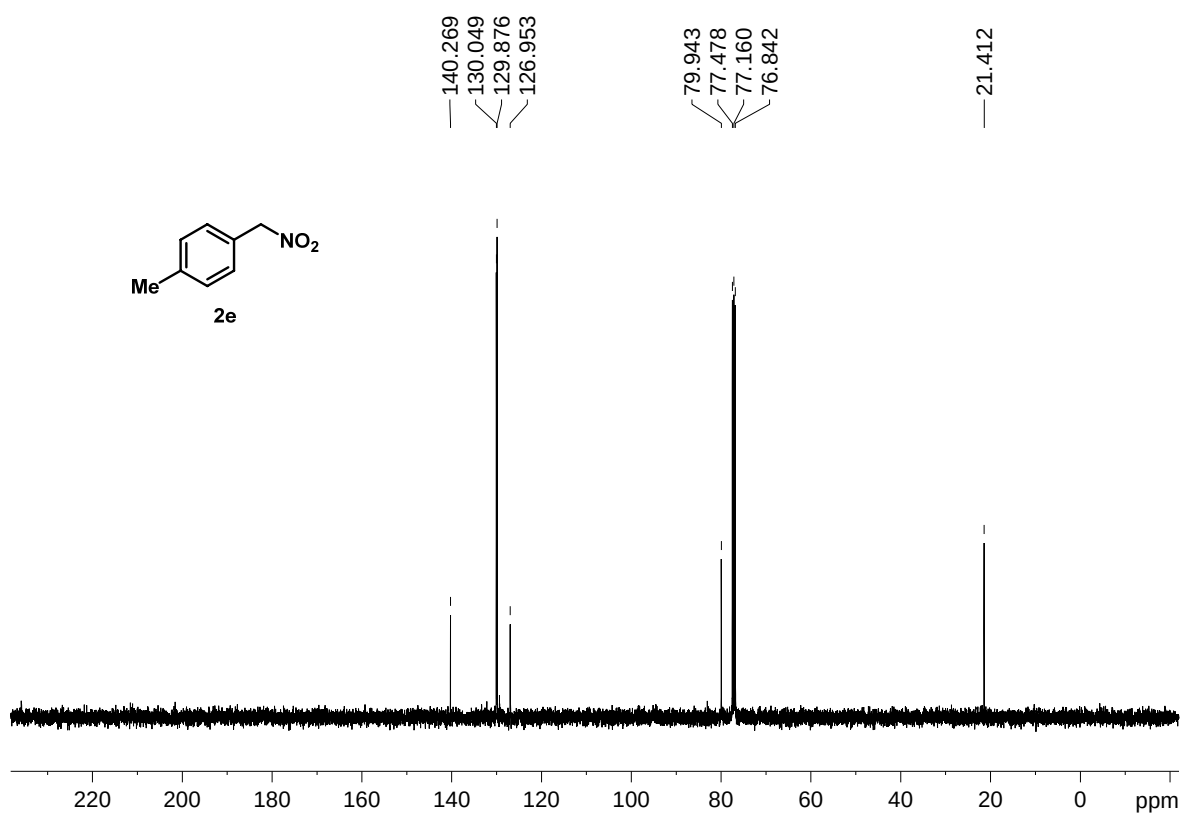
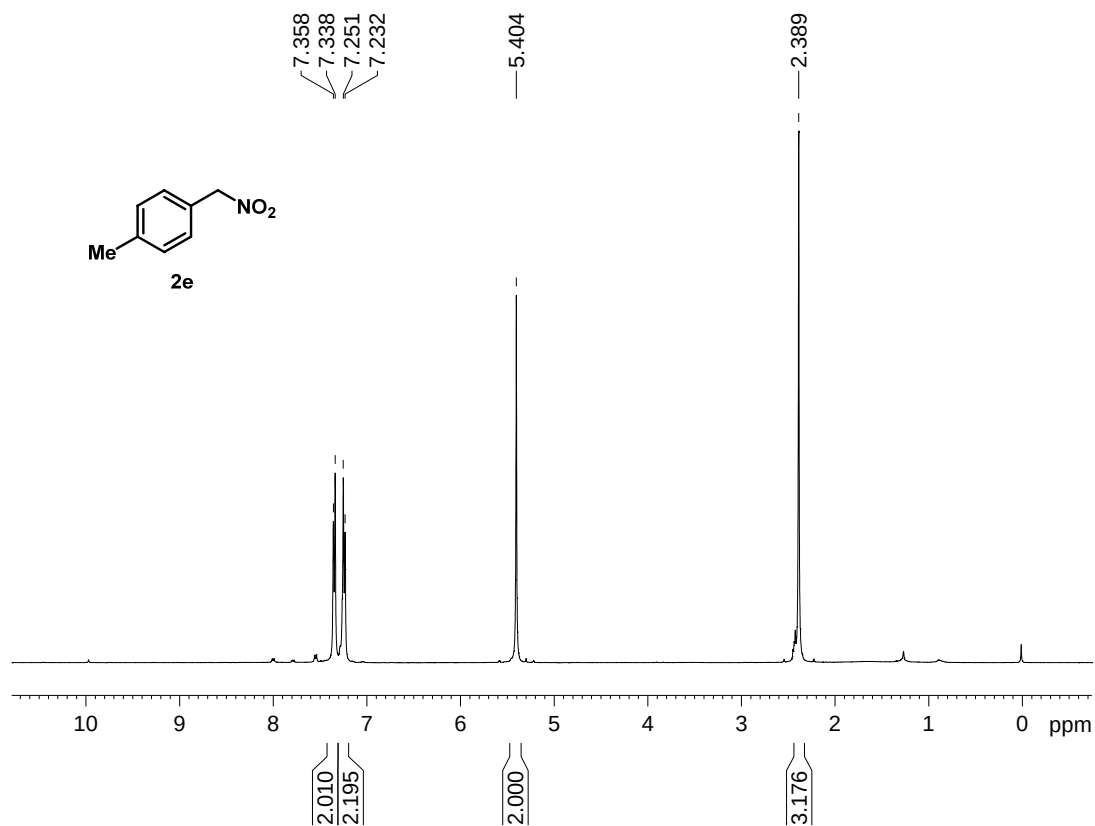


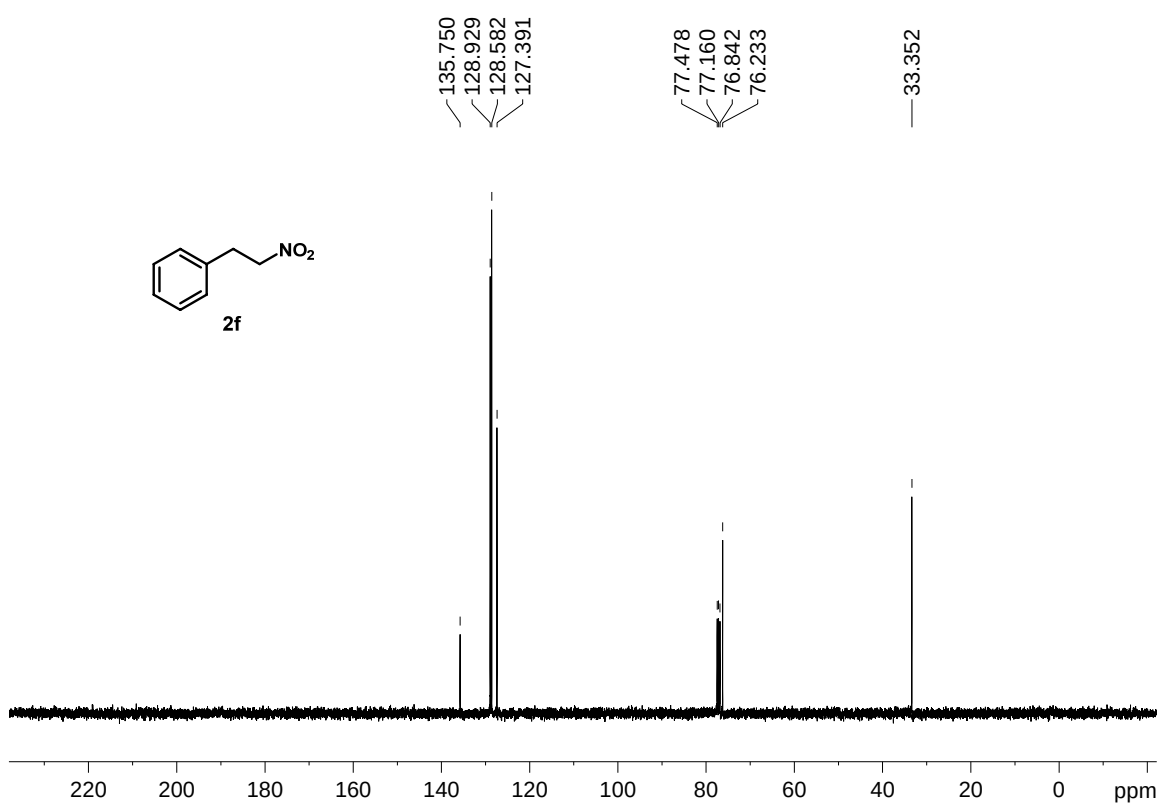
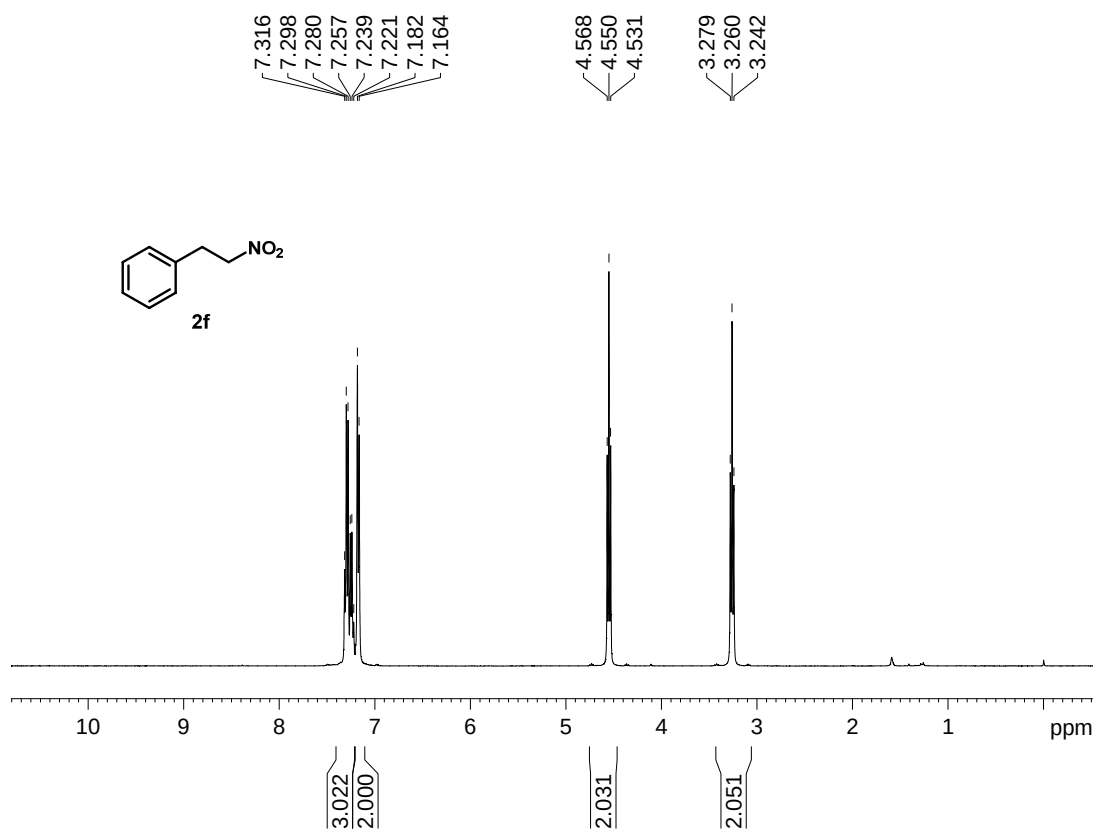


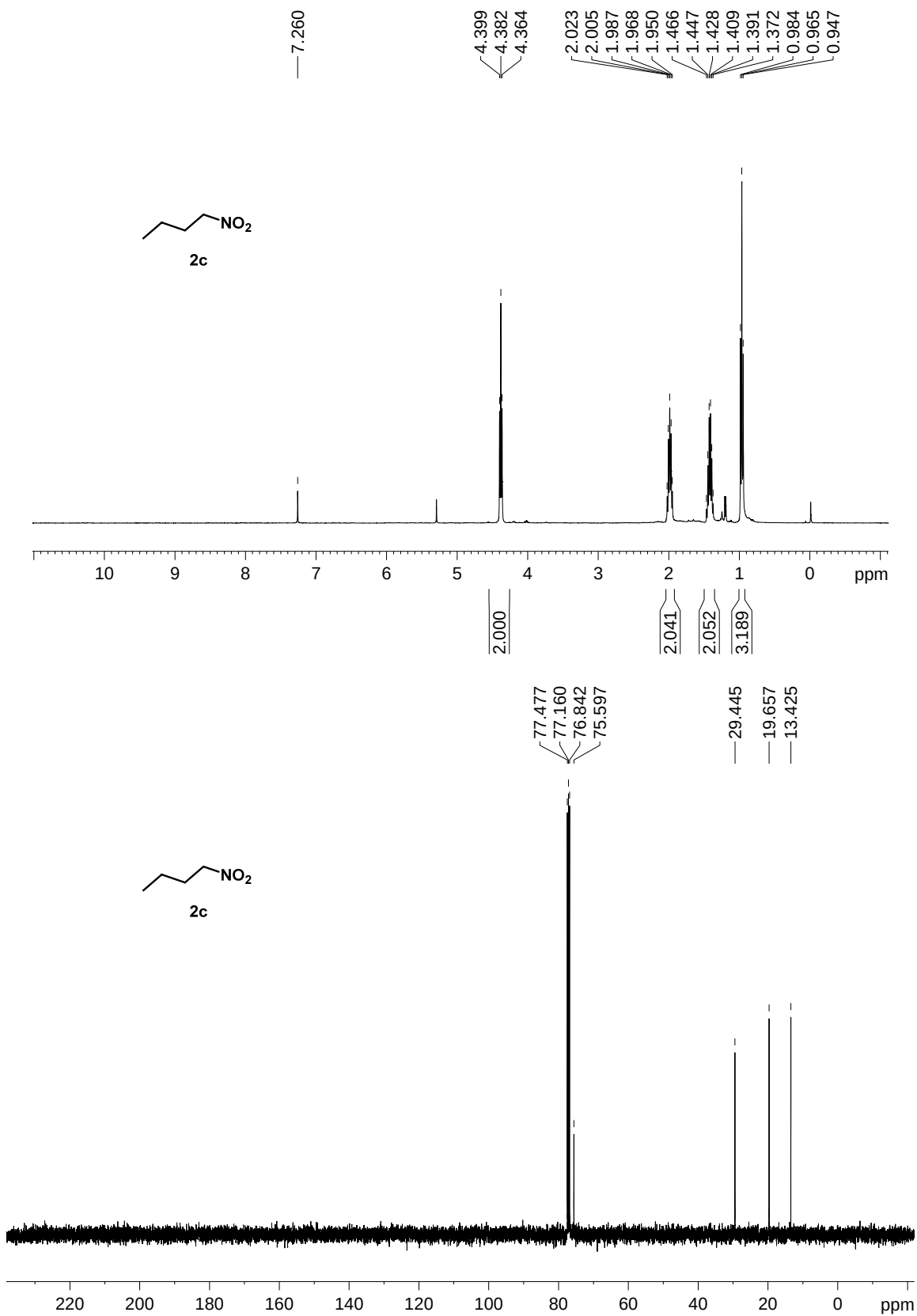


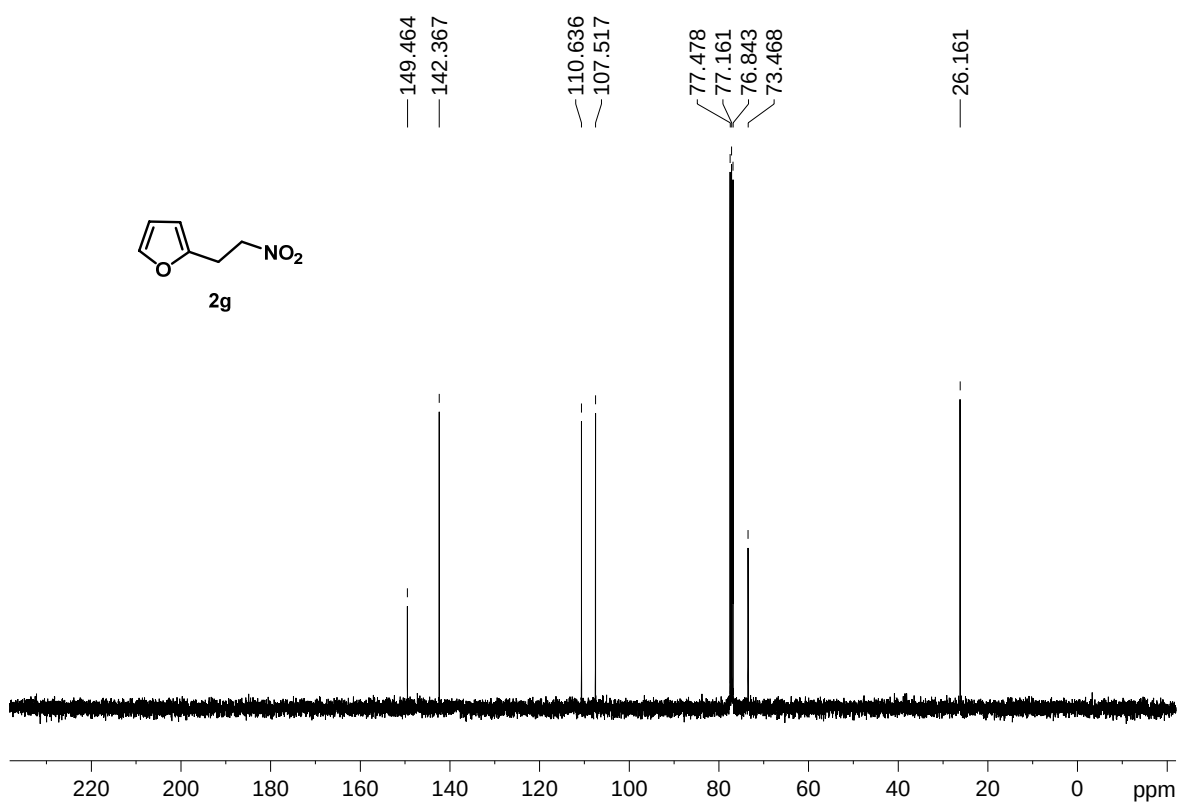
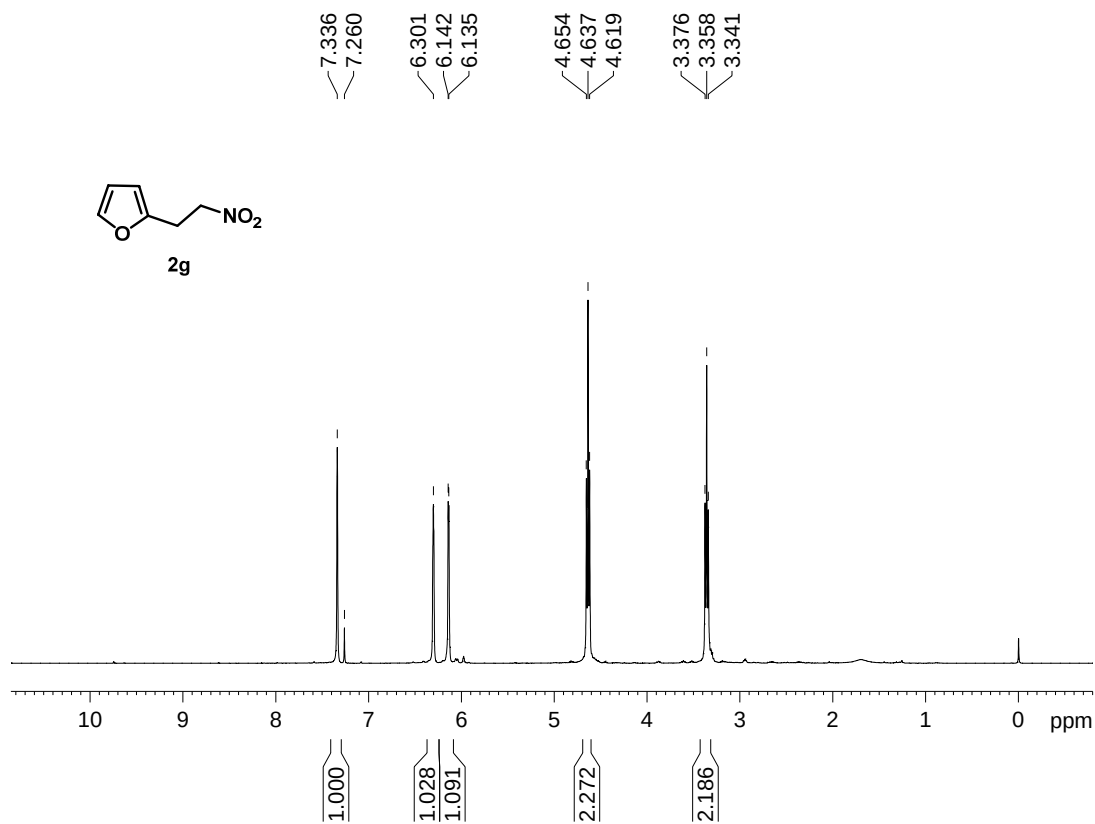


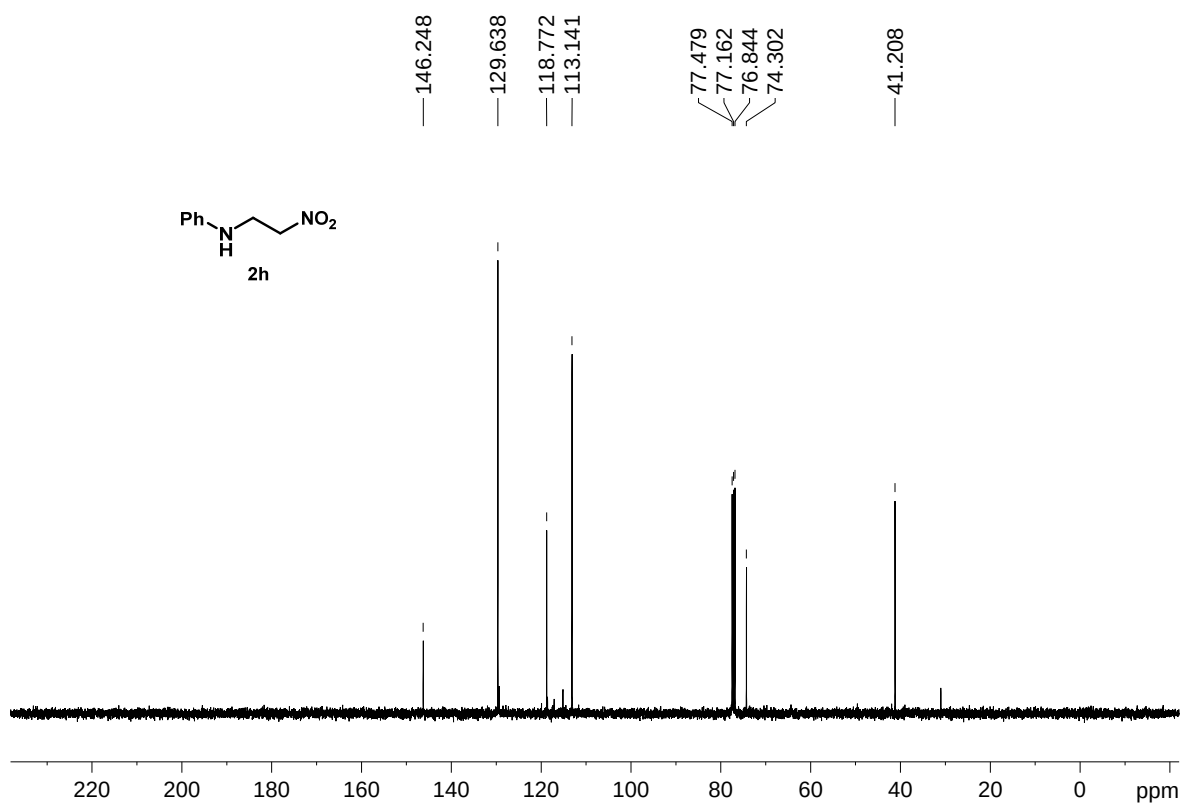
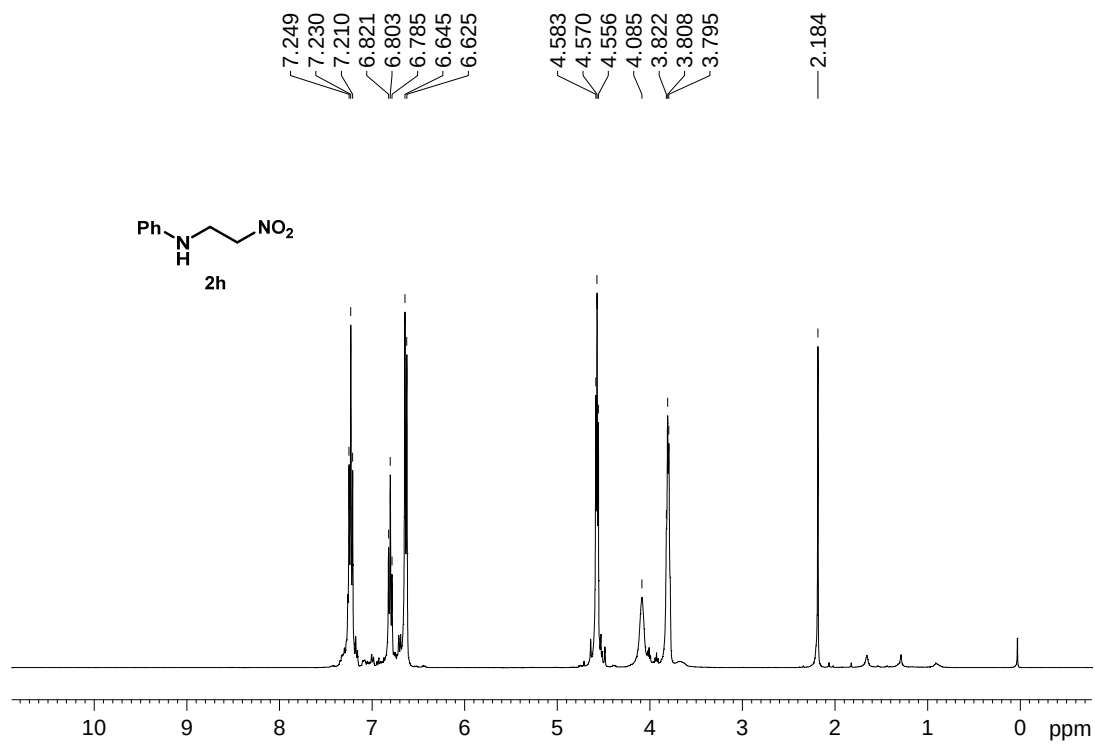


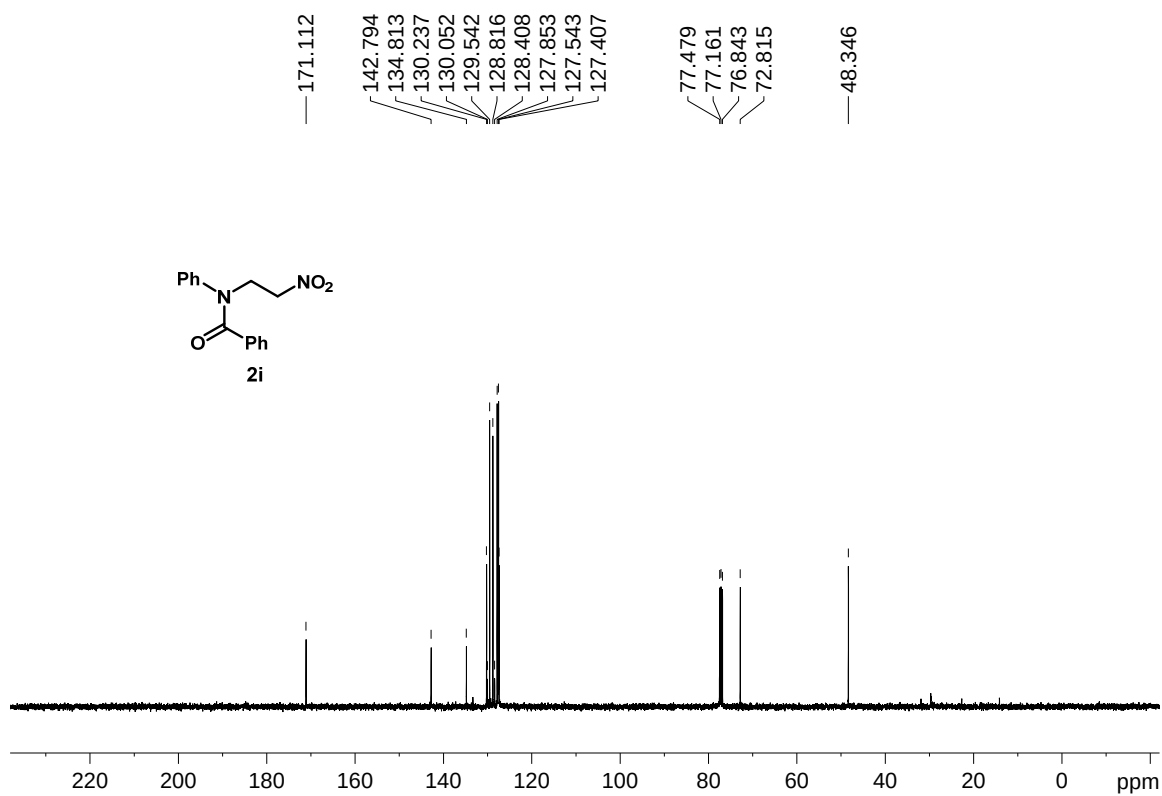
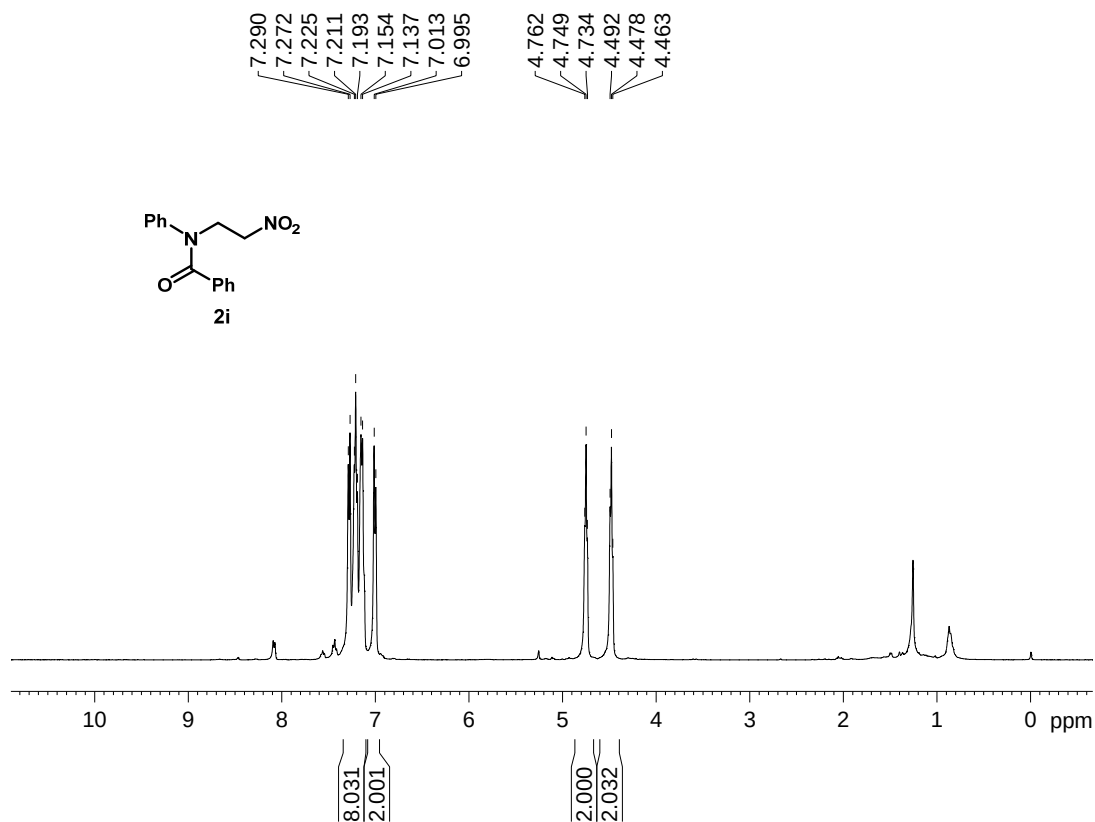


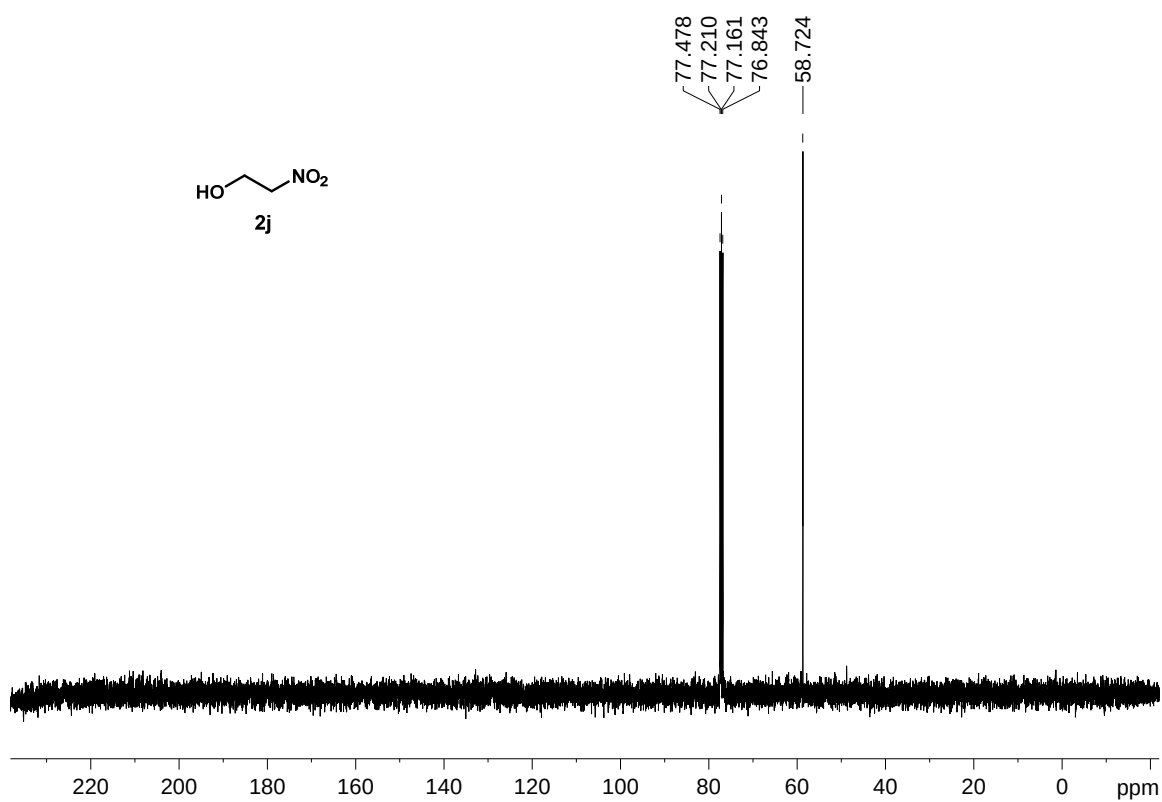
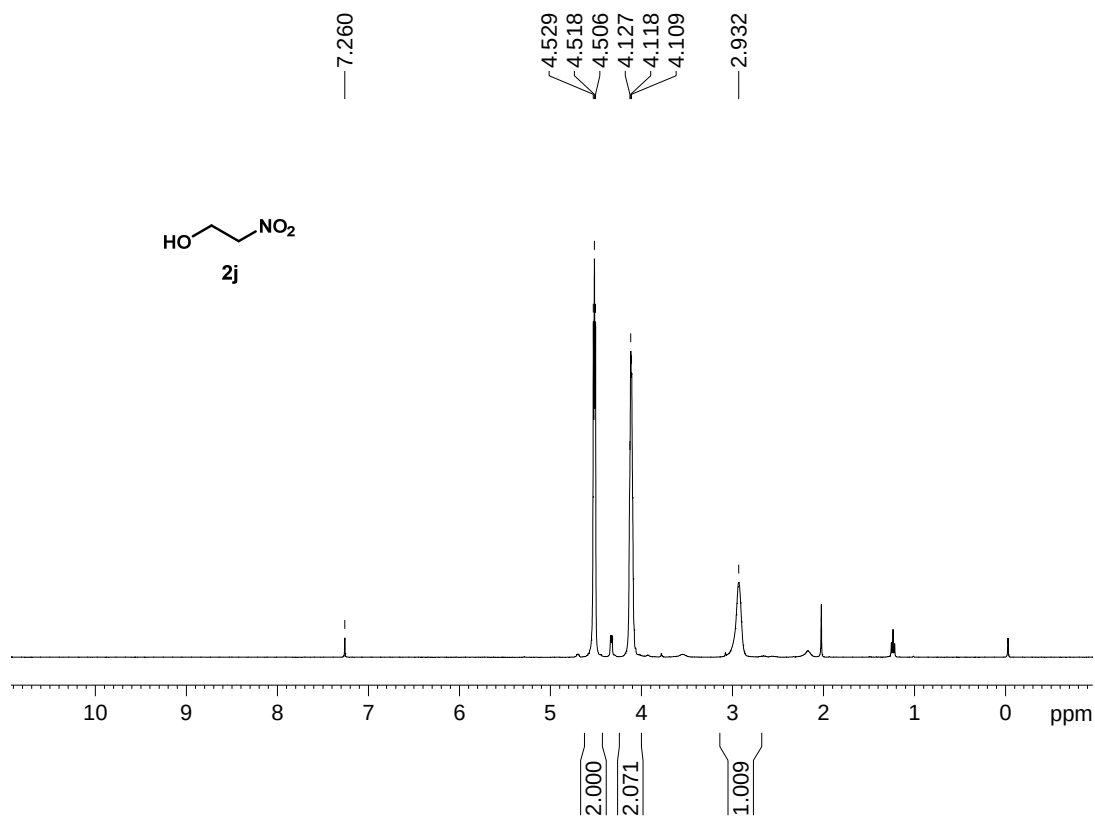


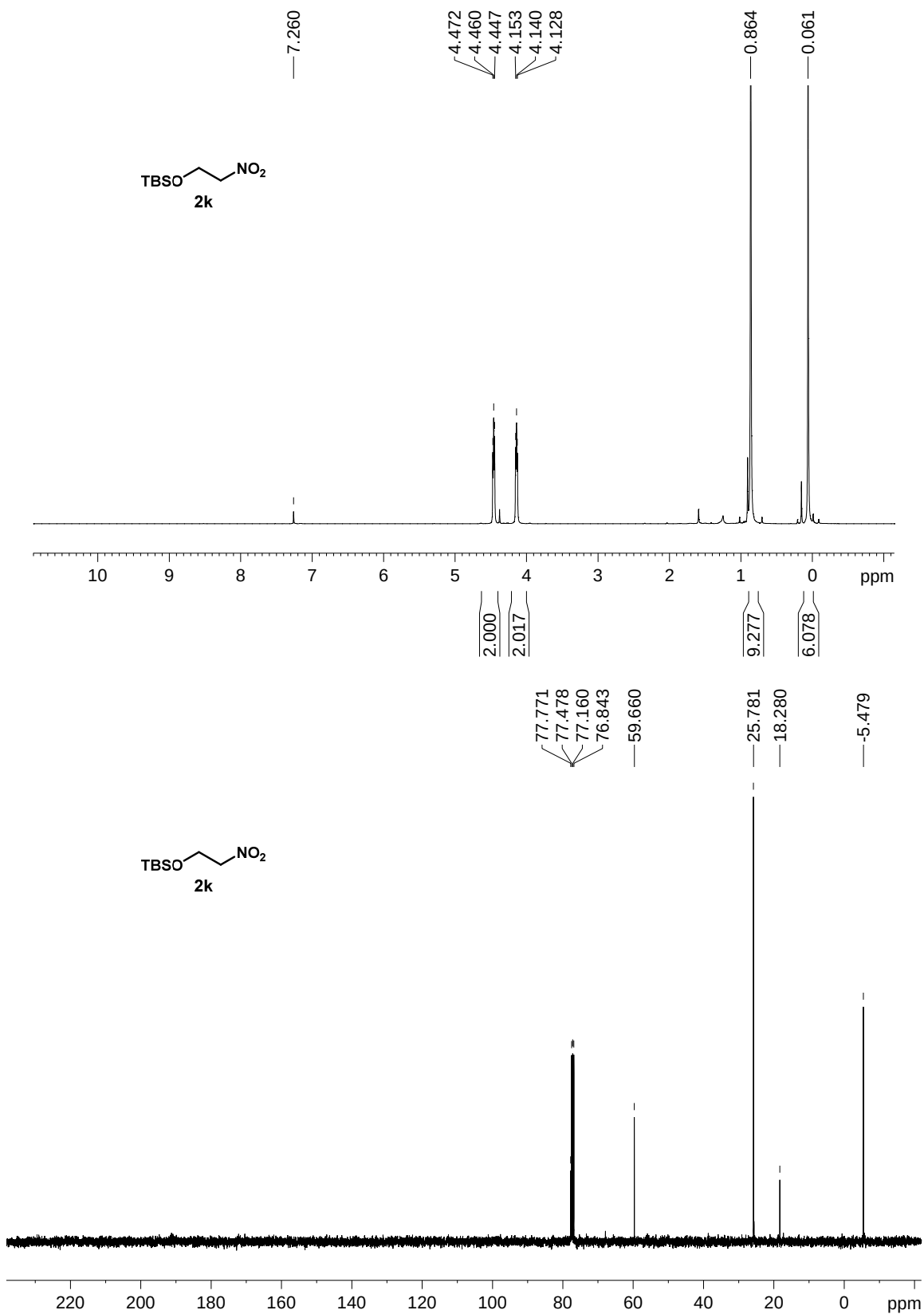


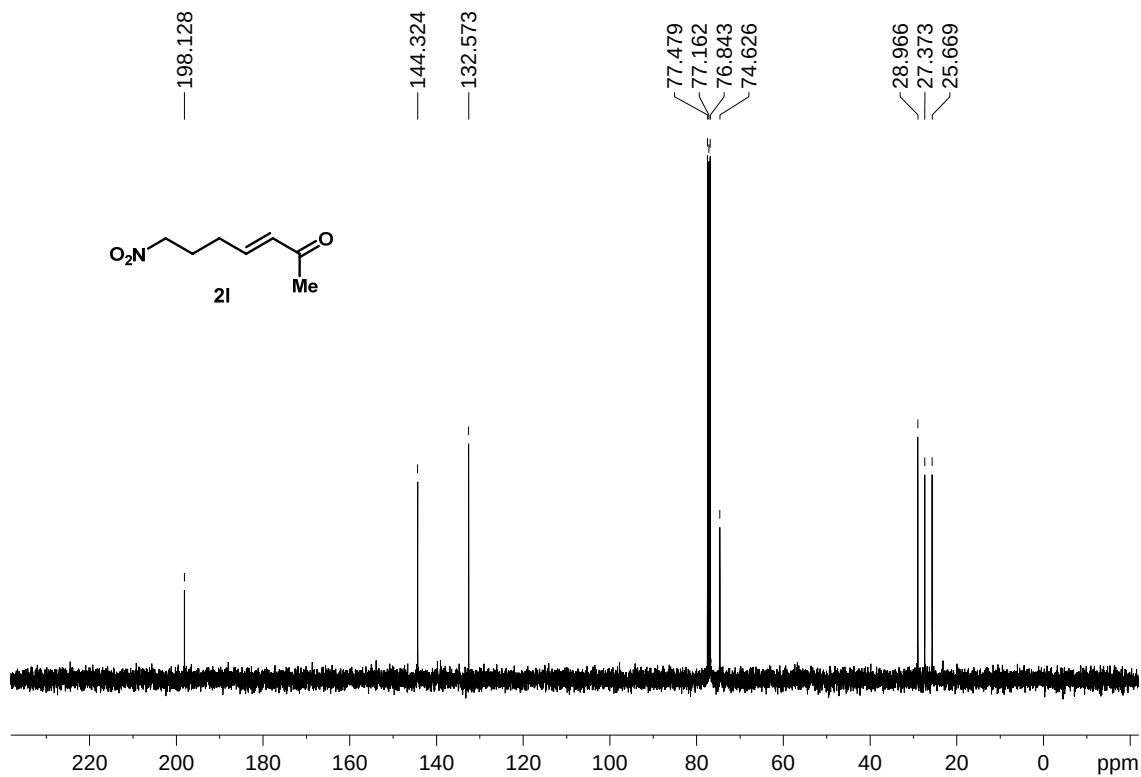
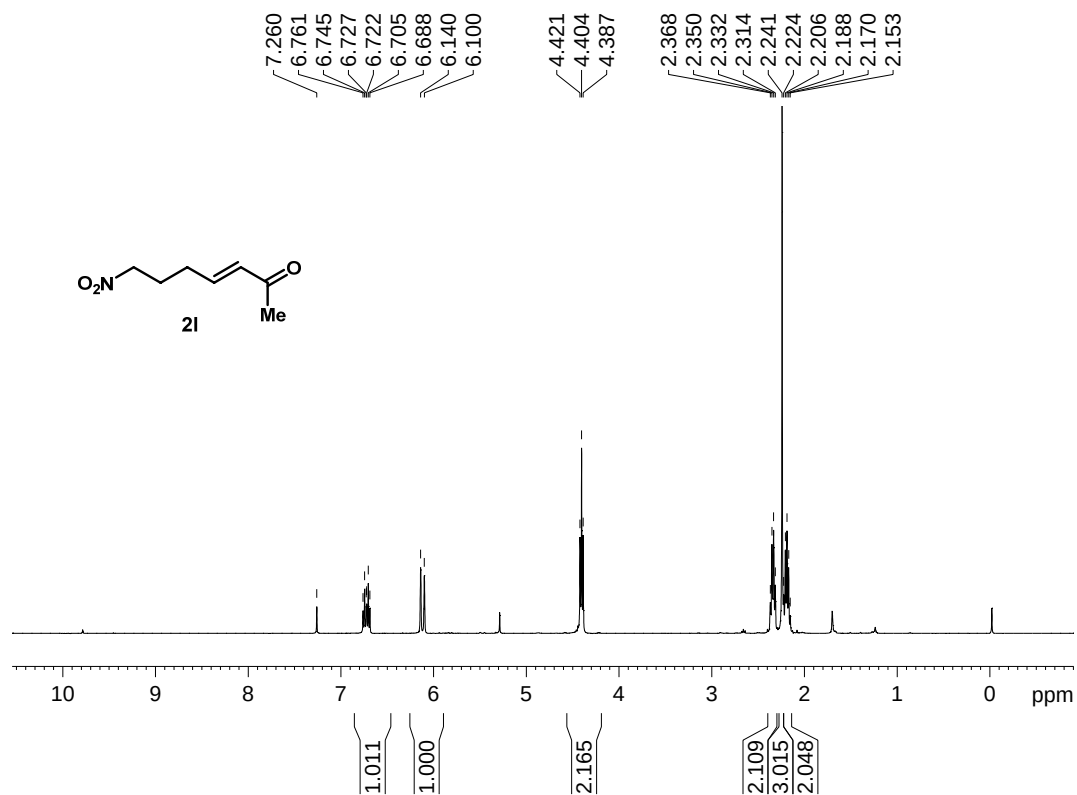


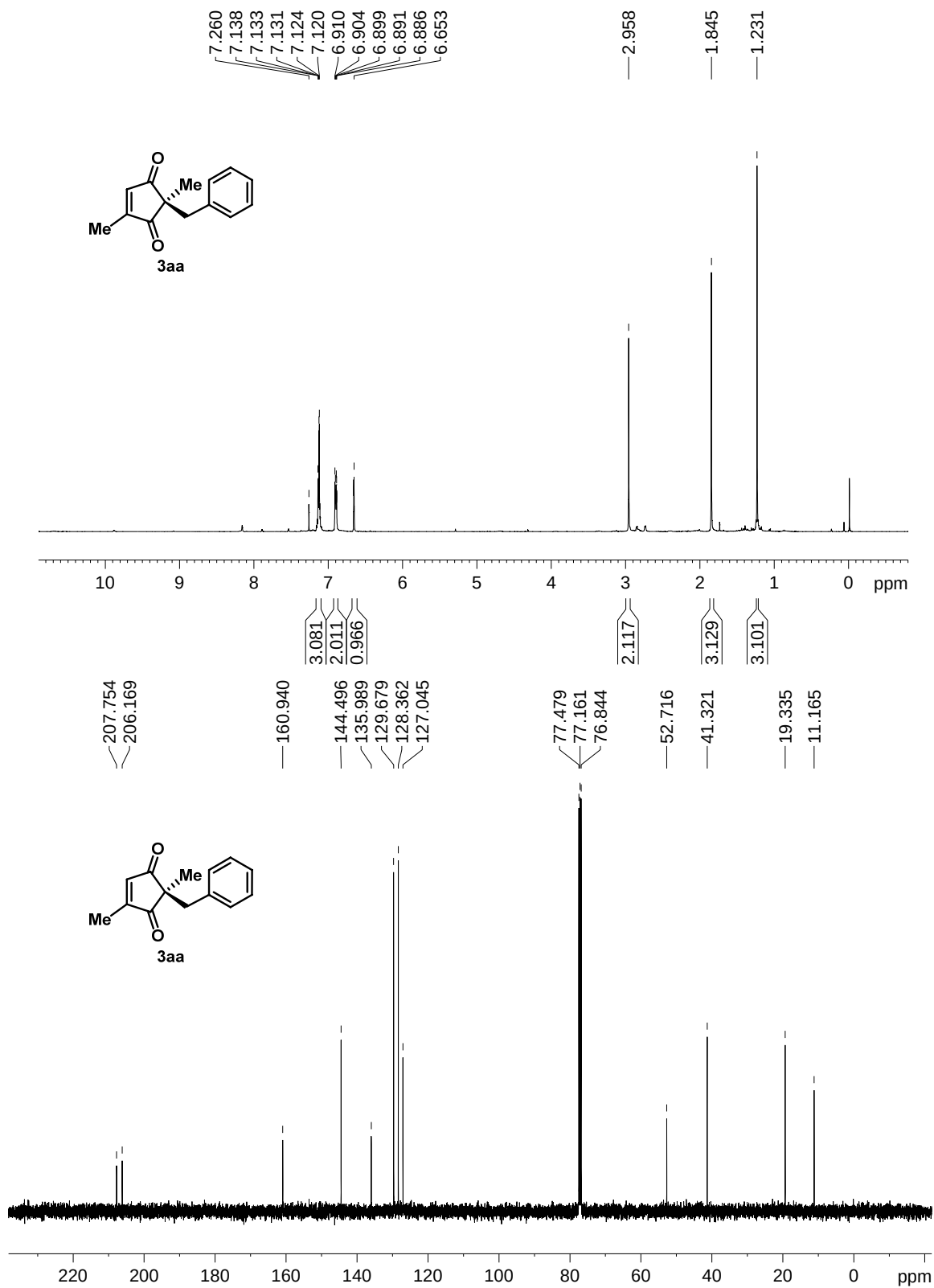


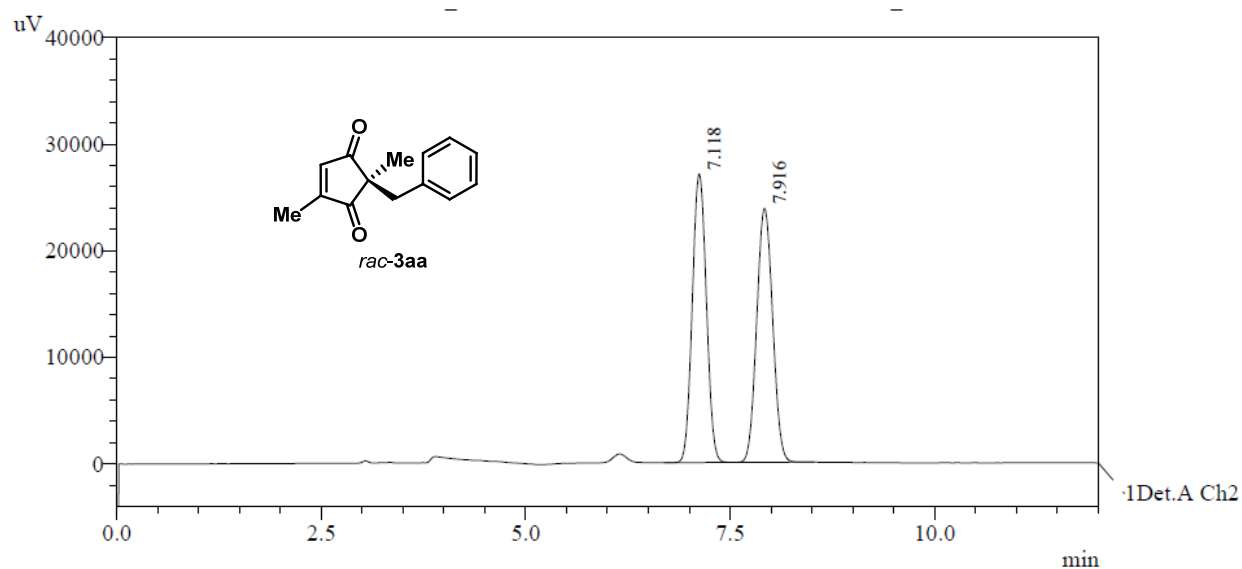








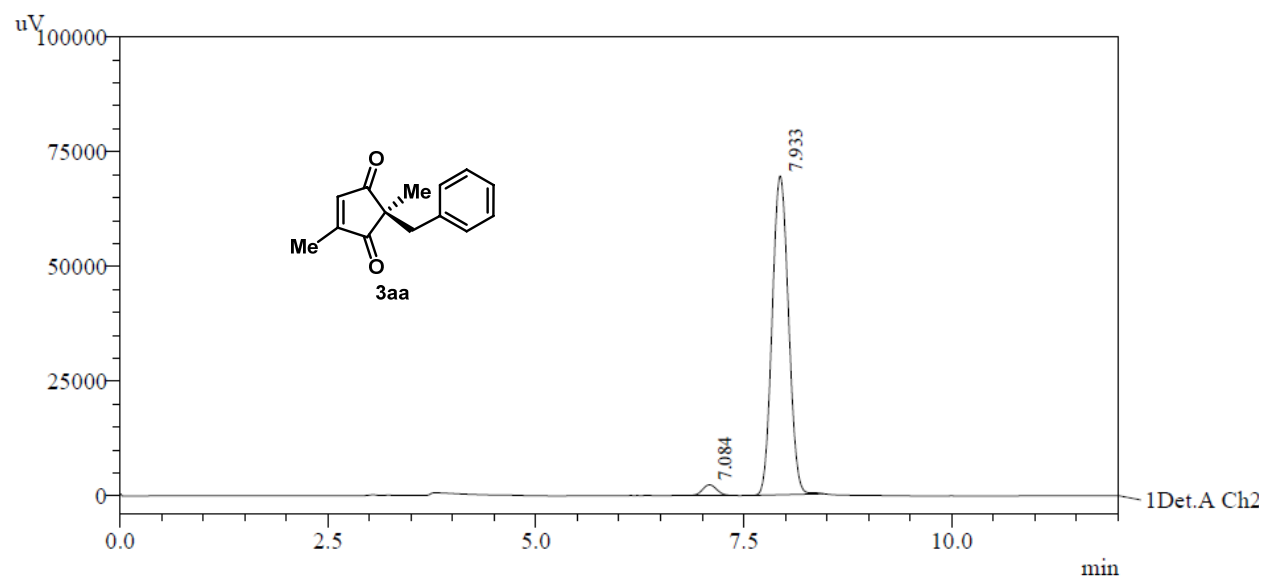




PeakTable

Detector A Ch2 254nm

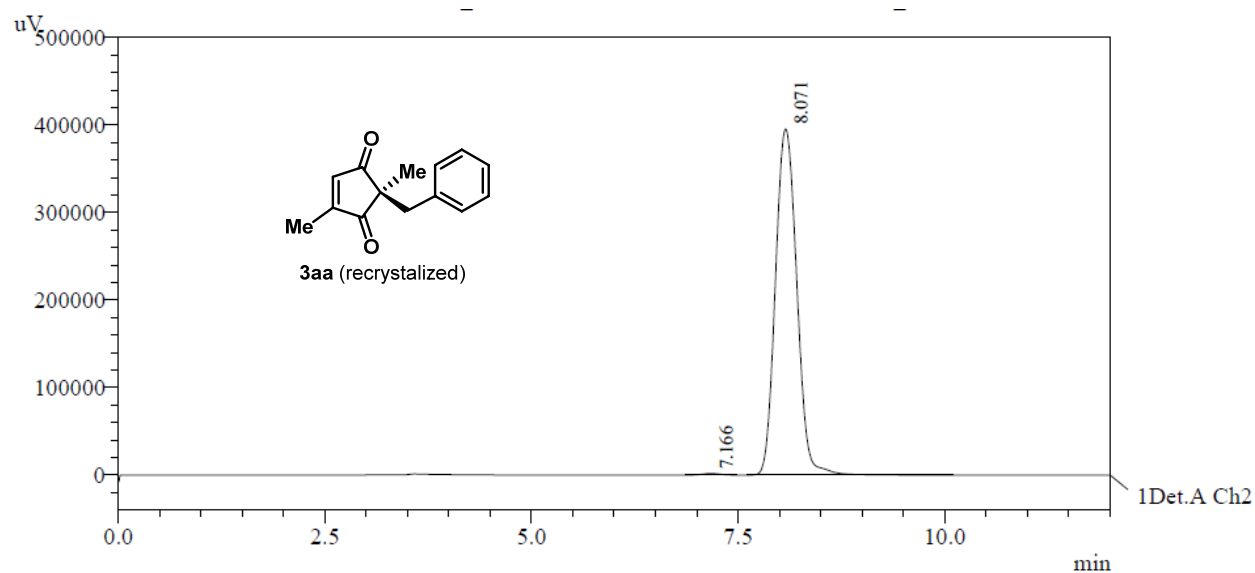
Peak#	Ret. Time	Area	Area %
1	7.118	323603	50.004
2	7.916	323549	49.996
Total		647152	100.000



PeakTable

Detector A Ch2 254nm

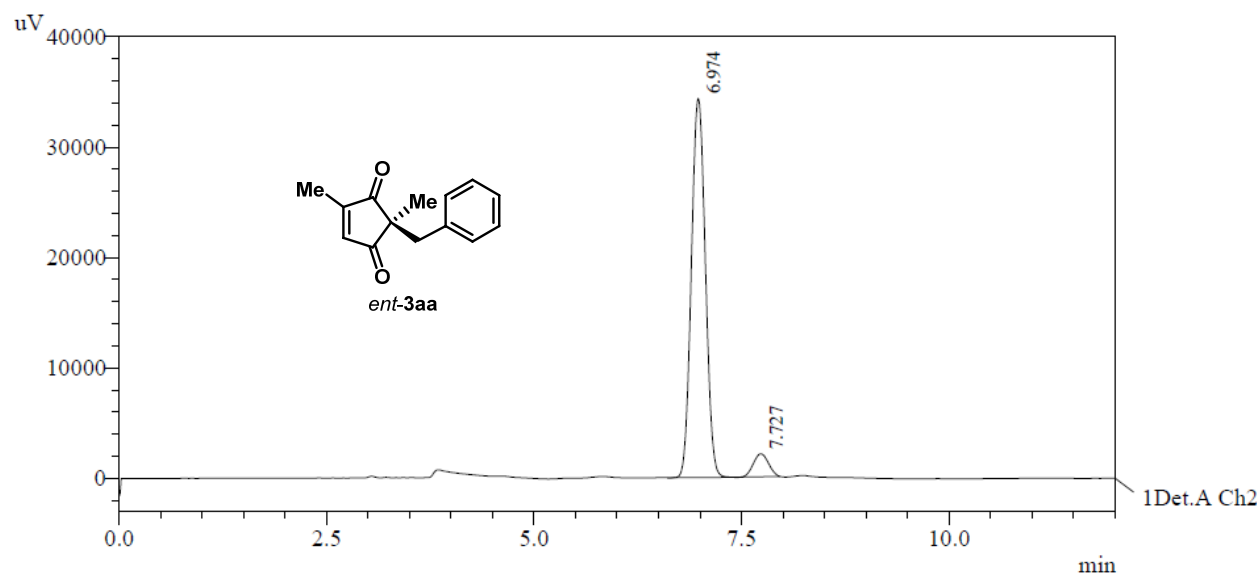
Peak#	Ret. Time	Area	Area %
1	7.084	27564	2.824
2	7.933	948595	97.176
Total		976158	100.000



PeakTable

Detector A Ch2 254nm

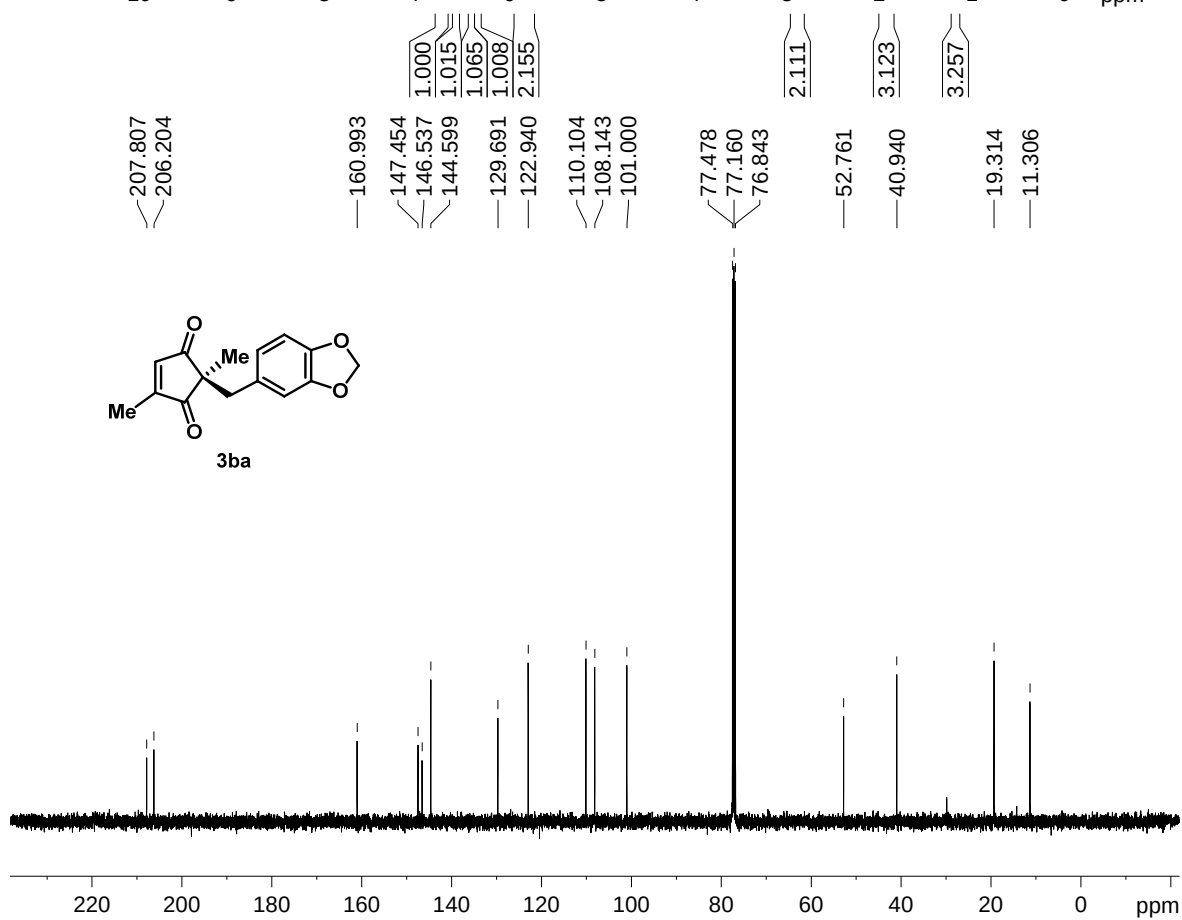
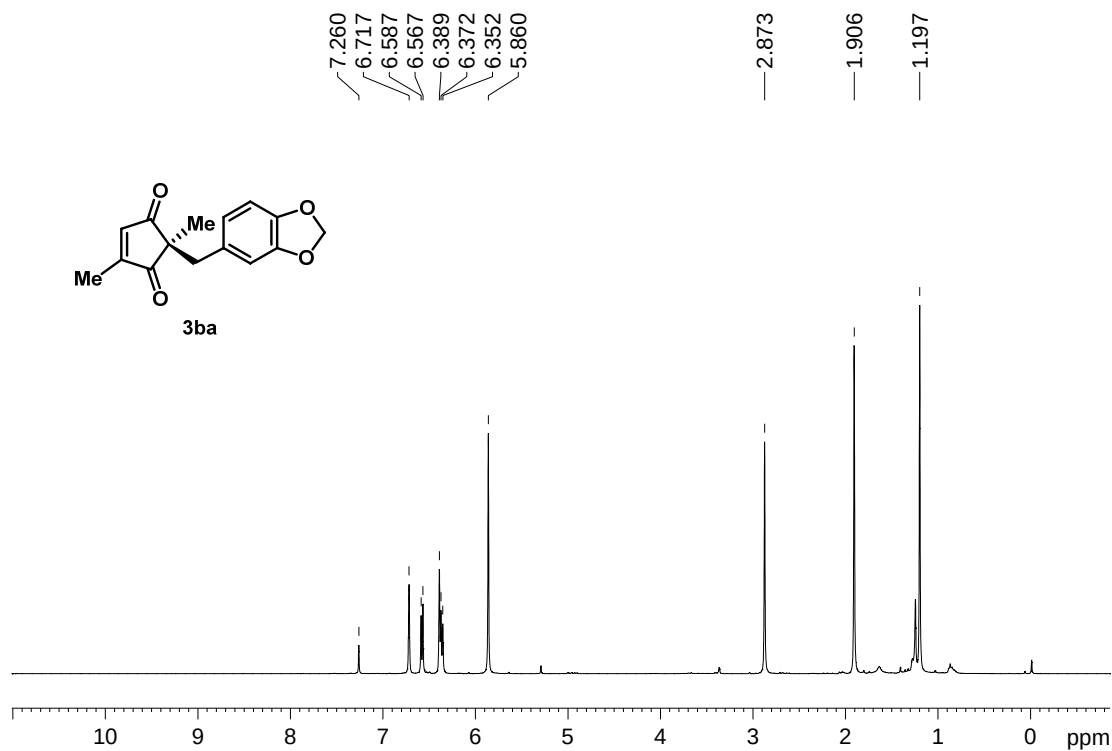
Peak#	Ret. Time	Area	Area %
1	7.166	25203	0.353
2	8.071	7118874	99.647
Total		7144078	100.000

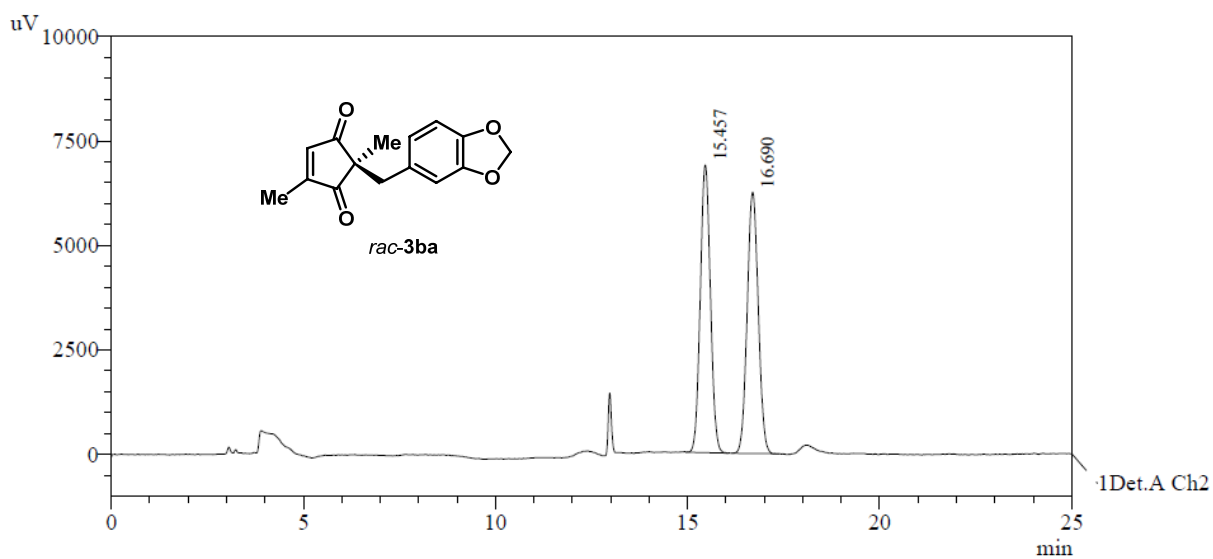


PeakTable

Detector A Ch2 254nm

Peak#	Ret. Time	Area	Area %
1	6.974	402797	93.803
2	7.727	26610	6.197
Total		429406	100.000

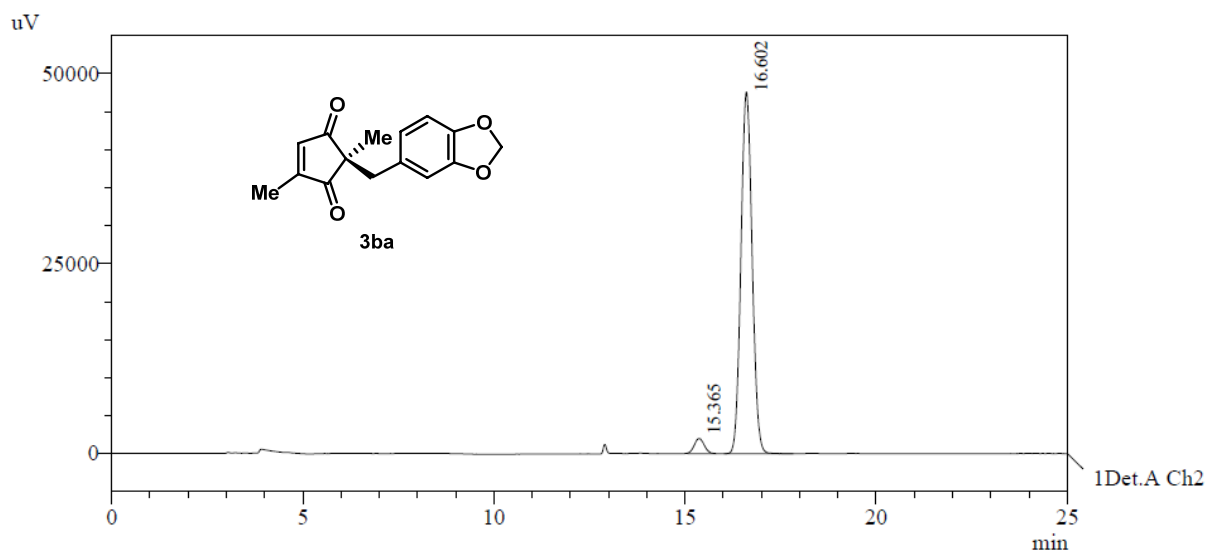




PeakTable

Detector A Ch2 254nm

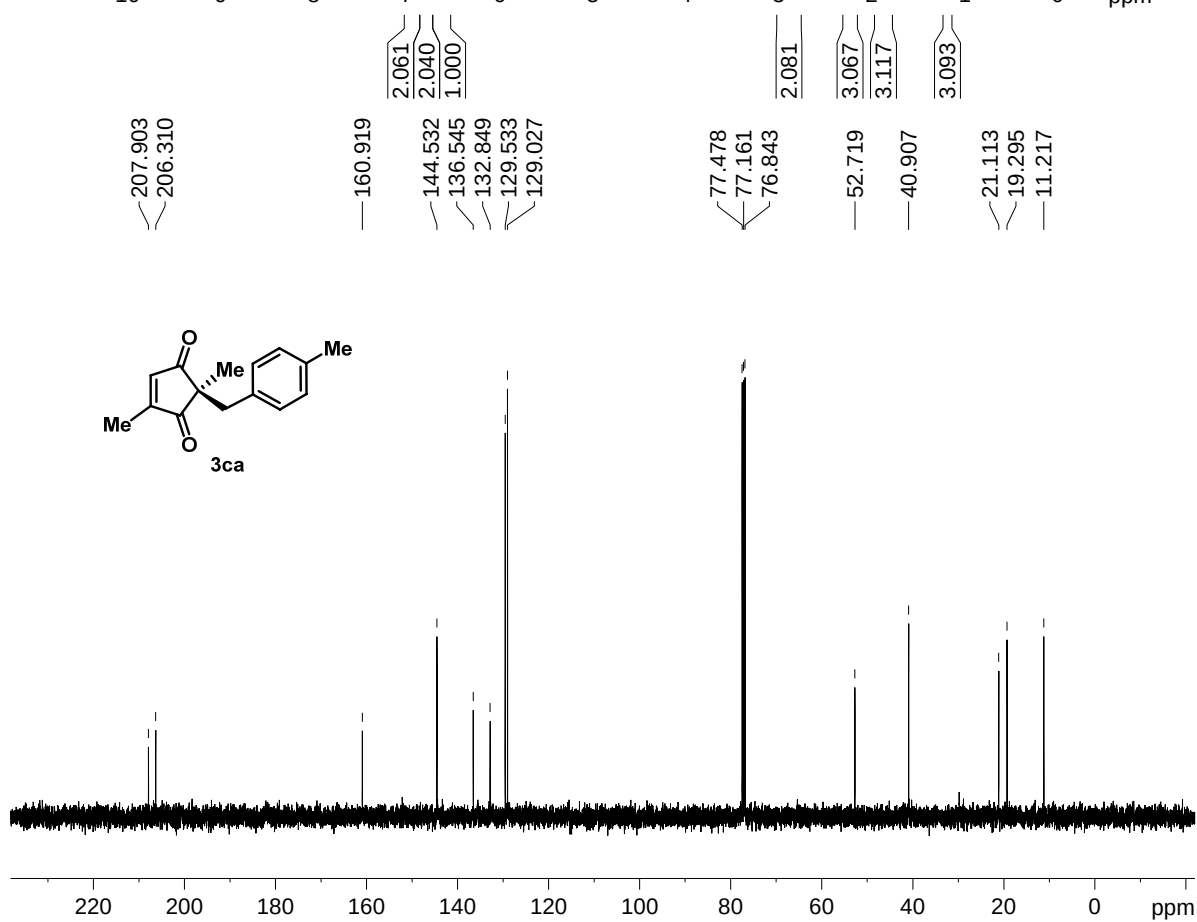
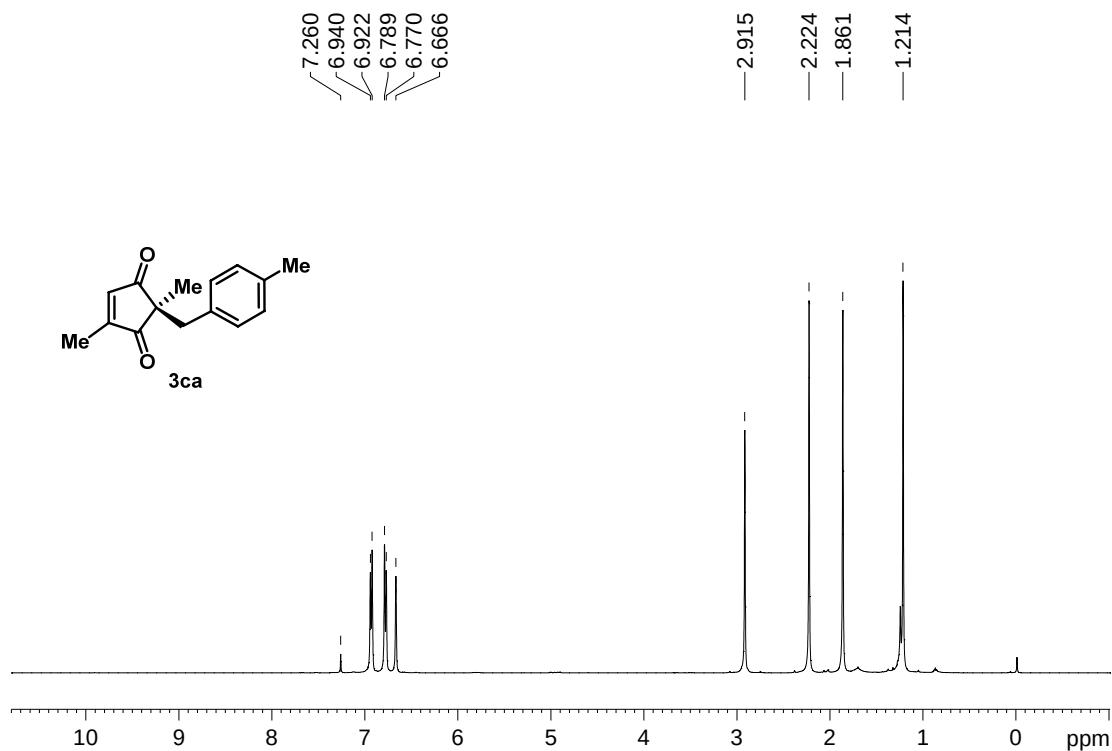
Peak#	Ret. Time	Area	Area %
1	15.457	126065	50.082
2	16.690	125654	49.918
Total		251719	100.000

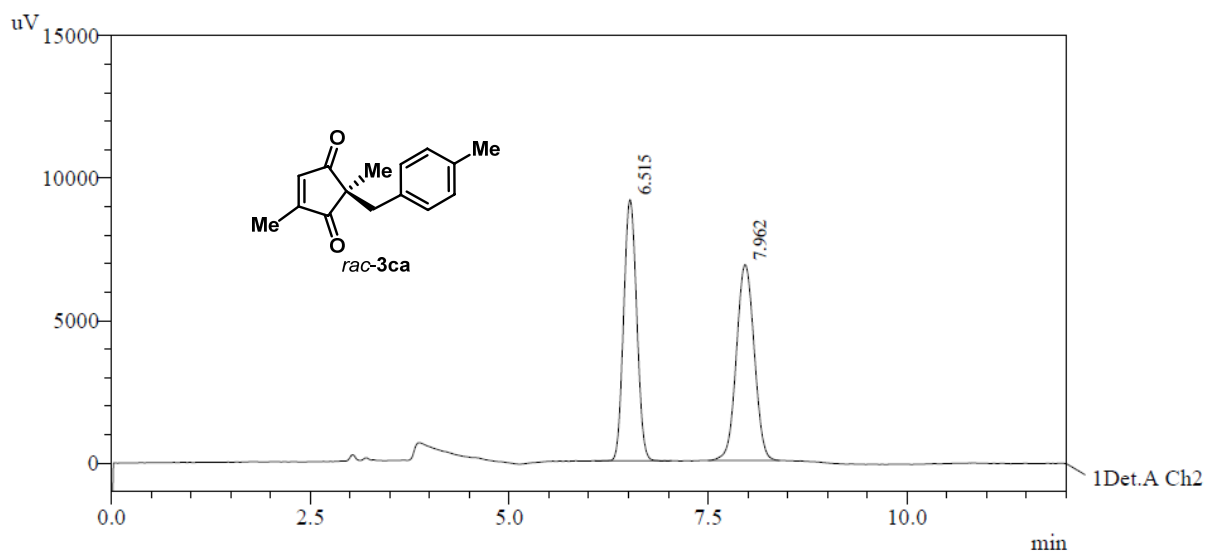


PeakTable

Detector A Ch2 254nm

Peak#	Ret. Time	Area	Area %
1	15.365	36290	3.604
2	16.602	970737	96.396
Total		1007028	100.000

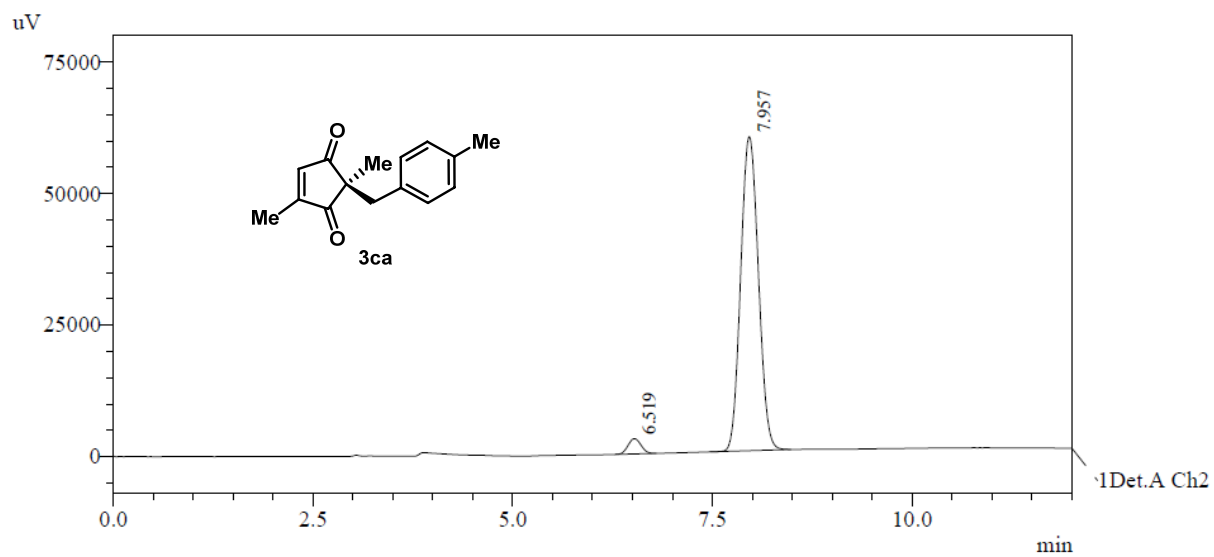




PeakTable

Detector A Ch2 254nm

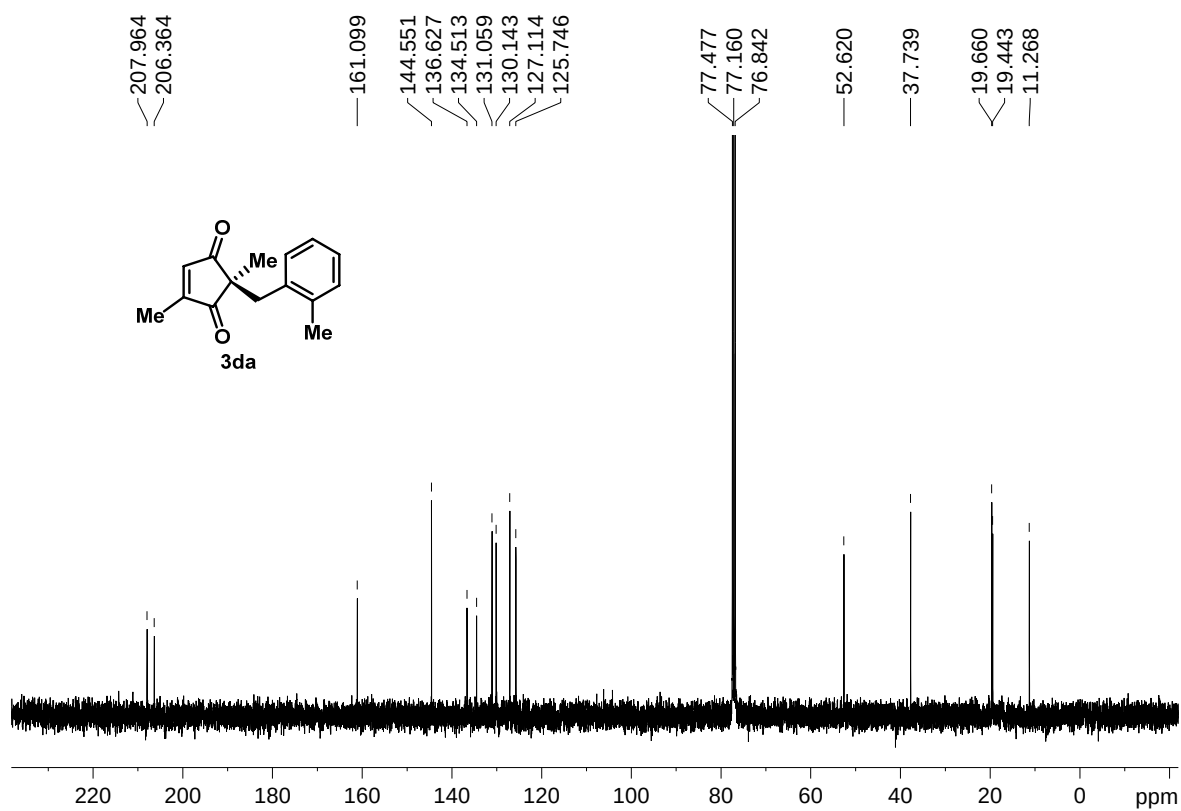
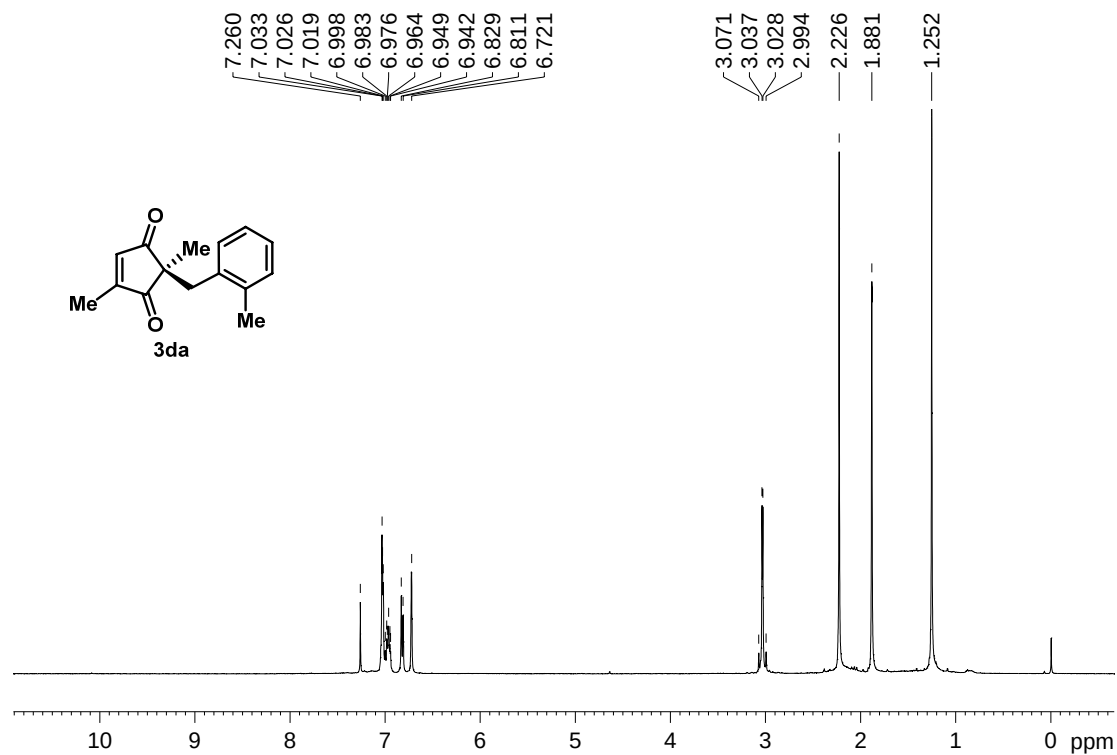
Peak#	Ret. Time	Area	Area %
1	6.515	104434	49.266
2	7.962	107546	50.734
Total		211980	100.000

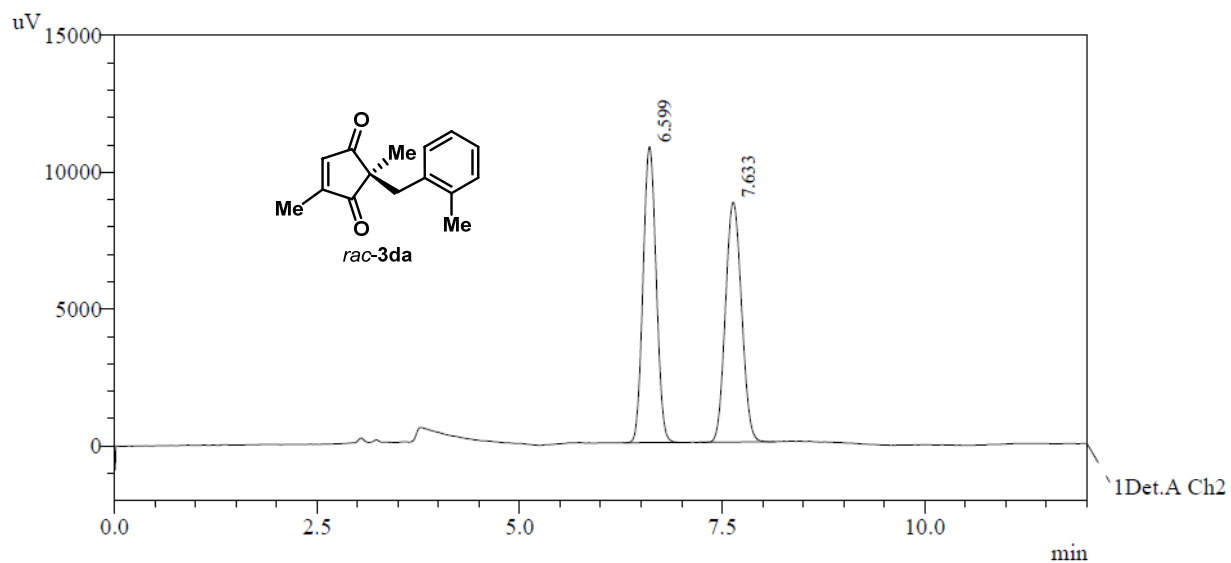


PeakTable

Detector A Ch2 254nm

Peak#	Ret. Time	Area	Area %
1	6.519	32592	3.420
2	7.957	920361	96.580
Total		952953	100.000

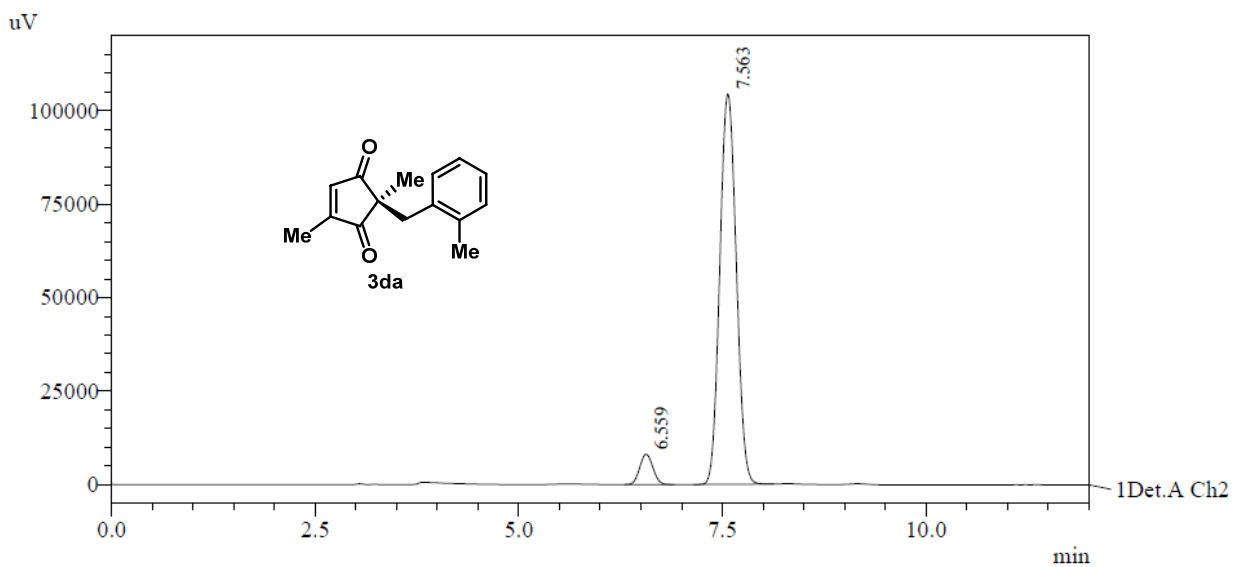




PeakTable

Detector A Ch2 254nm

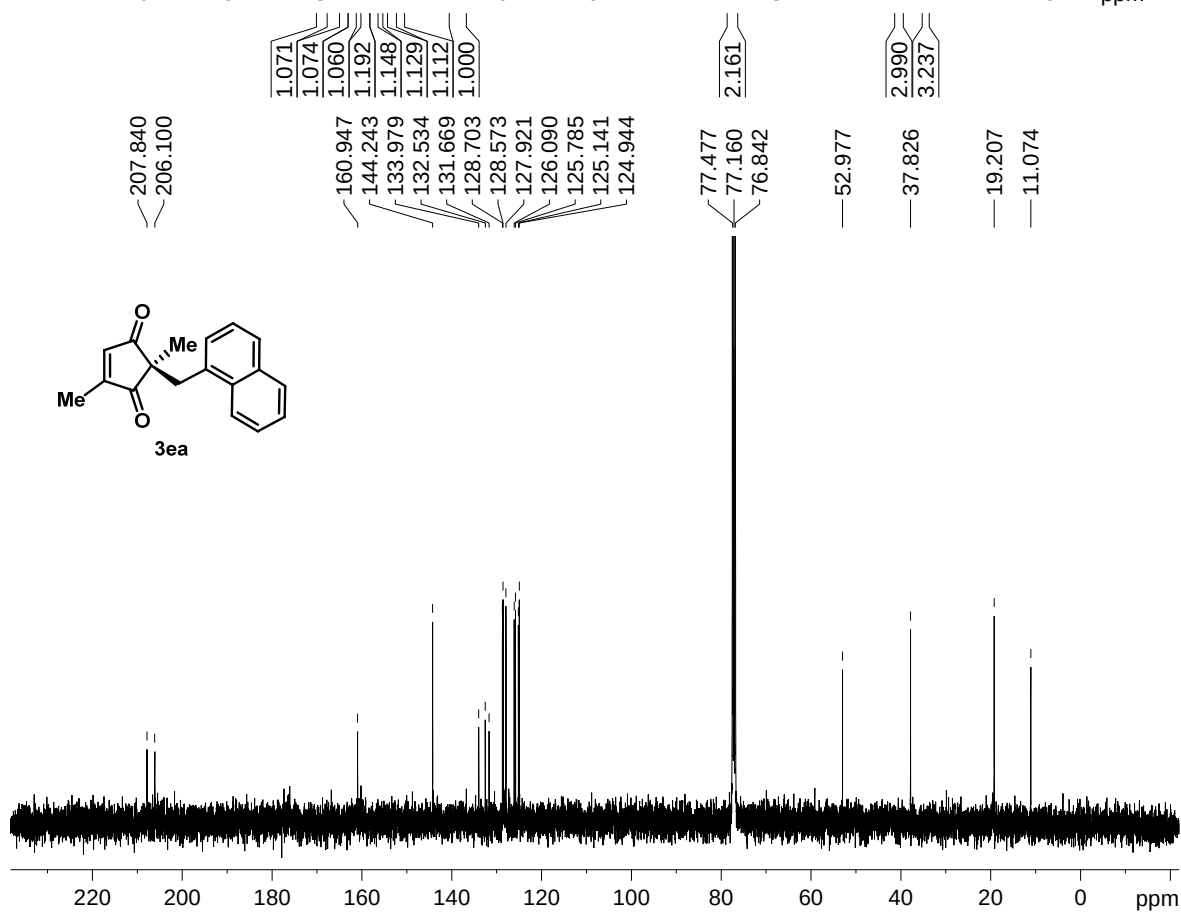
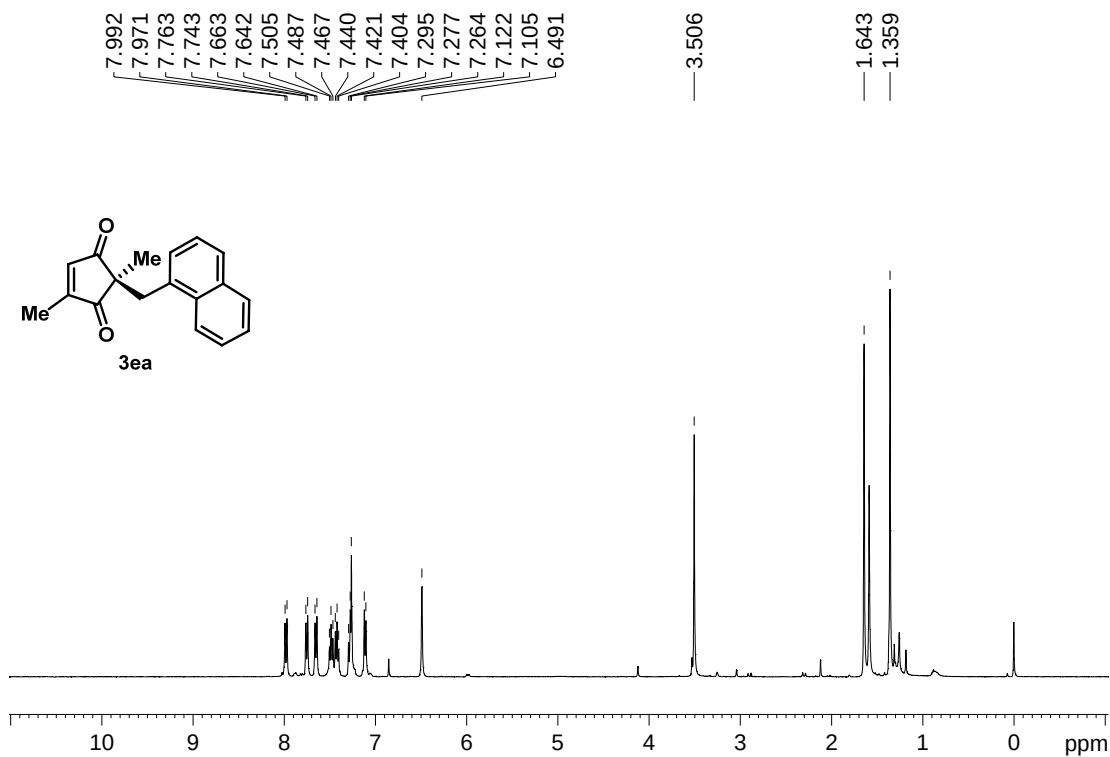
Peak#	Ret. Time	Area	Area %
1	6.599	121670	50.087
2	7.633	121246	49.913
Total		242915	100.000

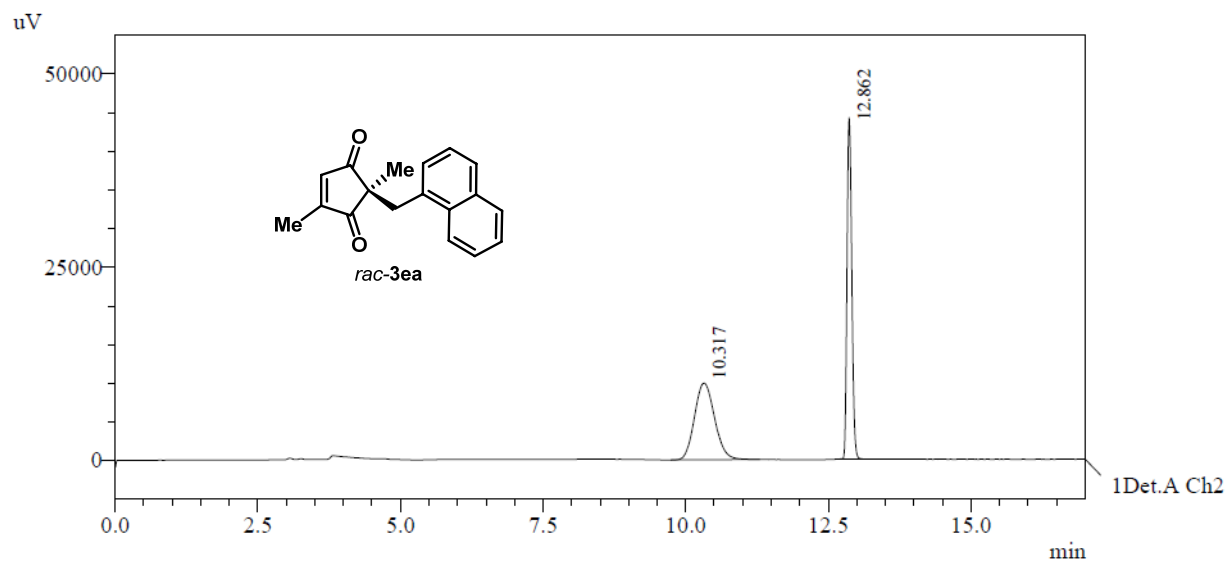


PeakTable

Detector A Ch2 254nm

Peak#	Ret. Time	Area	Area %
1	6.559	90579	5.815
2	7.563	1467183	94.185
Total		1557763	100.000

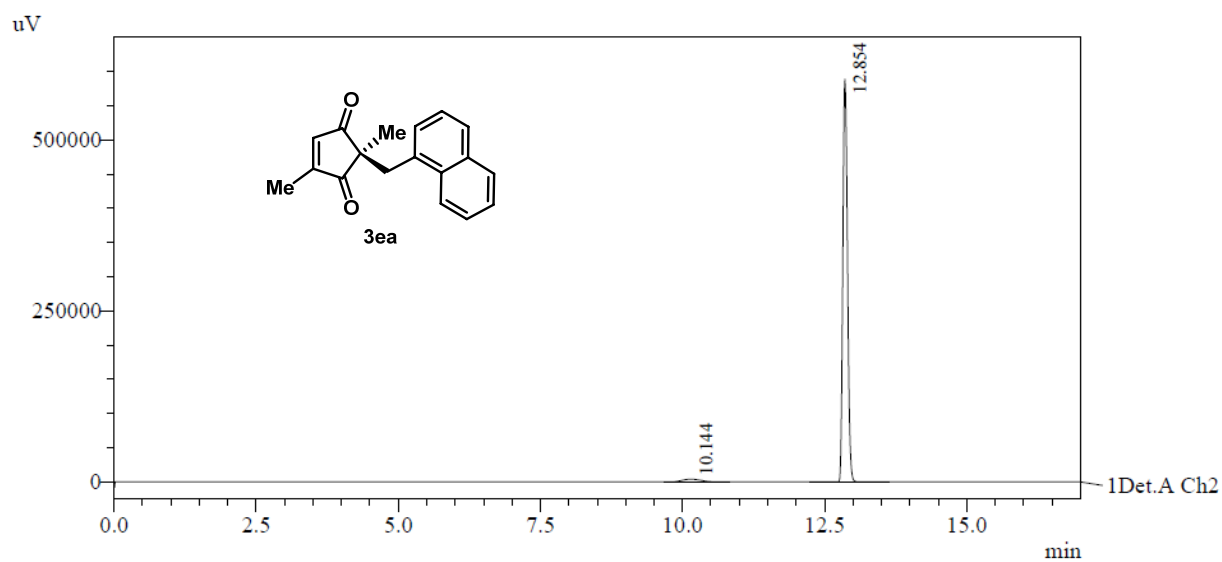




PeakTable

Detector A Ch2 254nm

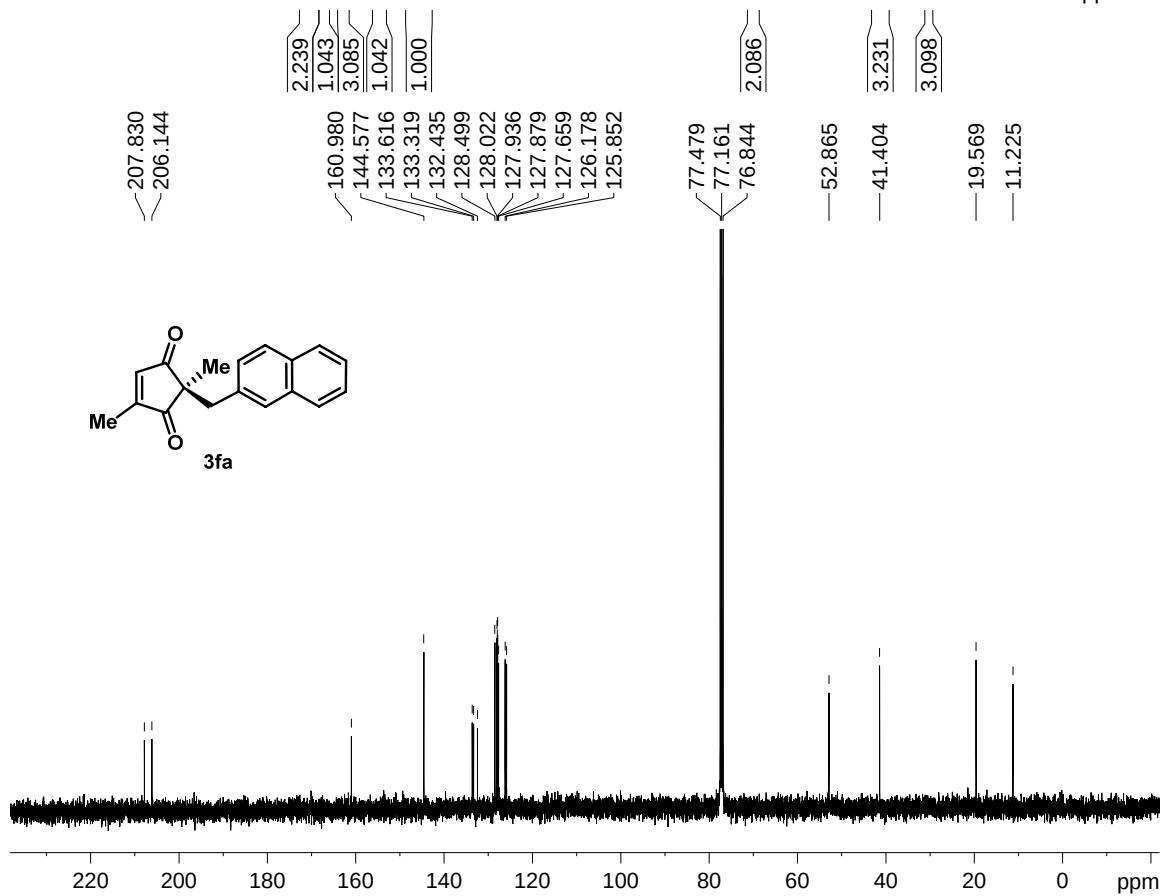
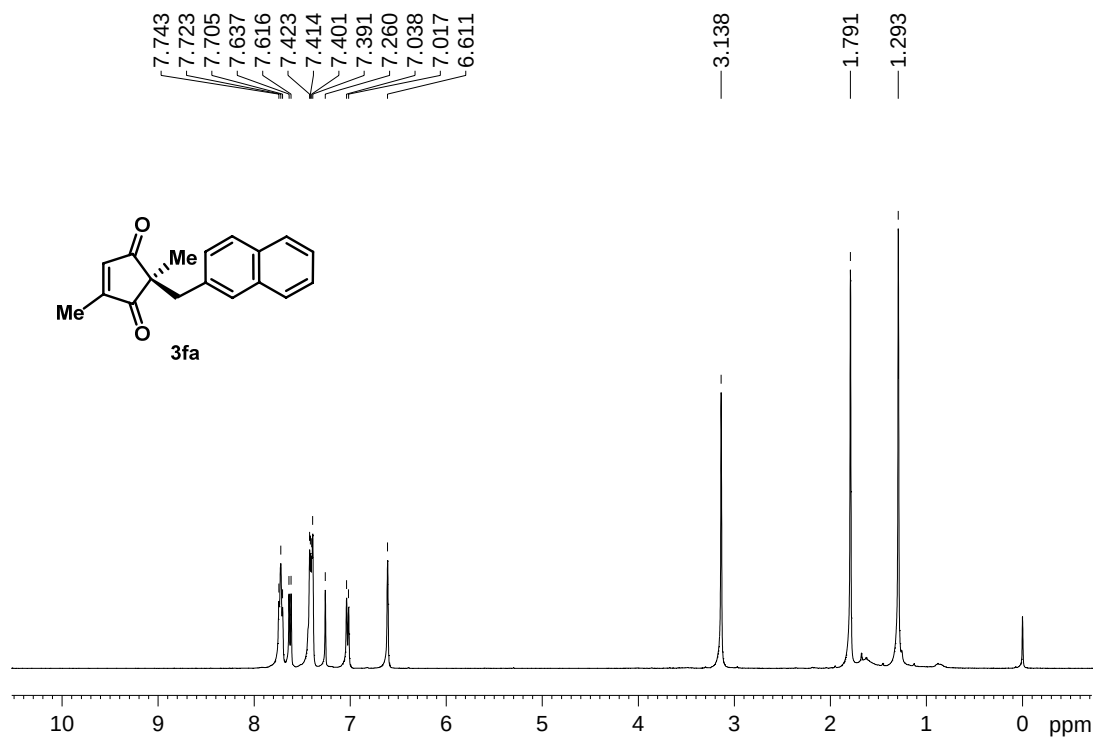
Peak#	Ret. Time	Area	Area %
1	10.317	243121	49.031
2	12.862	252727	50.969
Total		495848	100.000

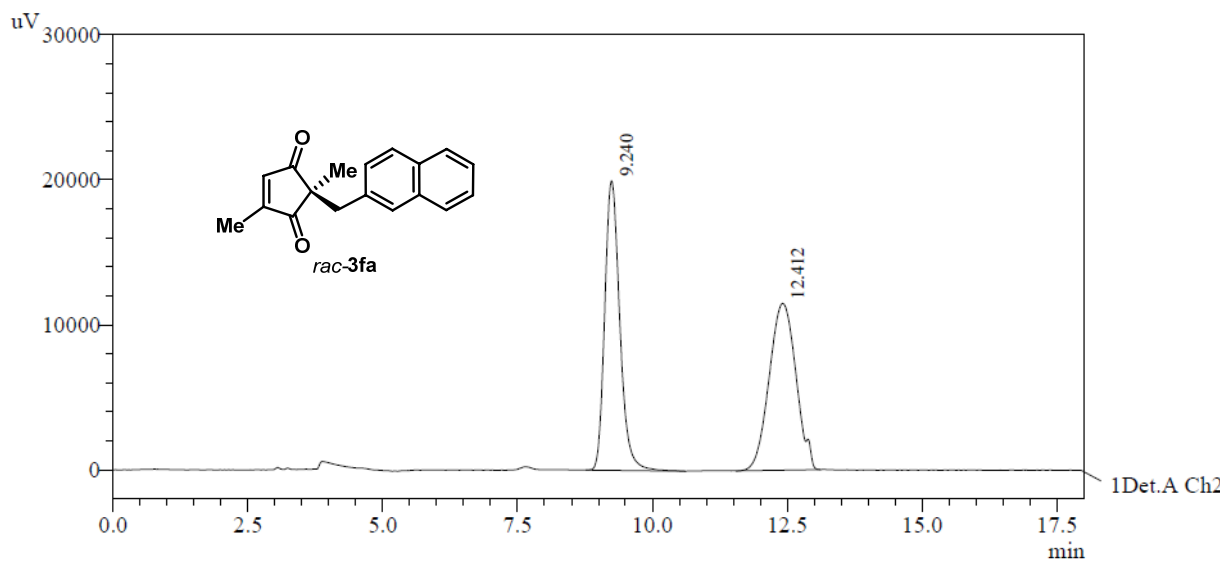


PeakTable

Detector A Ch2 254nm

Peak#	Ret. Time	Area	Area %
1	10.144	97446	2.857
2	12.854	3313376	97.143
Total		3410822	100.000

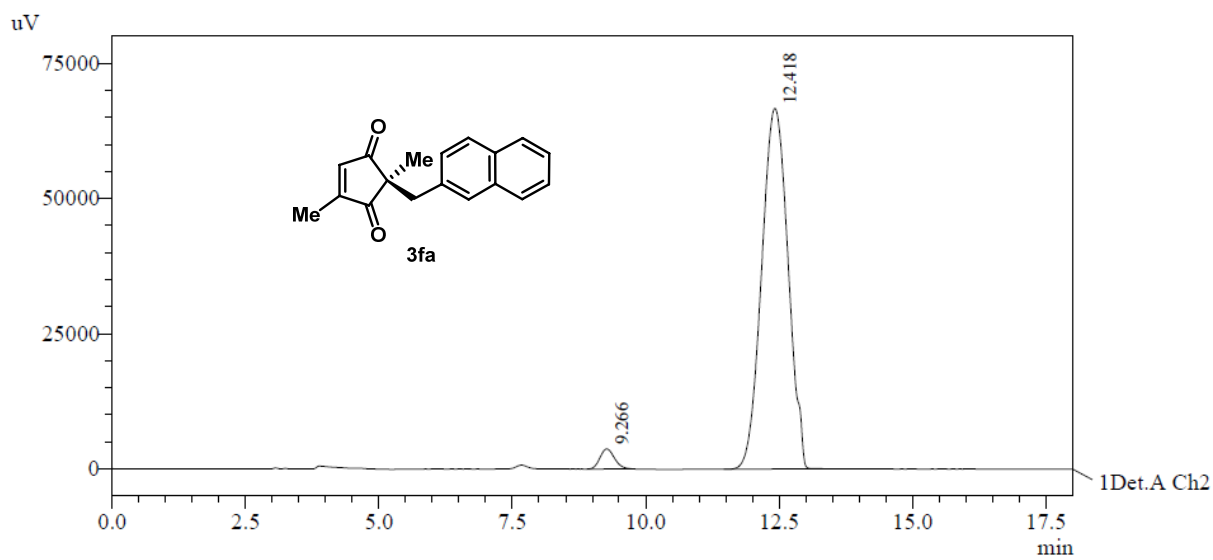




PeakTable

Detector A Ch2 254nm

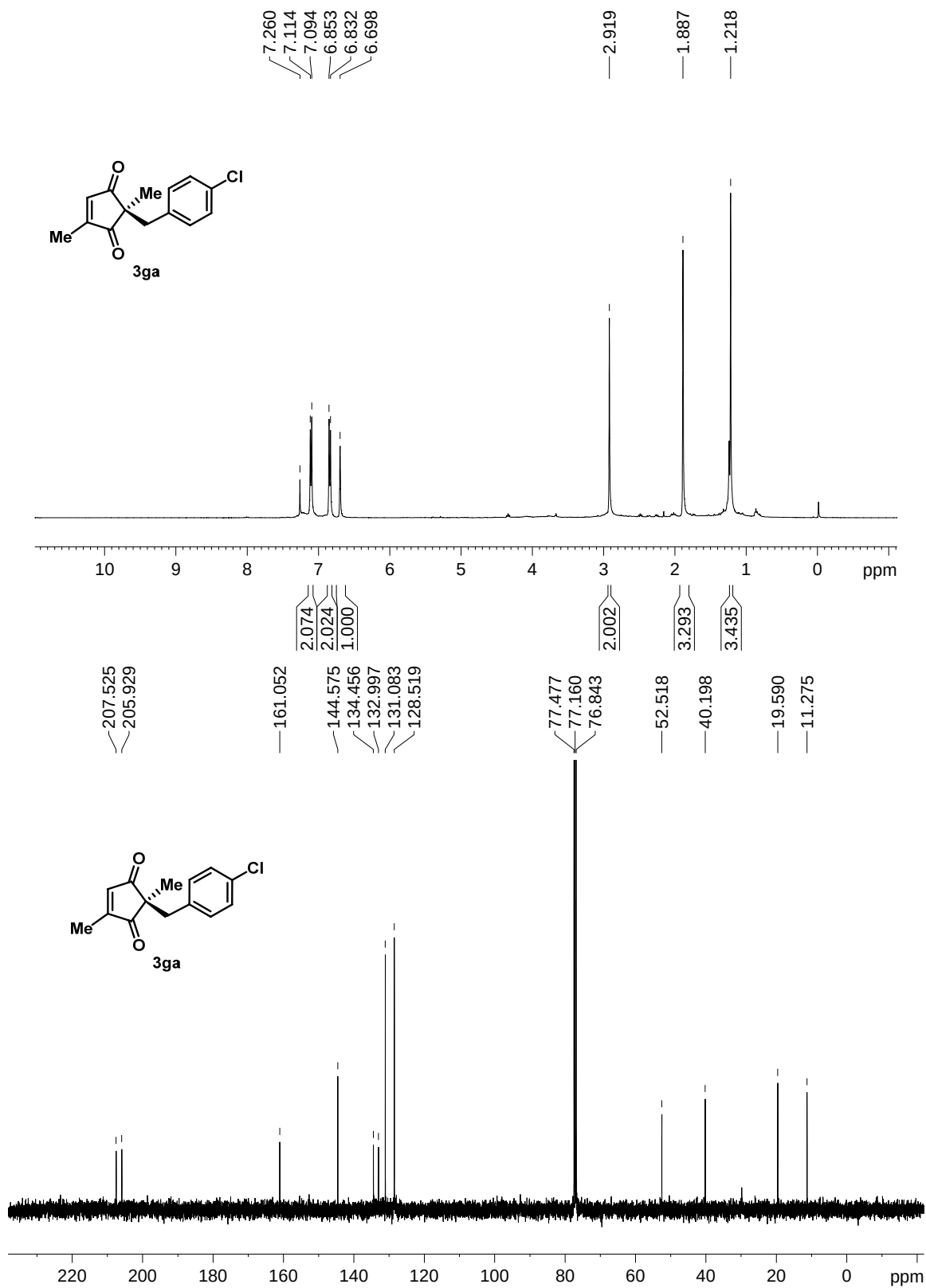
Peak#	Ret. Time	Area	Area %
1	9.240	388215	49.390
2	12.412	397812	50.610
Total		786027	100.000

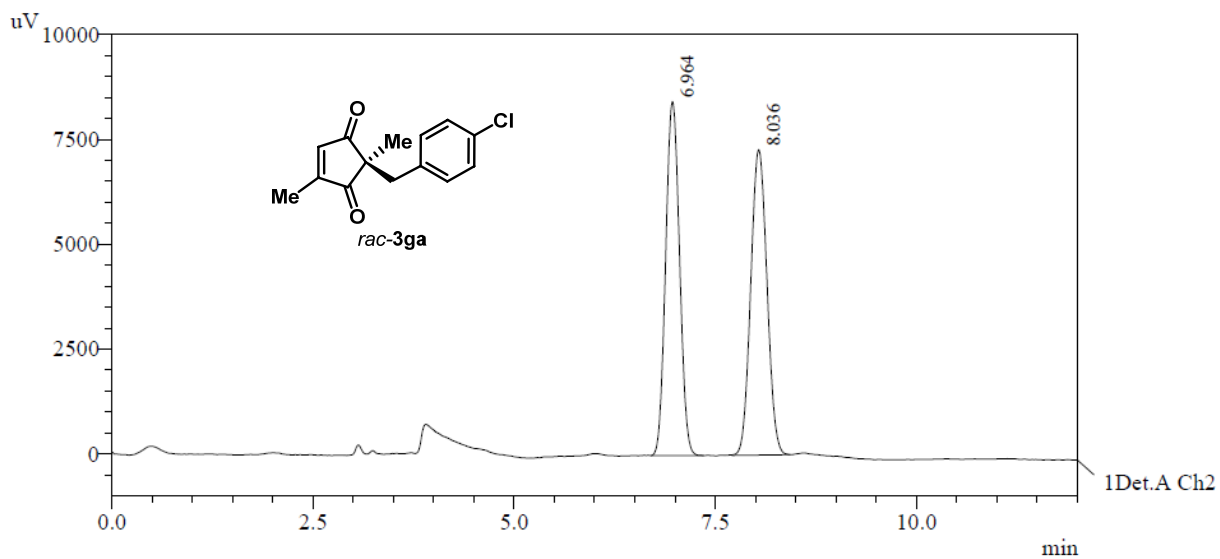


PeakTable

Detector A Ch2 254nm

Peak#	Ret. Time	Area	Area %
1	9.266	70186	2.971
2	12.418	2292516	97.029
Total		2362702	100.000

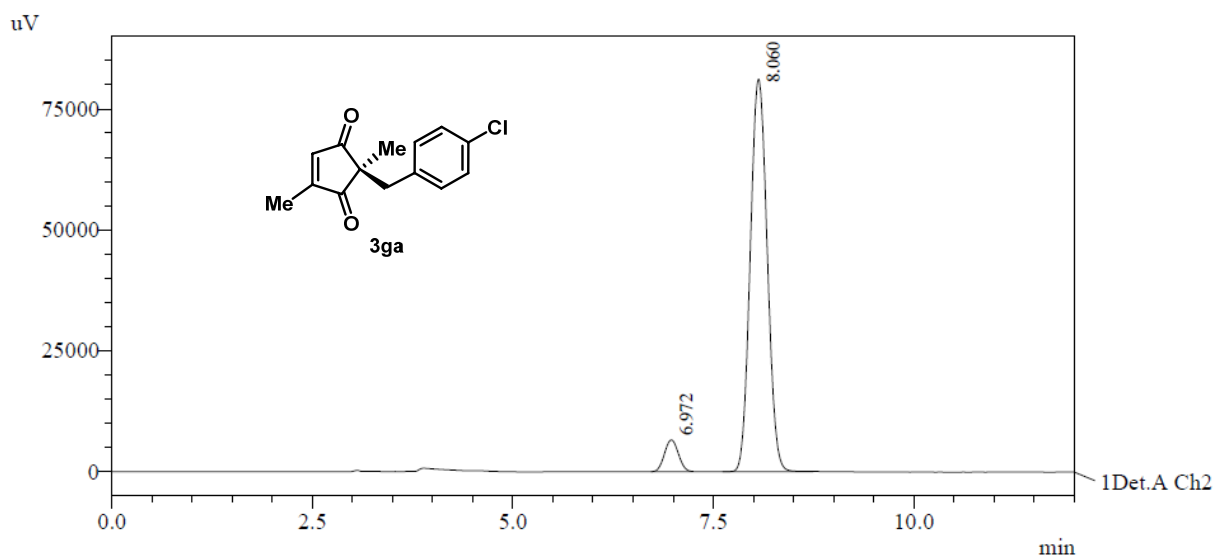




PeakTable

Detector A Ch2 254nm

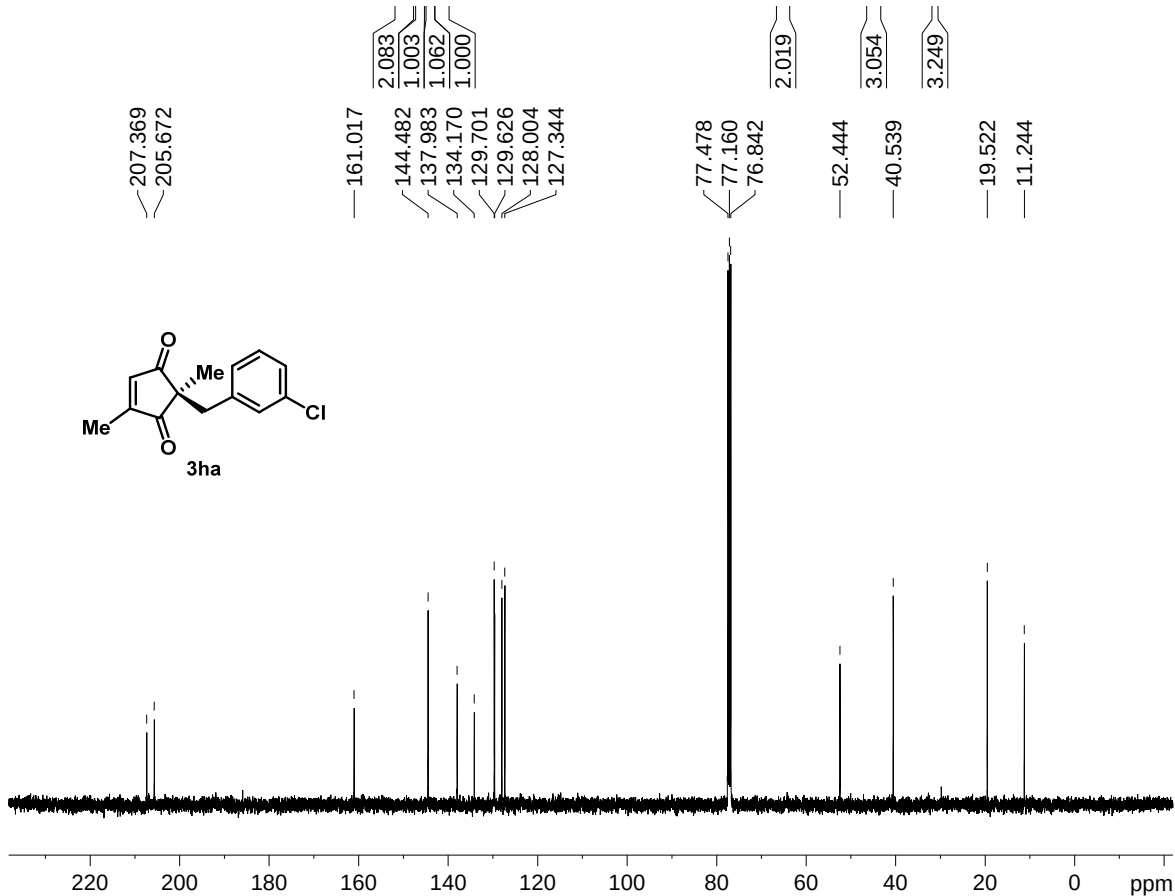
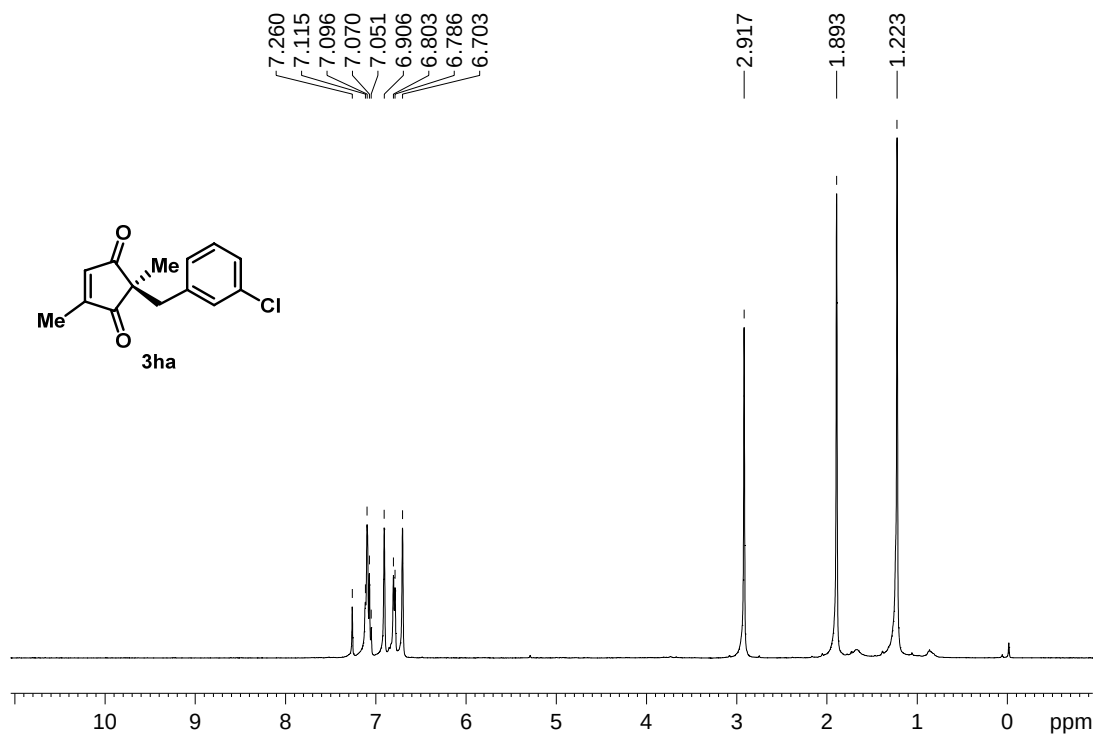
Peak#	Ret. Time	Area	Area %
1	6.964	101129	49.698
2	8.036	102359	50.302
Total		203488	100.000

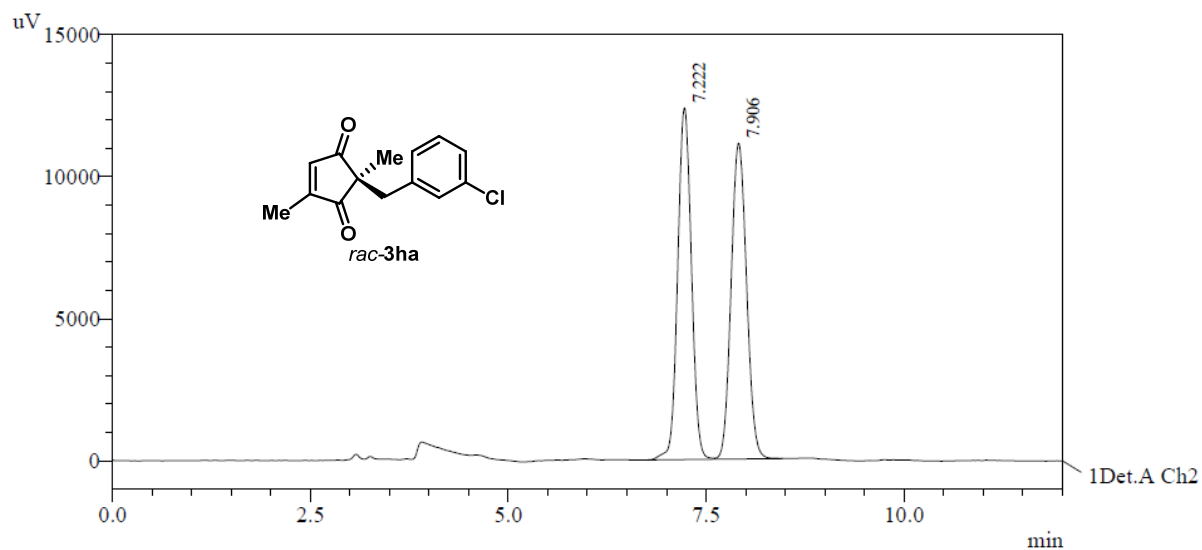


PeakTable

Detector A Ch2 254nm

Peak#	Ret. Time	Area	Area %
1	6.972	78807	6.196
2	8.060	1193180	93.804
Total		1271988	100.000

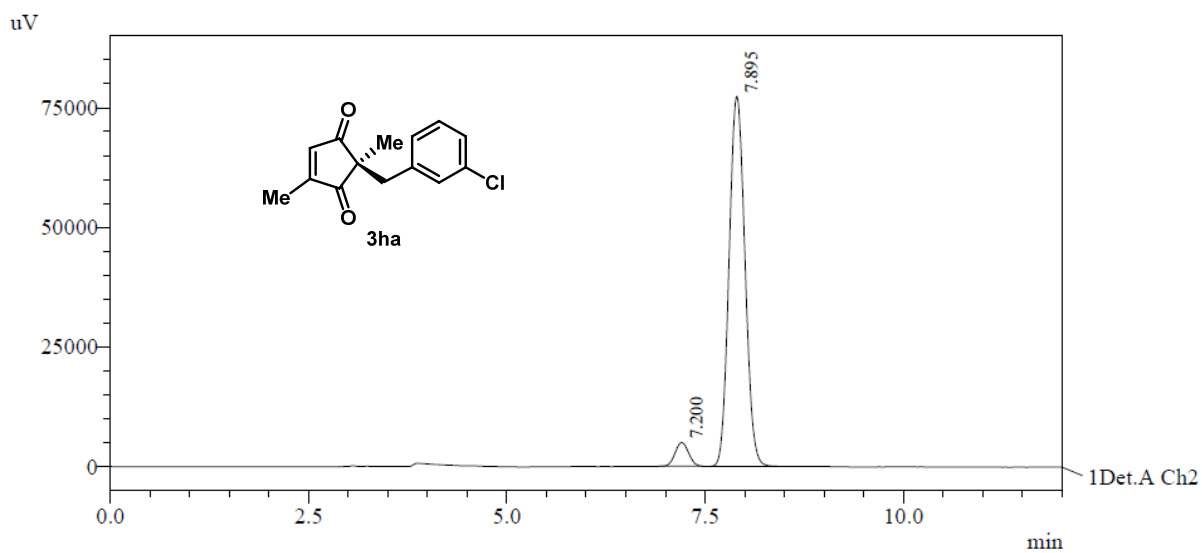




PeakTable

Detector A Ch2 254nm

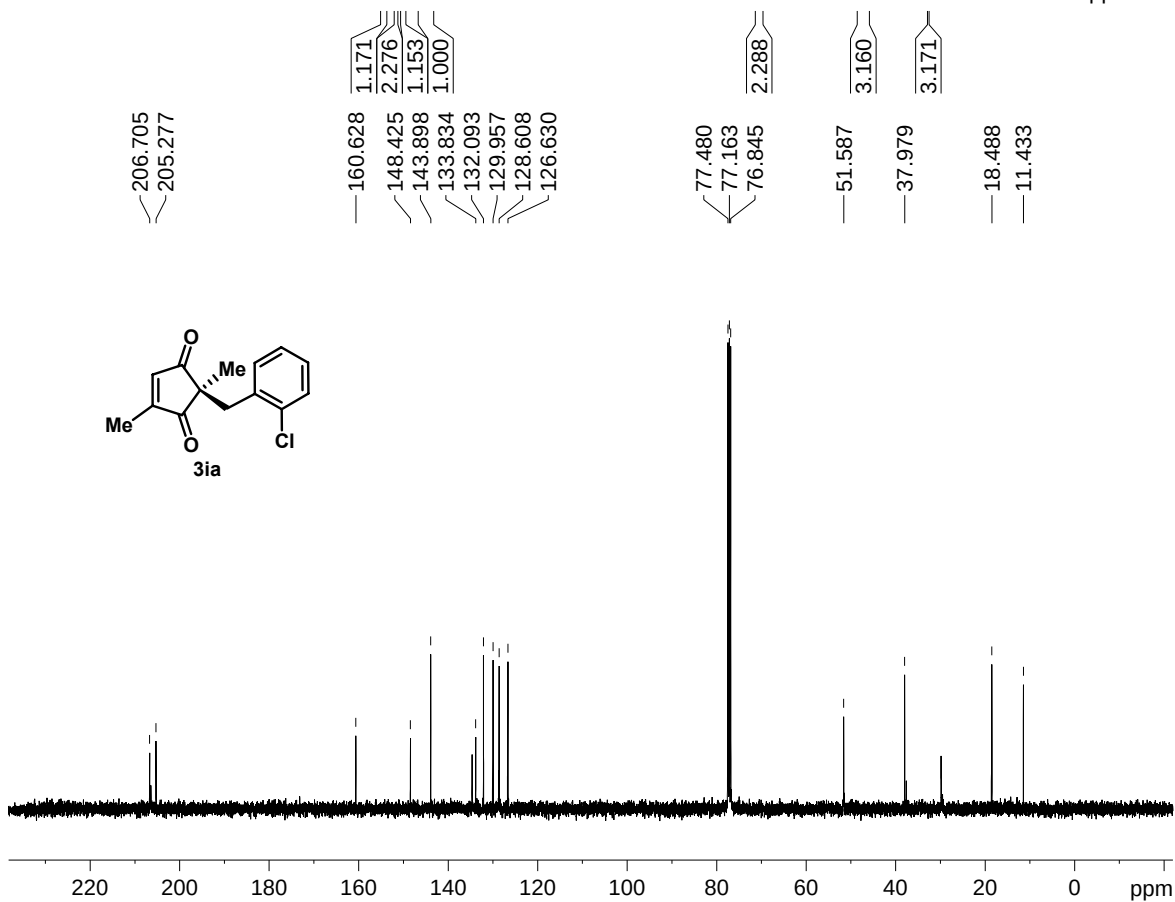
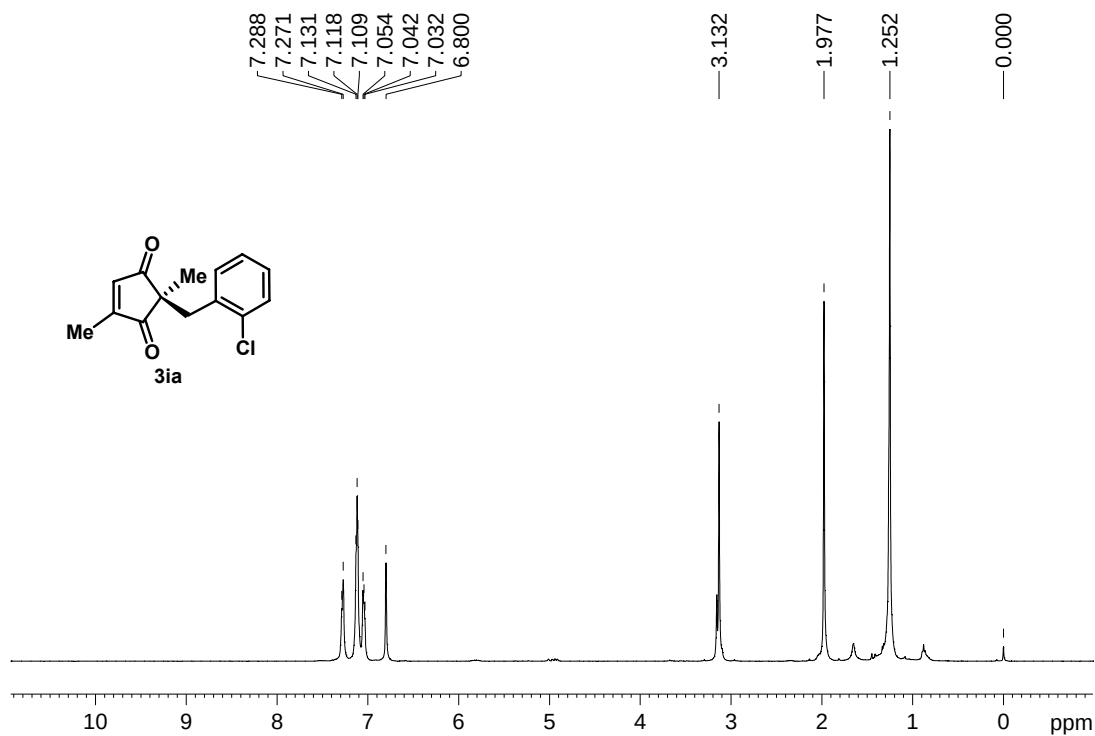
Peak#	Ret. Time	Area	Area %
1	7.222	149502	49.760
2	7.906	150947	50.240
Total		300449	100.000

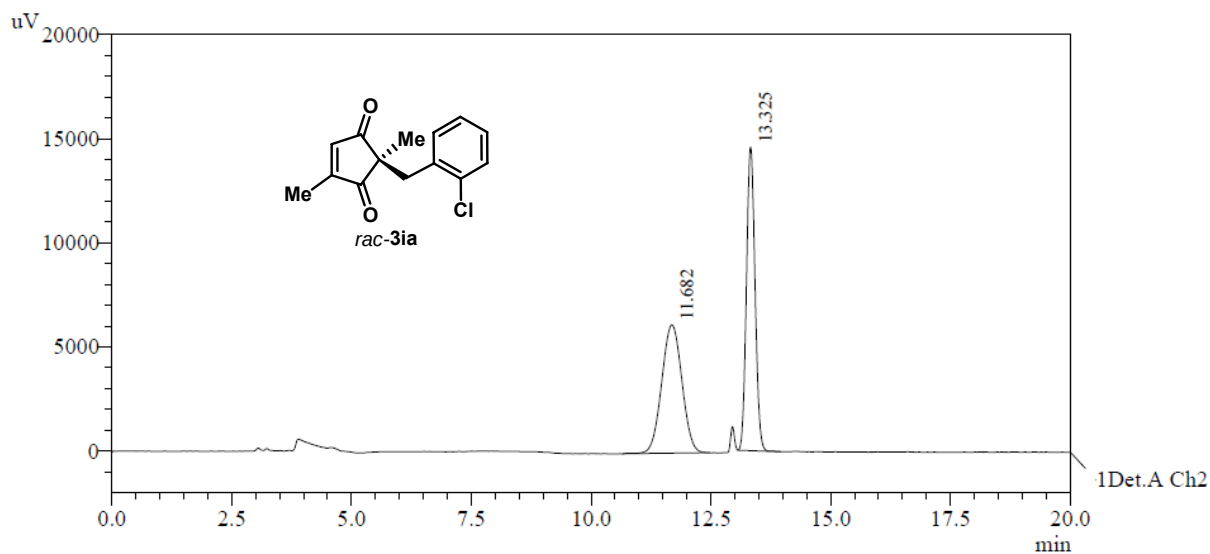


PeakTable

Detector A Ch2 254nm

Peak#	Ret. Time	Area	Area %
1	7.200	58836	5.173
2	7.895	1078474	94.827
Total		1137310	100.000

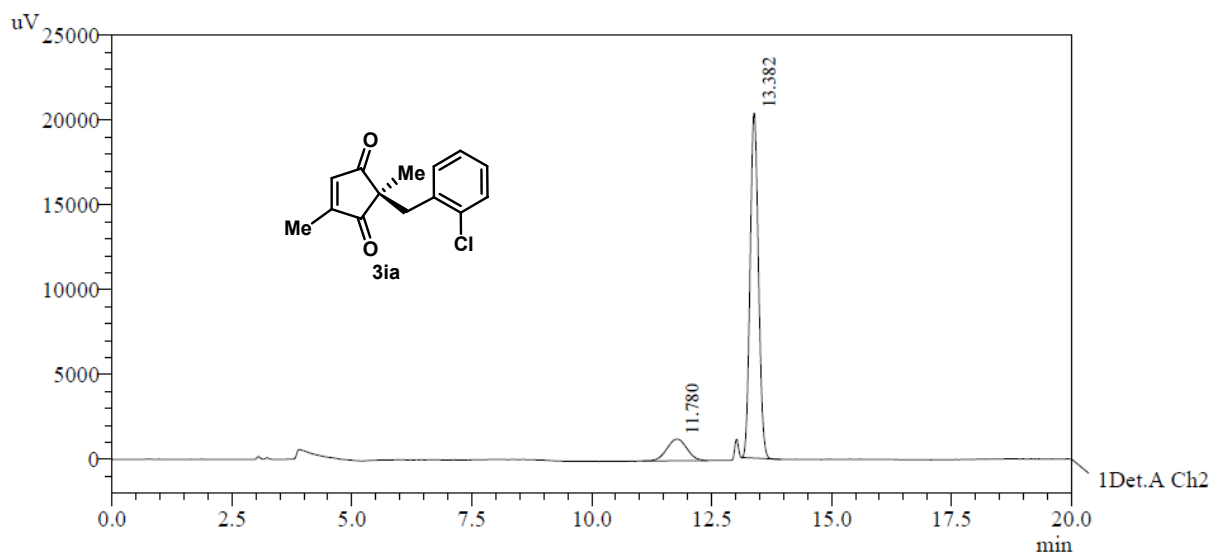




PeakTable

Detector A Ch2 254nm

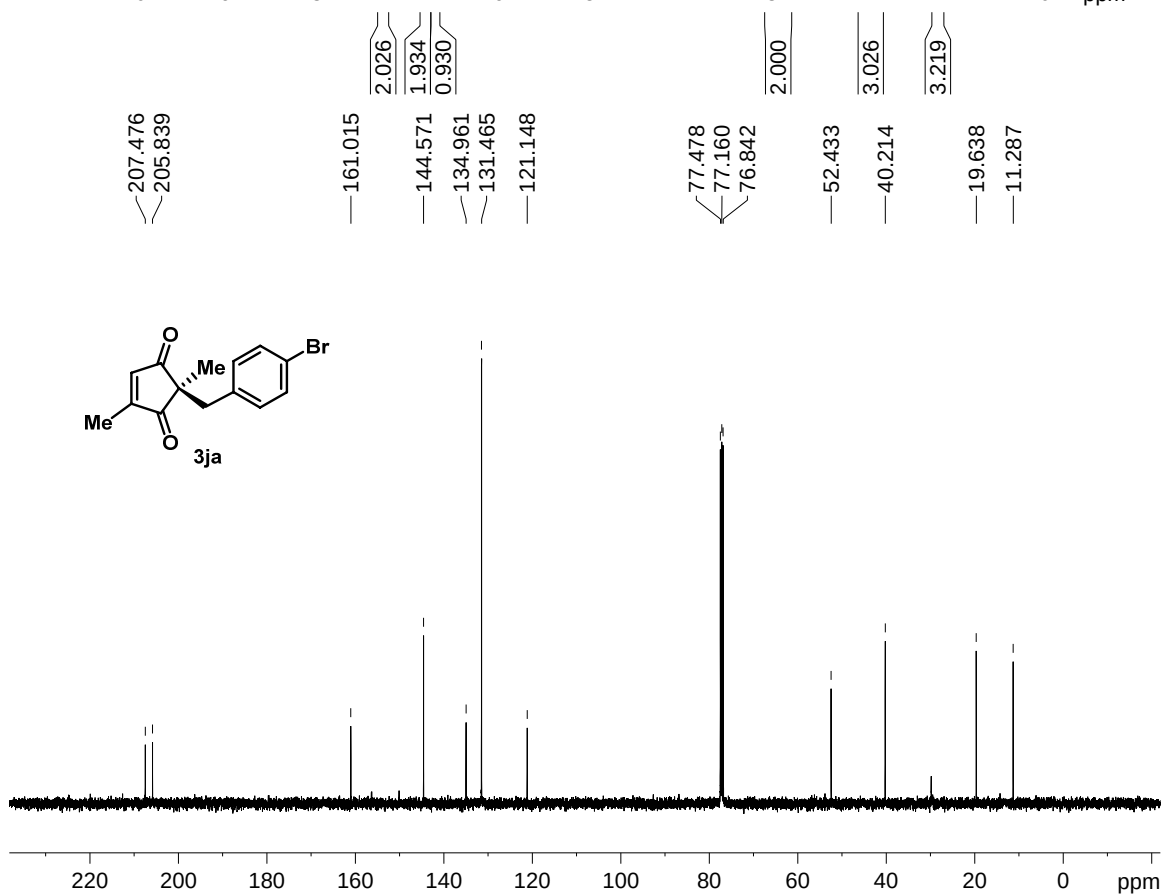
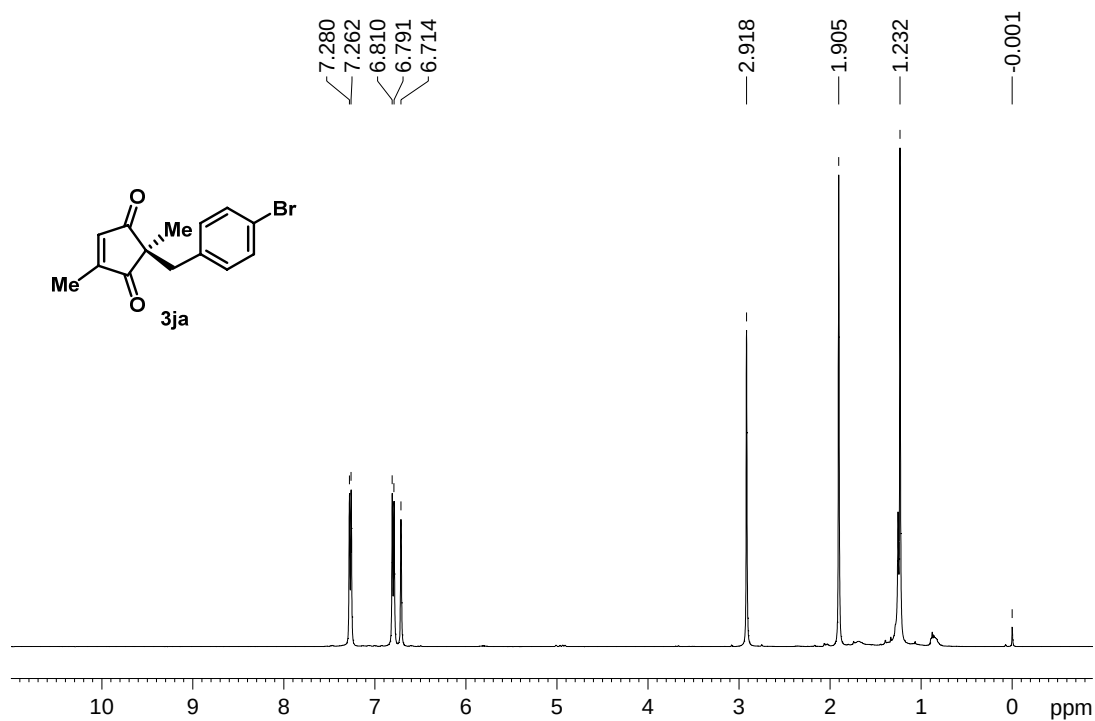
Peak#	Ret. Time	Area	Area %
1	11.682	180955	50.005
2	13.325	180920	49.995
Total		361876	100.000

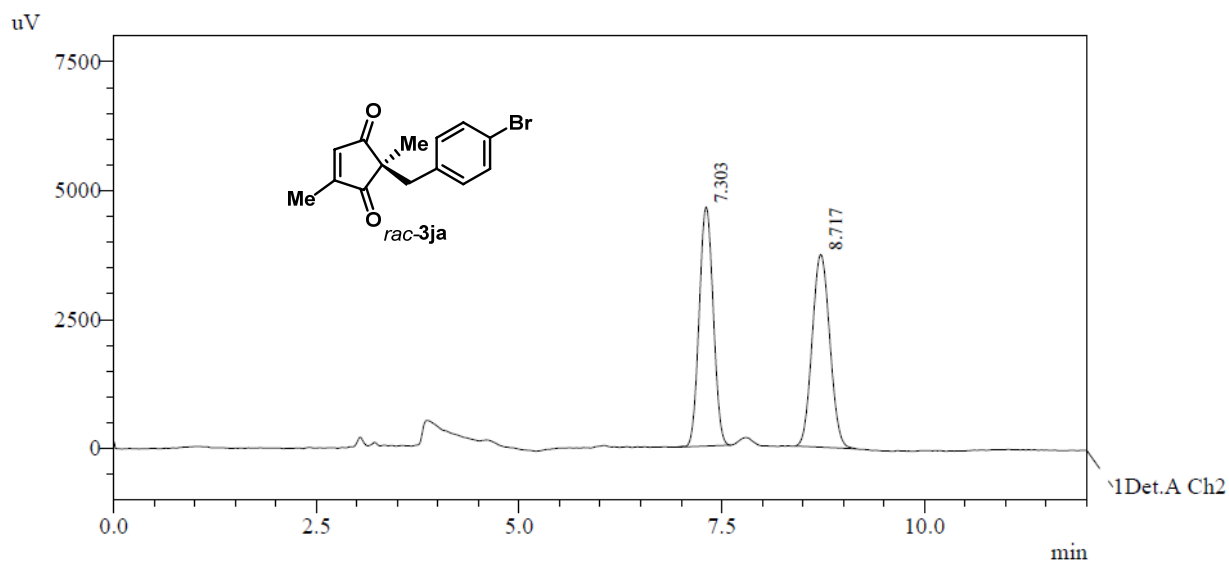


PeakTable

Detector A Ch2 254nm

Peak#	Ret. Time	Area	Area %
1	11.780	37158	13.067
2	13.382	247201	86.933
Total		284359	100.000

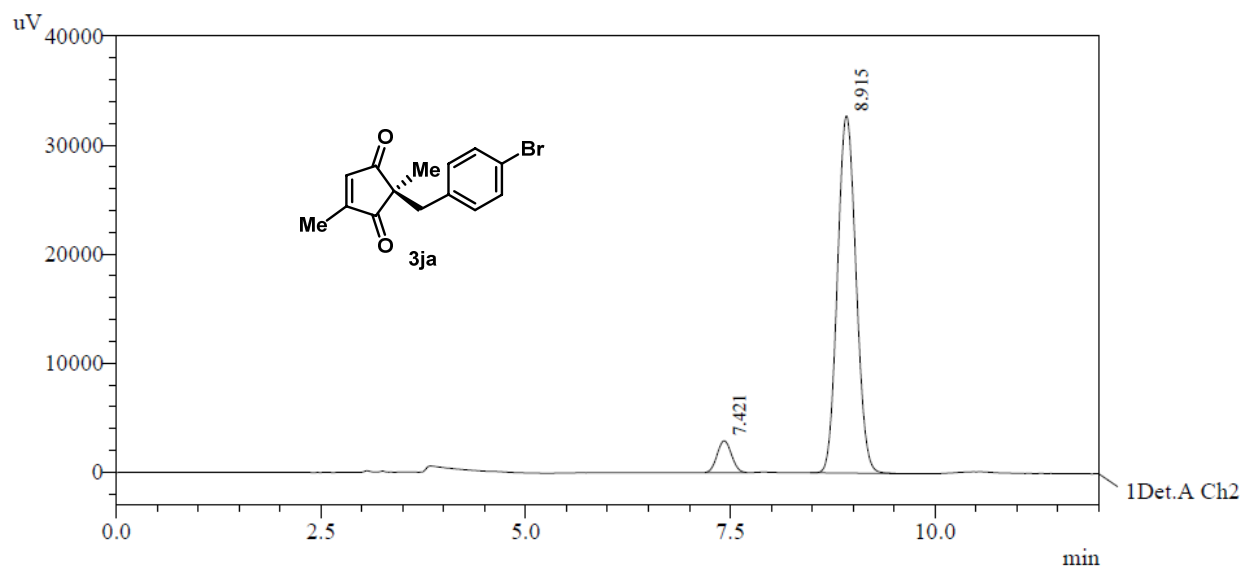




PeakTable

Detector A Ch2 254nm

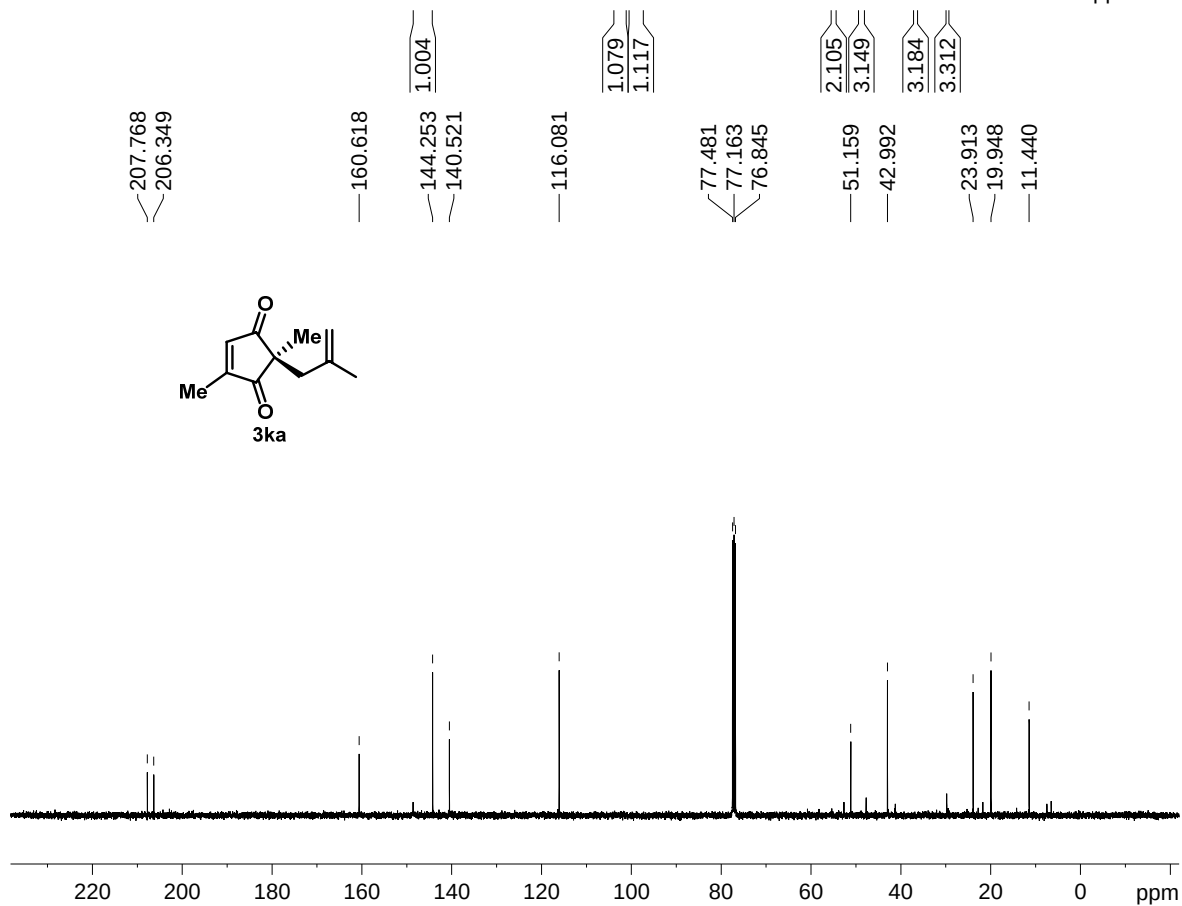
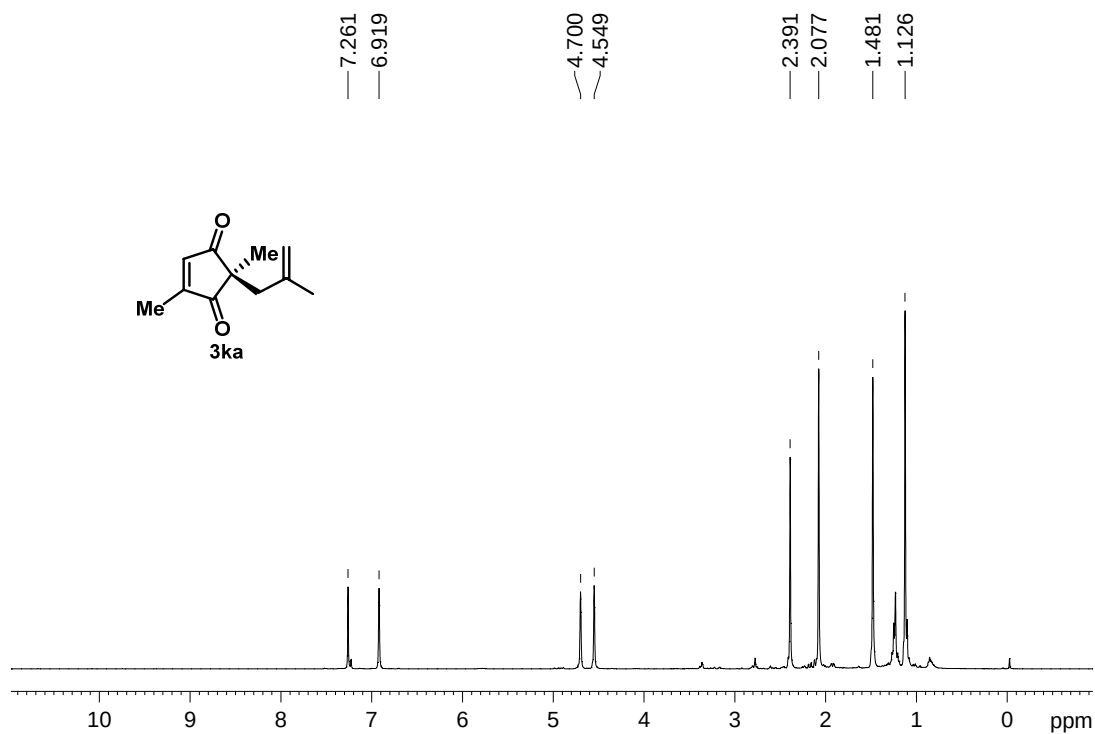
Peak#	Ret. Time	Area	Area %
1	7.303	55937	49.675
2	8.717	56668	50.325
Total		112605	100.000

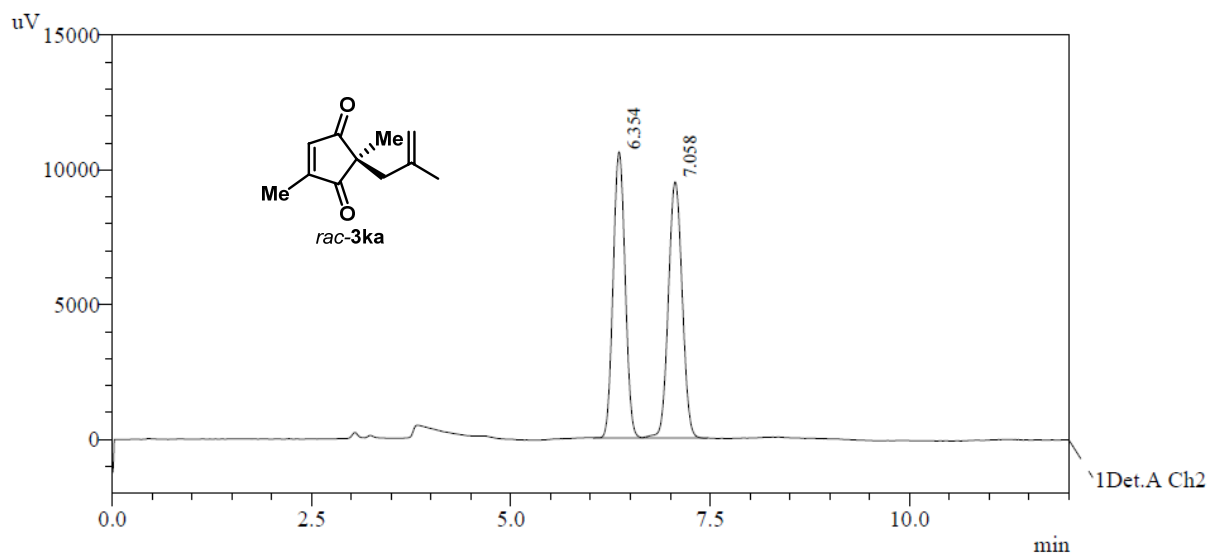


PeakTable

Detector A Ch2 254nm

Peak#	Ret. Time	Area	Area %
1	7.421	35328	6.398
2	8.915	516854	93.602
Total		552183	100.000

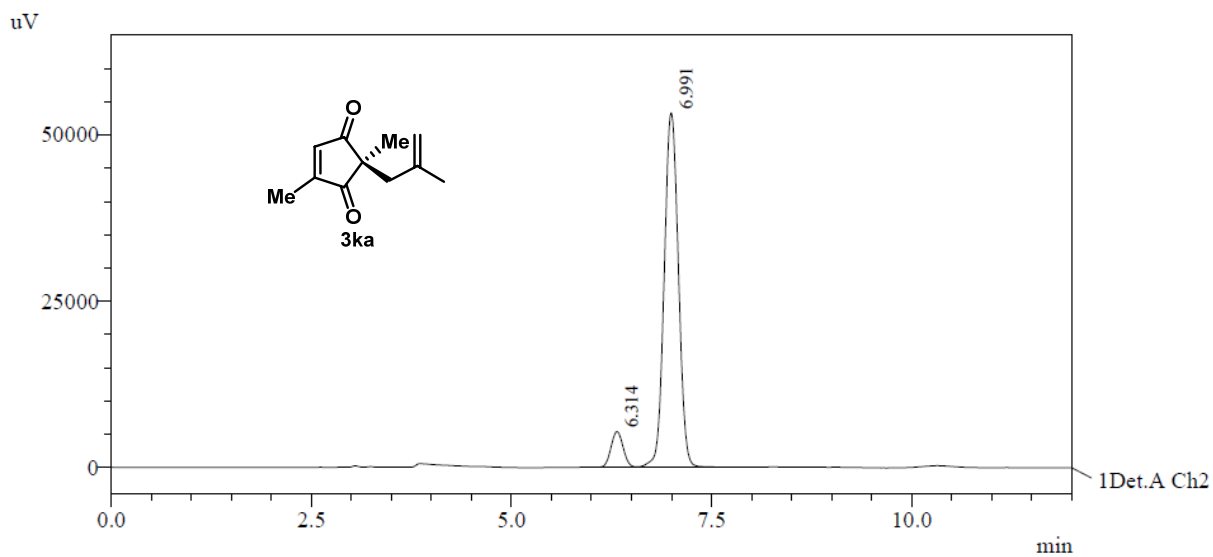




PeakTable

Detector A Ch2 254nm

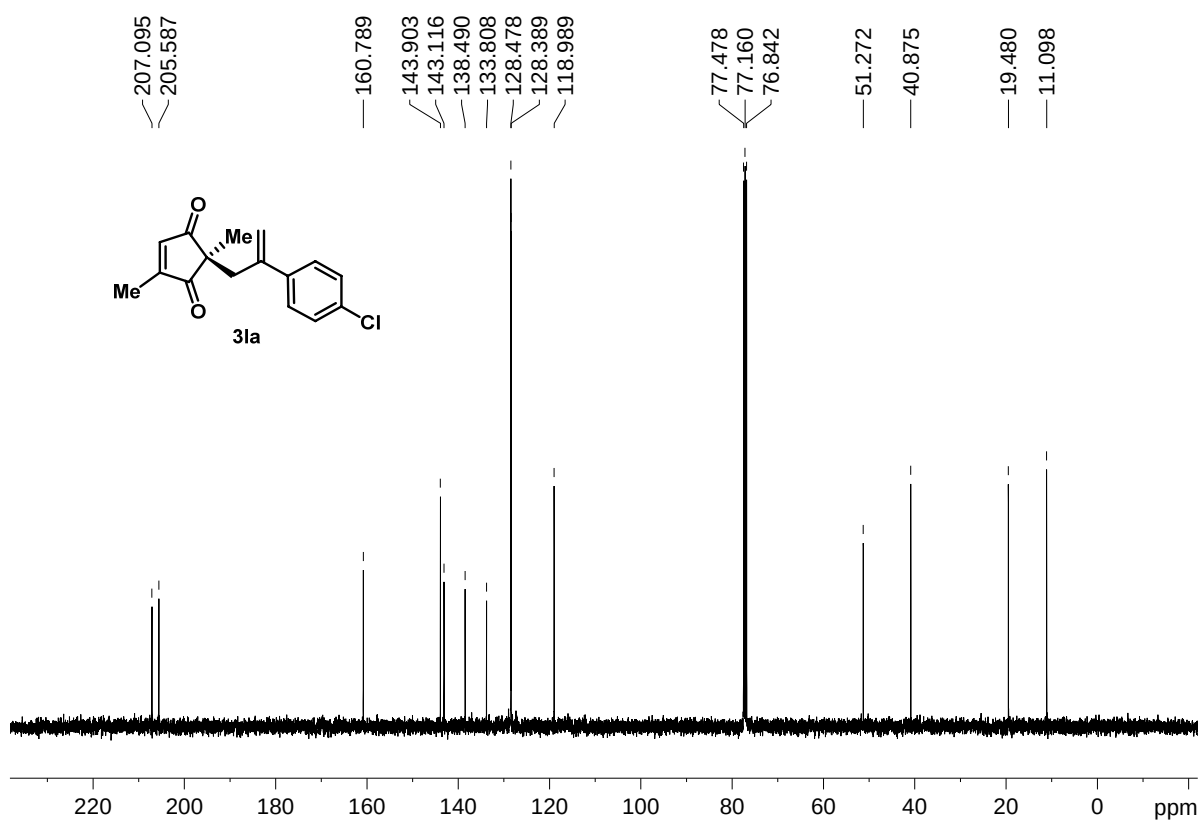
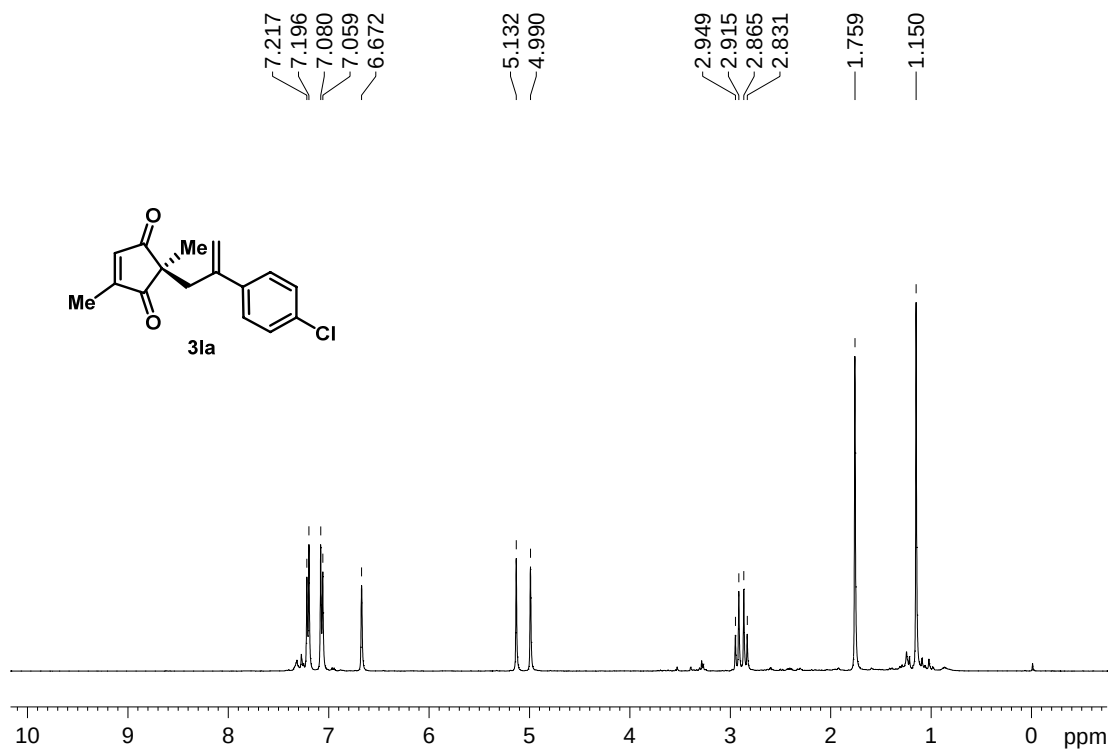
Peak#	Ret. Time	Area	Area %
1	6.354	111358	49.282
2	7.058	114602	50.718
Total		225960	100.000

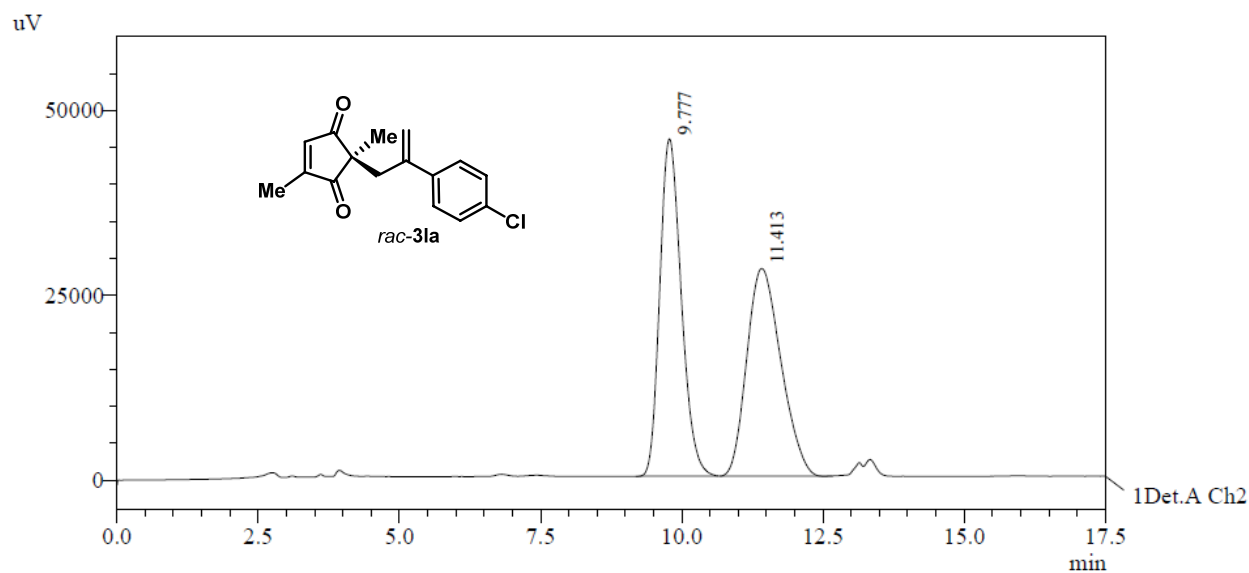


PeakTable

Detector A Ch2 254nm

Peak#	Ret. Time	Area	Area %
1	6.314	56115	7.880
2	6.991	655978	92.120
Total		712093	100.000

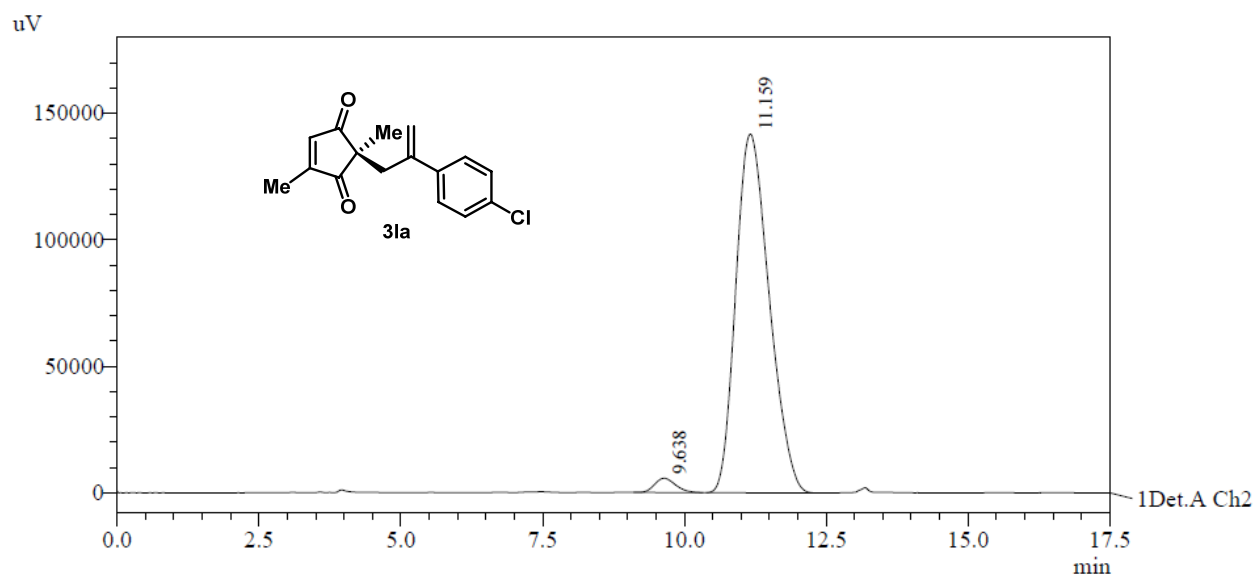




PeakTable

Detector A Ch2 254nm

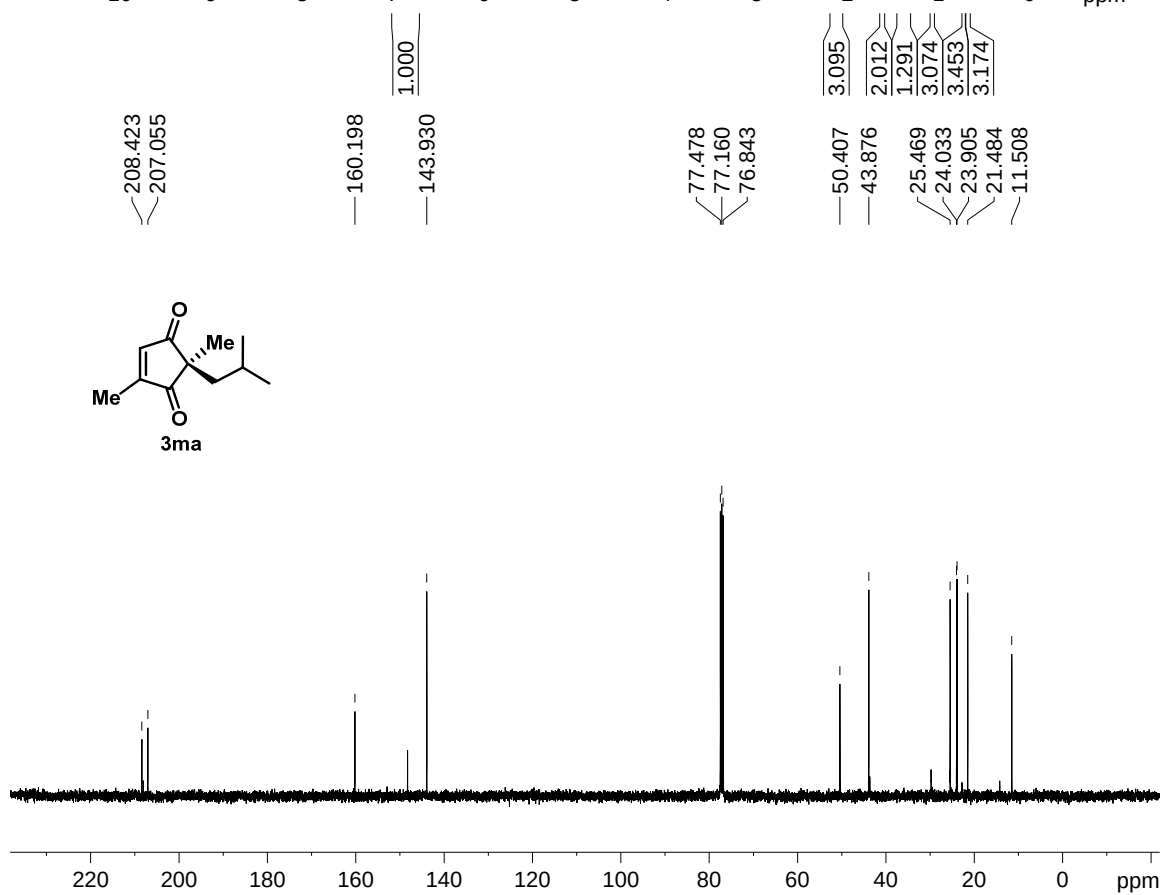
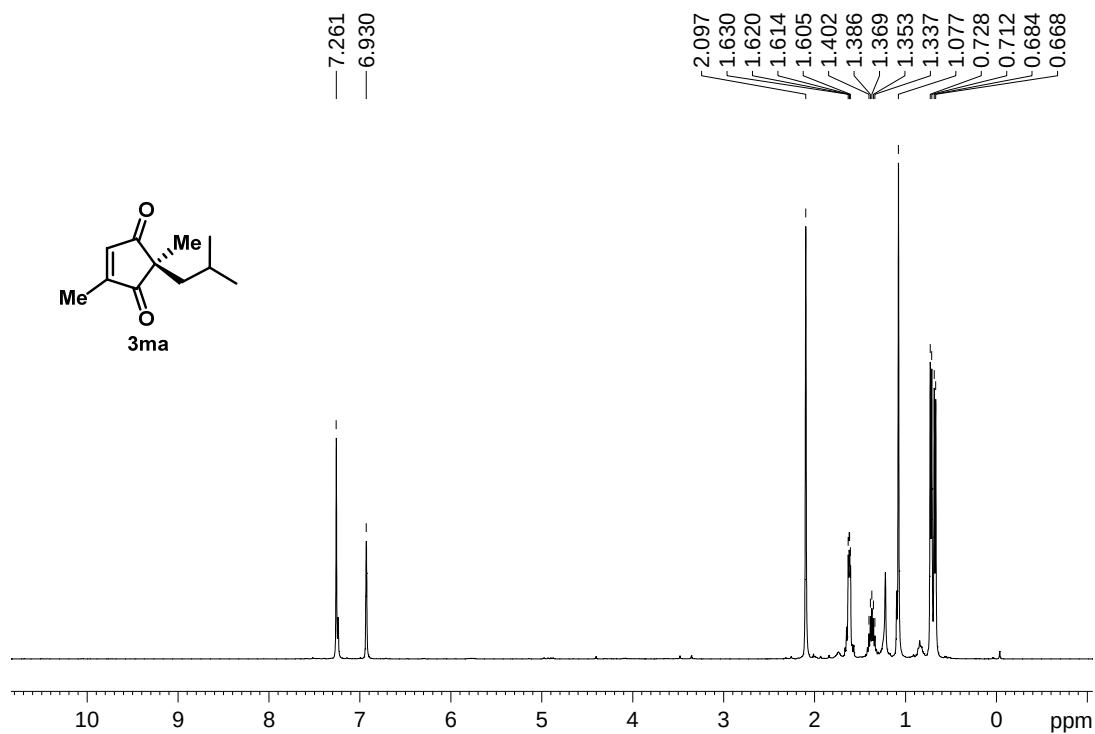
Peak#	Ret. Time	Area	Area %
1	9.777	1206421	50.541
2	11.413	1180574	49.459
Total		2386995	100.000

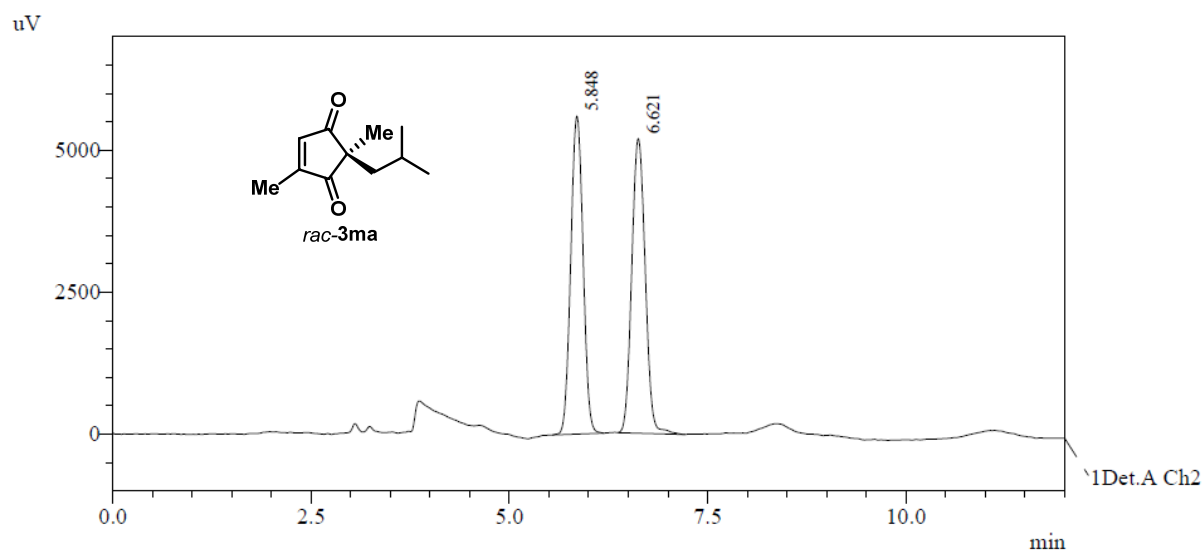


PeakTable

Detector A Ch2 254nm

Peak#	Ret. Time	Area	Area %
1	9.638	144794	2.432
2	11.159	5808654	97.568
Total		5953448	100.000

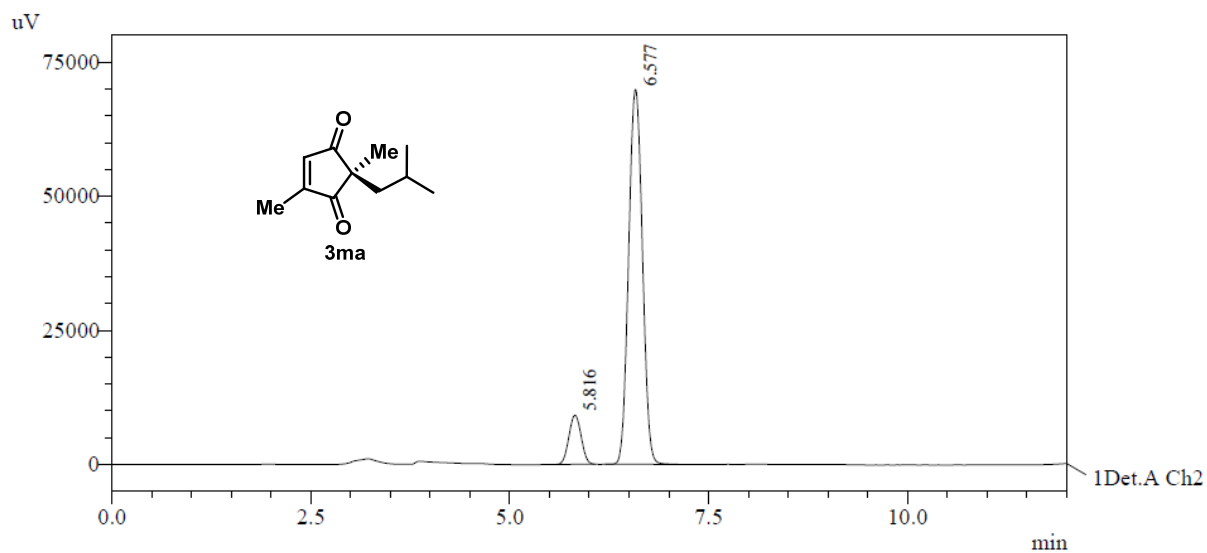




PeakTable

Detector A Ch2 254nm

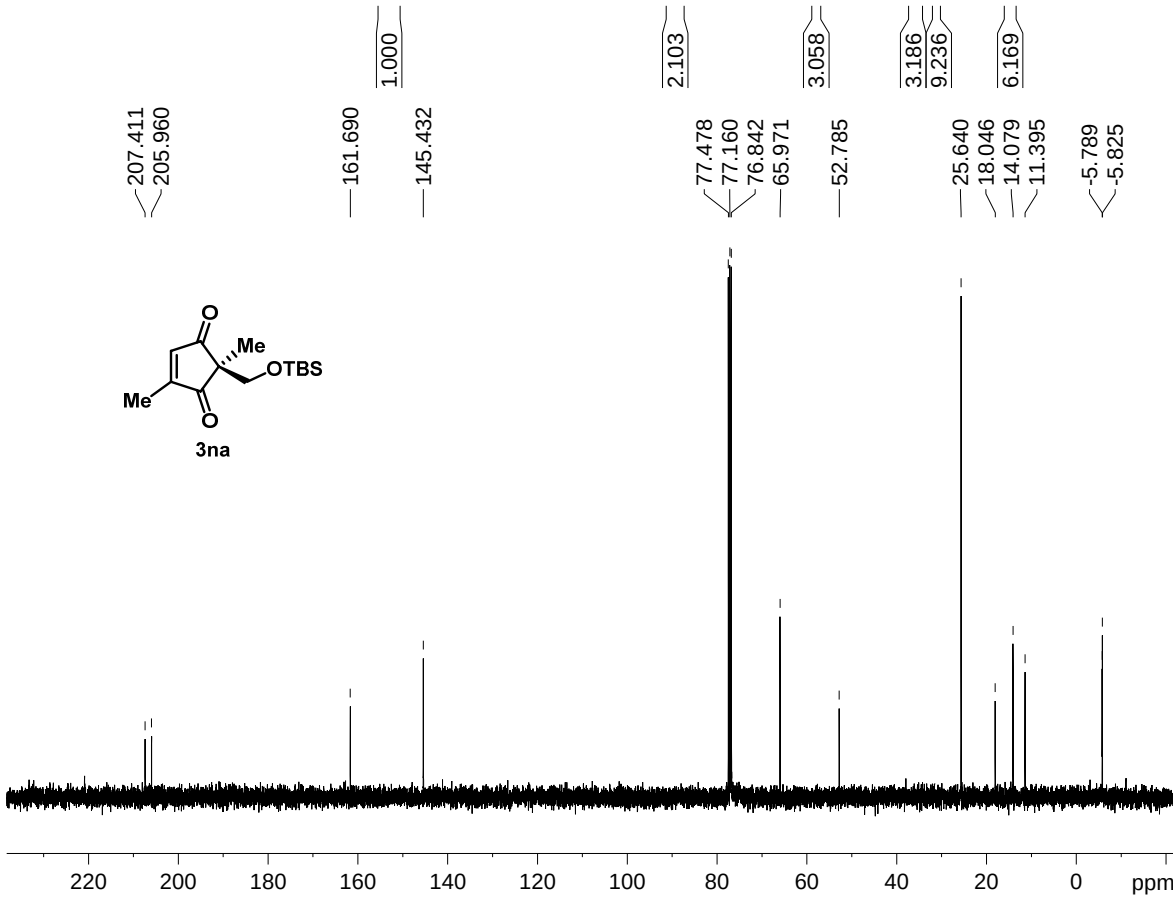
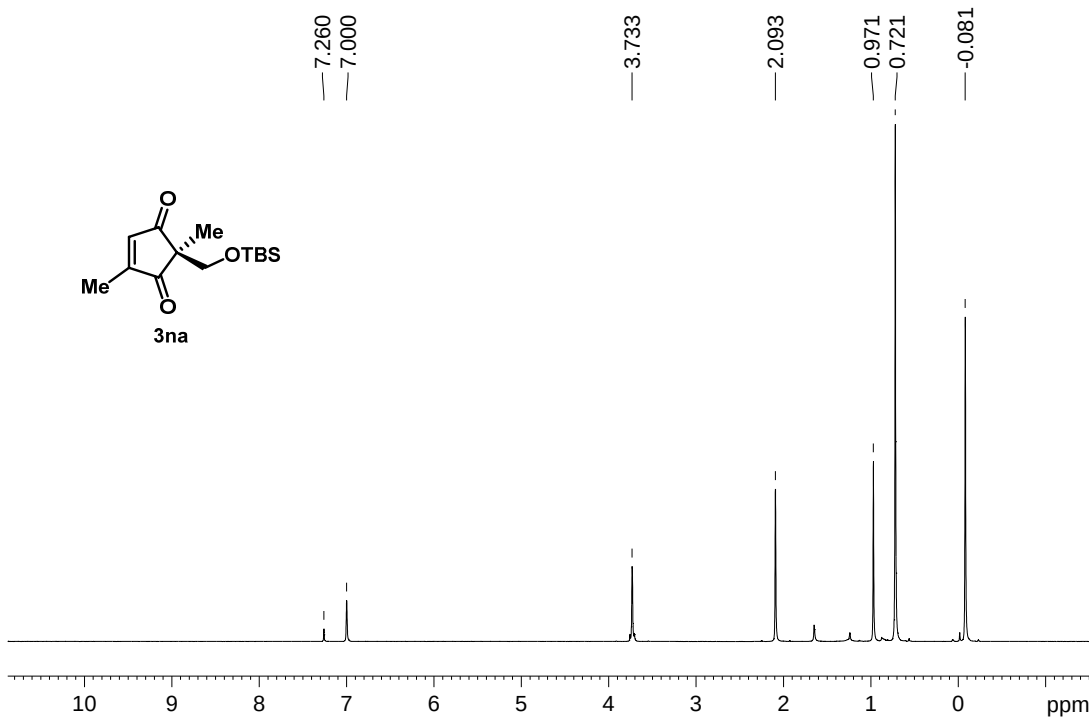
Peak#	Ret. Time	Area	Area %
1	5.848	60630	49.686
2	6.621	61396	50.314
Total		122026	100.000

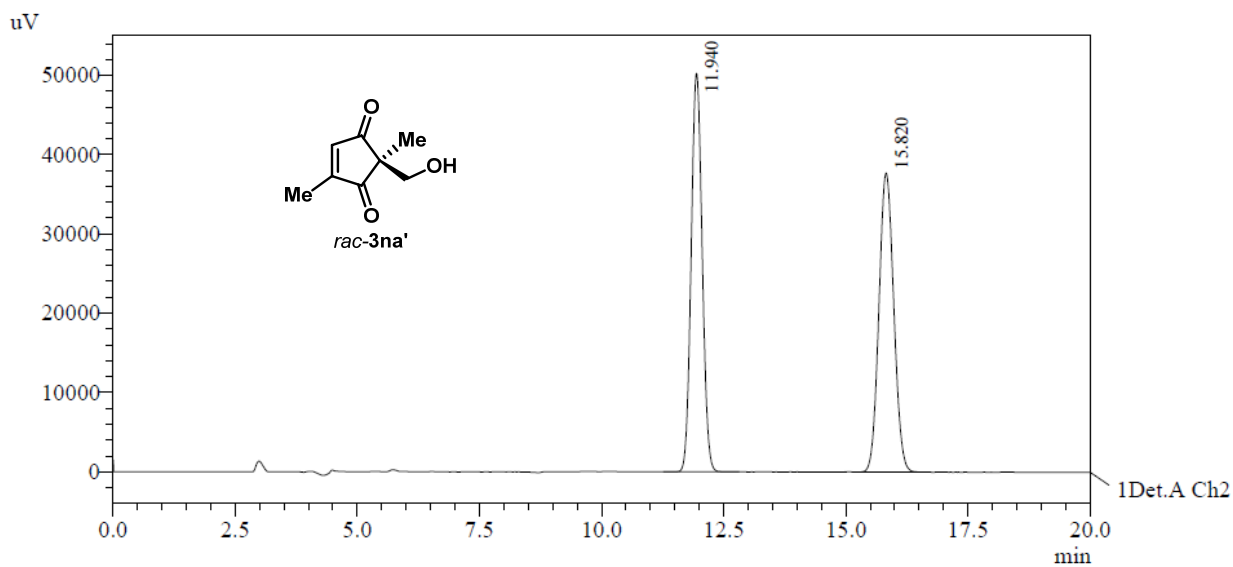


PeakTable

Detector A Ch2 254nm

Peak#	Ret. Time	Area	Area %
1	5.816	98234	10.442
2	6.577	842514	89.558
Total		940748	100.000

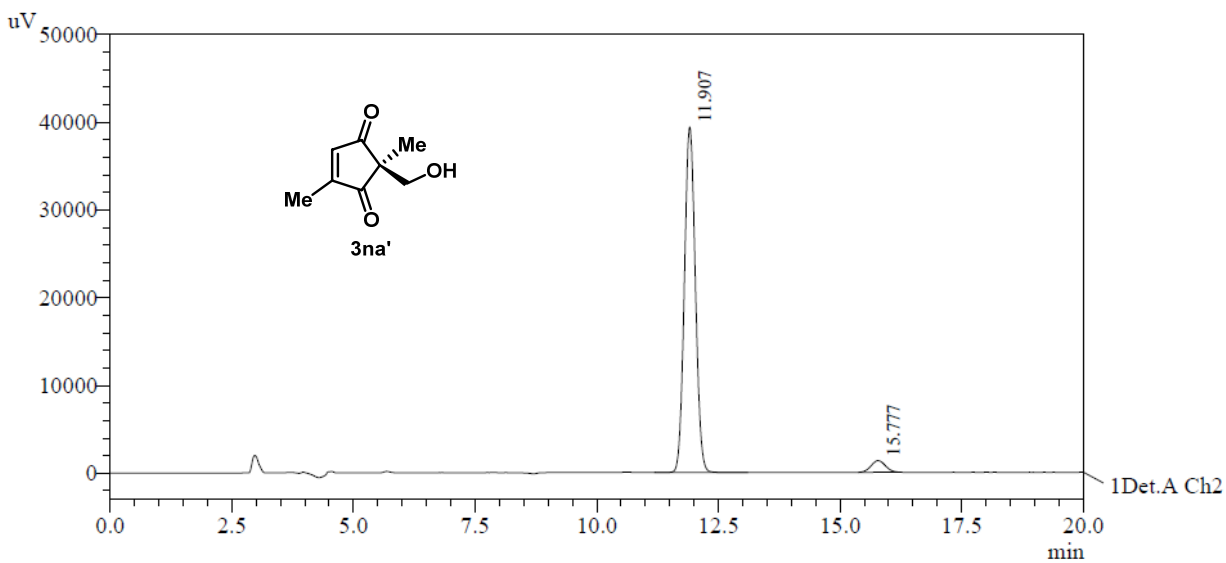




PeakTable

Detector A Ch2 254nm

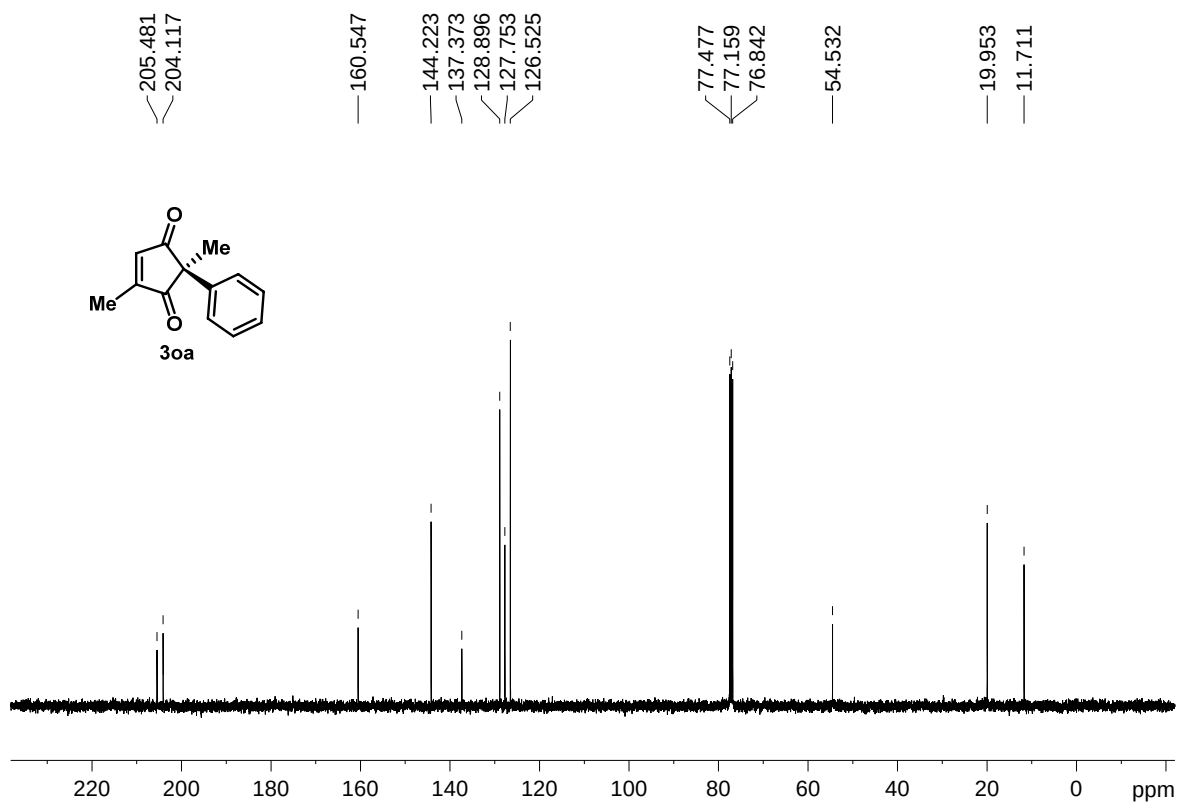
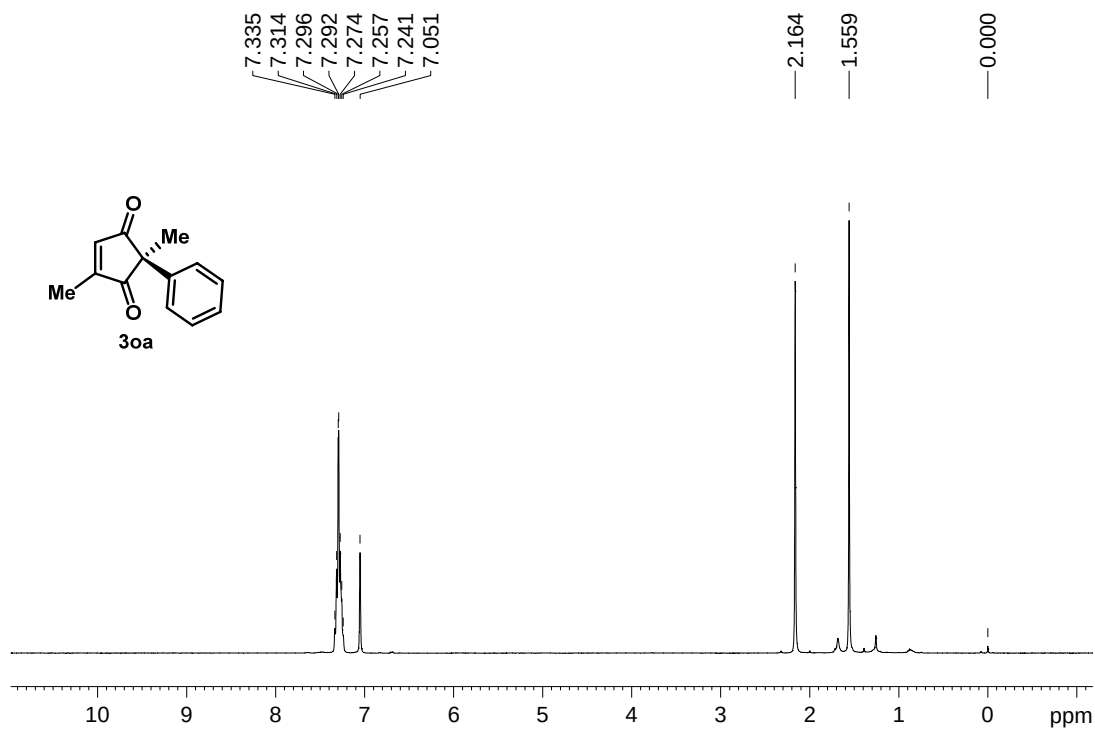
Peak#	Ret. Time	Area	Area %
1	11.940	787755	49.704
2	15.820	797130	50.296
Total		1584885	100.000

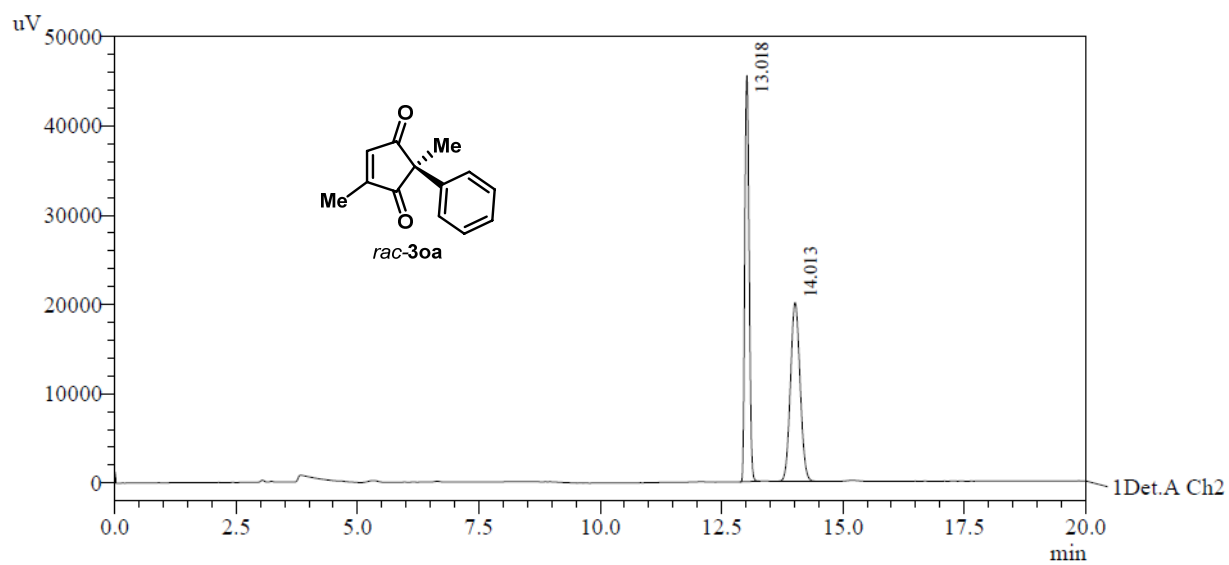


PeakTable

Detector A Ch2 254nm

Peak#	Ret. Time	Area	Area %
1	11.907	616981	95.772
2	15.777	27235	4.228
Total		644216	100.000

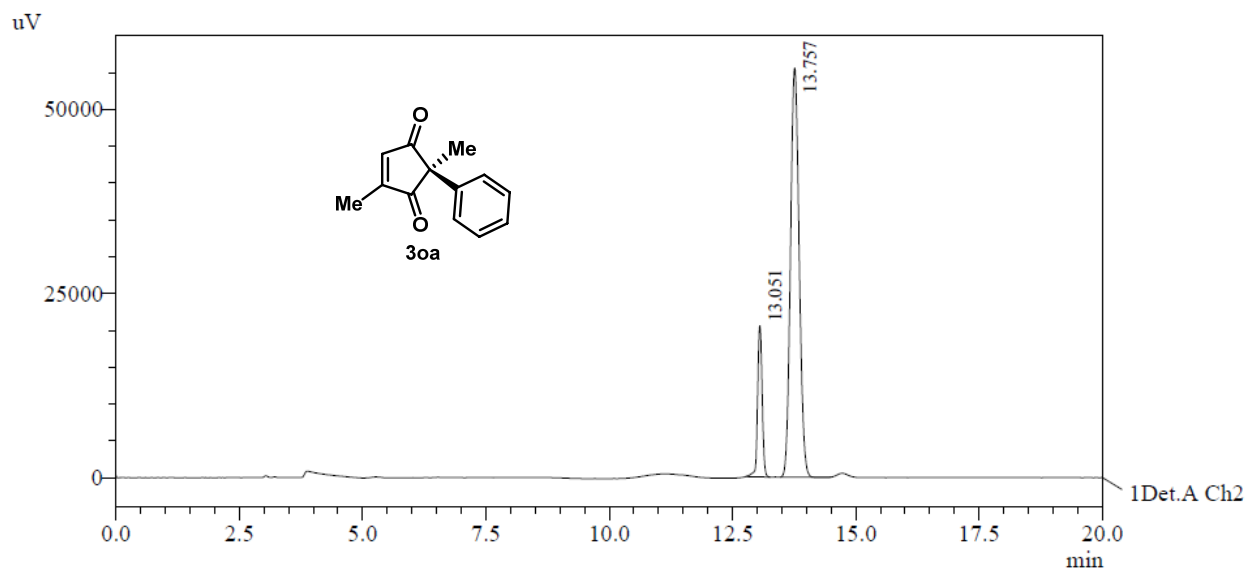




PeakTable

Detector A Ch2 254nm

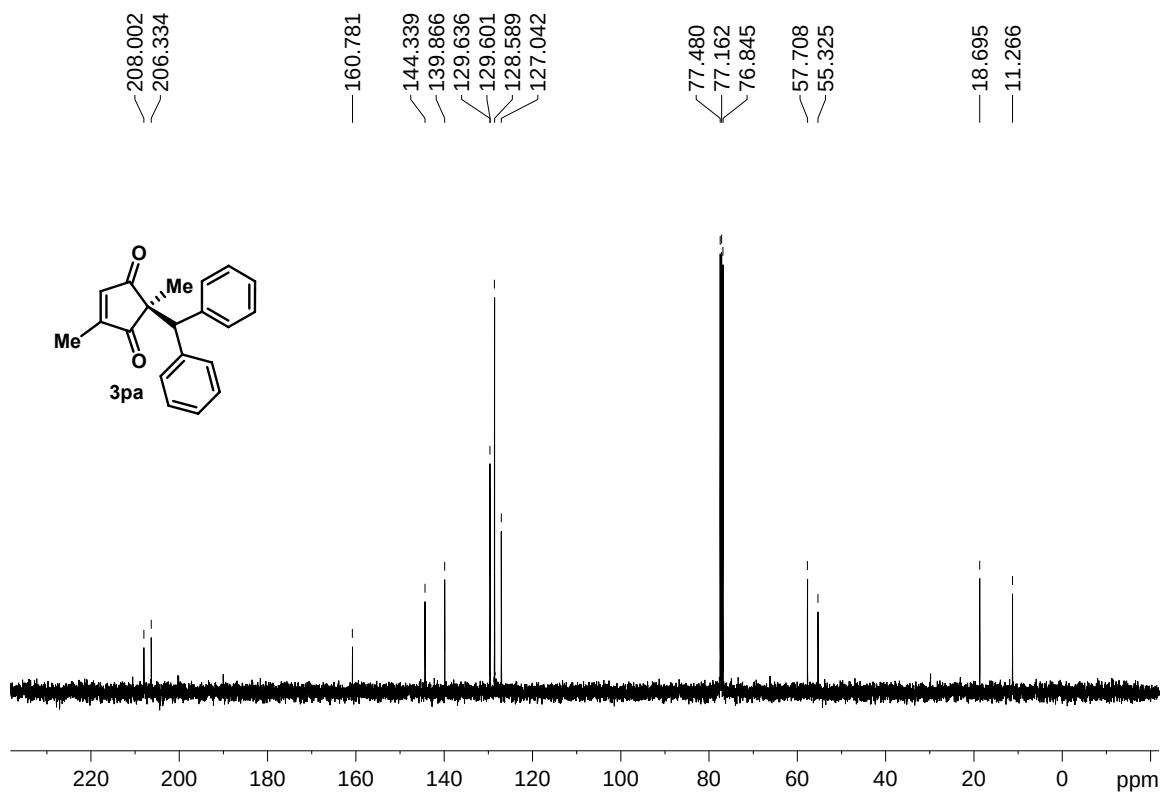
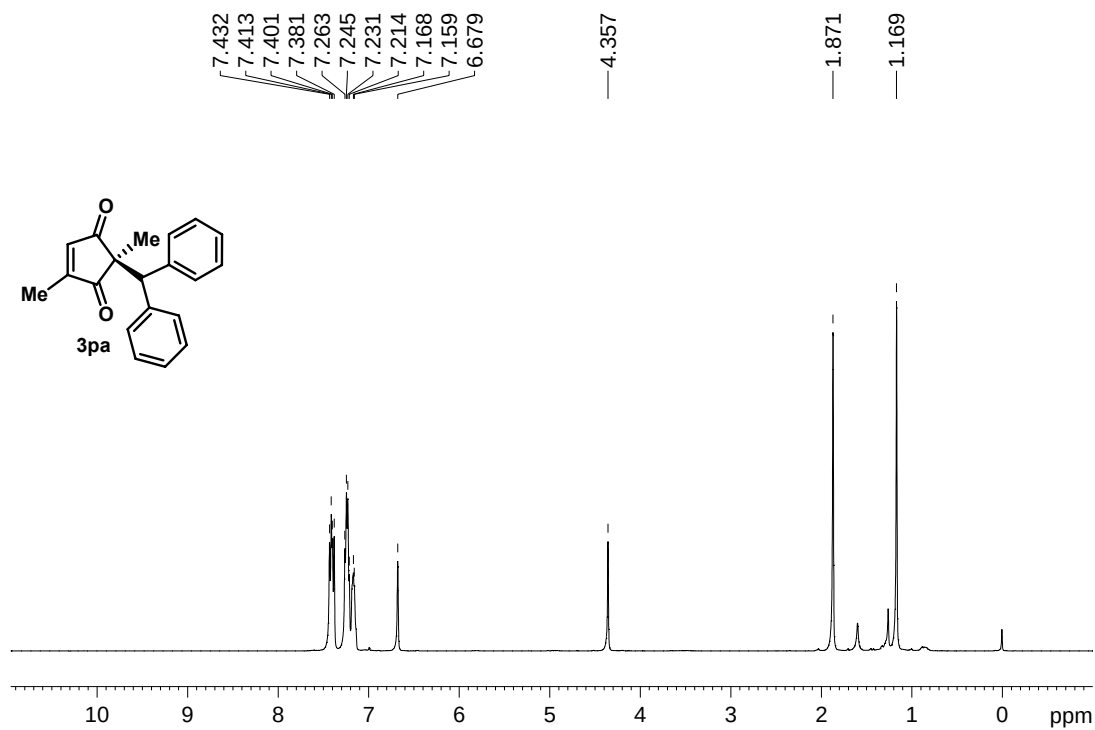
Peak#	Ret. Time	Area	Area %
1	13.018	283946	50.578
2	14.013	277457	49.422
Total		561403	100.000

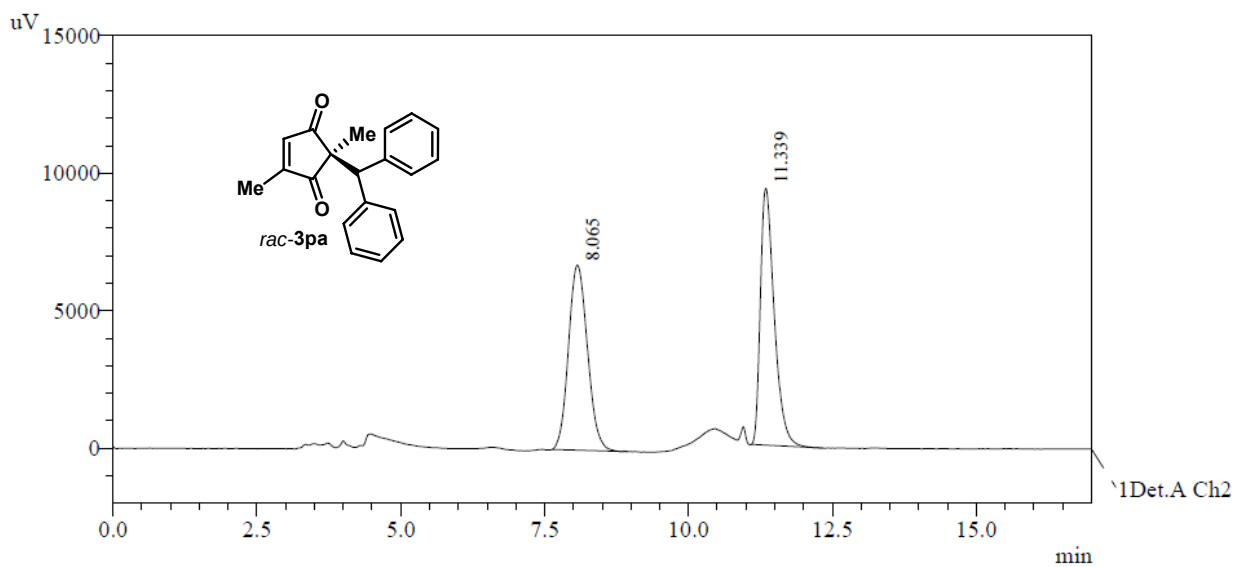


PeakTable

Detector A Ch2 254nm

Peak#	Ret. Time	Area	Area %
1	13.051	132861	16.400
2	13.757	677257	83.600
Total		810119	100.000

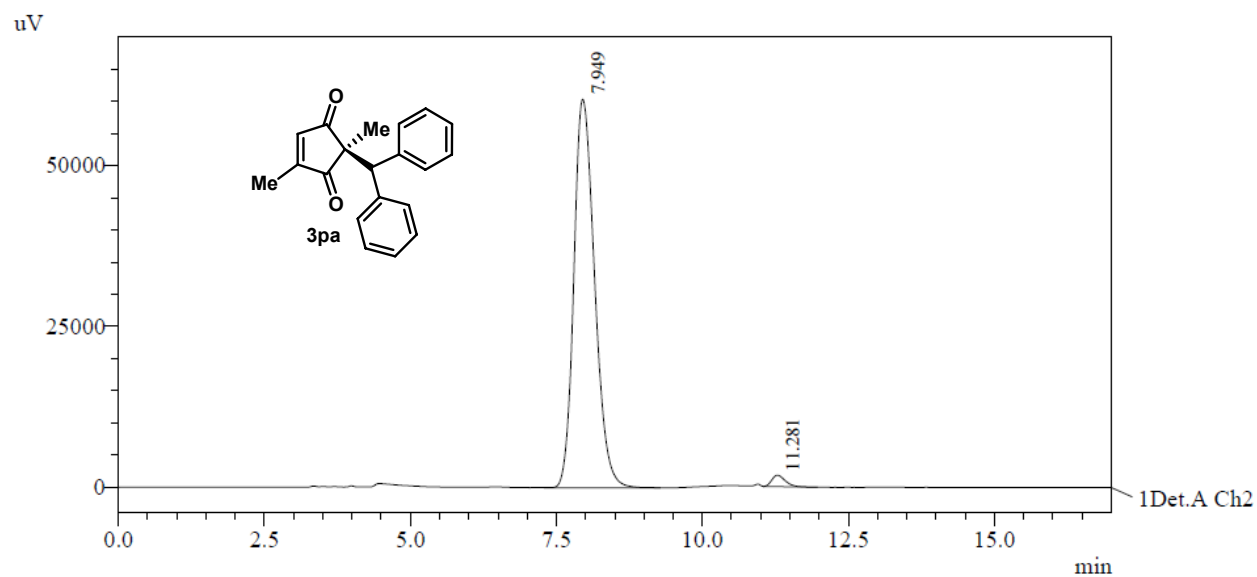




PeakTable

Detector A Ch2 254nm

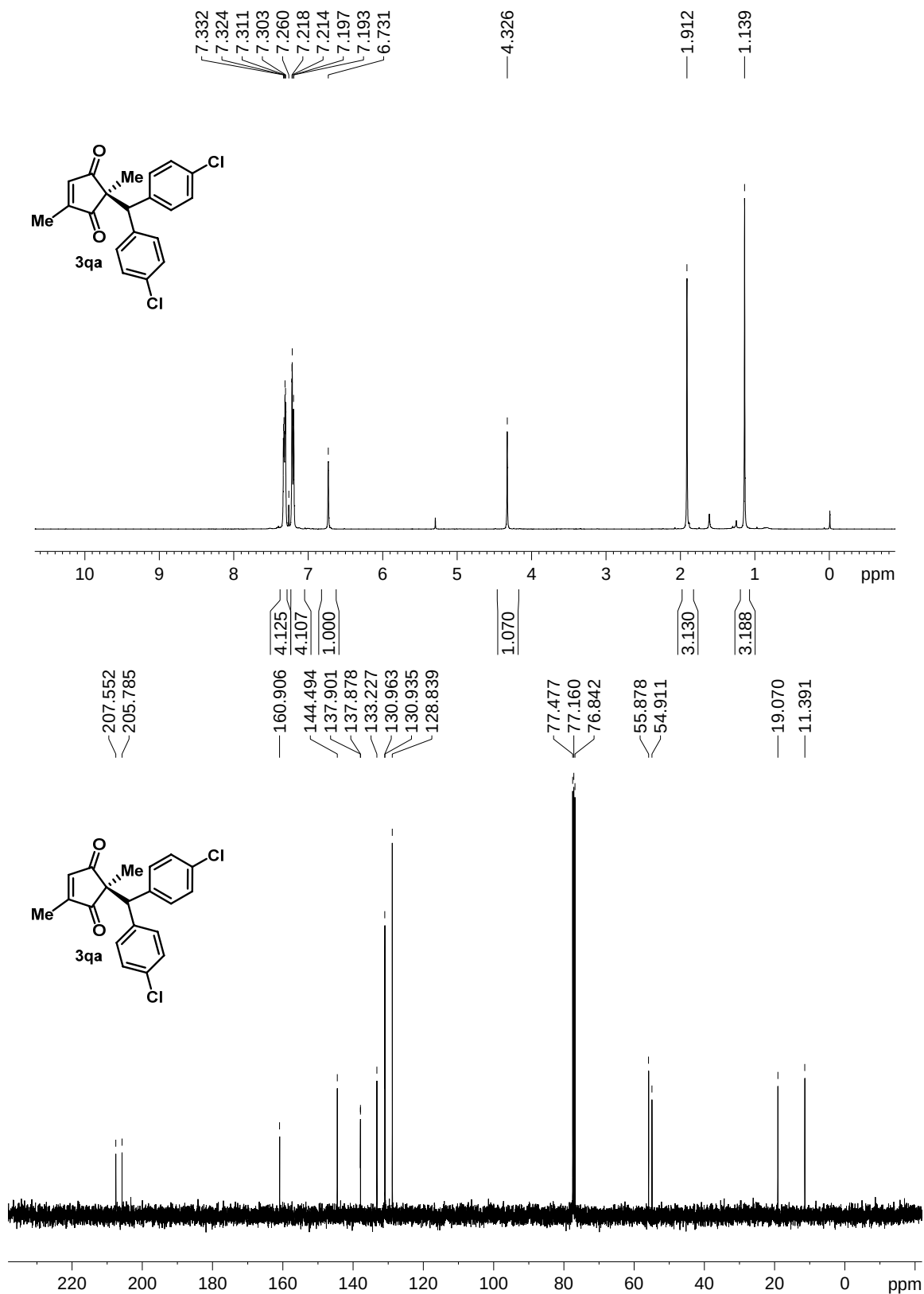
Peak#	Ret. Time	Area	Area %
1	8.065	154594	49.712
2	11.339	156385	50.288
Total		310978	100.000

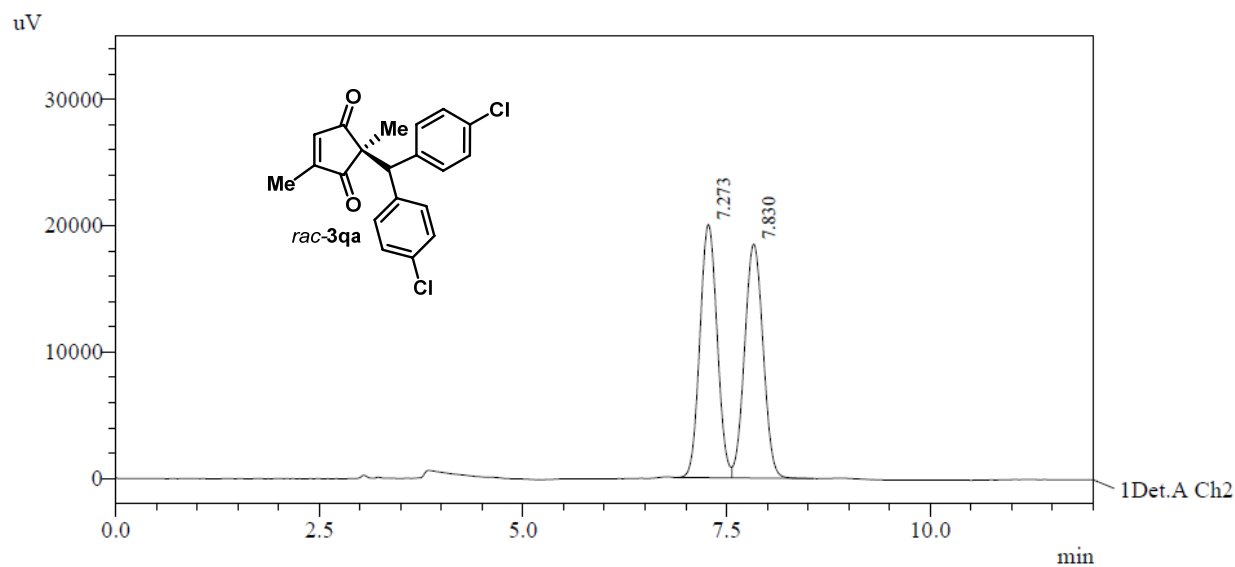


PeakTable

Detector A Ch2 254nm

Peak#	Ret. Time	Area	Area %
1	7.949	1493901	98.178
2	11.281	27726	1.822
Total		1521627	100.000

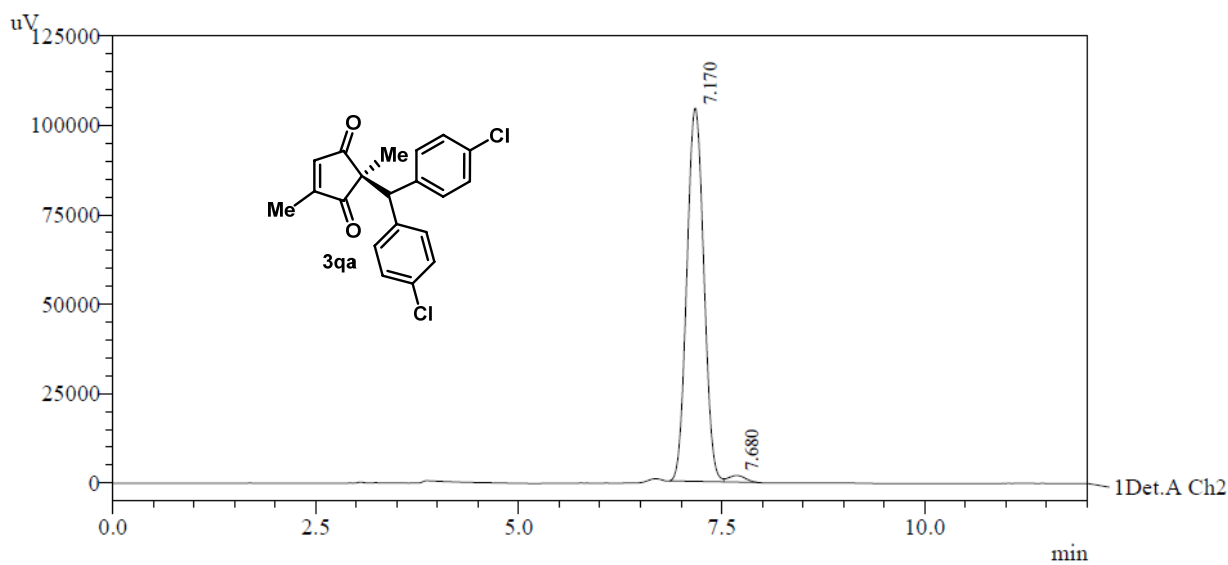




PeakTable

Detector A Ch2 254nm

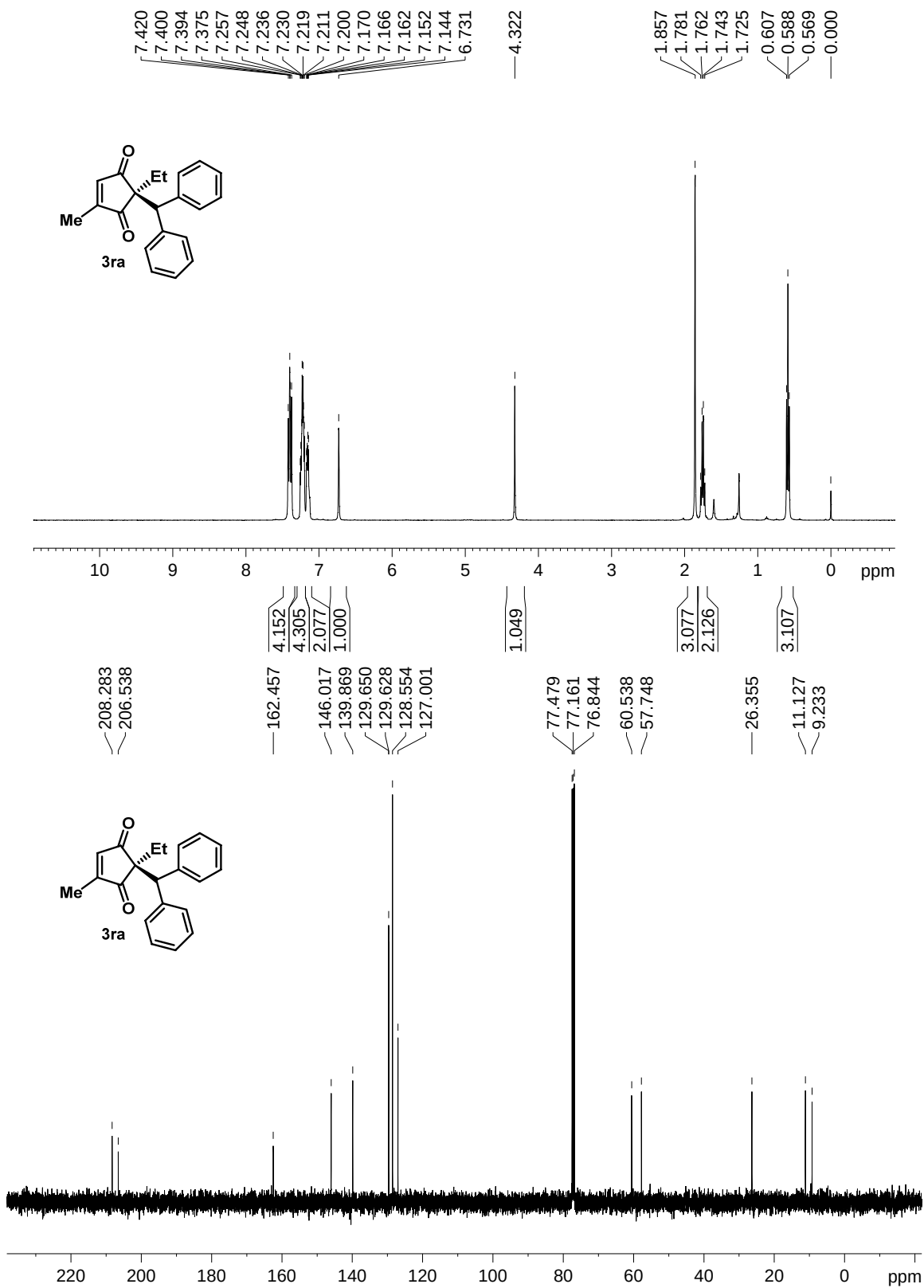
Peak#	Ret. Time	Area	Area %
1	7.273	295336	50.276
2	7.830	292089	49.724
Total		587425	100.000

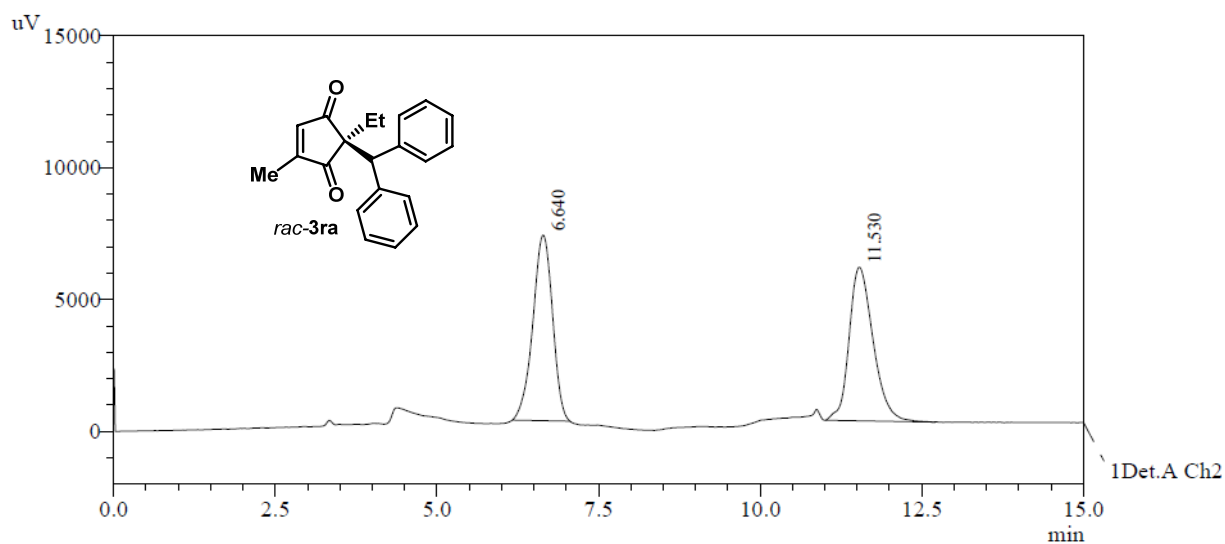


PeakTable

Detector A Ch2 254nm

Peak#	Ret. Time	Area	Area %
1	7.170	1519523	98.267
2	7.680	26798	1.733
Total		1546322	100.000

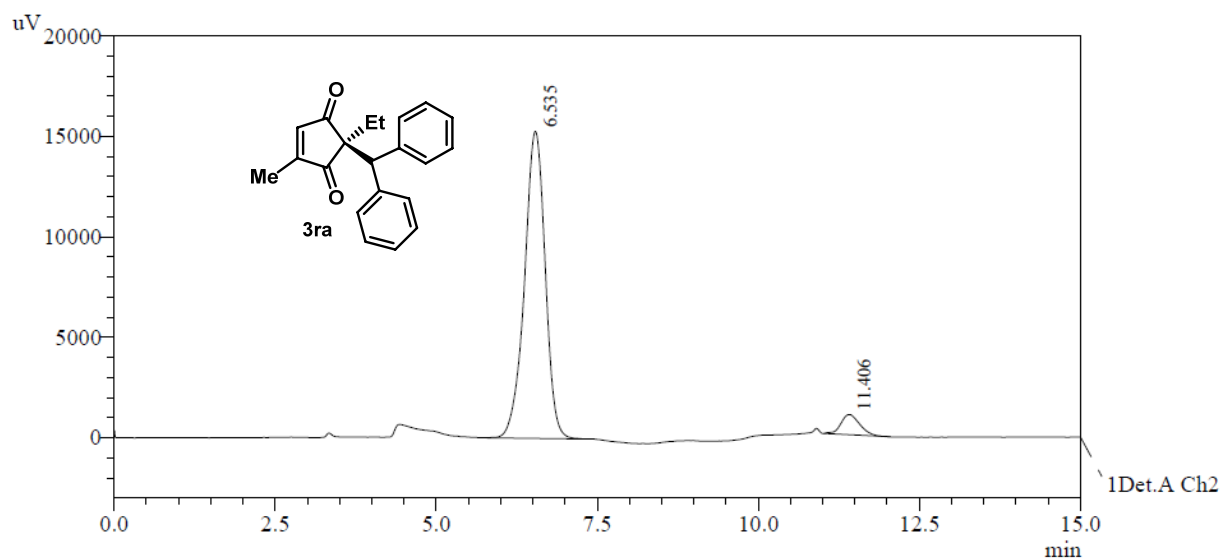




PeakTable

Detector A Ch2 254nm

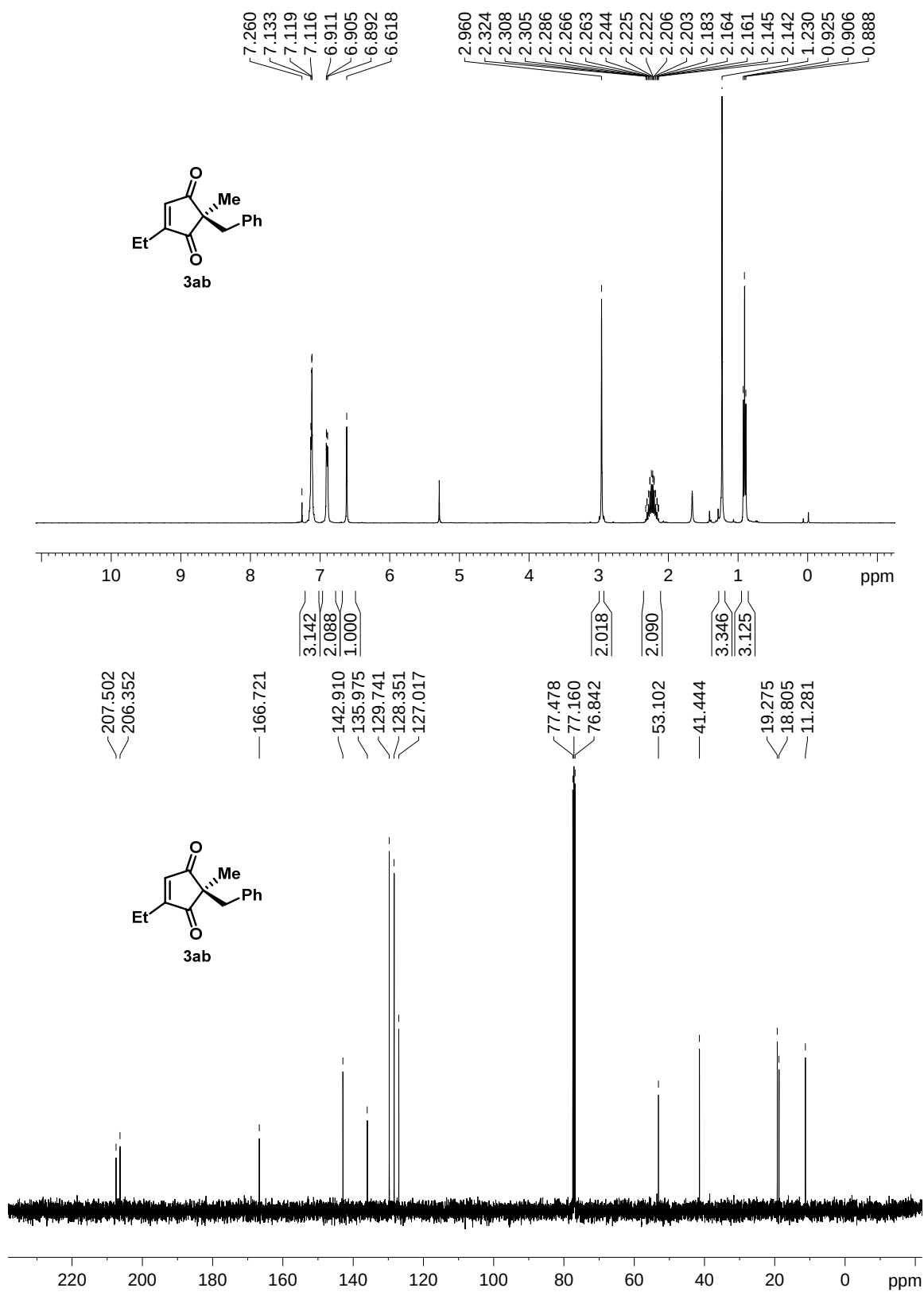
Peak#	Ret. Time	Area	Area %
1	6.640	149476	49.781
2	11.530	150790	50.219
Total		300266	100.000

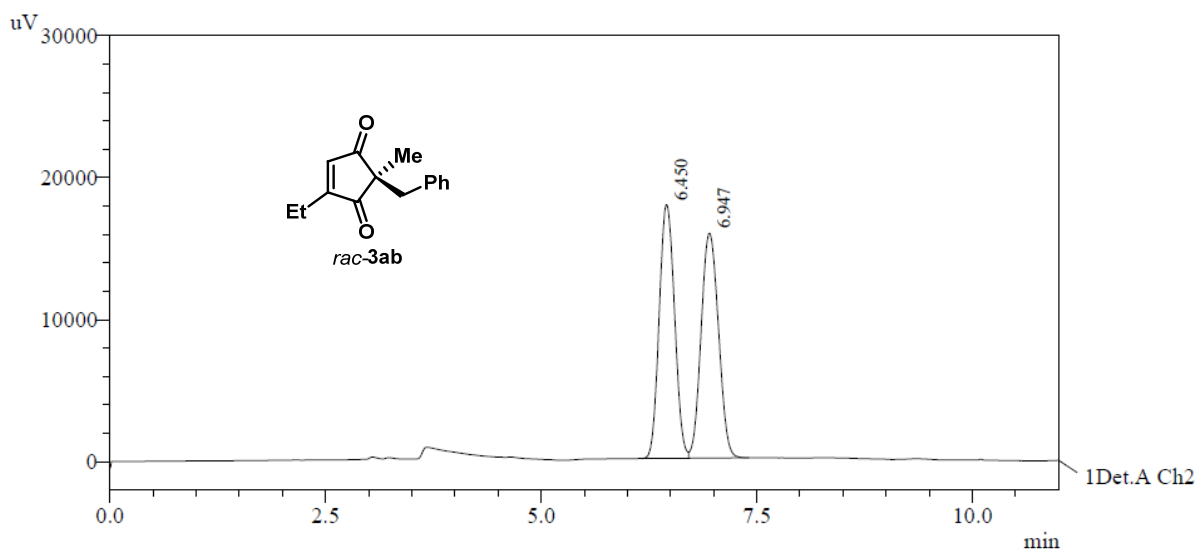


PeakTable

Detector A Ch2 254nm

Peak#	Ret. Time	Area	Area %
1	6.535	342273	94.353
2	11.406	20486	5.647
Total		362759	100.000

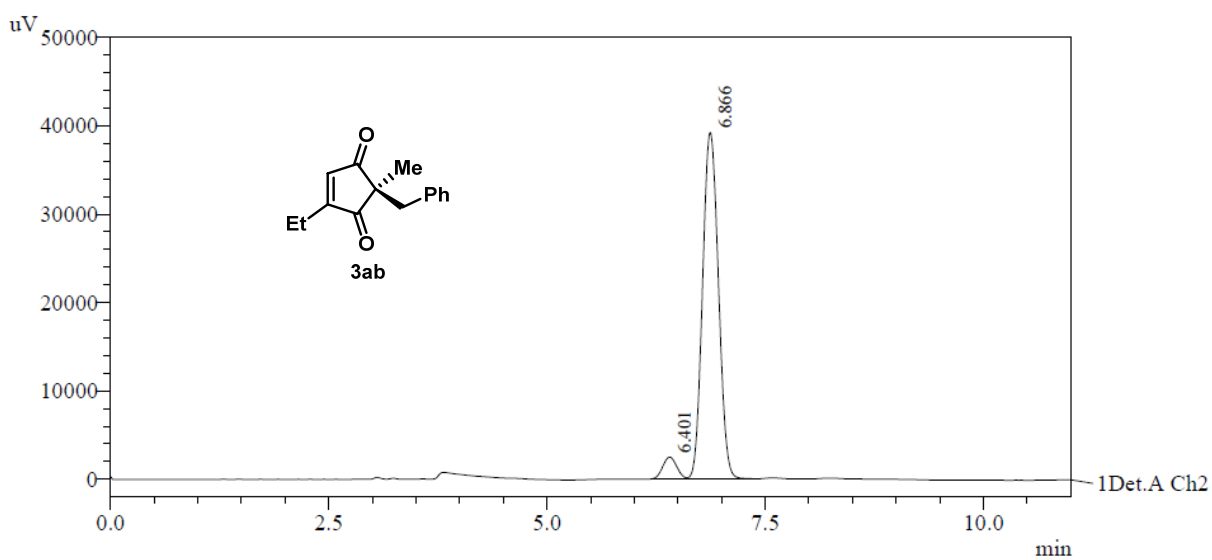




PeakTable

Detector A Ch2 254nm

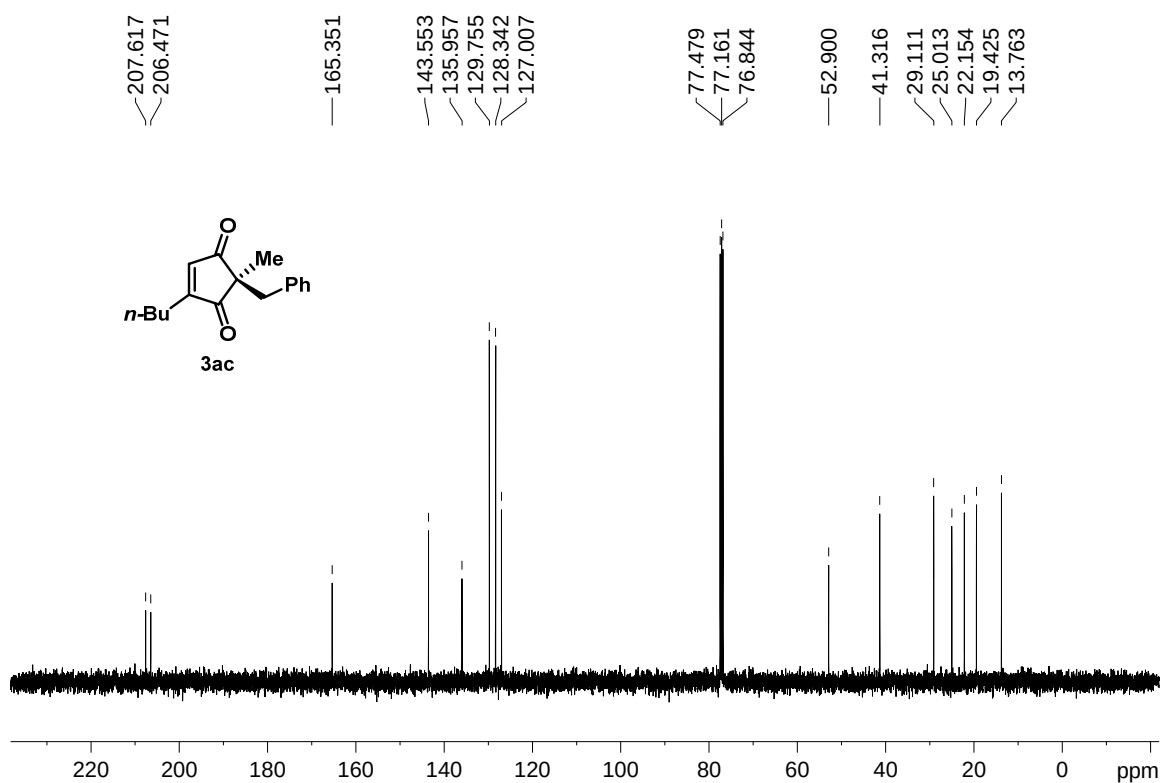
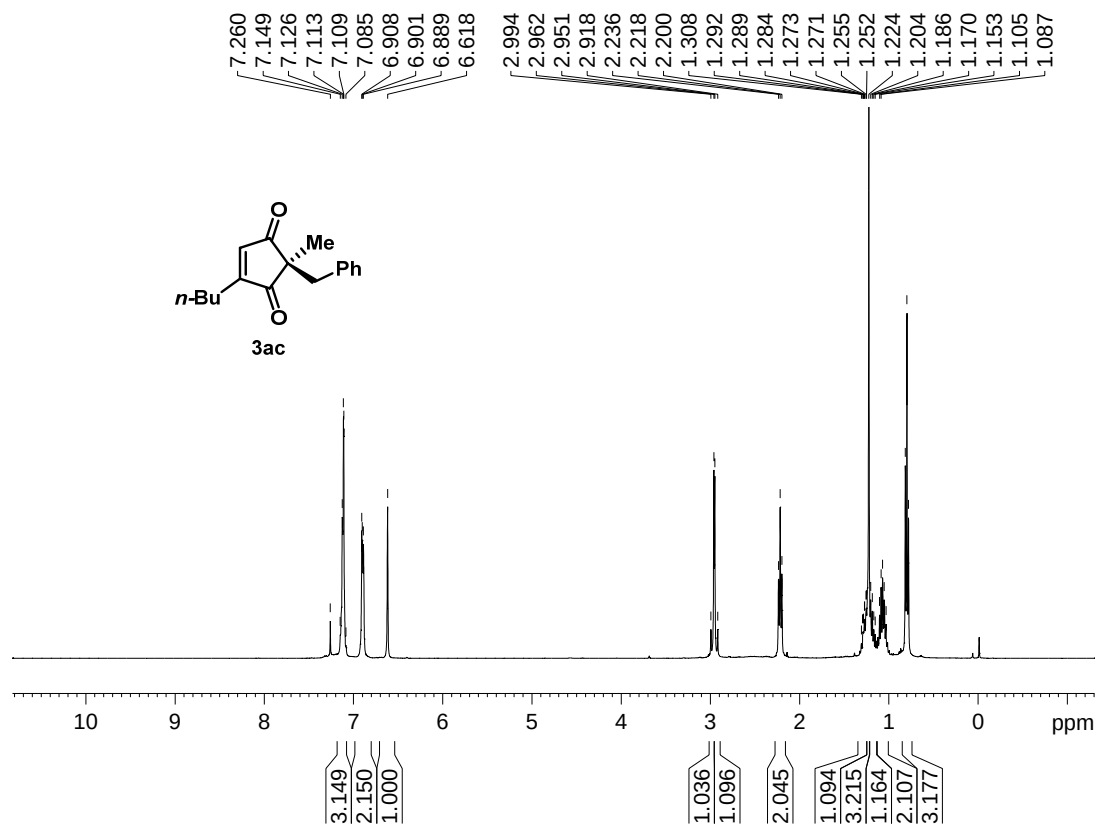
Peak#	Ret. Time	Area	Area %
1	6.450	221932	49.970
2	6.947	222196	50.030
Total		444128	100.000

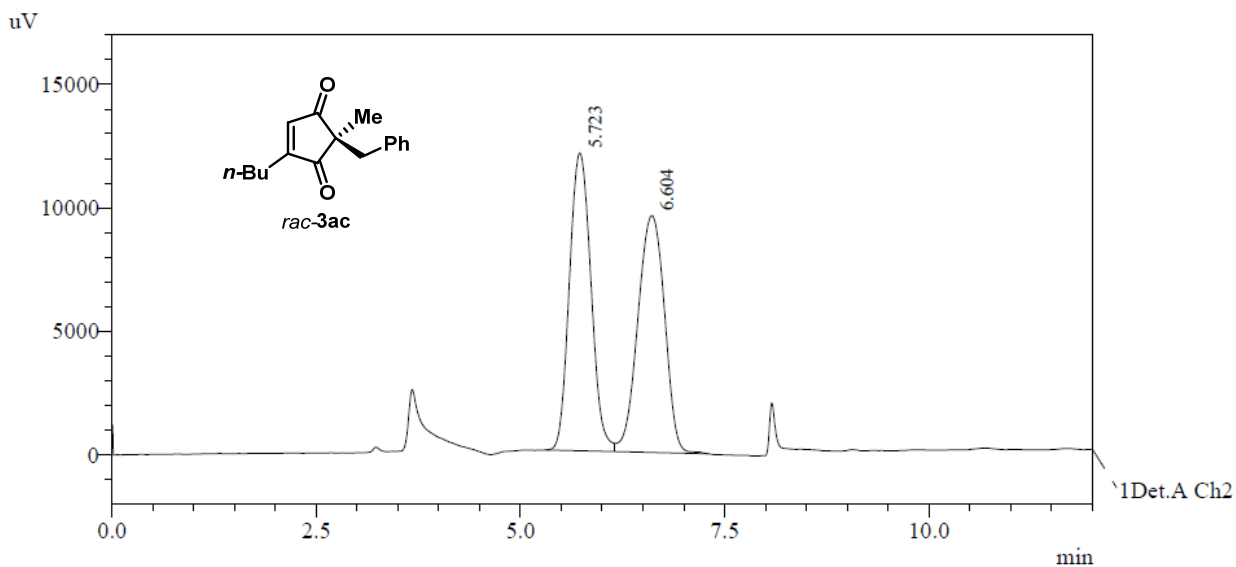


PeakTable

Detector A Ch2 254nm

Peak#	Ret. Time	Area	Area %
1	6.401	27349	5.239
2	6.866	494638	94.761
Total		521987	100.000

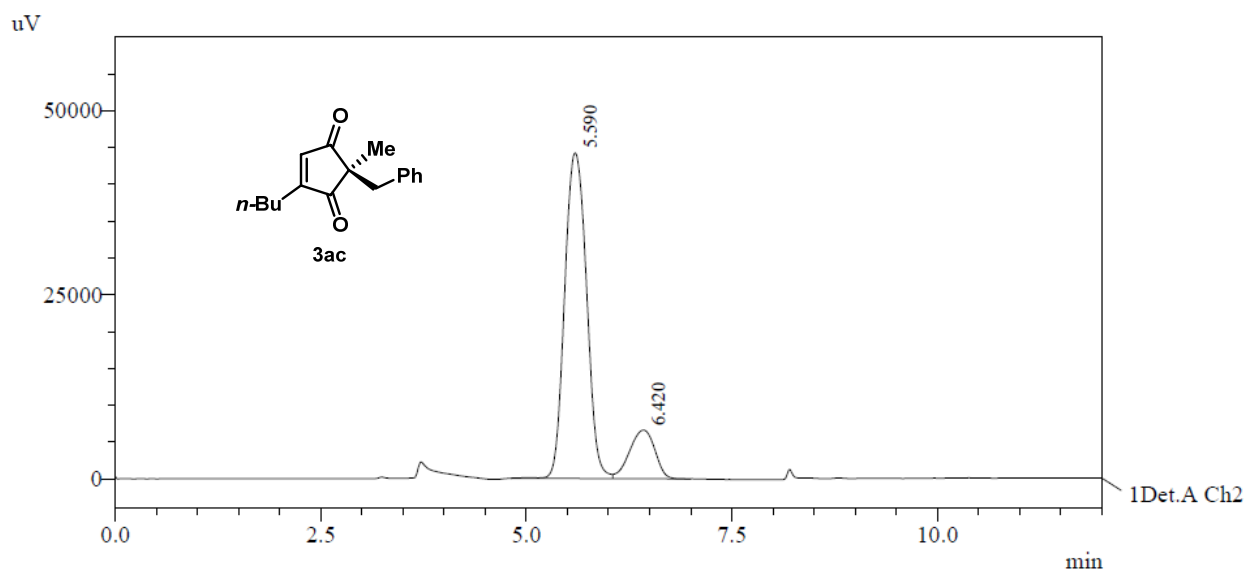




PeakTable

Detector A Ch2 254nm

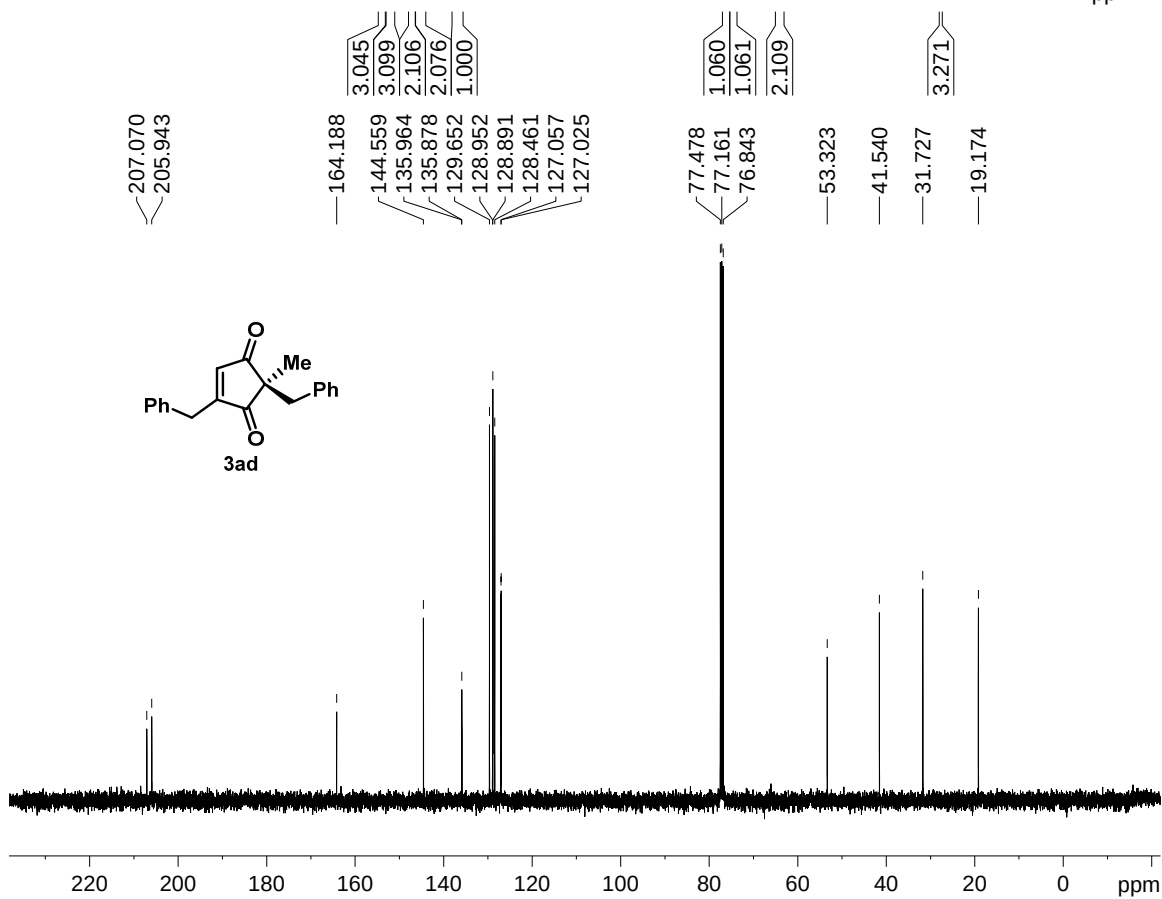
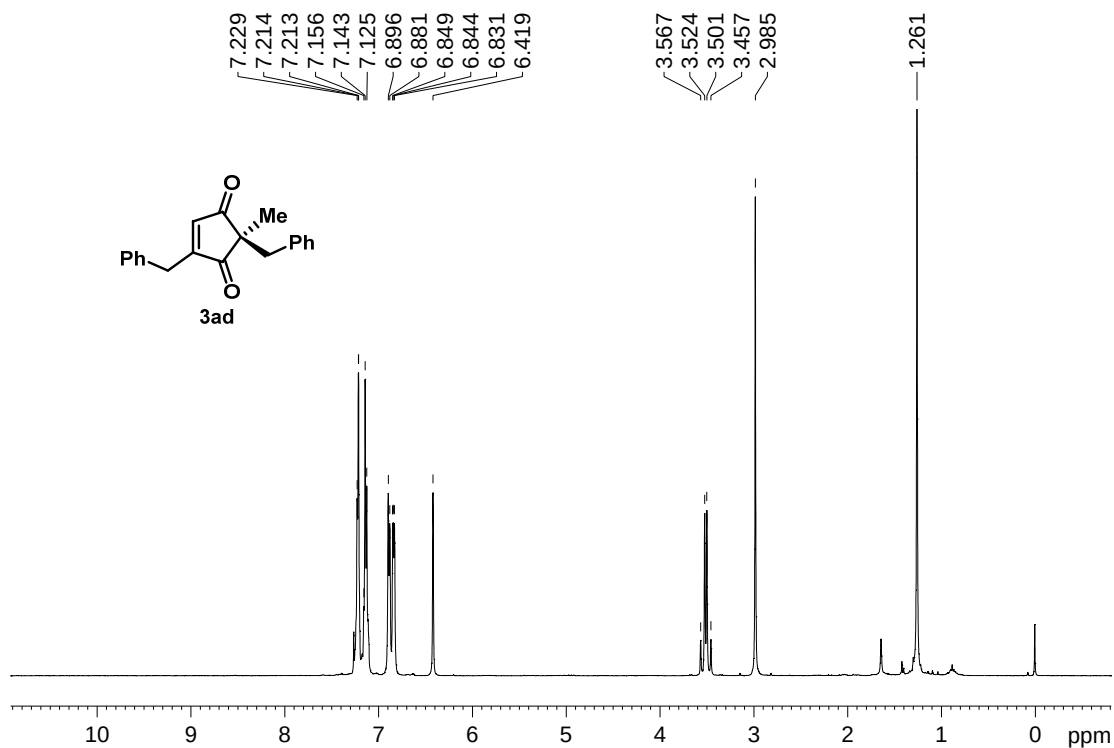
Peak#	Ret. Time	Area	Area %
1	5.723	221531	50.360
2	6.604	218366	49.640
Total		439896	100.000

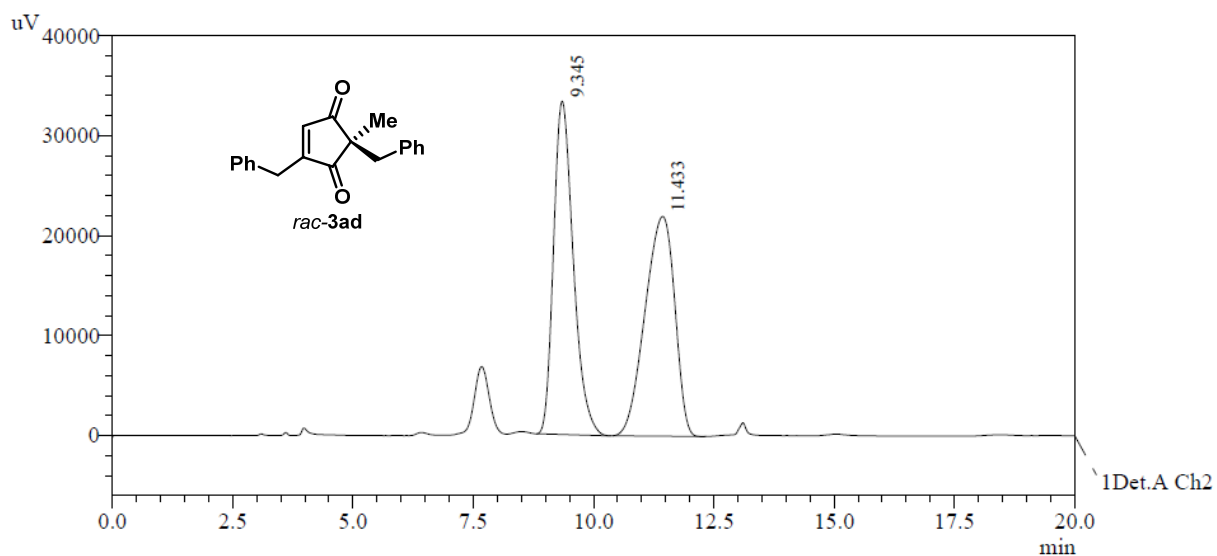


PeakTable

Detector A Ch2 254nm

Peak#	Ret. Time	Area	Area %
1	5.590	817704	85.291
2	6.420	141015	14.709
Total		958718	100.000

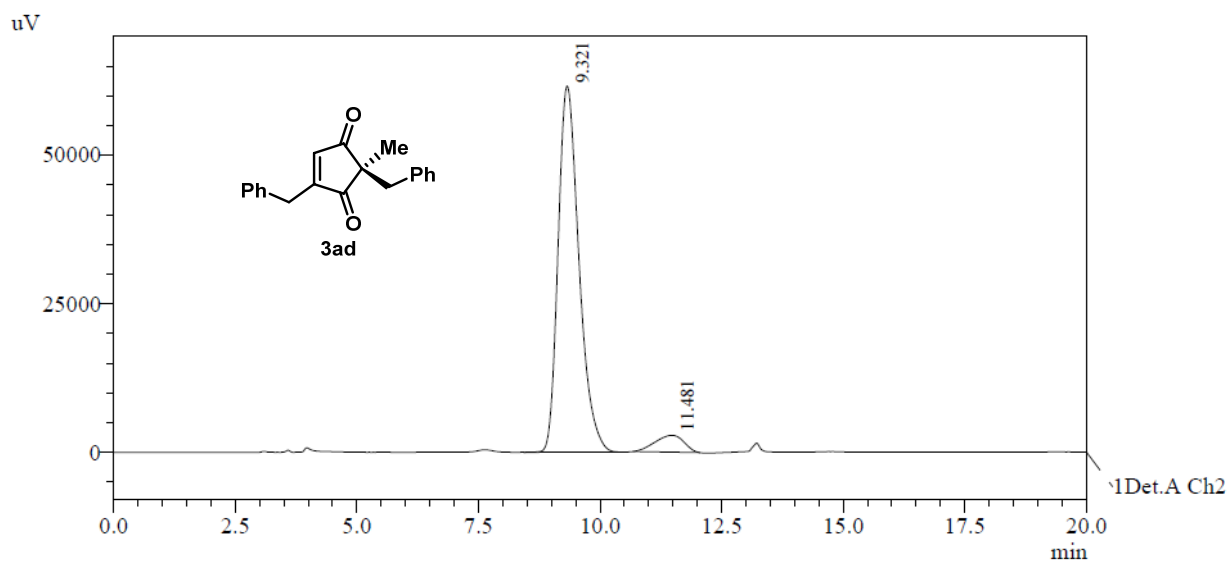




PeakTable

Detector A Ch2 254nm

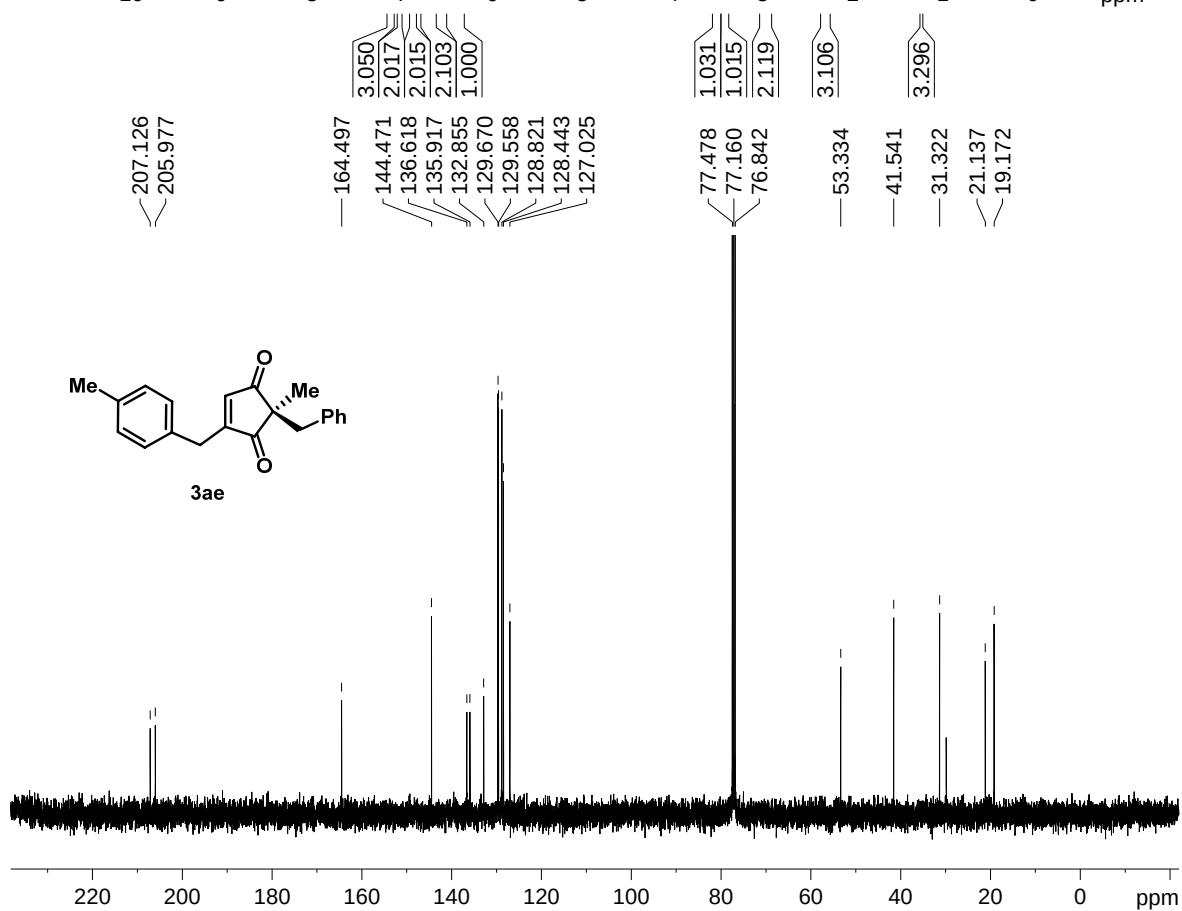
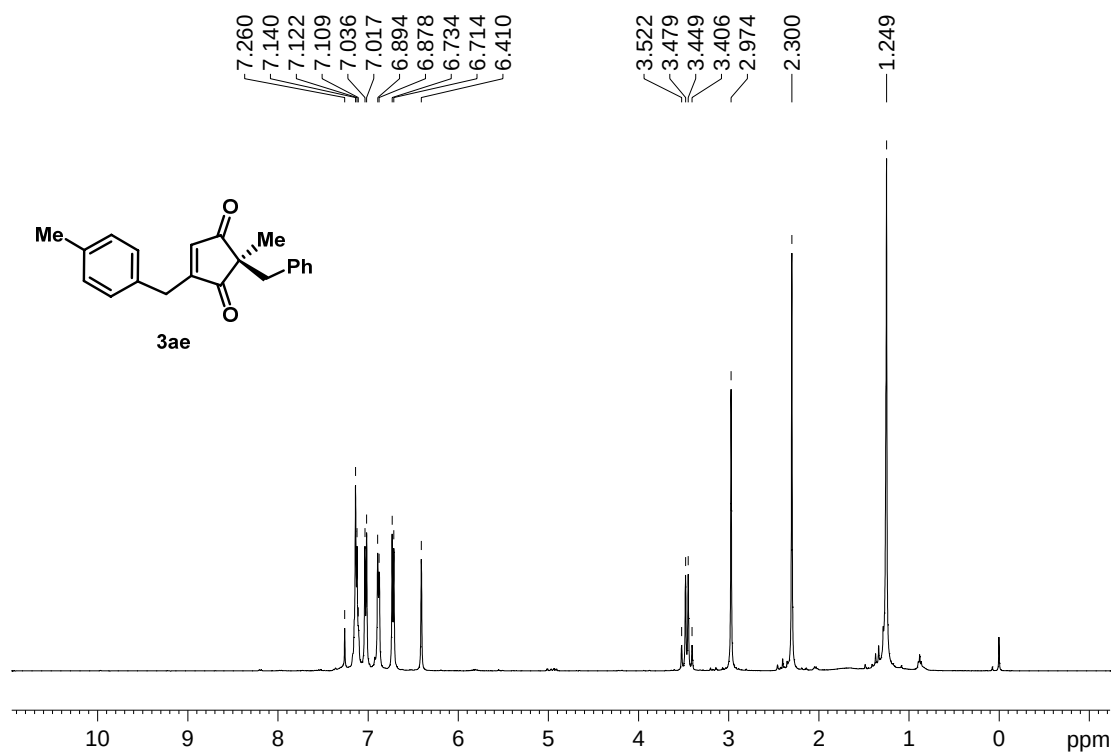
Peak#	Ret. Time	Area	Area %
1	9.345	953560	50.220
2	11.433	945193	49.780
Total		1898753	100.000

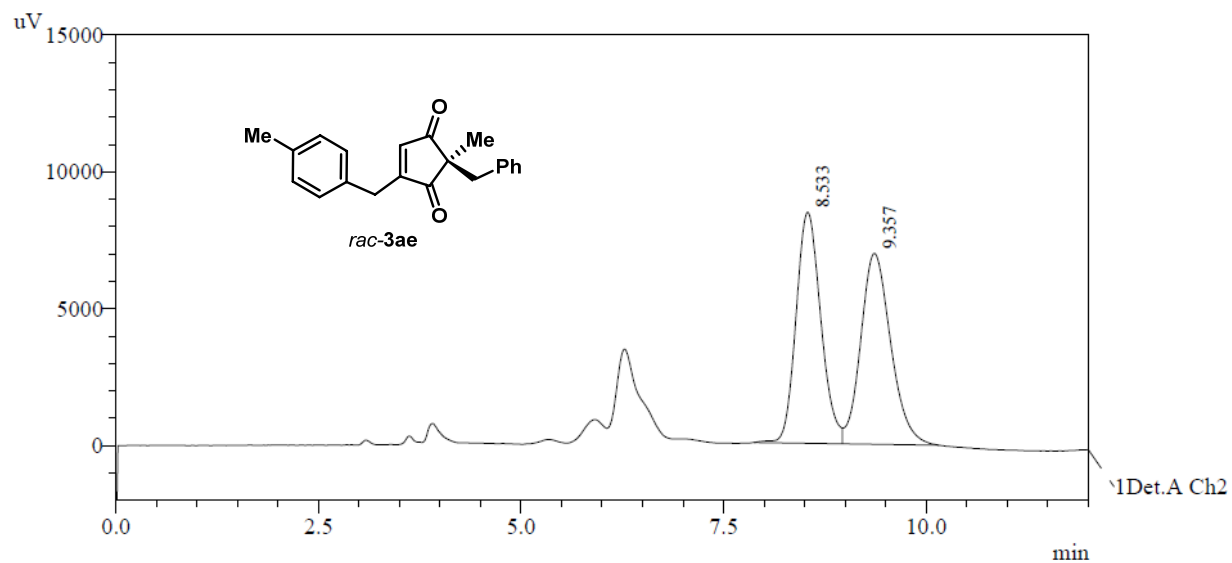


PeakTable

Detector A Ch2 254nm

Peak#	Ret. Time	Area	Area %
1	9.321	1842250	94.017
2	11.481	117245	5.983
Total		1959494	100.000

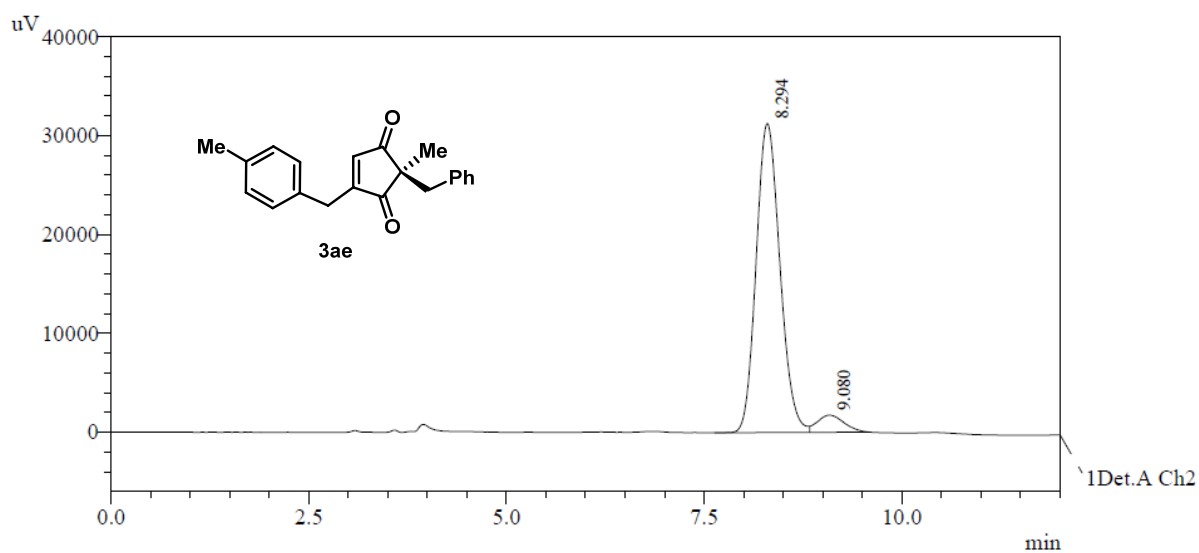




PeakTable

Detector A Ch2 254nm

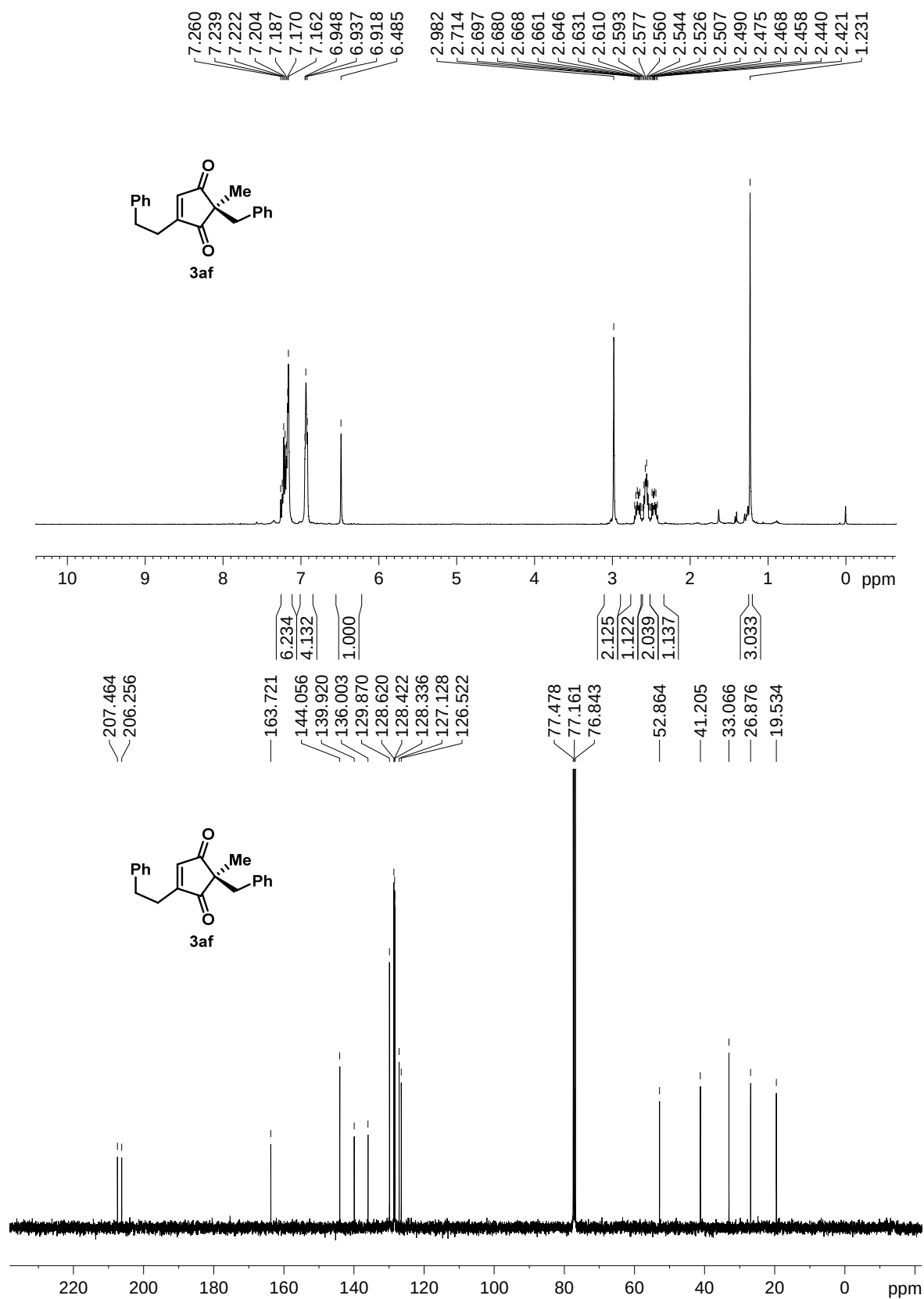
Peak#	Ret. Time	Area	Area %
1	8.533	179579	49.974
2	9.357	179763	50.026
Total		359342	100.000

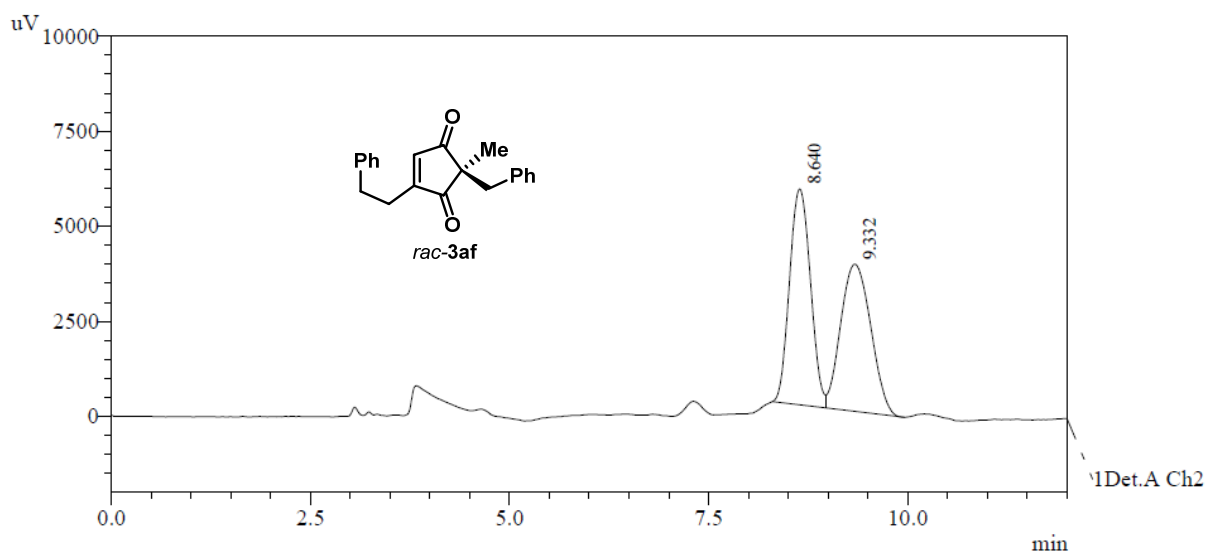


PeakTable

Detector A Ch2 254nm

Peak#	Ret. Time	Area	Area %
1	8.294	654881	94.160
2	9.080	40615	5.840
Total		695496	100.000

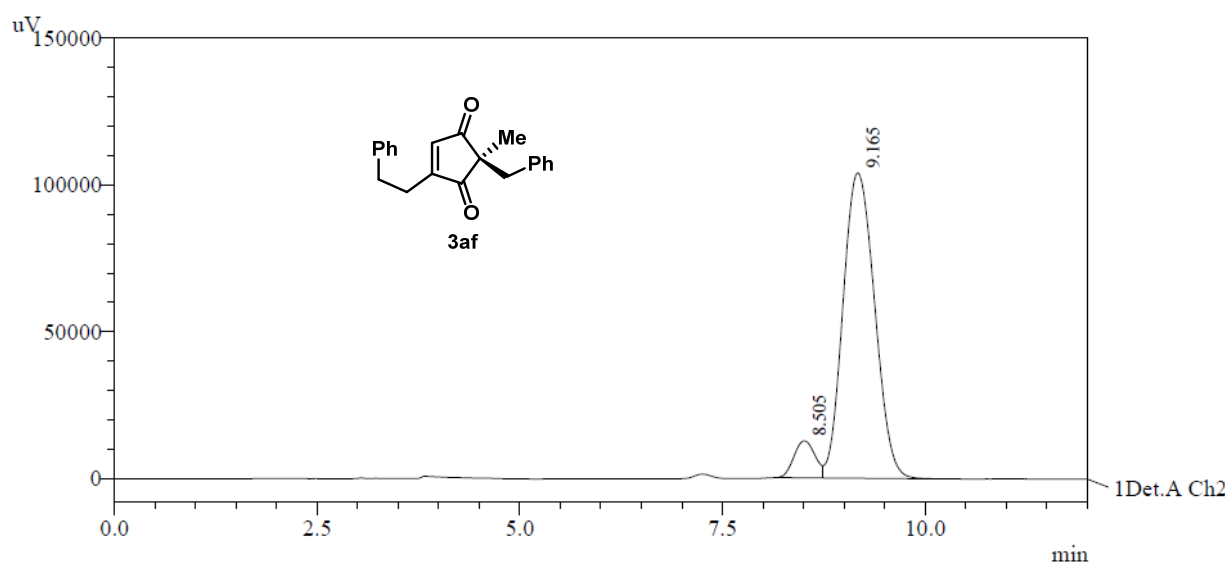




PeakTable

Detector A Ch2 254nm

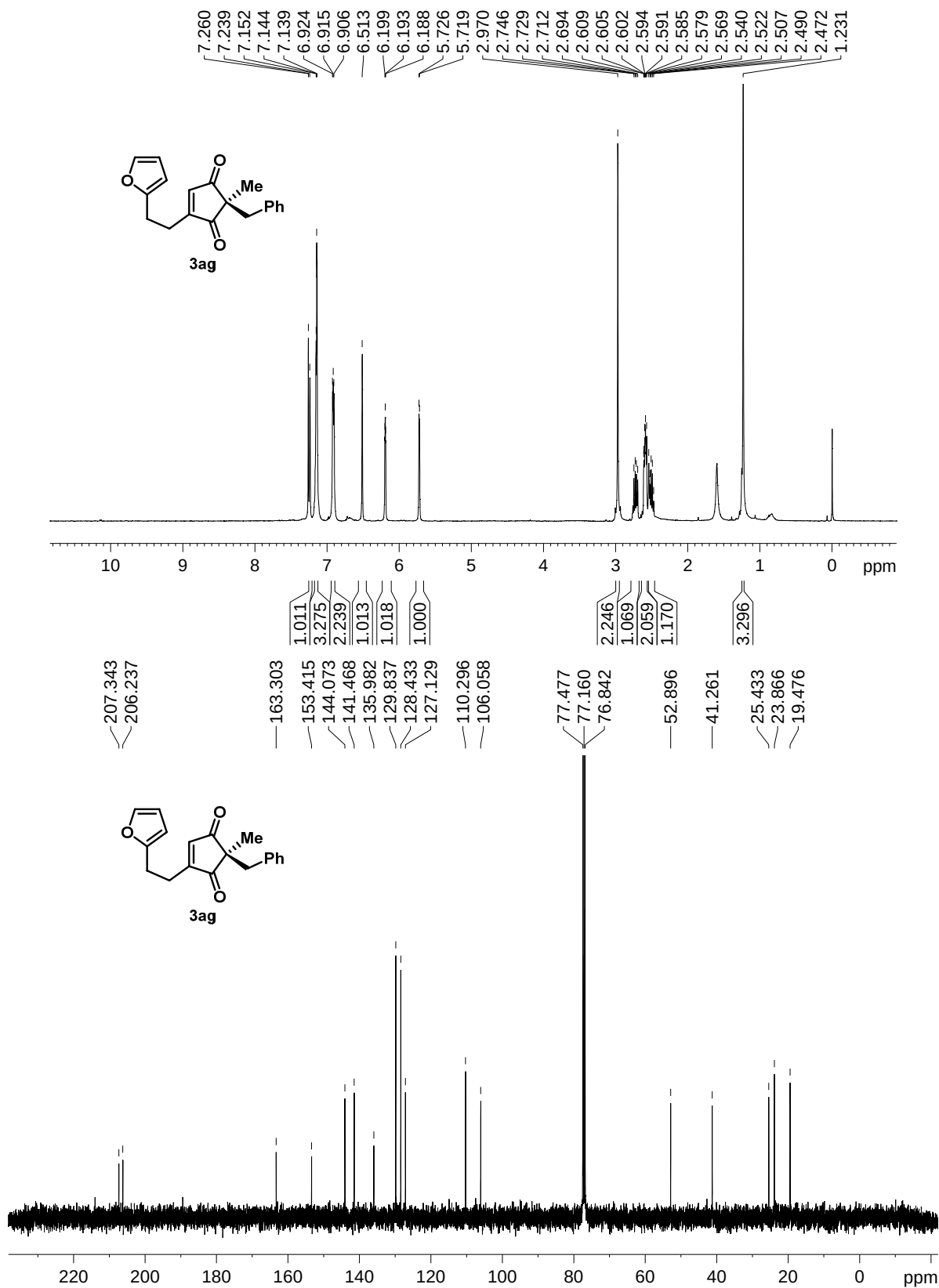
Peak#	Ret. Time	Area	Area %
1	8.640	104087	50.577
2	9.332	101712	49.423
Total		205799	100.000

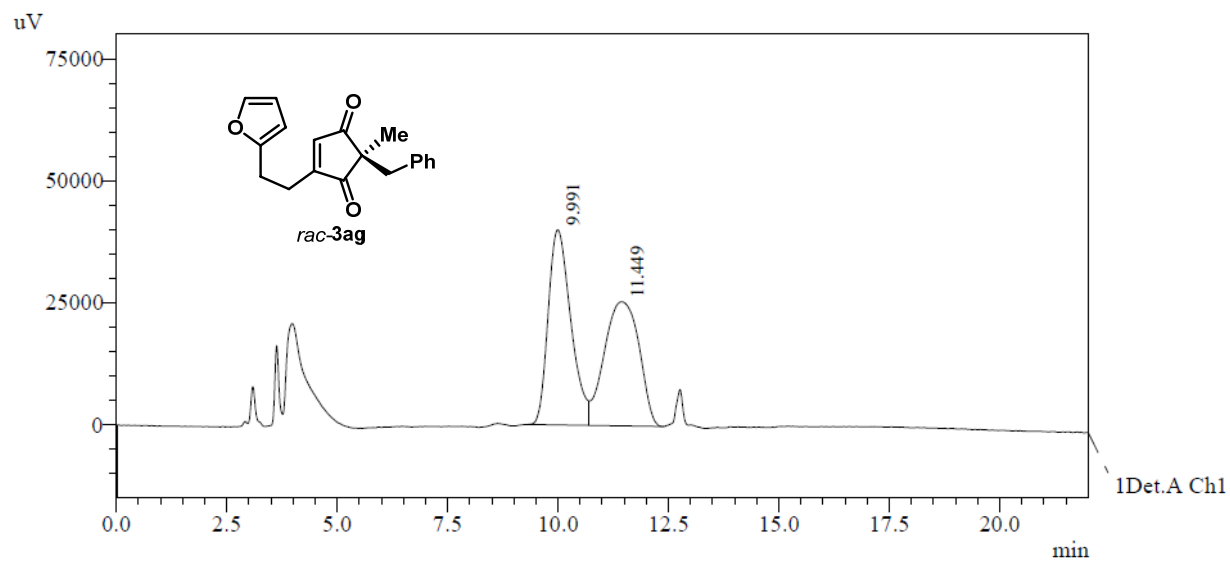


PeakTable

Detector A Ch2 254nm

Peak#	Ret. Time	Area	Area %
1	8.505	227676	7.465
2	9.165	2822251	92.535
Total		3049927	100.000

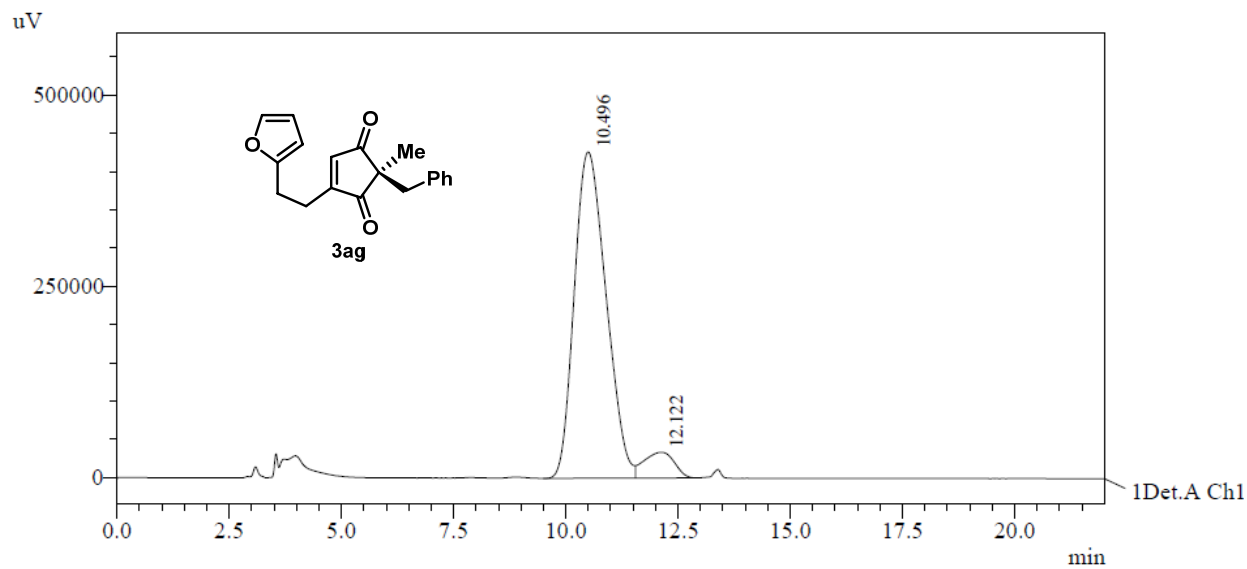




PeakTable

Detector A Ch1 210nm

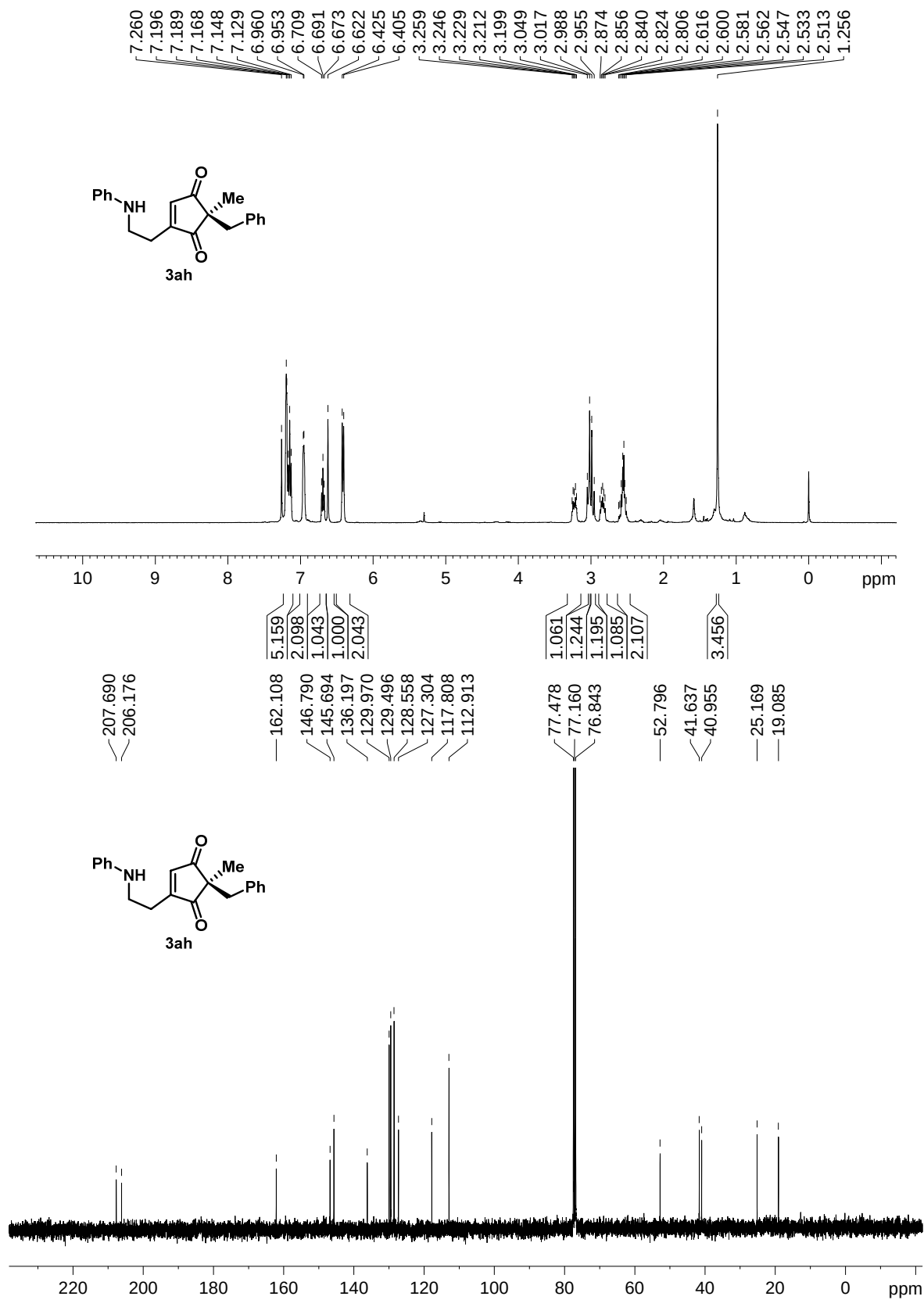
Peak#	Ret. Time	Area	Area %
1	9.991	1429551	50.614
2	11.449	1394889	49.386
Total		2824440	100.000

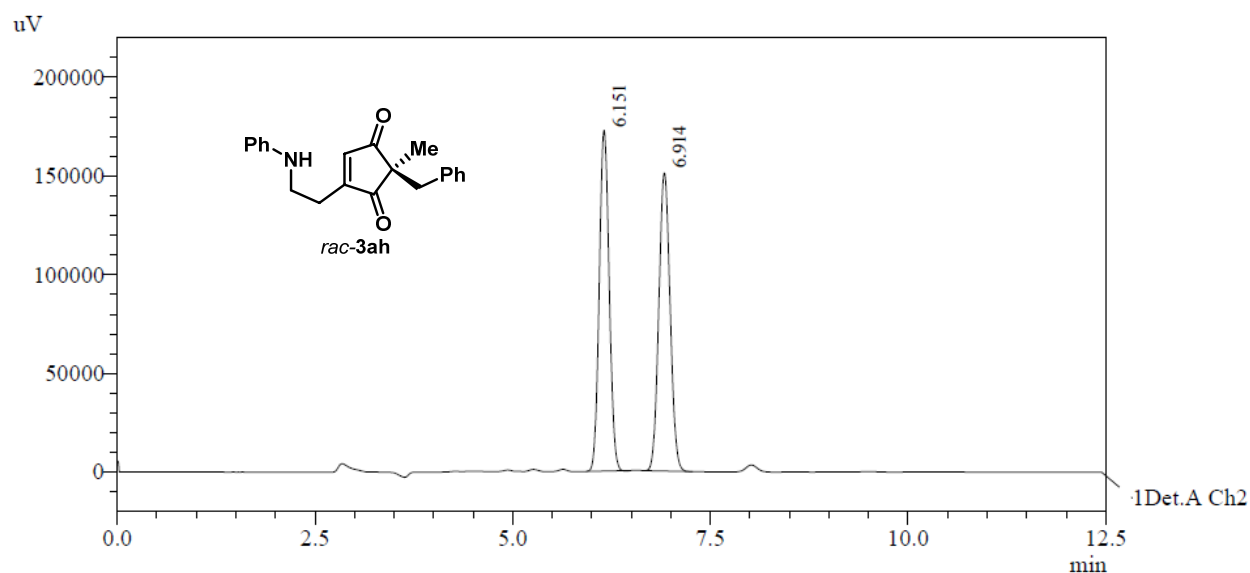


PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Area %
1	10.496	20997343	93.016
2	12.122	1576599	6.984
Total		22573942	100.000

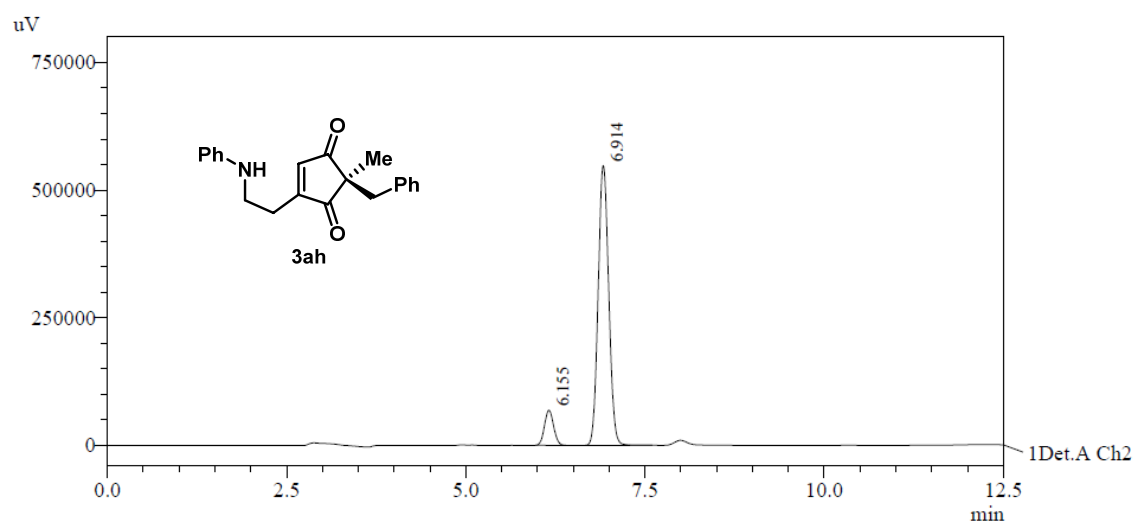




PeakTable

Detector A Ch2 254nm

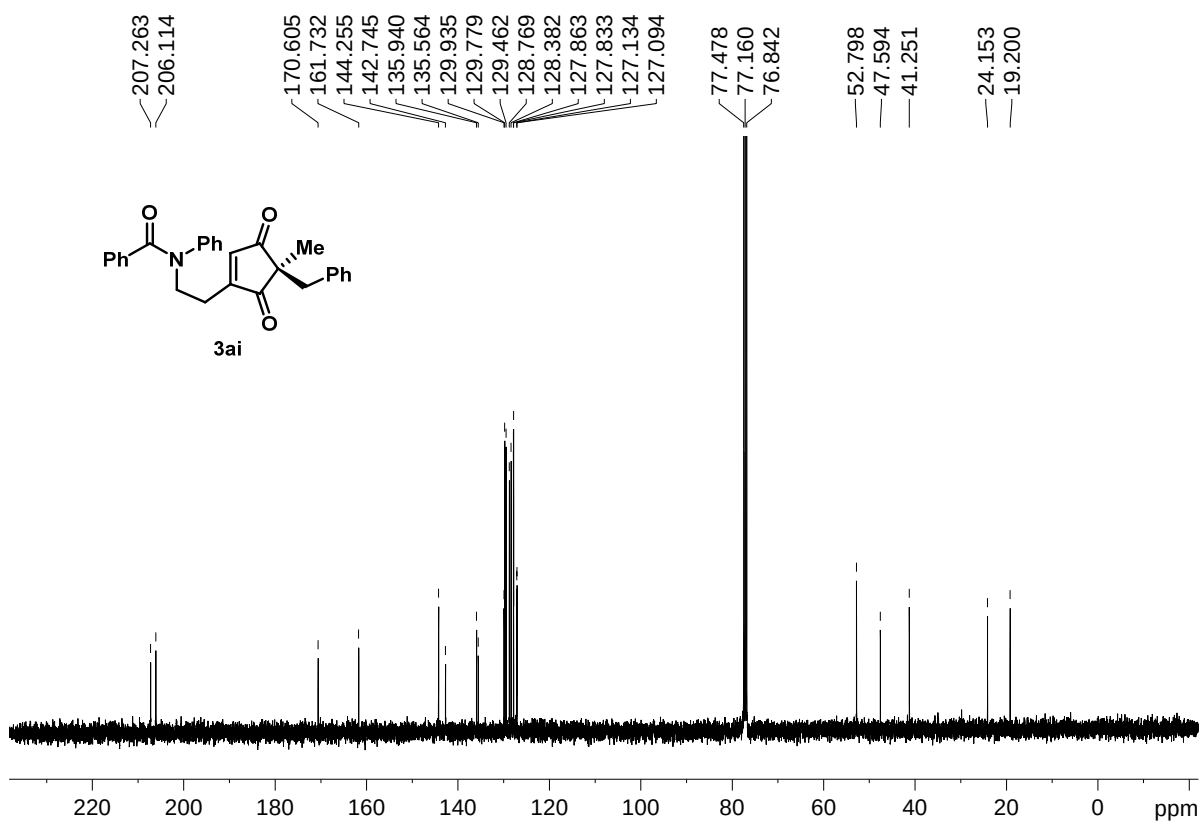
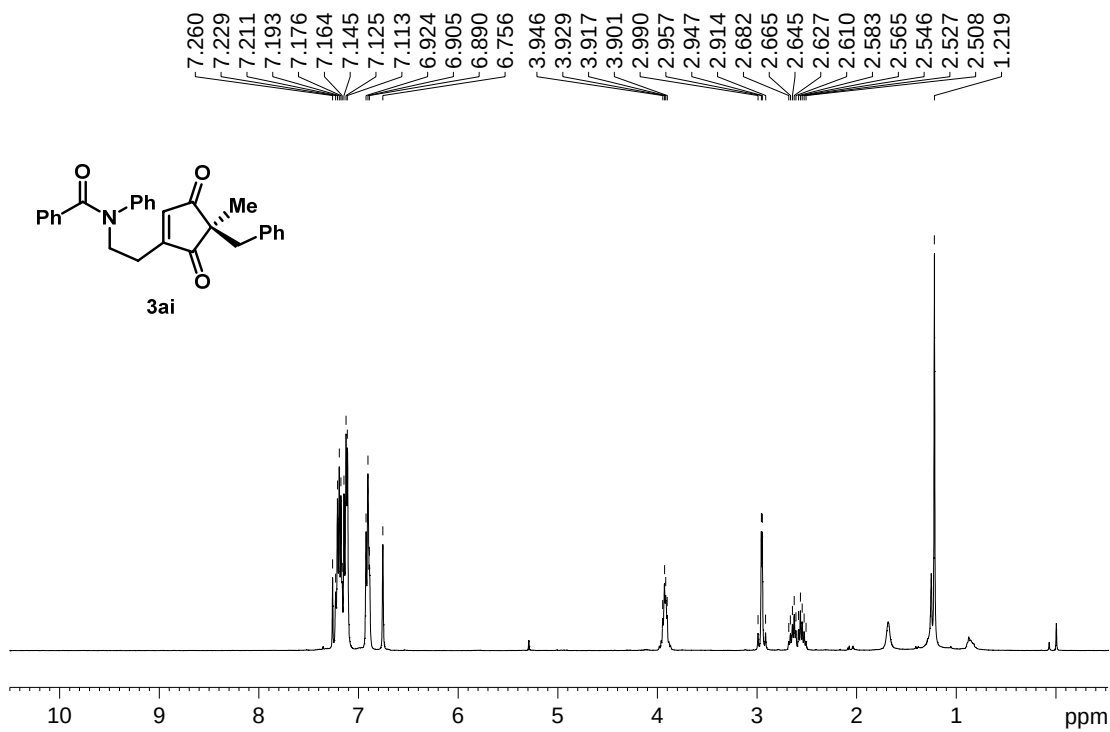
Peak#	Ret. Time	Area	Area %
1	6.151	1505445	50.103
2	6.914	1499241	49.897
Total		3004686	100.000

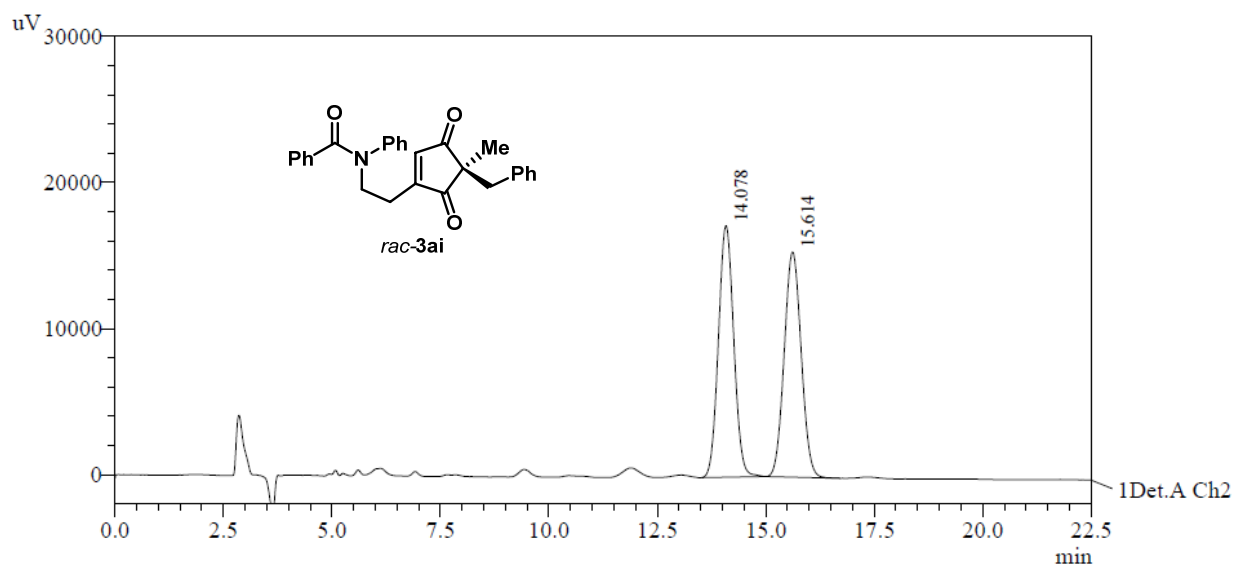


PeakTable

Detector A Ch2 254nm

Peak#	Ret. Time	Area	Area %
1	6.155	610403	9.819
2	6.914	5606346	90.181
Total		6216749	100.000

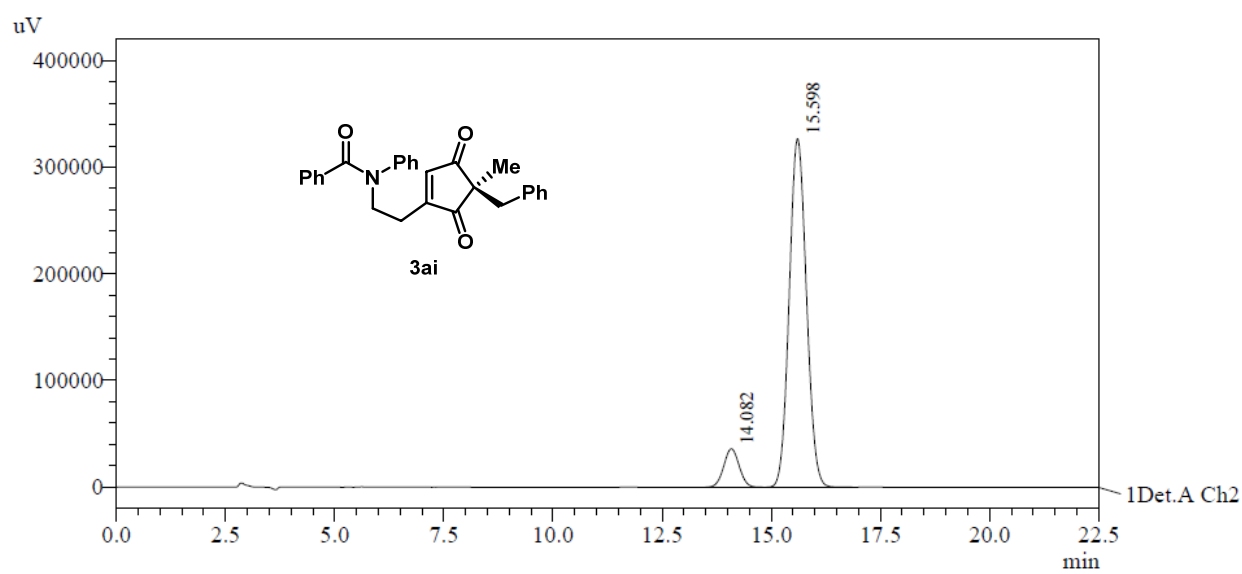




PeakTable

Detector A Ch2 254nm

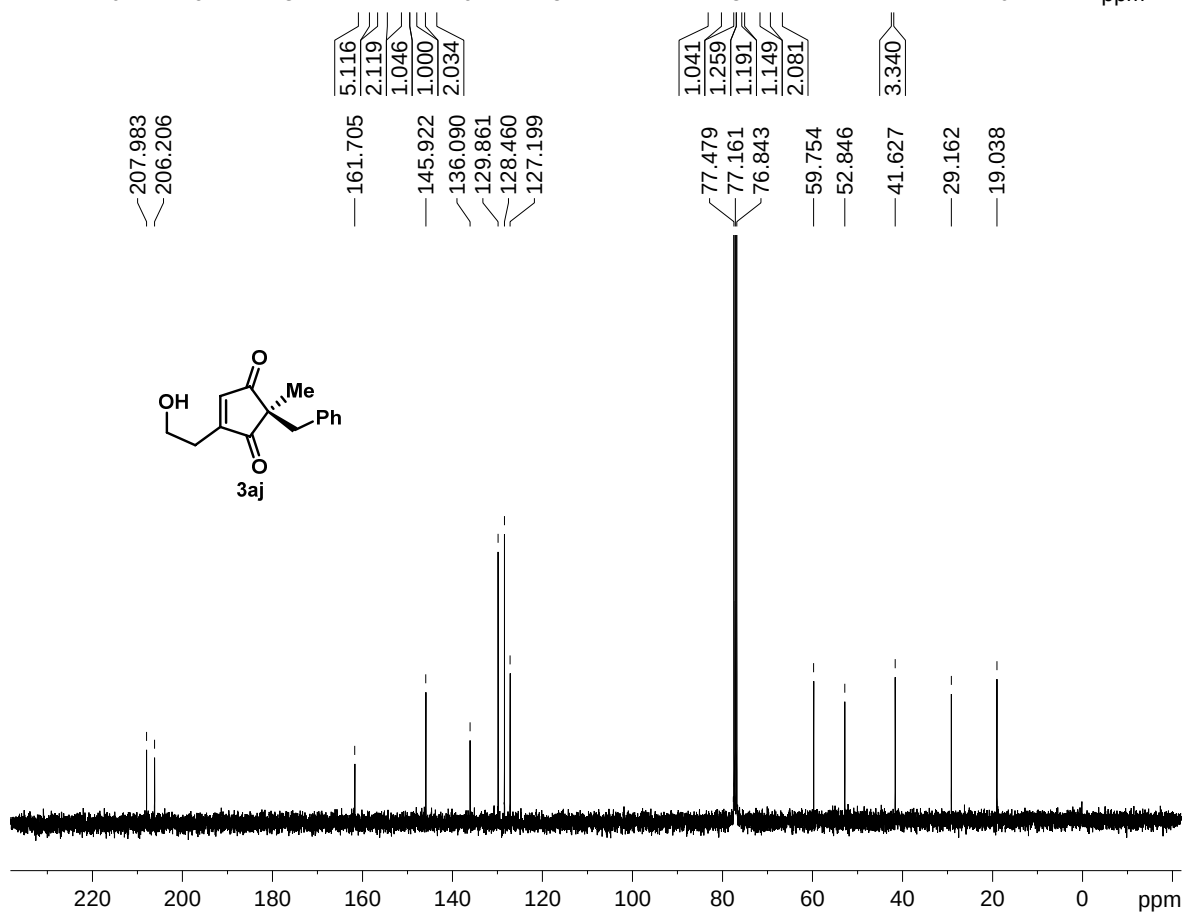
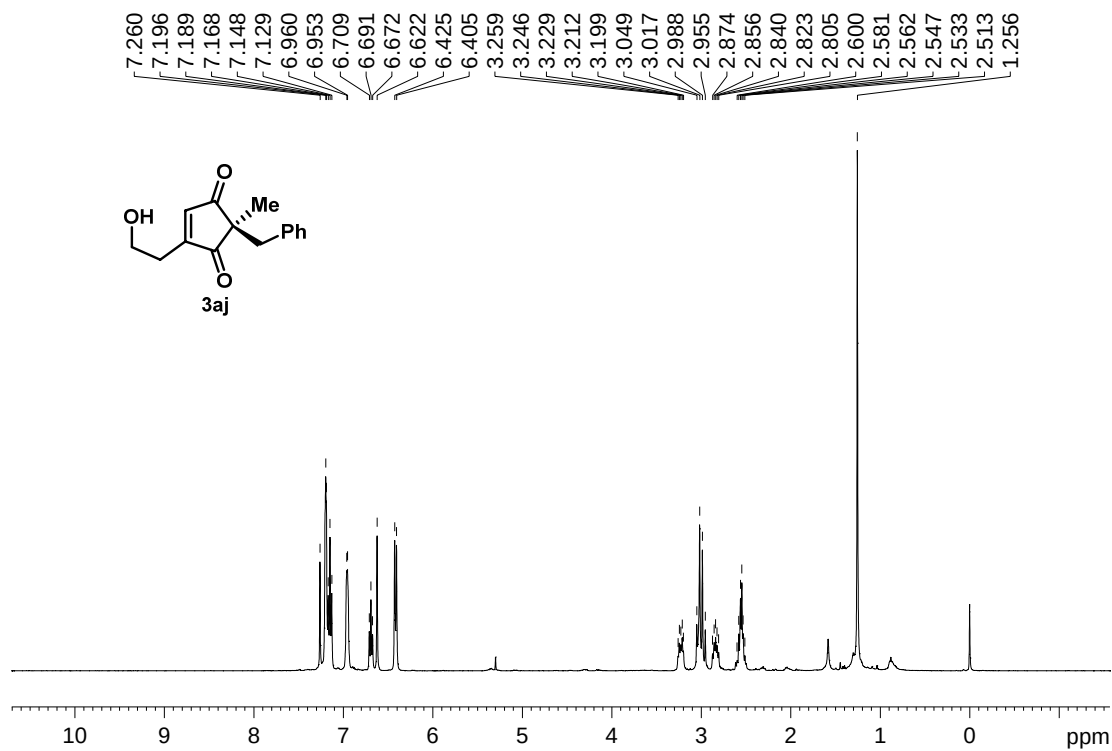
Peak#	Ret. Time	Area	Area %
1	14.078	423084	50.190
2	15.614	419873	49.810
Total		842957	100.000

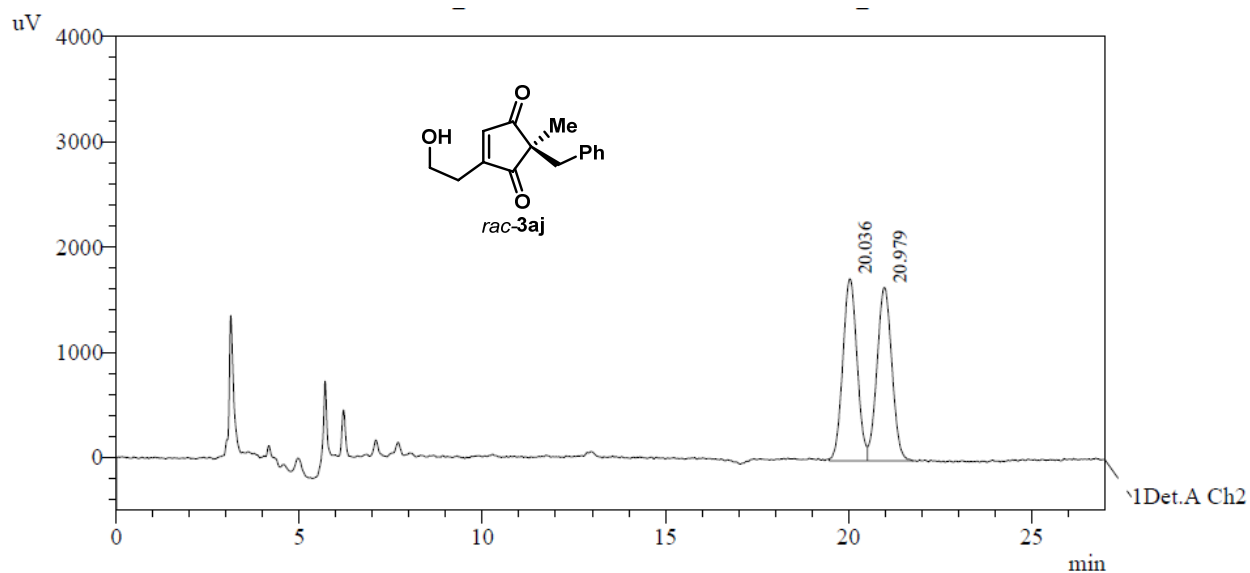


PeakTable

Detector A Ch2 254nm

Peak#	Ret. Time	Area	Area %
1	14.082	894975	9.071
2	15.598	8971662	90.929
Total		9866637	100.000

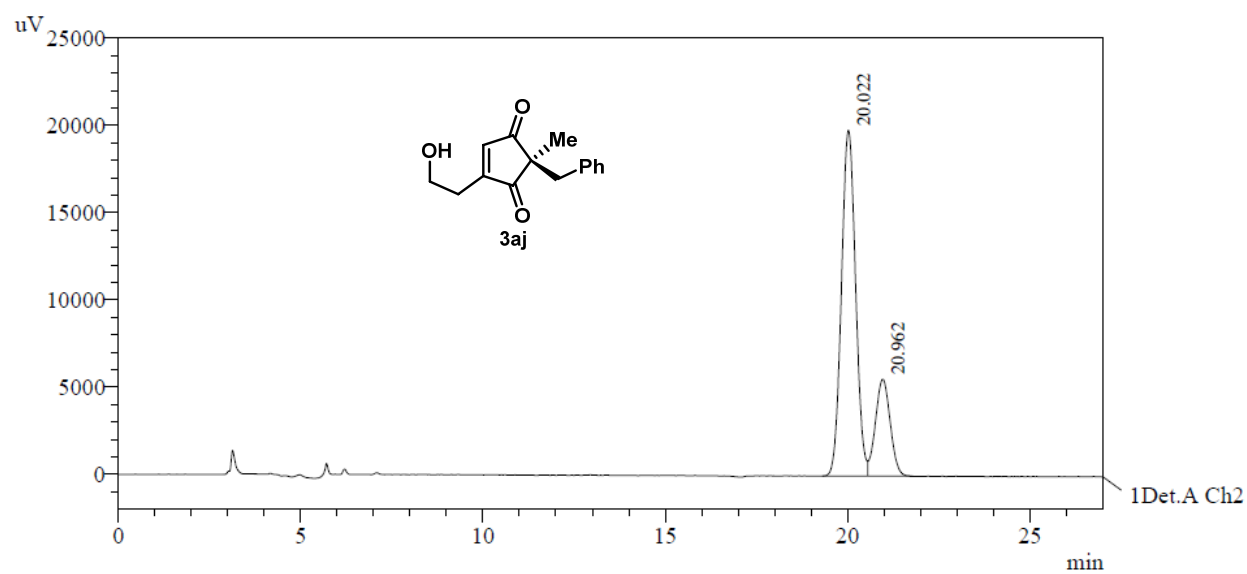




PeakTable

Detector A Ch2 254nm

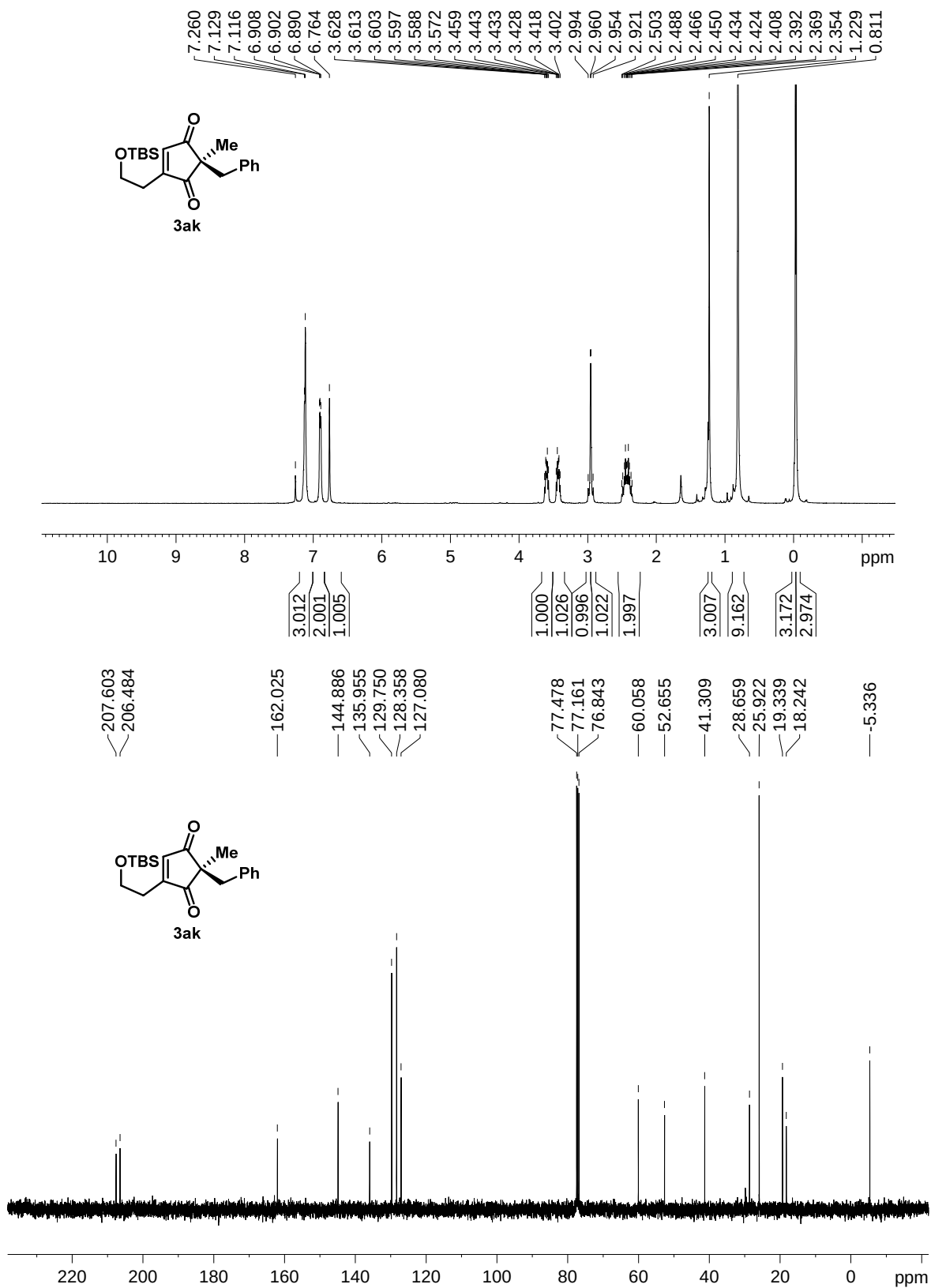
Peak#	Ret. Time	Area	Area %
1	20.036	46840	50.085
2	20.979	46680	49.915
Total		93520	100.000

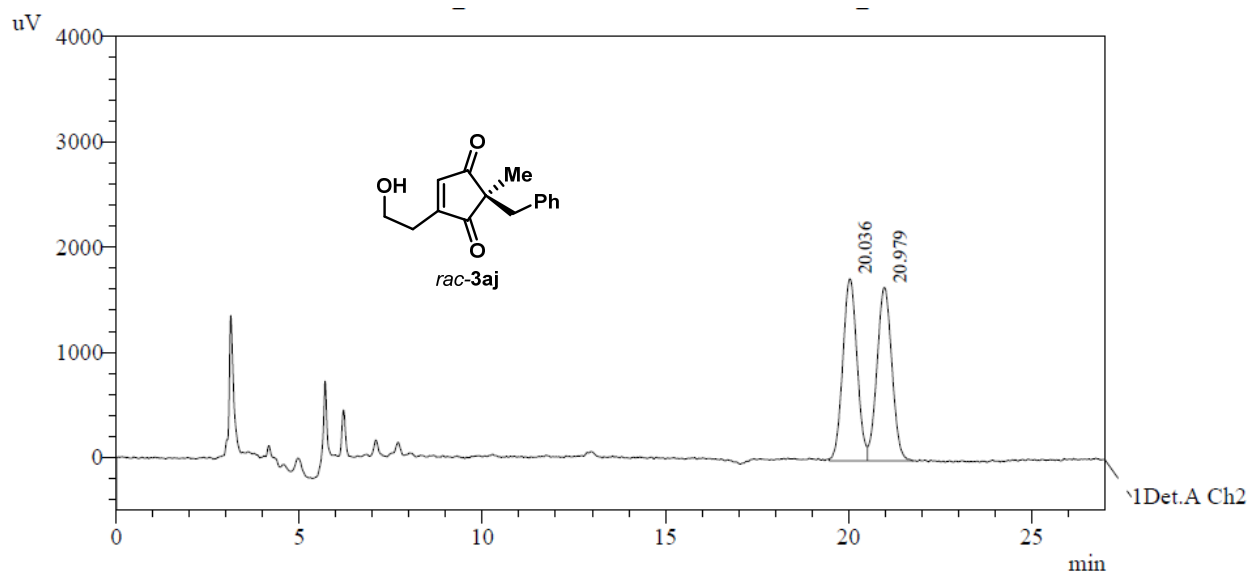


PeakTable

Detector A Ch2 254nm

Peak#	Ret. Time	Area	Area %
1	20.022	534404	77.318
2	20.962	156771	22.682
Total		691175	100.000

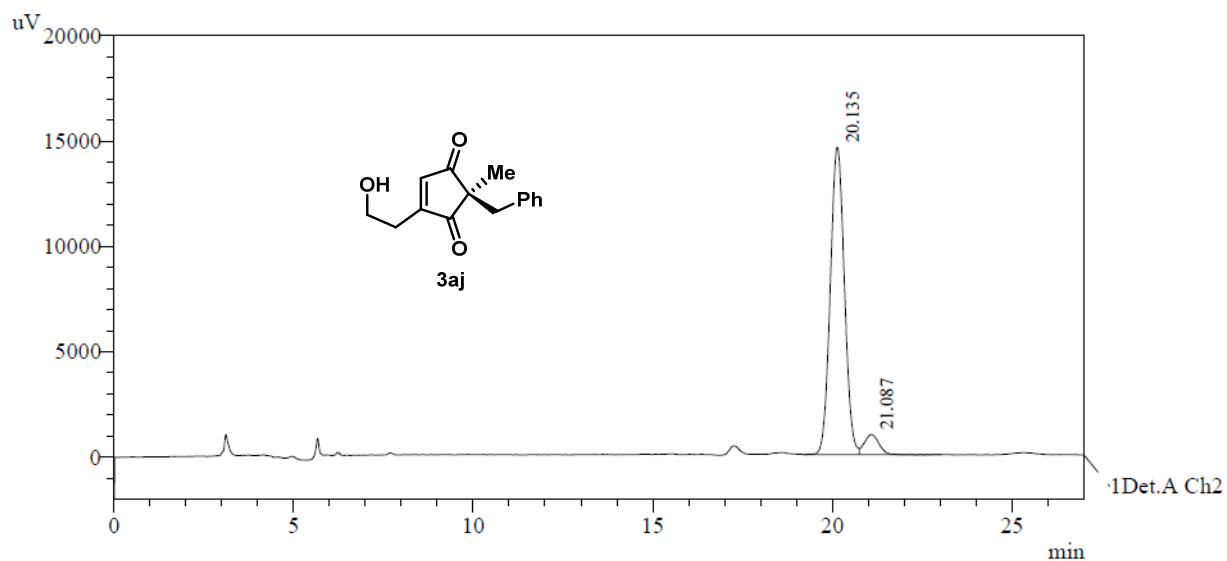




PeakTable

Detector A Ch2 254nm

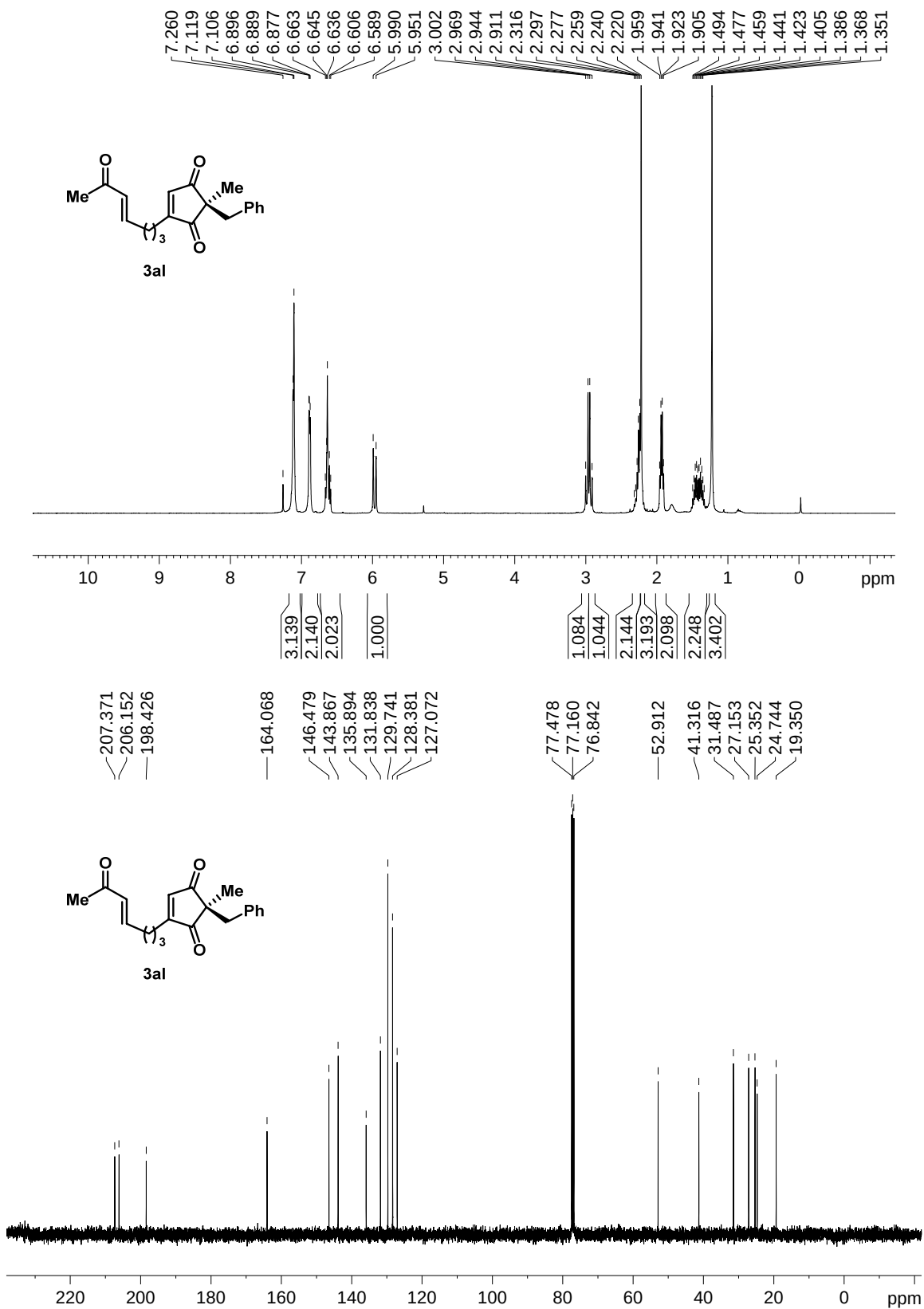
Peak#	Ret. Time	Area	Area %
1	20.036	46840	50.085
2	20.979	46680	49.915
Total		93520	100.000

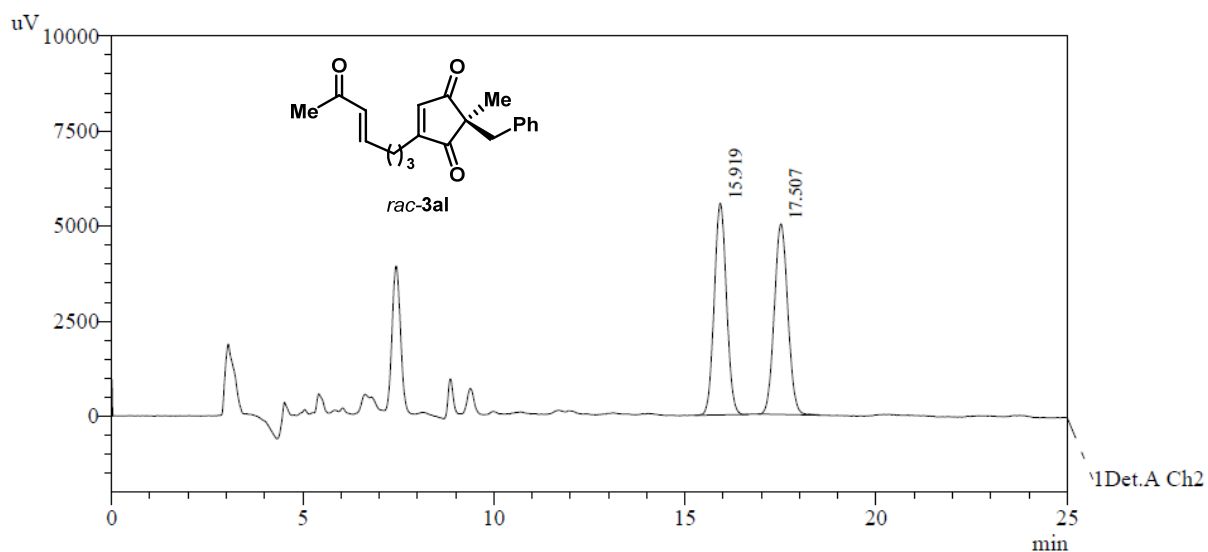


PeakTable

Detector A Ch2 254nm

Peak#	Ret. Time	Area	Area %
1	20.135	398261	93.680
2	21.087	26870	6.320
Total		425131	100.000

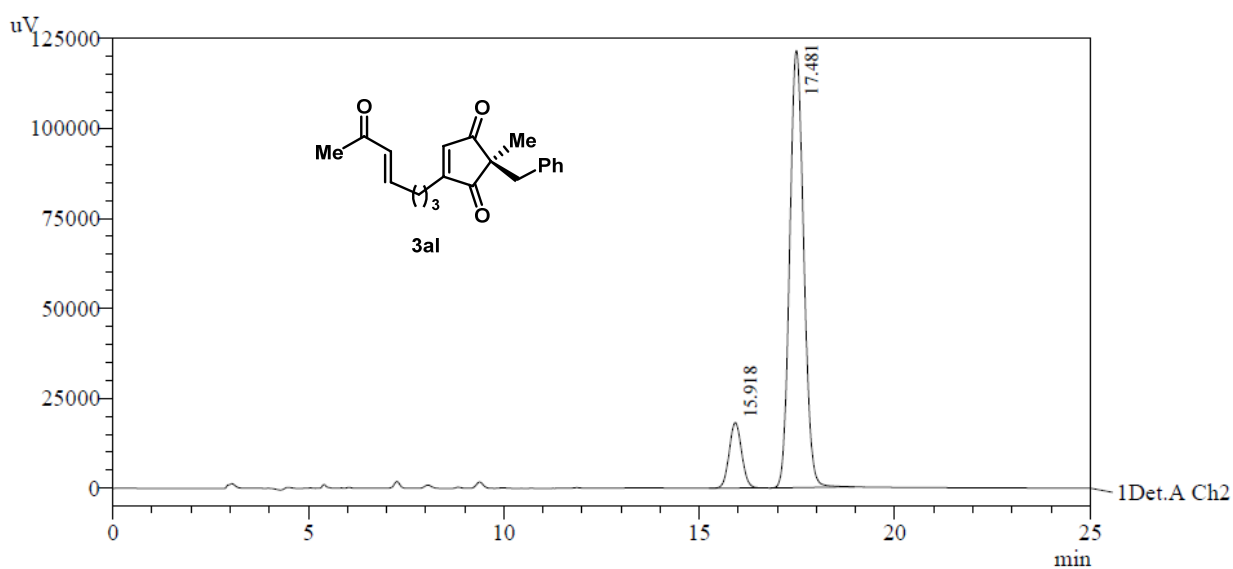




PeakTable

Detector A Ch2 254nm

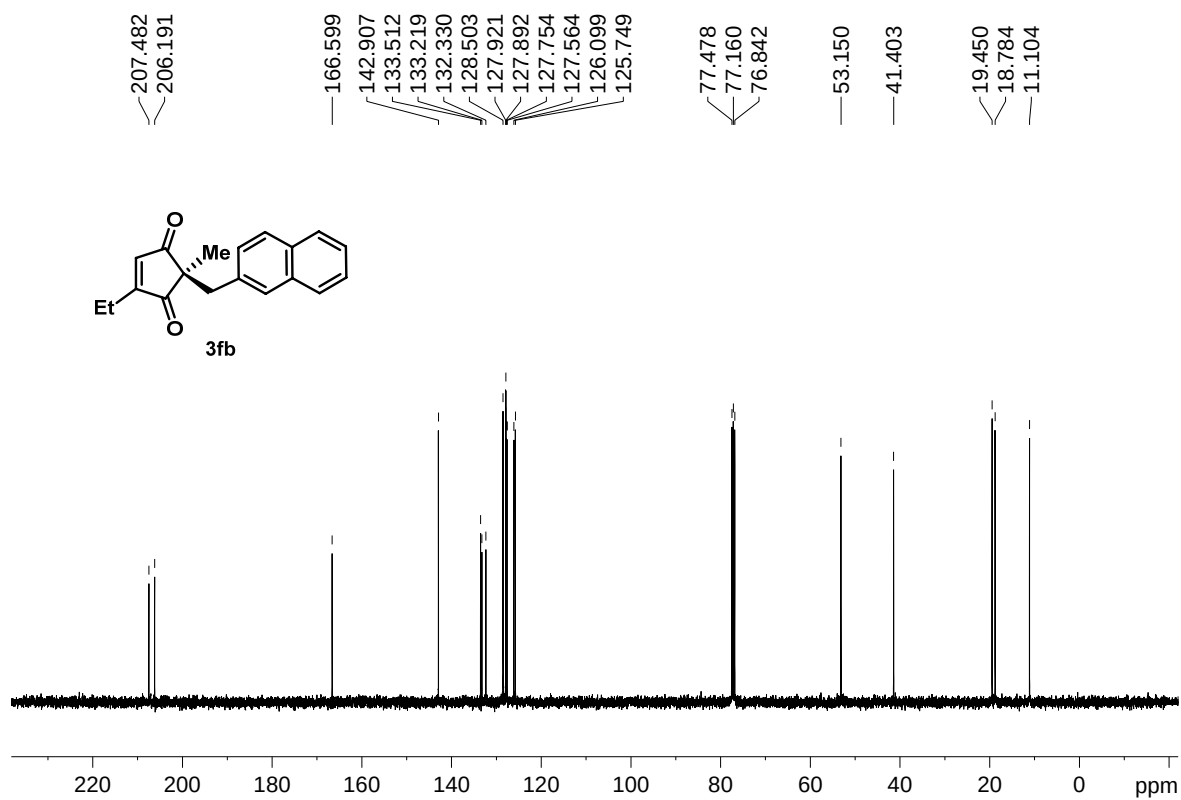
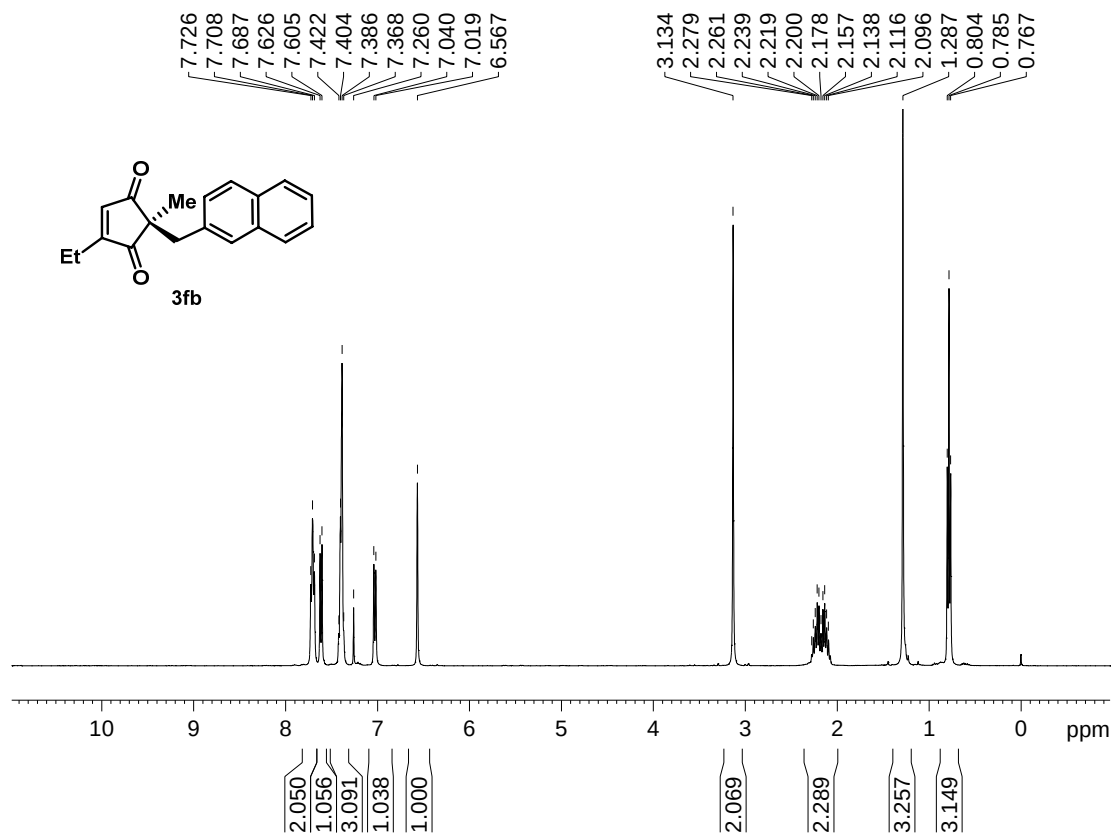
Peak#	Ret. Time	Area	Area %
1	15.919	124426	50.171
2	17.507	123577	49.829
Total		248003	100.000

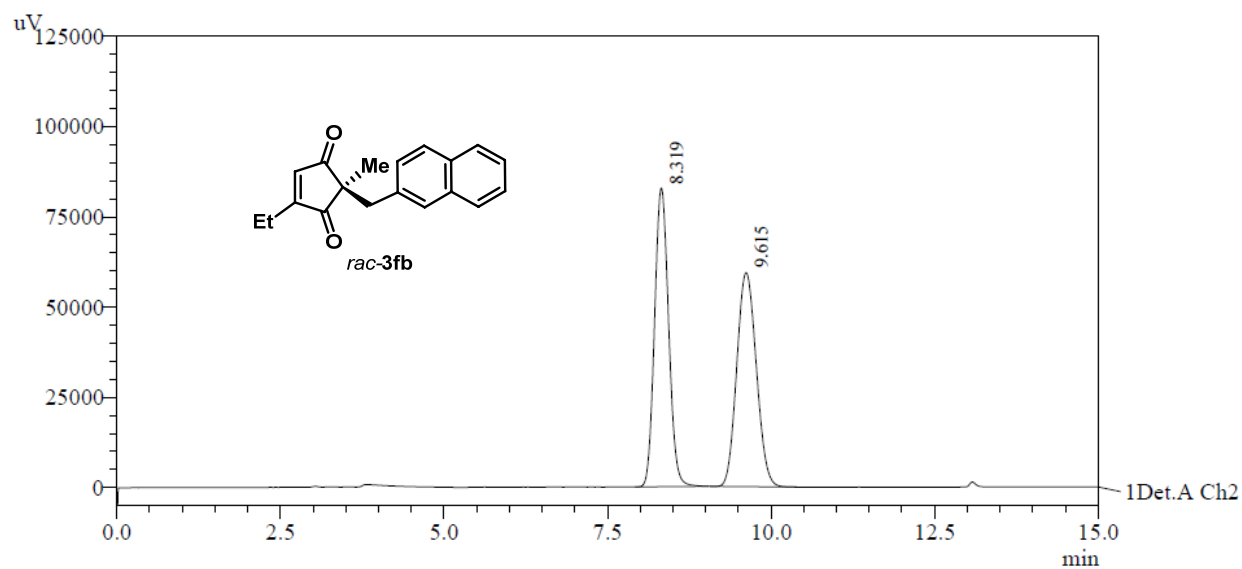


PeakTable

Detector A Ch2 254nm

Peak#	Ret. Time	Area	Area %
1	15.918	404022	11.755
2	17.481	3032919	88.245
Total		3436940	100.000

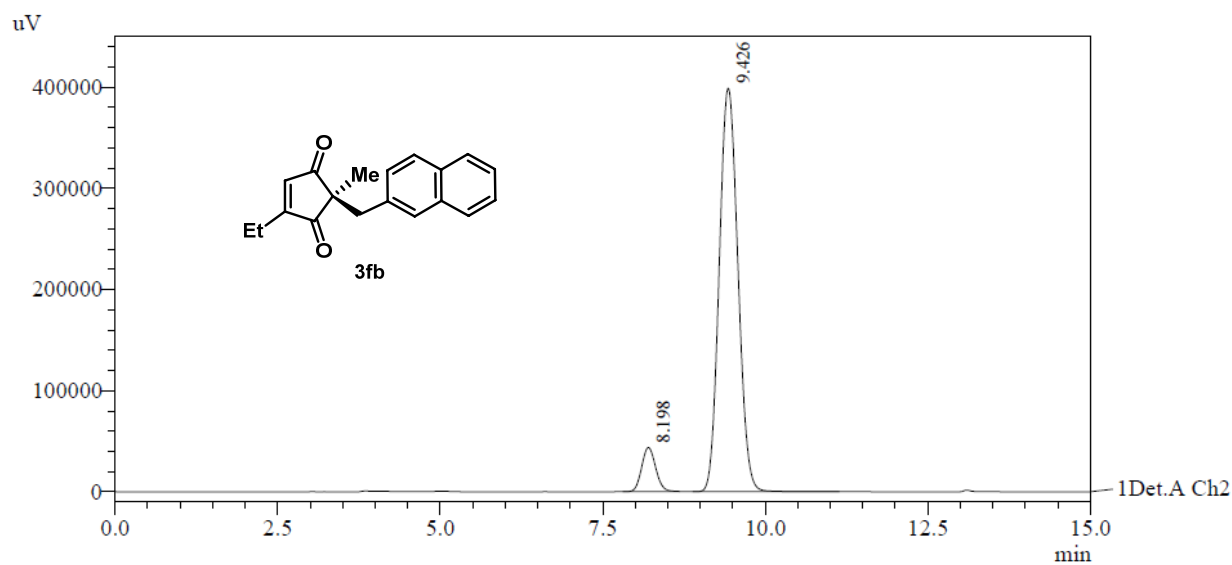




PeakTable

Detector A Ch2 254nm

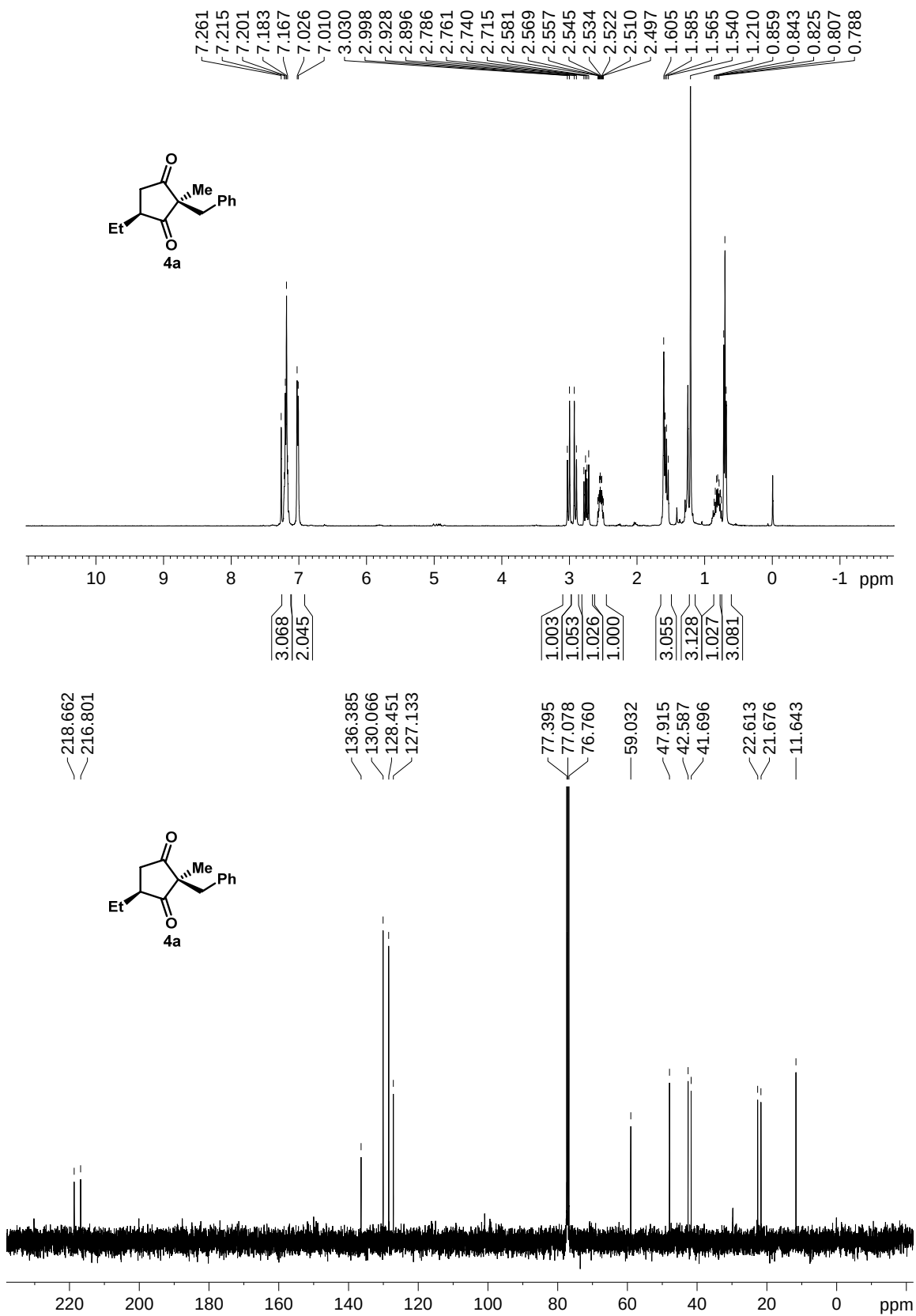
Peak#	Ret. Time	Area	Area %
1	8.319	1233517	50.022
2	9.615	1232411	49.978
Total		2465928	100.000

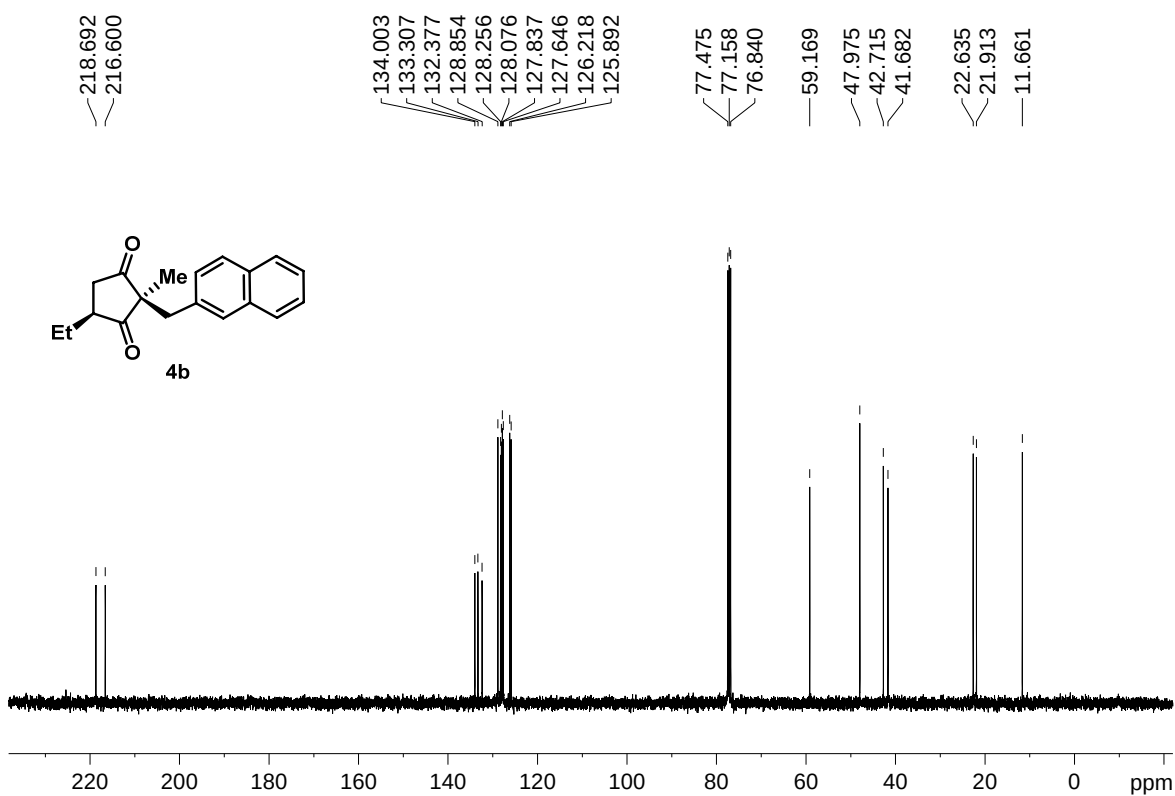
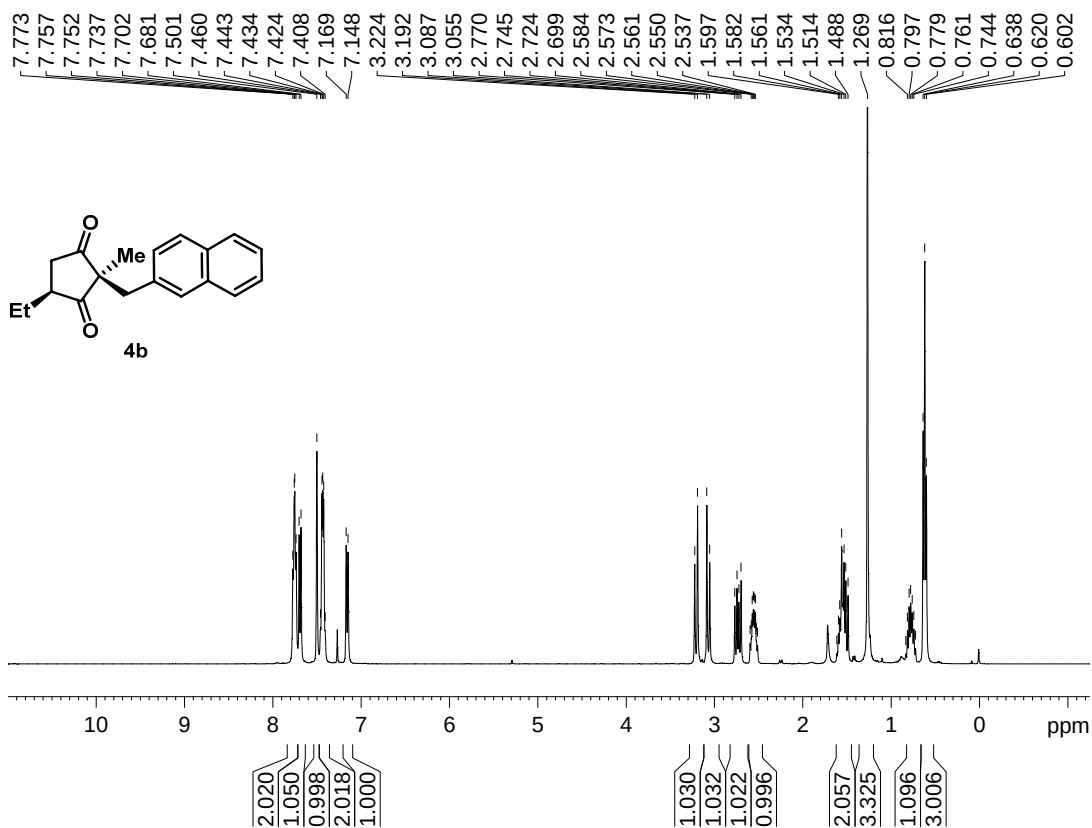


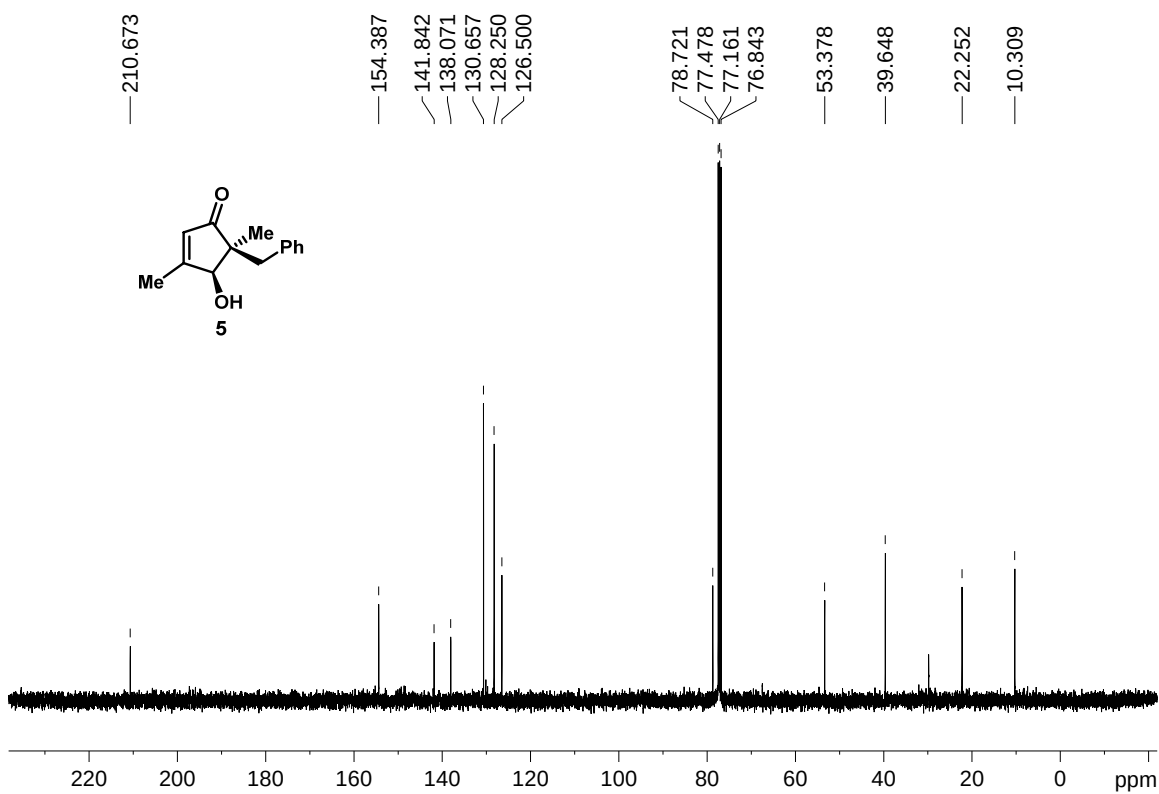
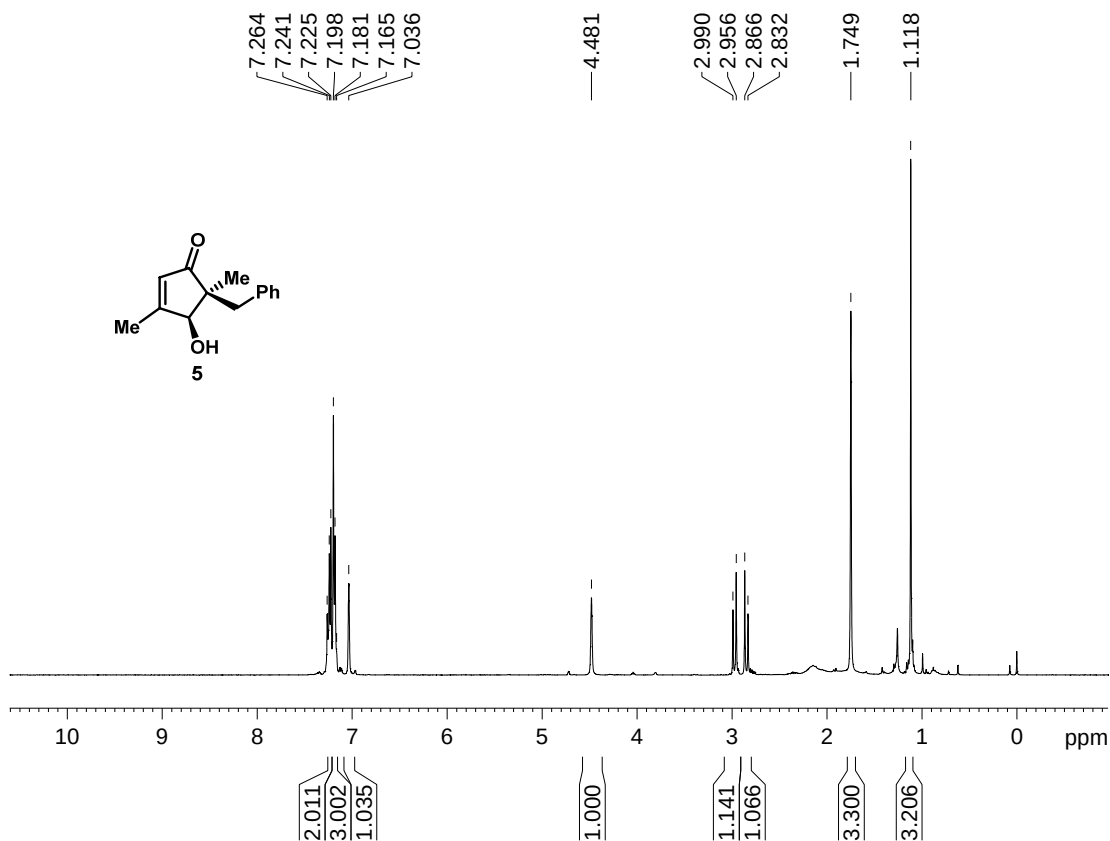
PeakTable

Detector A Ch2 254nm

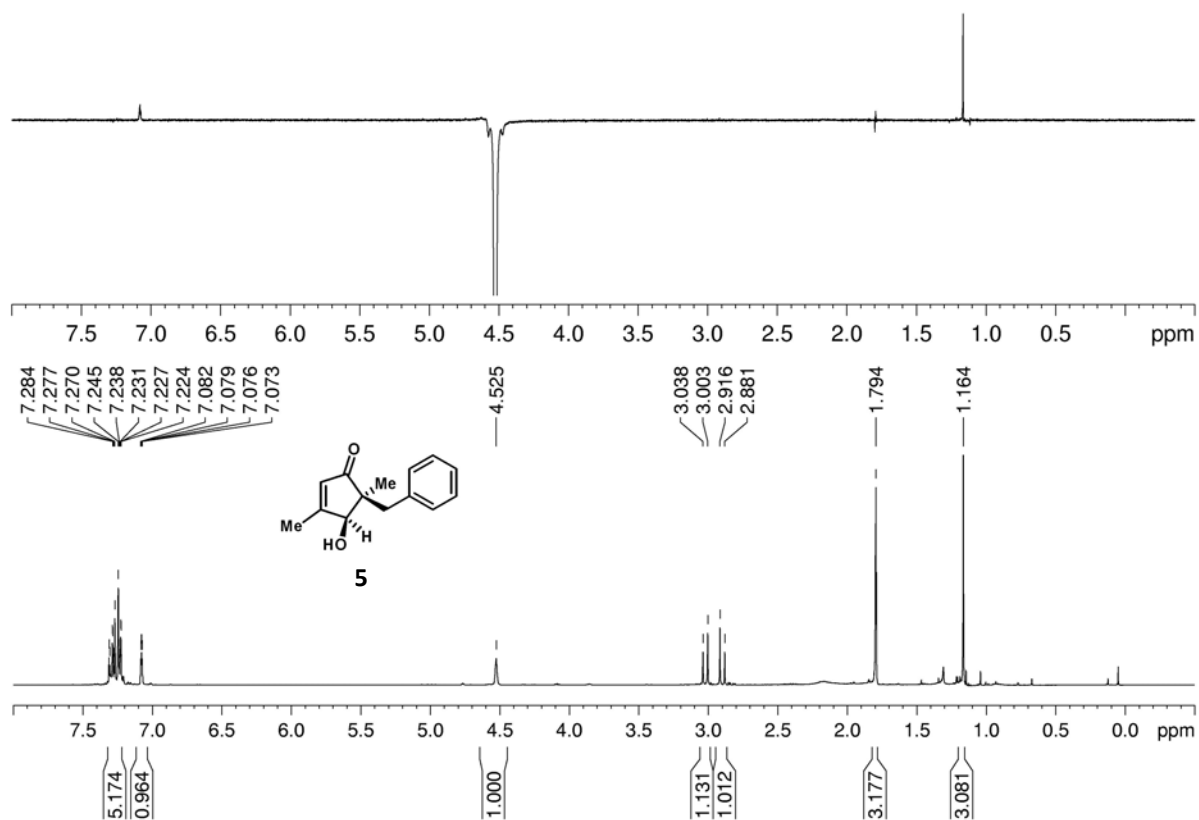
Peak#	Ret. Time	Area	Area %
1	8.198	648247	7.526
2	9.426	7964874	92.474
Total		8613121	100.000

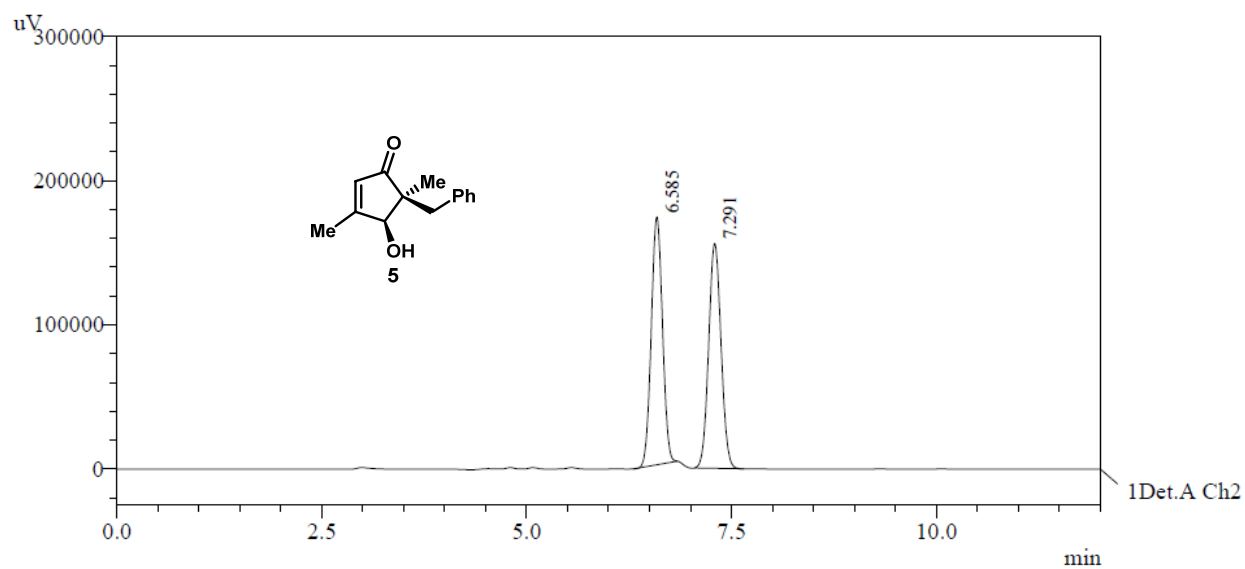






1D NOE of 5:

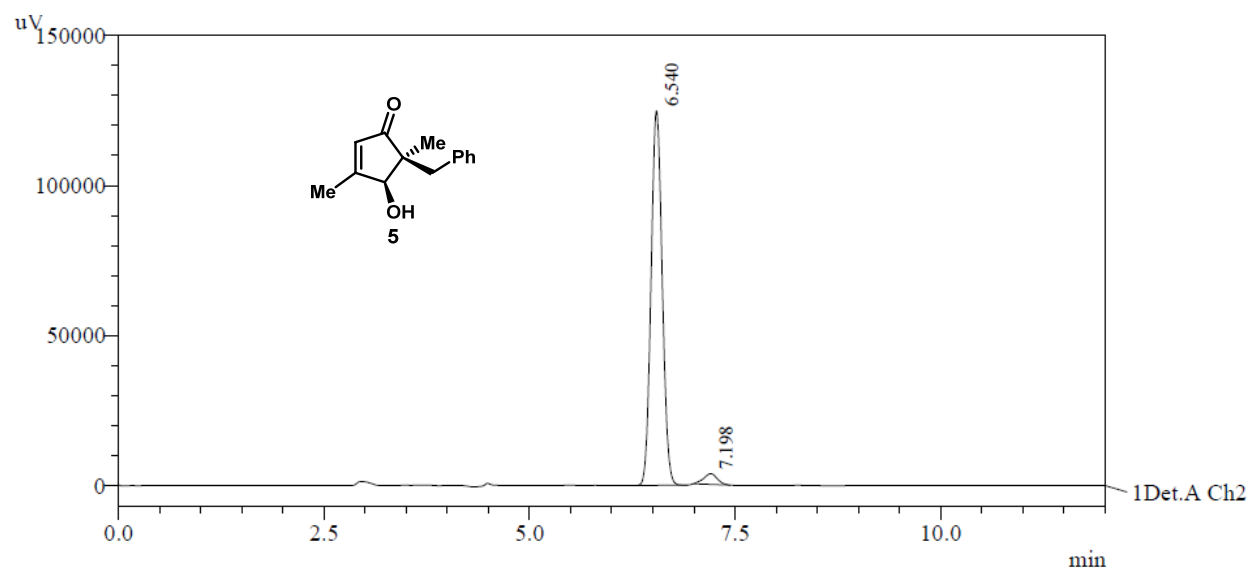




PeakTable

Detector A Ch2 254nm

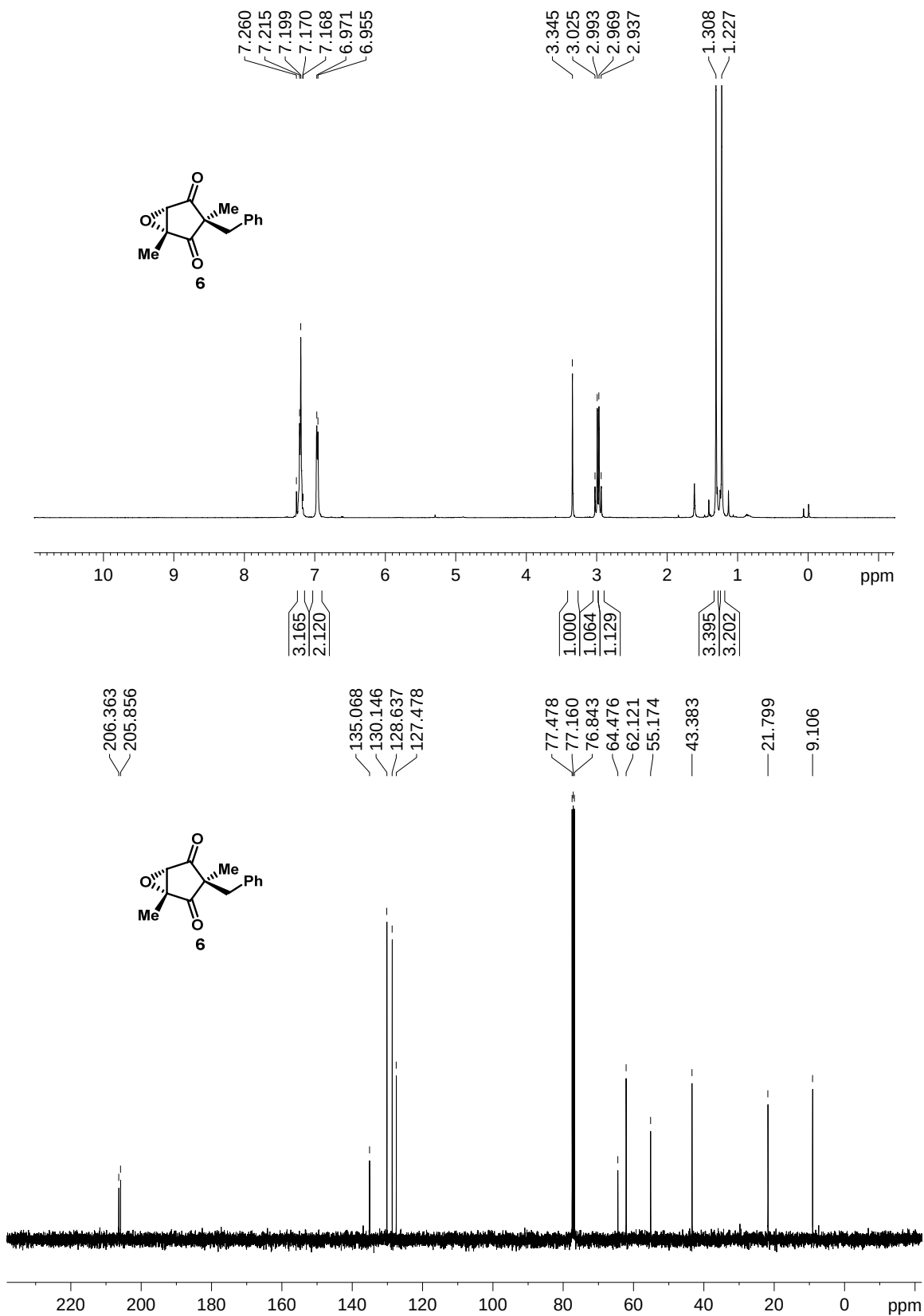
Peak#	Ret. Time	Area	Area %
1	6.585	1636486	49.911
2	7.291	1642306	50.089
Total		3278792	100.000



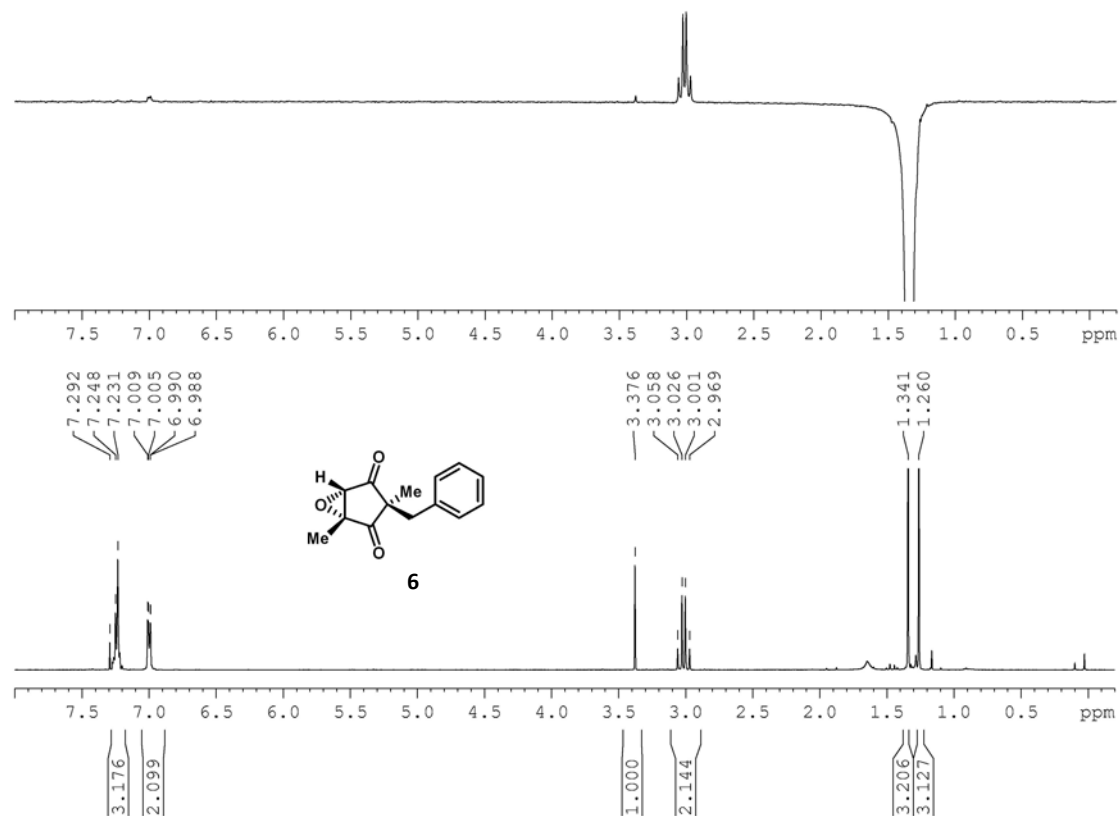
PeakTable

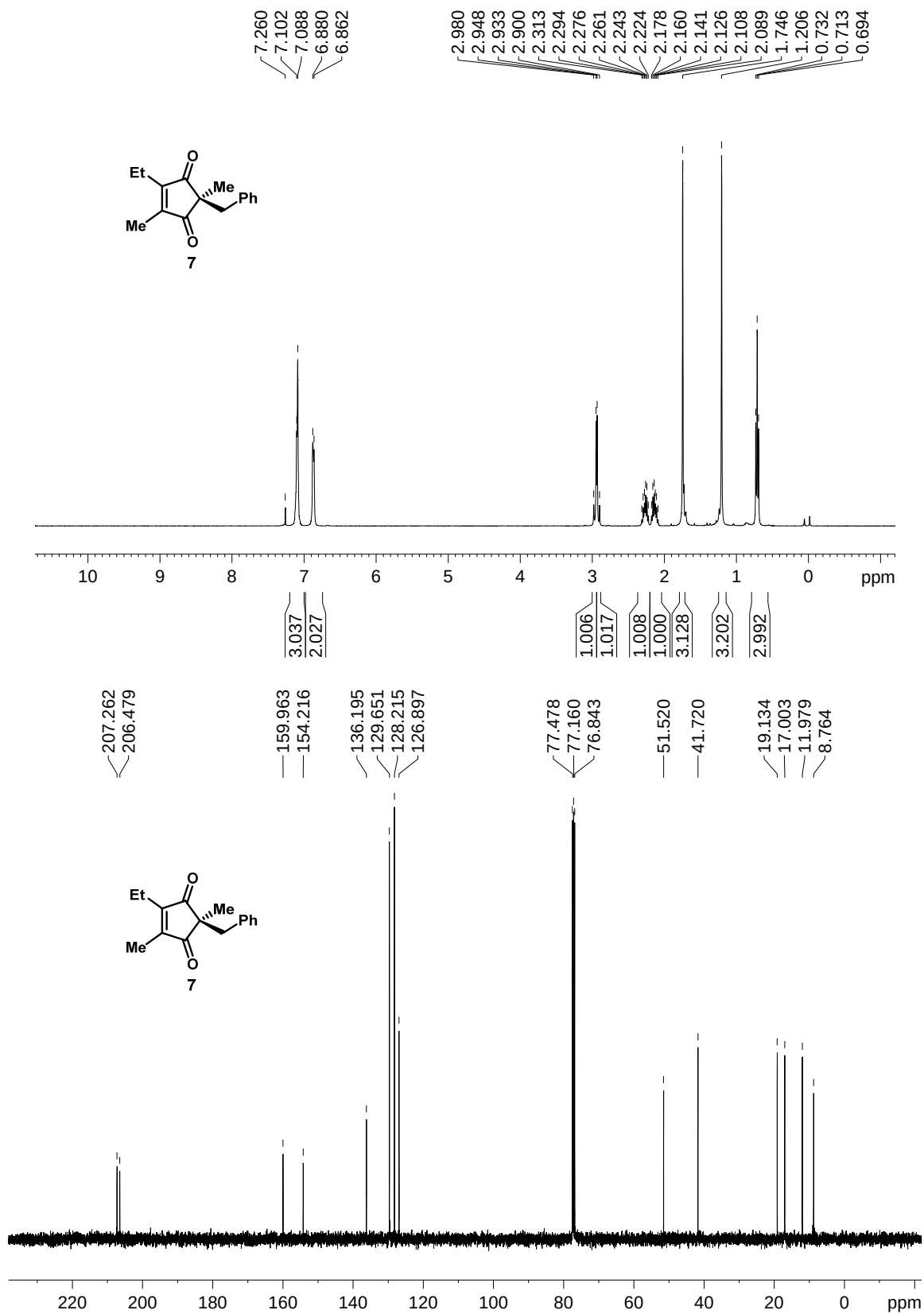
Detector A Ch2 254nm

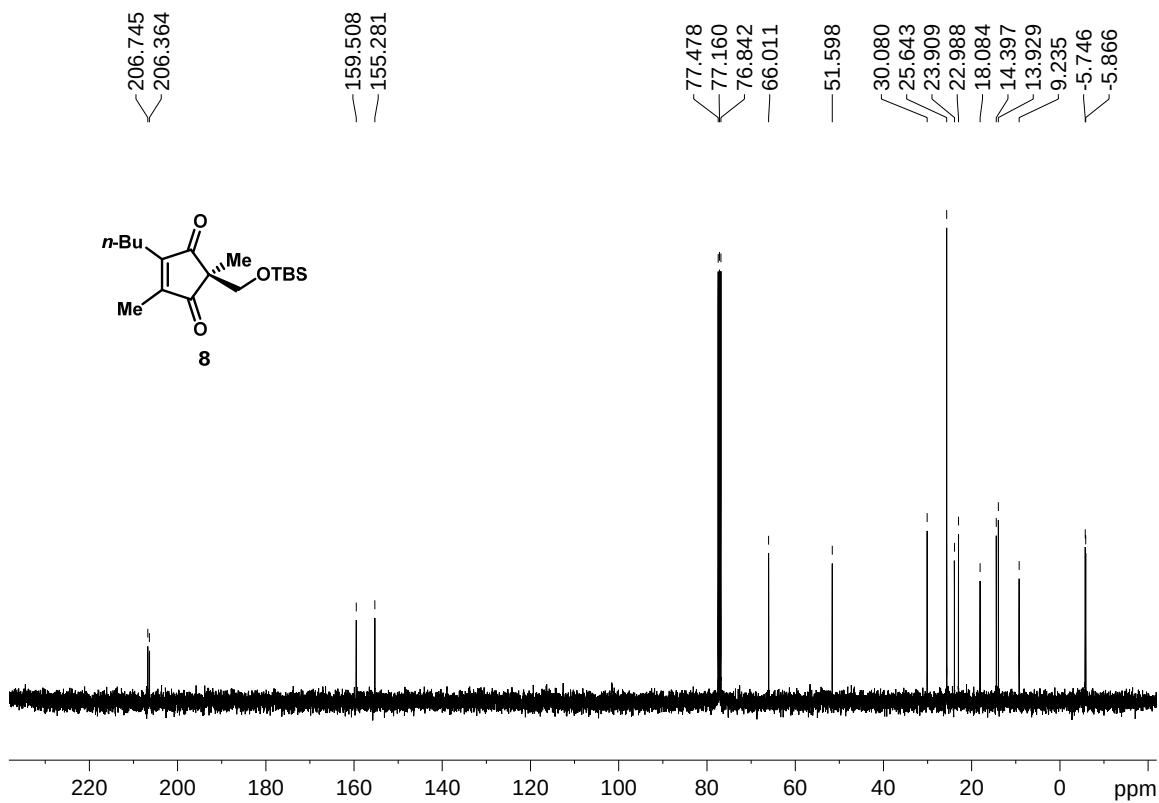
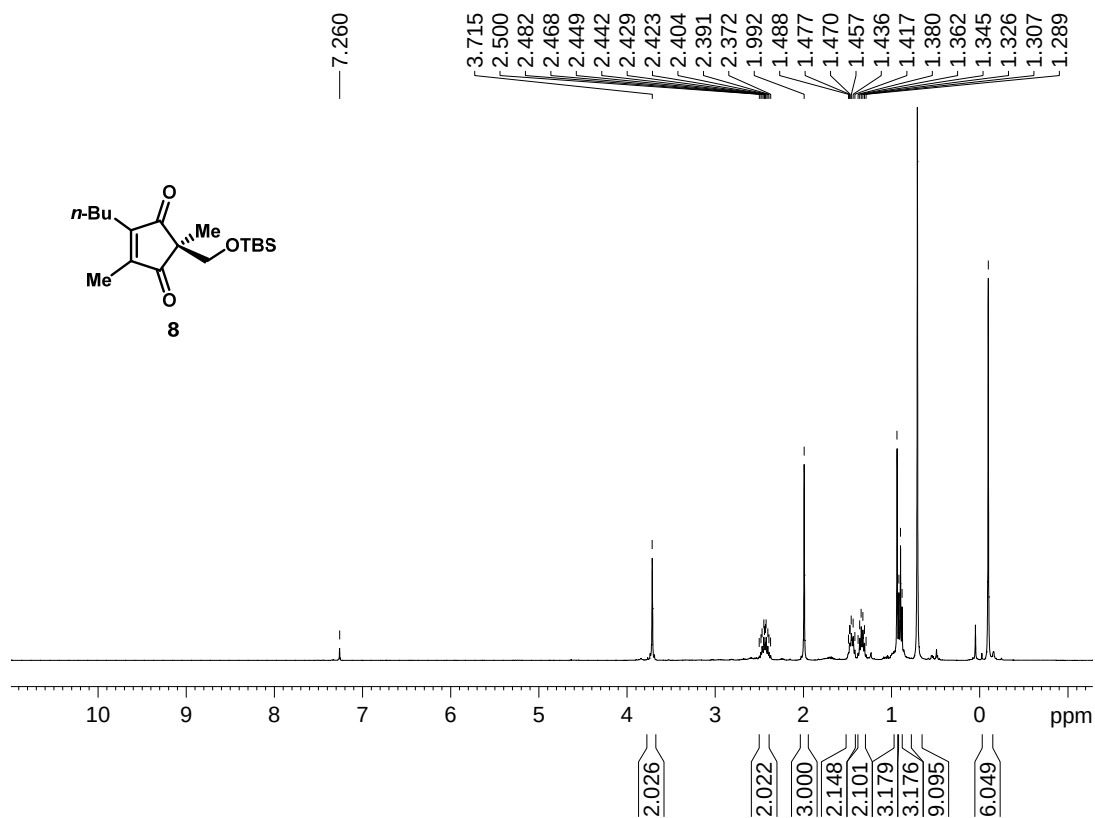
Peak#	Ret. Time	Area	Area %
1	6.540	1177273	96.617
2	7.198	41228	3.383
Total		1218501	100.000

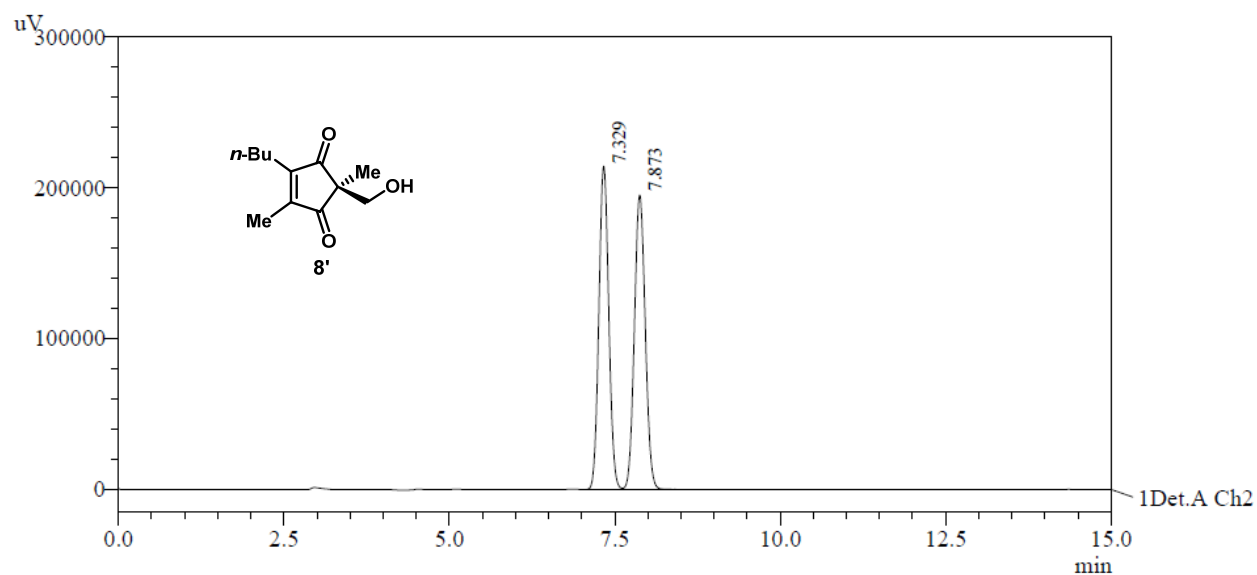


1D NOE of 6:





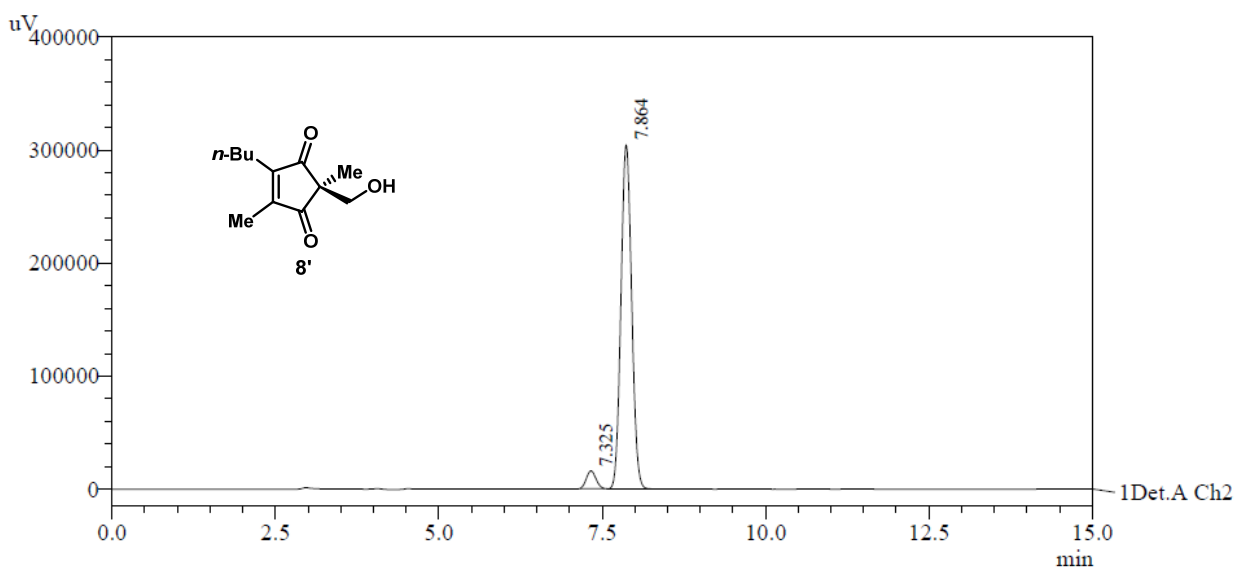




PeakTable

Detector A Ch2 254nm

Peak#	Ret. Time	Area	Area %
1	7.329	2221076	49.867
2	7.873	2232943	50.133
Total		4454019	100.000



PeakTable

Detector A Ch2 254nm

Peak#	Ret. Time	Area	Area %
1	7.325	158690	4.375
2	7.864	3468788	95.625
Total		3627478	100.000