

Nitro-enabled catalytic enantioselective formal umpolung alkenylation of β -ketoesters

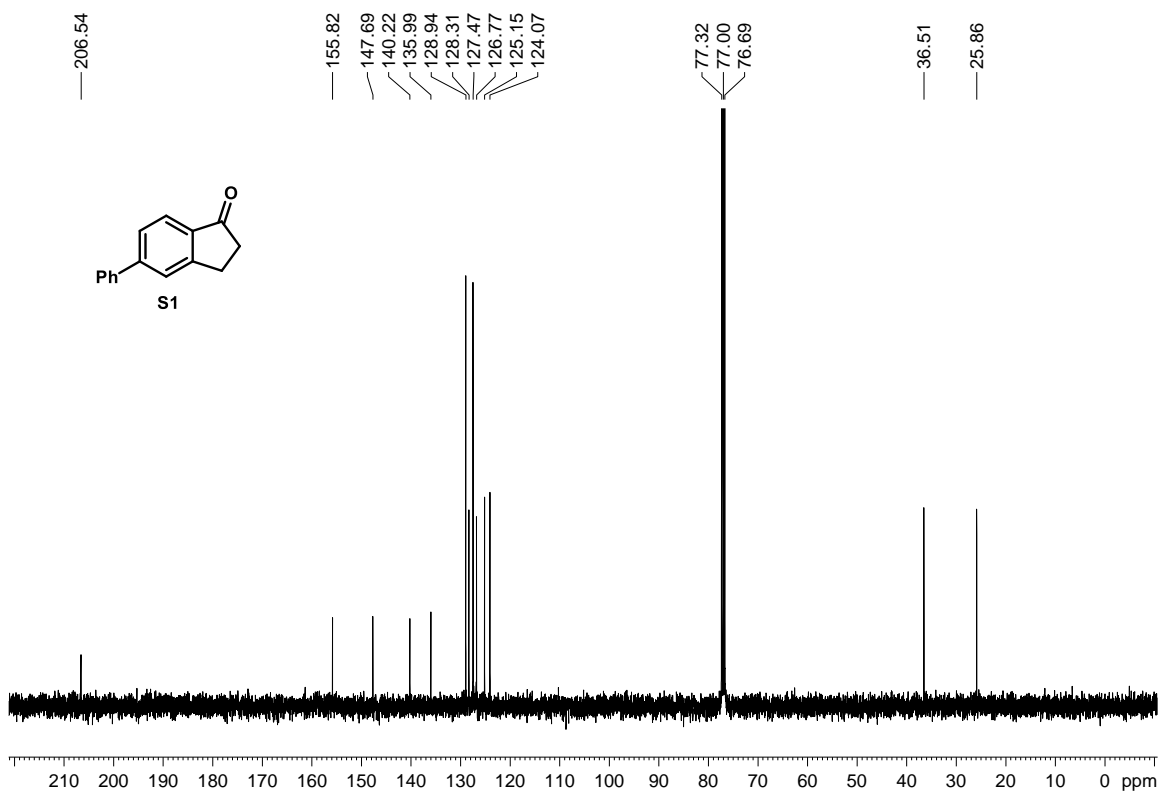
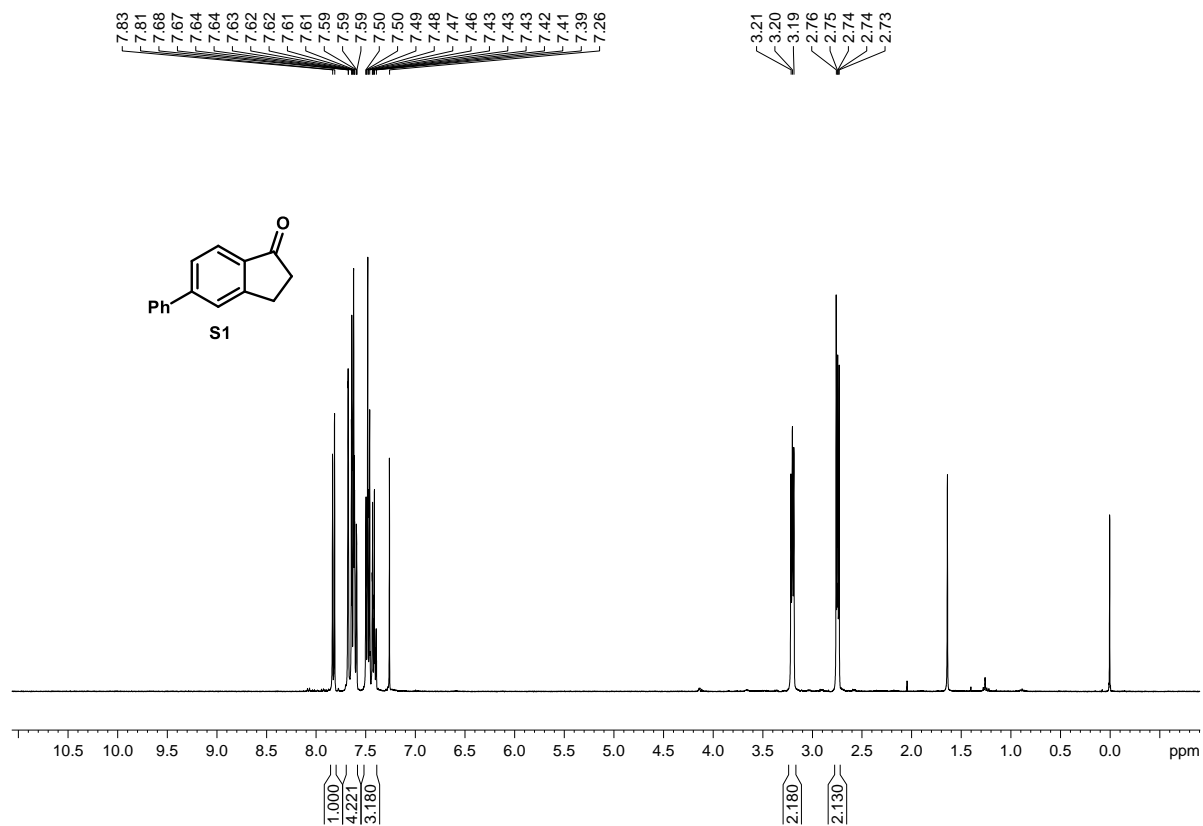
Abhijnan Ray Choudhury[‡], Madhu Sudan Manna[‡] and Santanu Mukherjee*

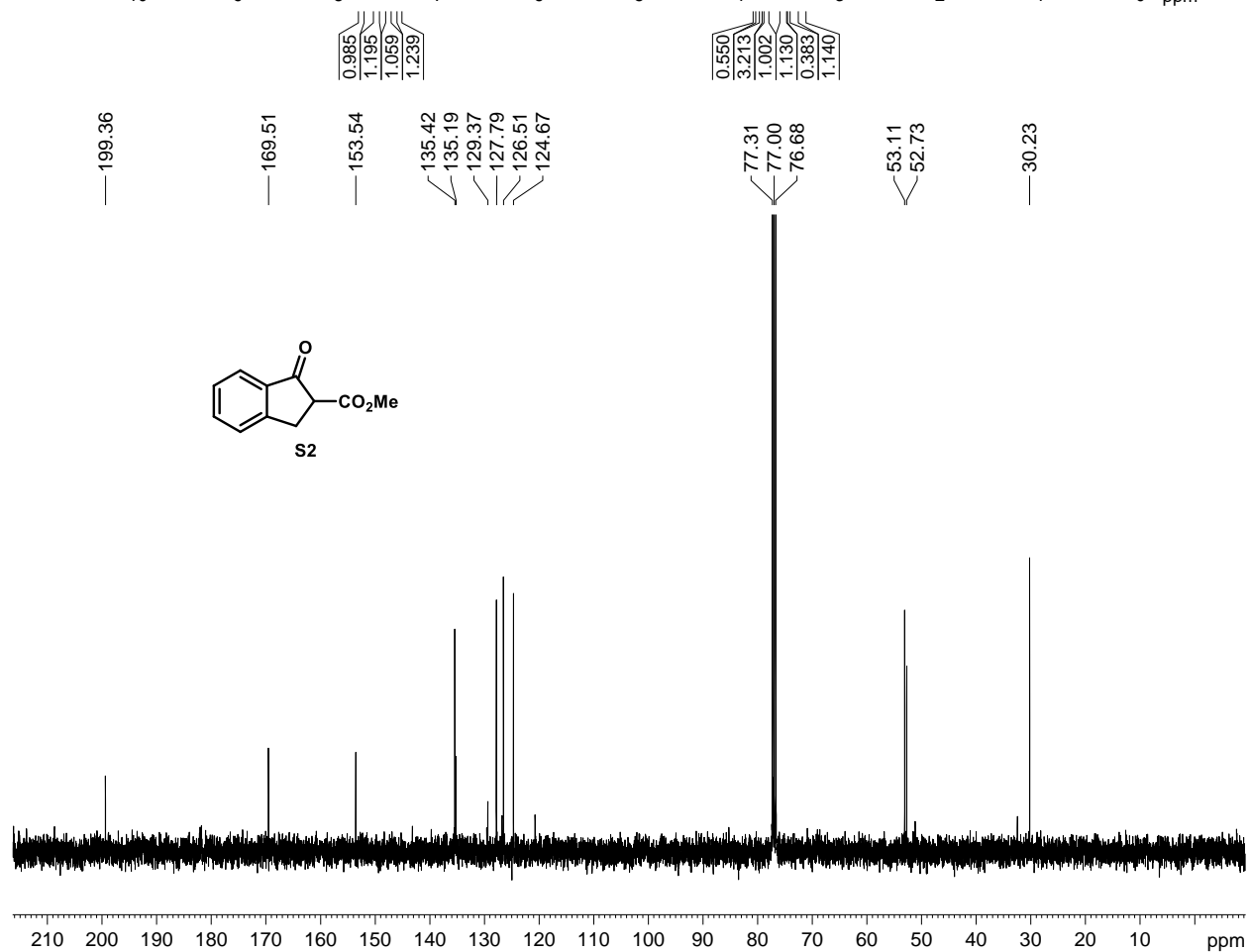
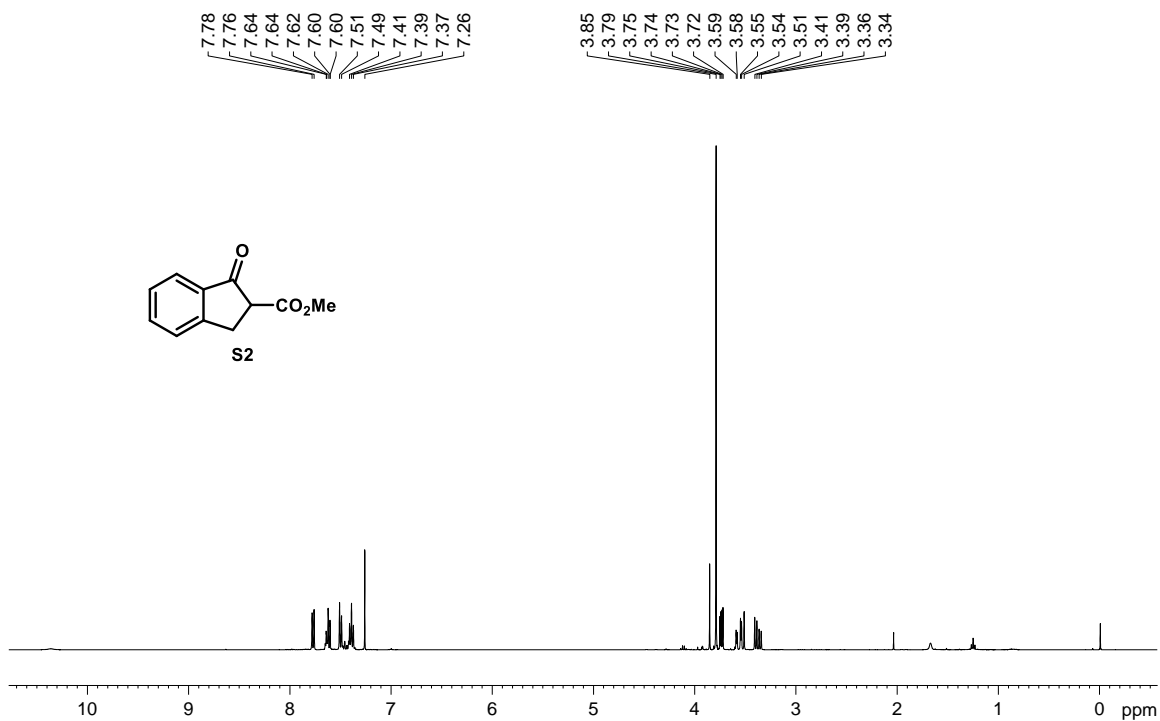
Department of Organic Chemistry, Indian Institute of Science, Bangalore 560 012, INDIA

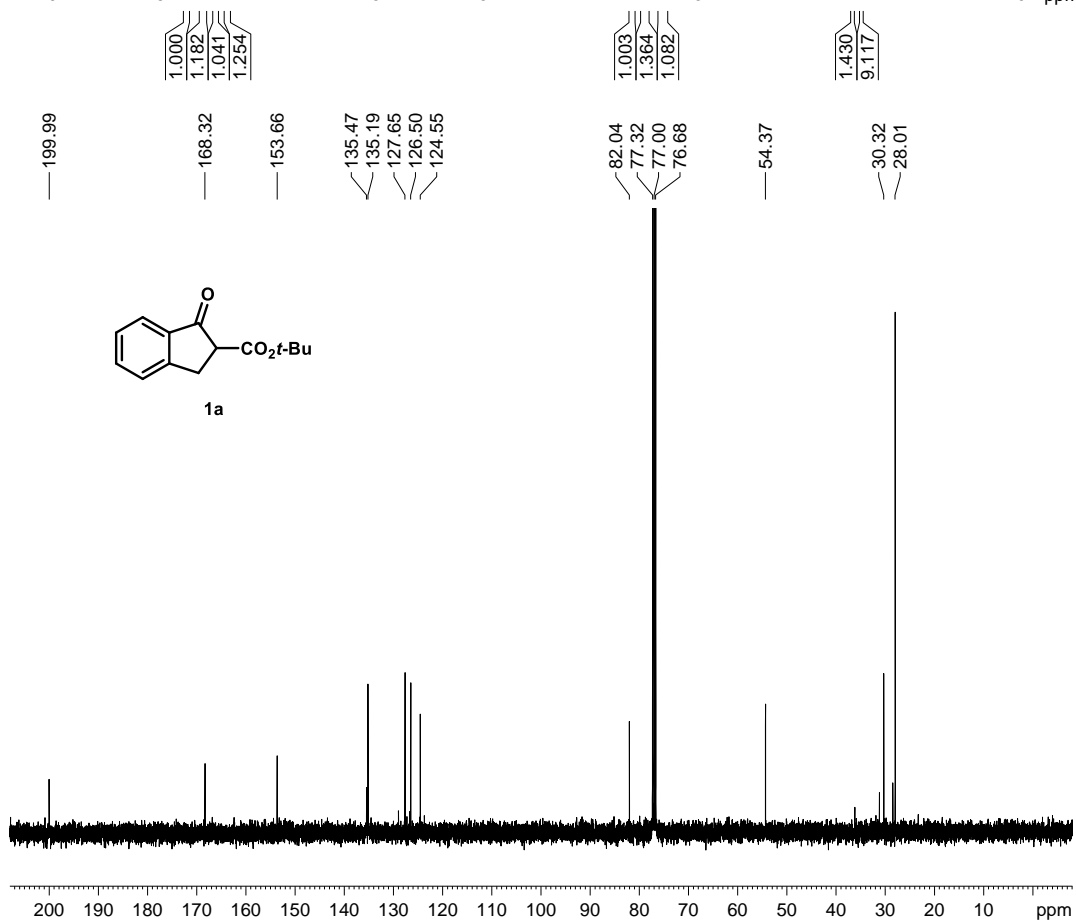
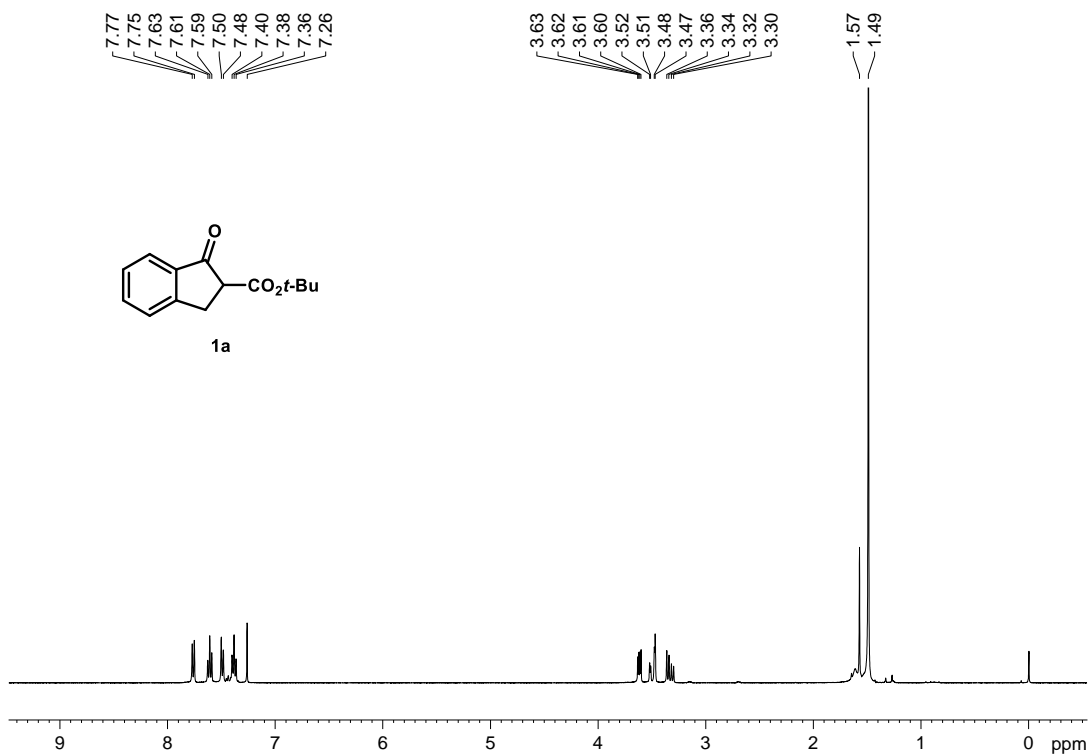
sm@orgchem.iisc.ernet.in

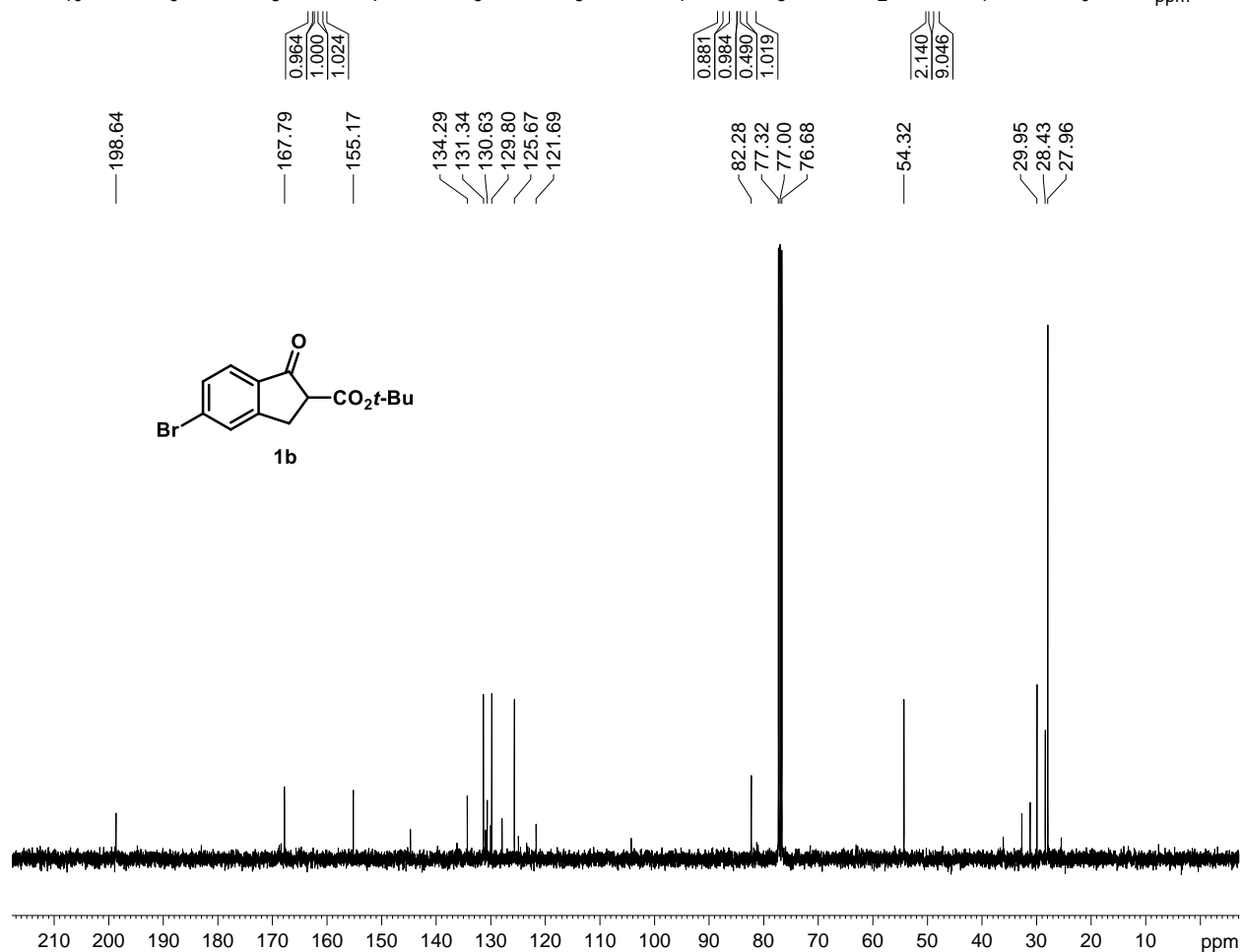
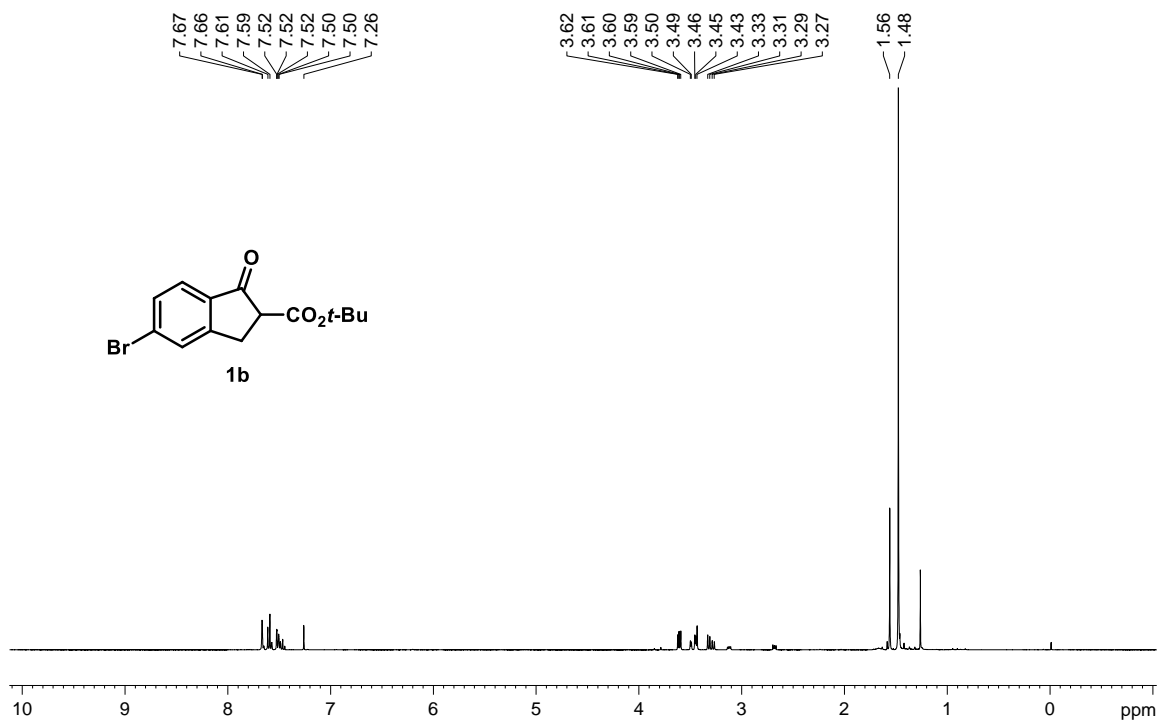
SUPPORTING INFORMATION: PART B

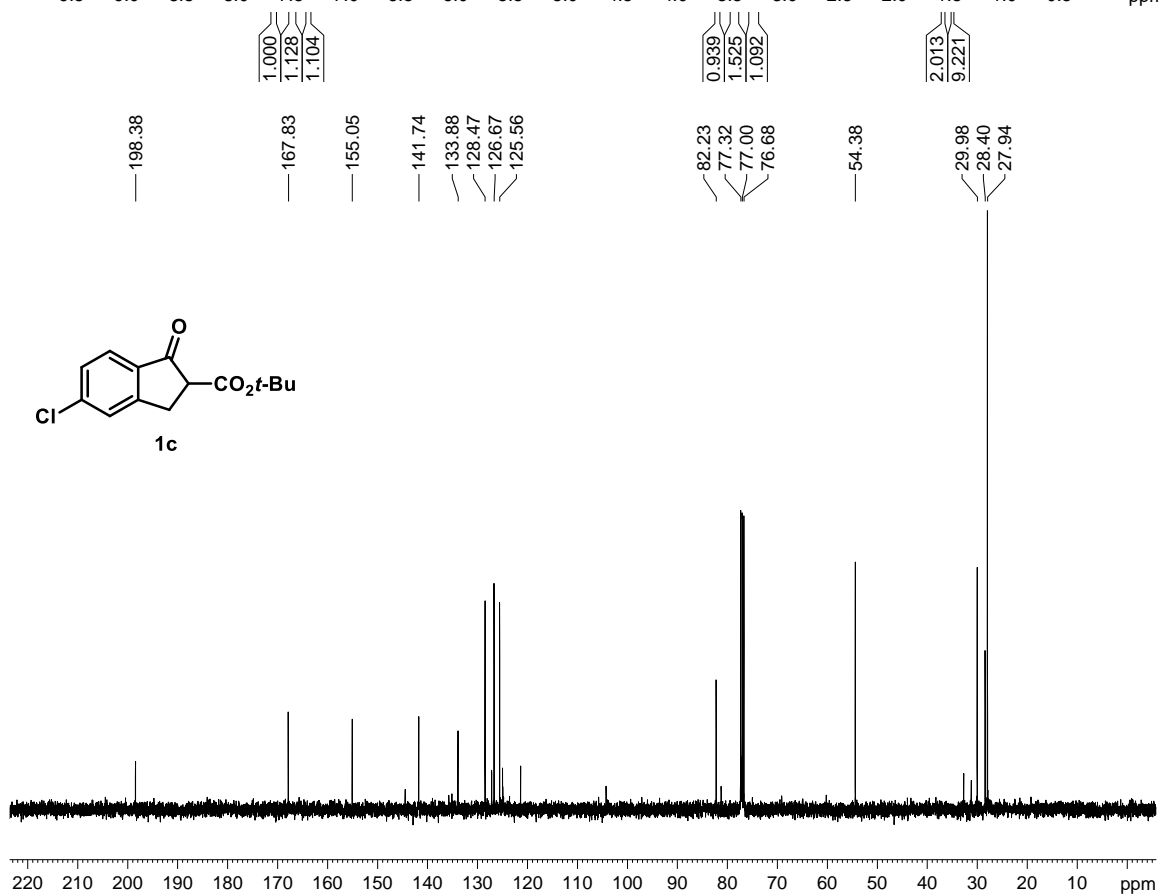
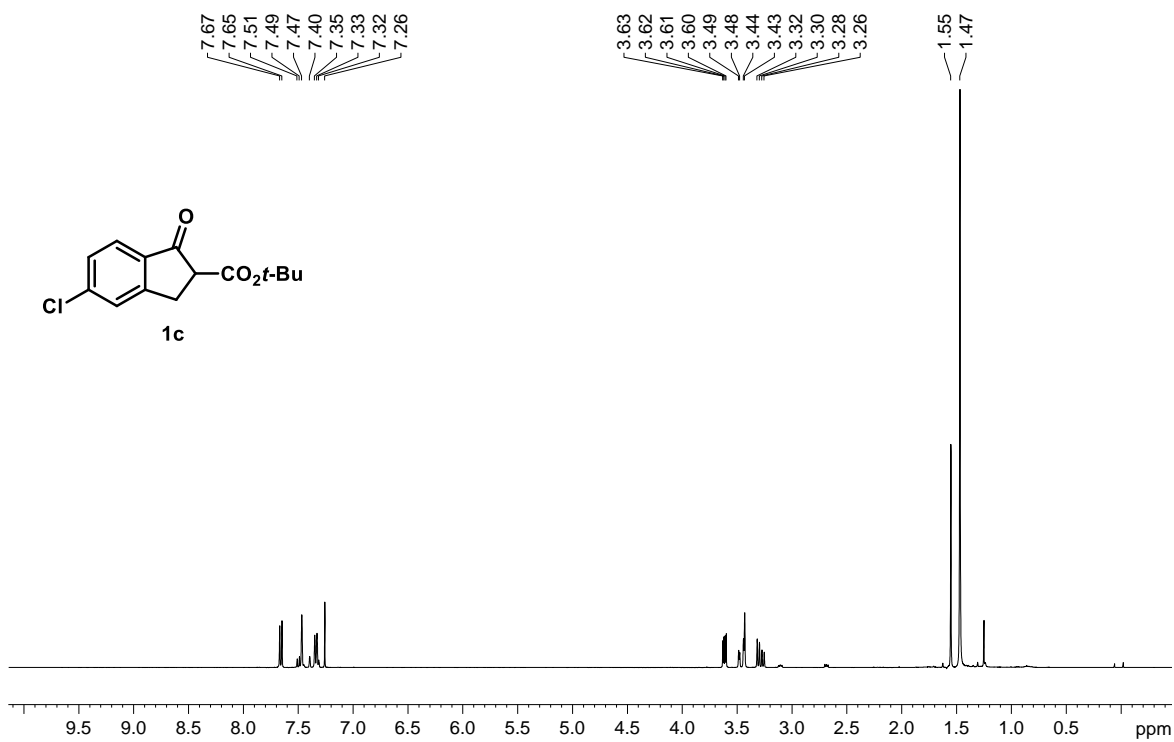
[‡] These authors contributed equally to this work

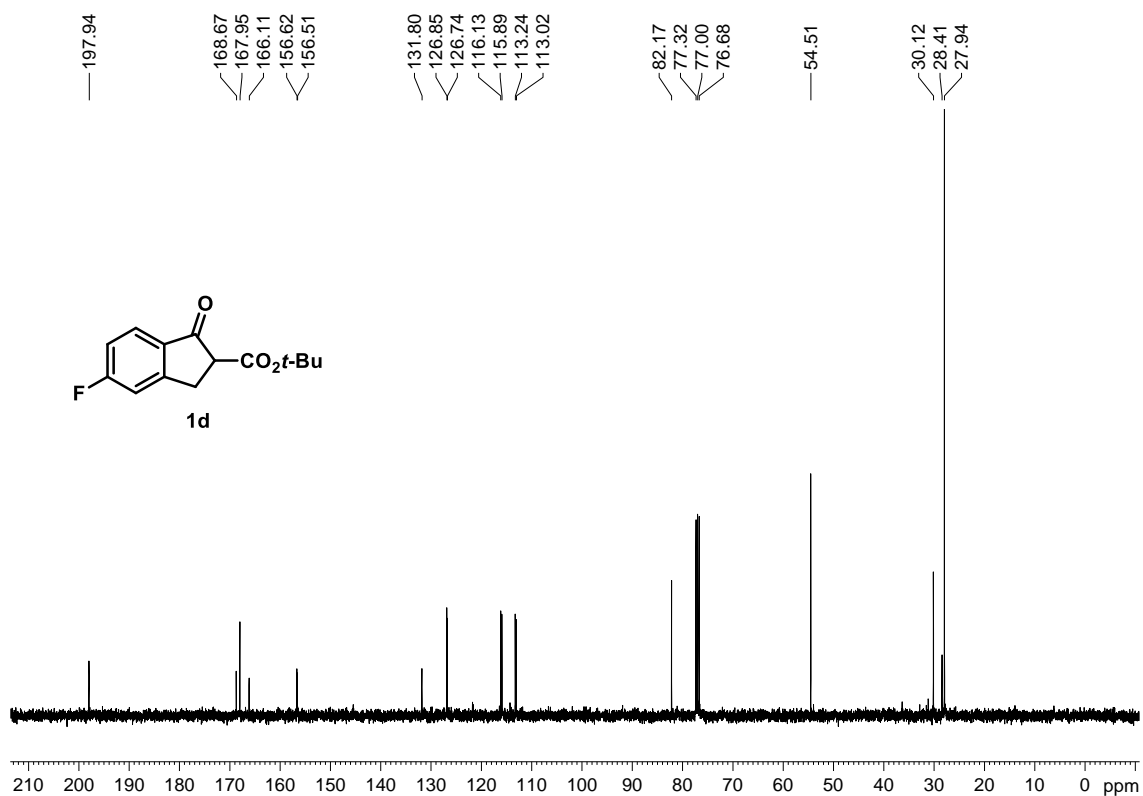
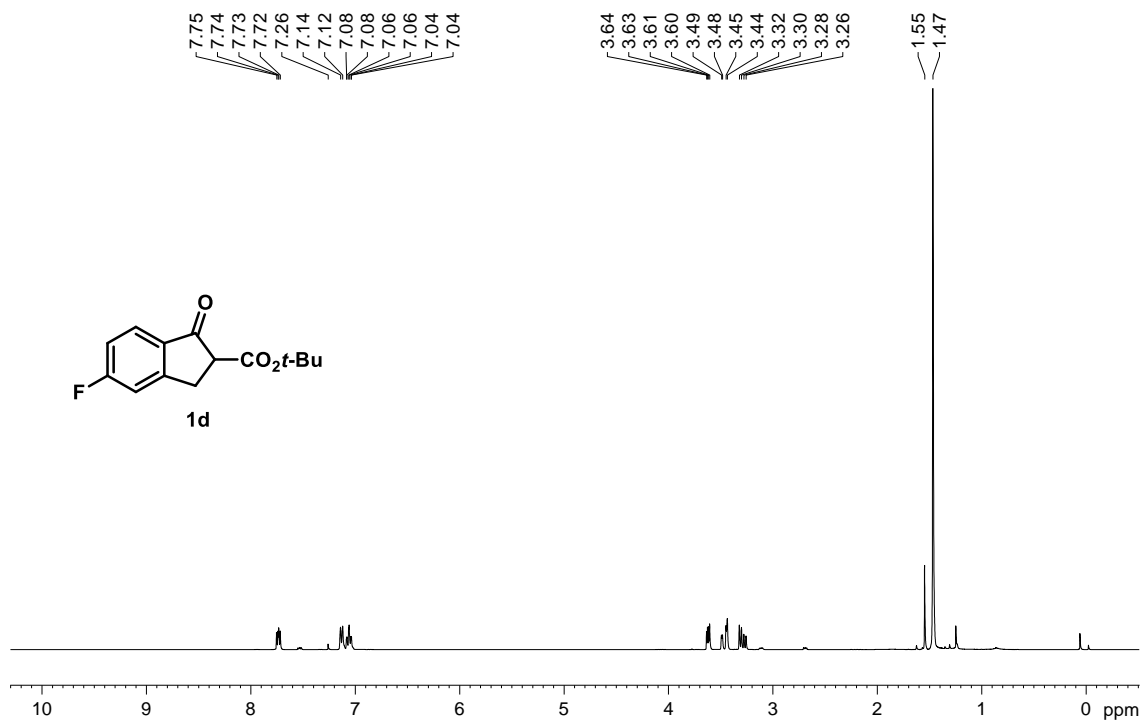


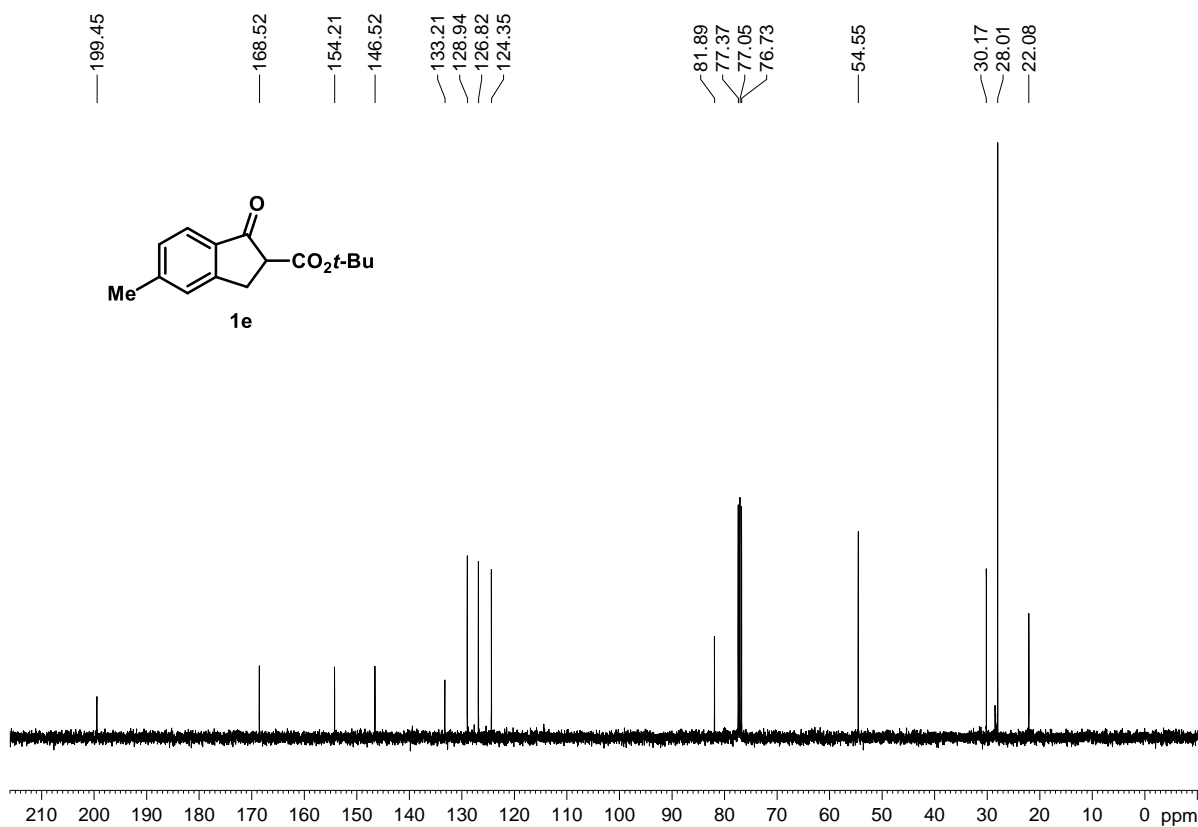
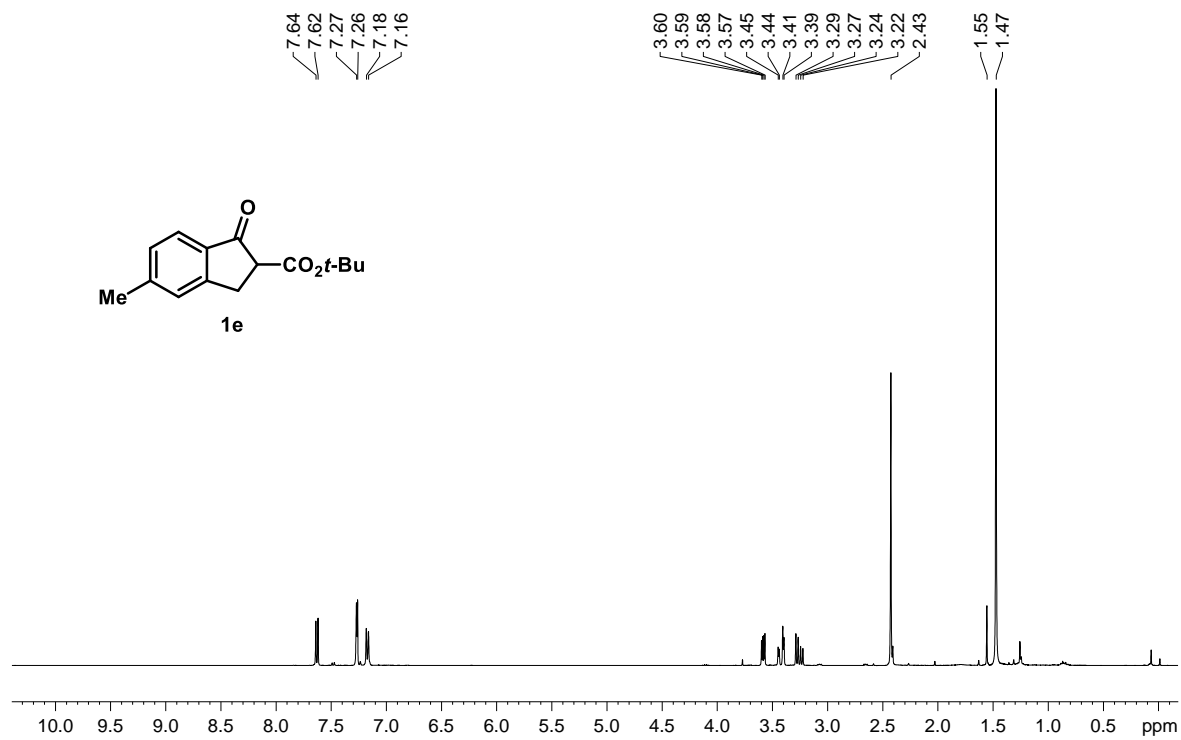


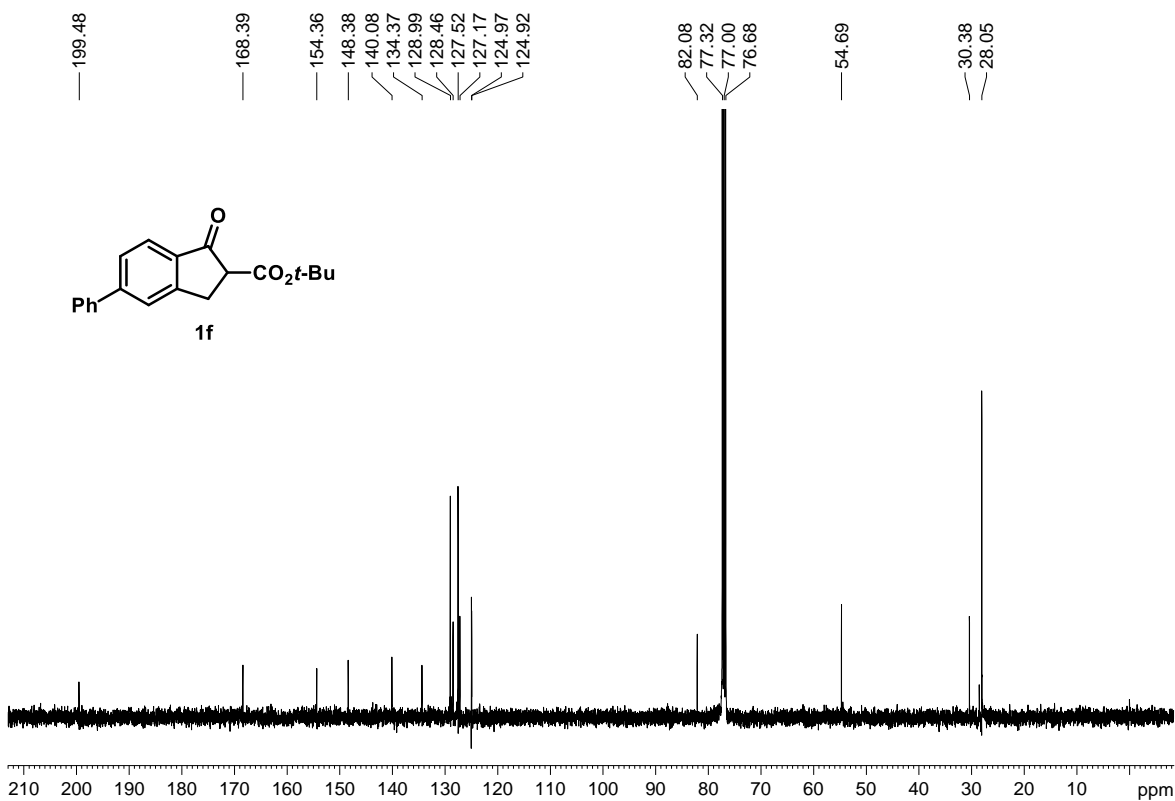
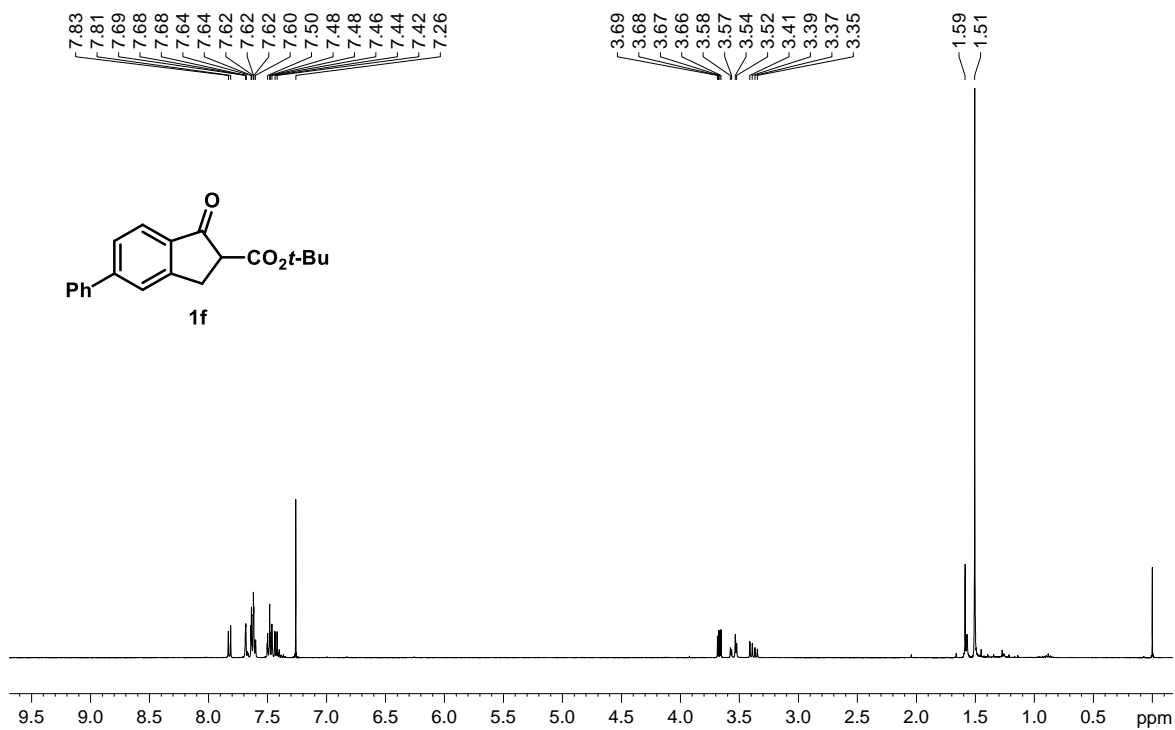


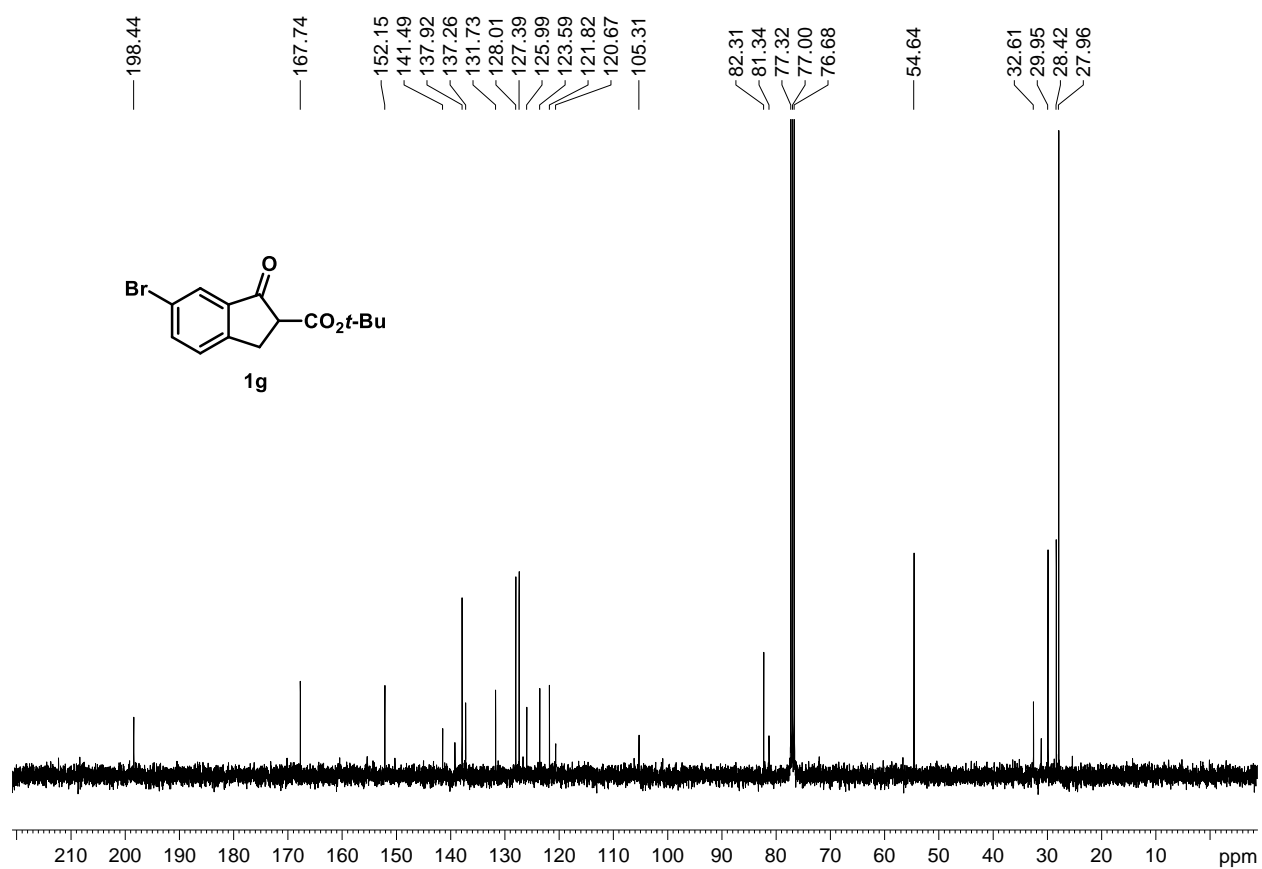
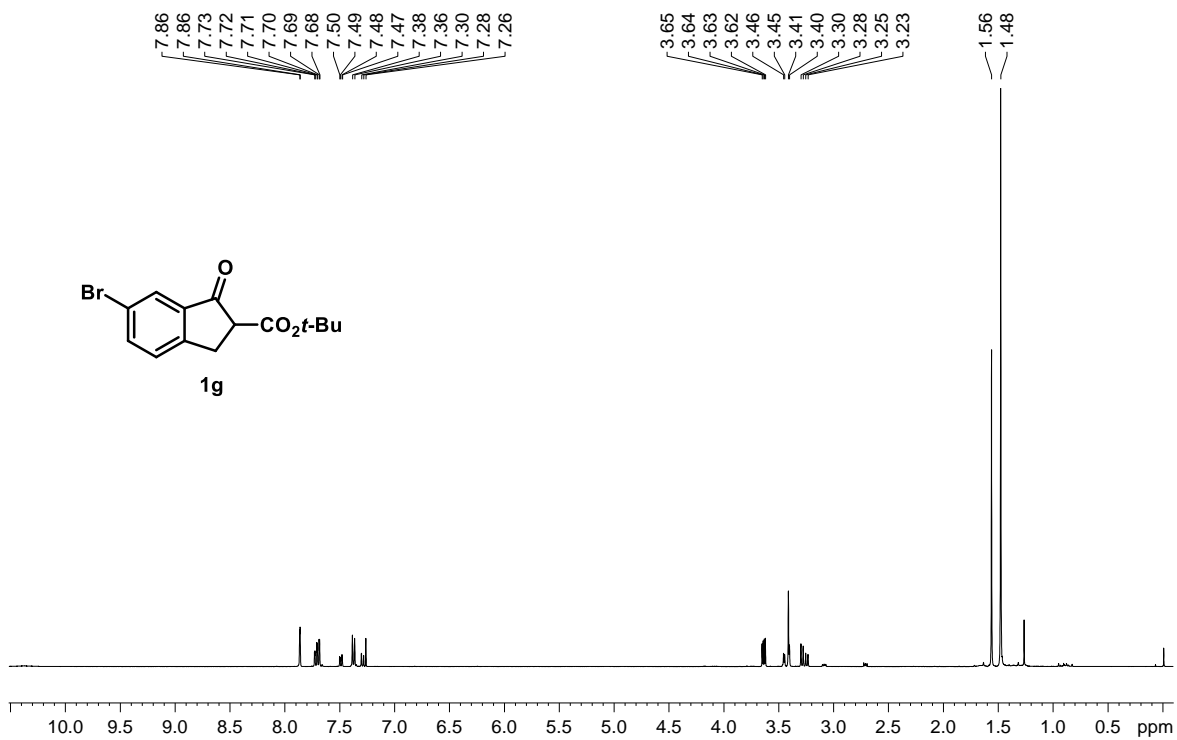


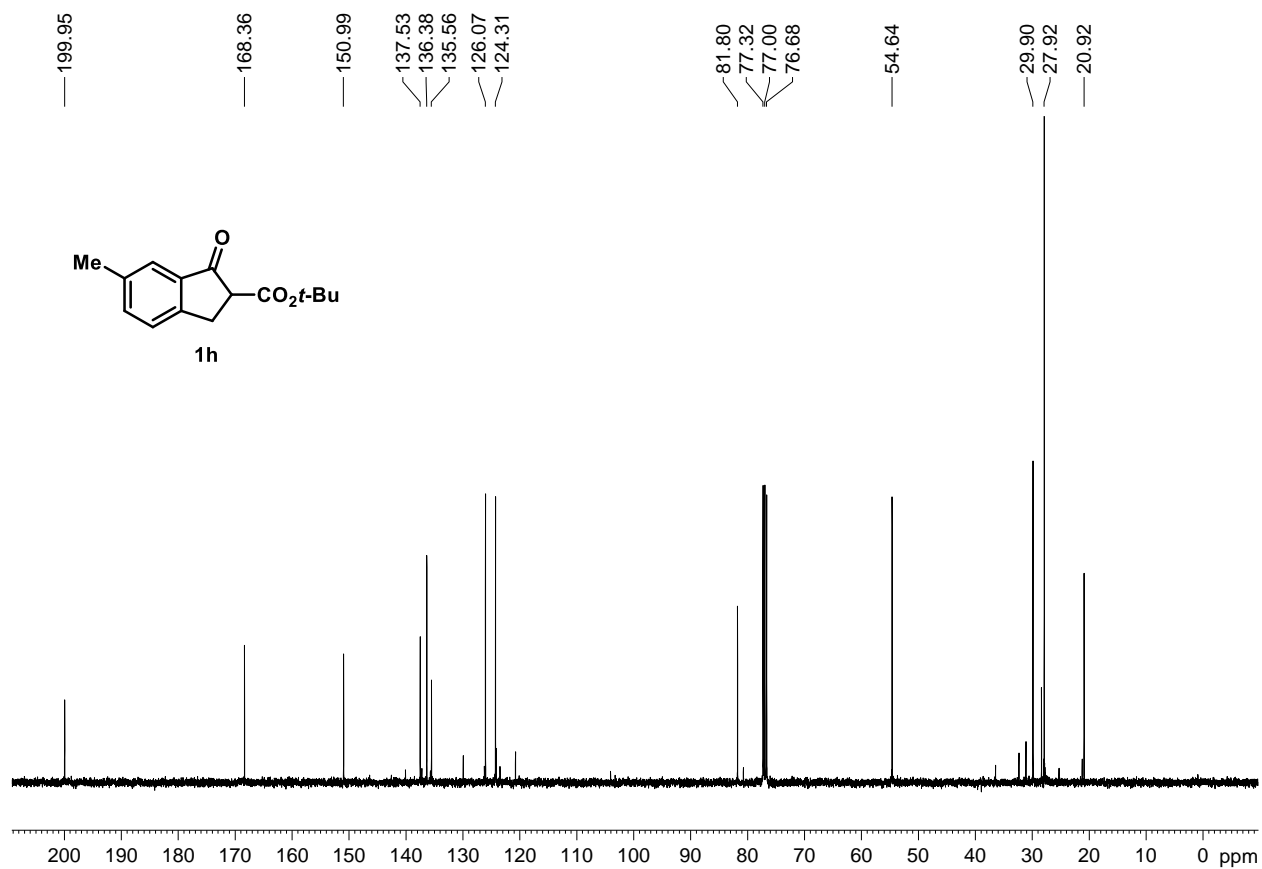
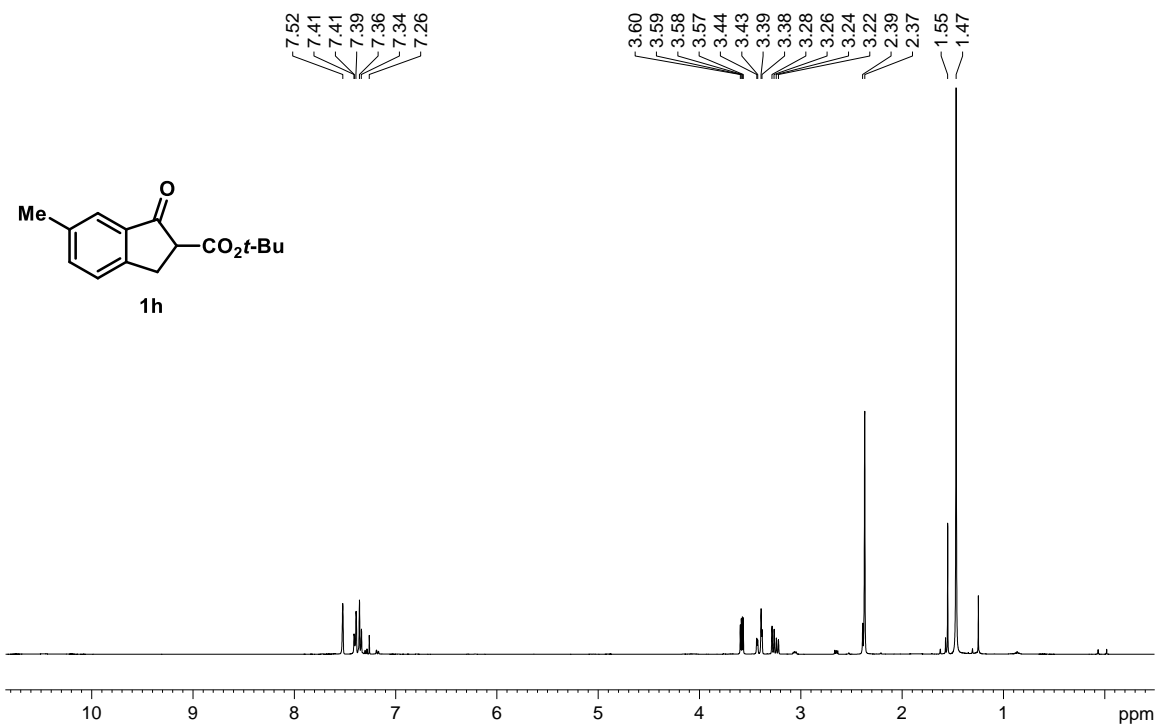


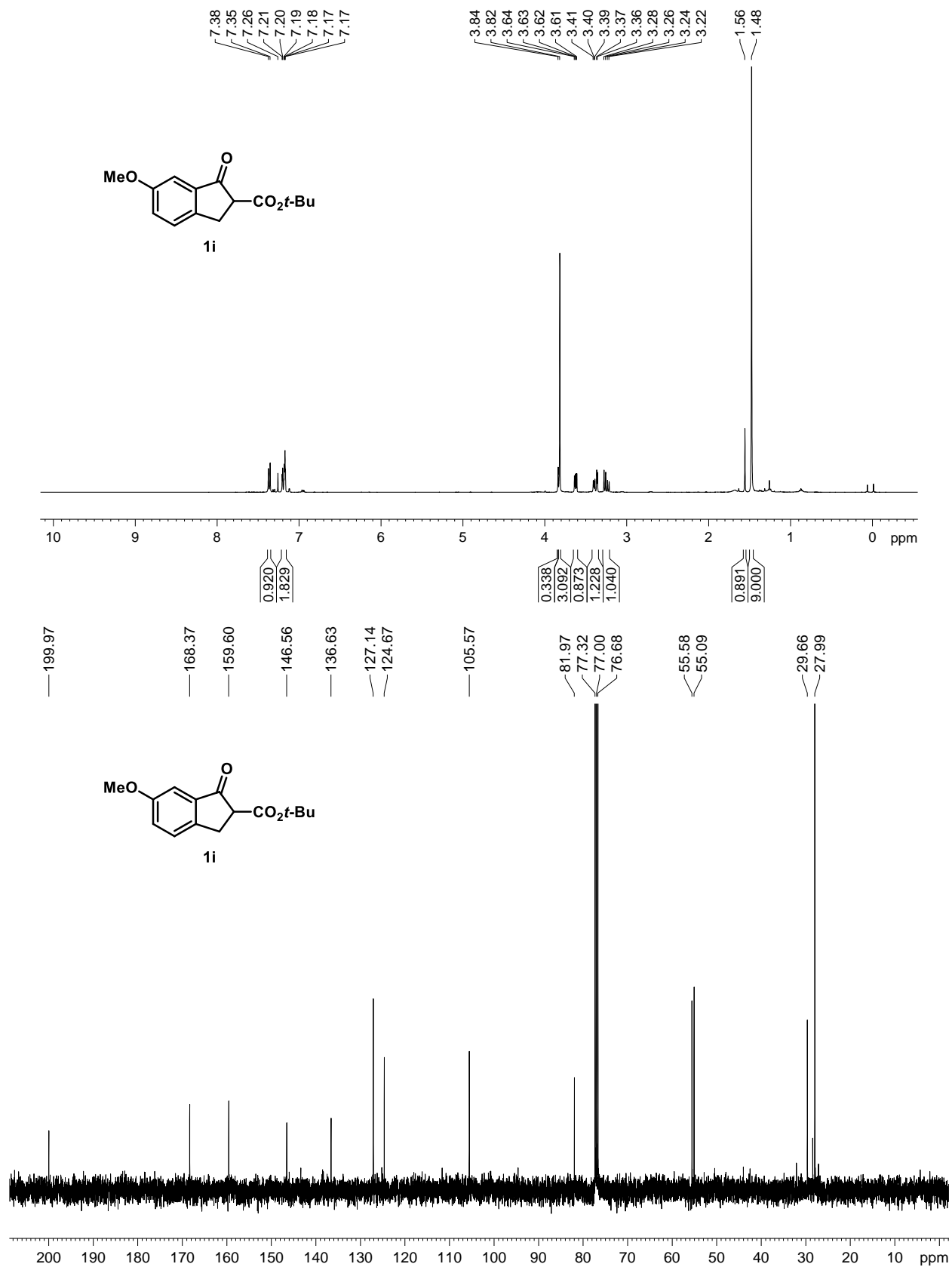


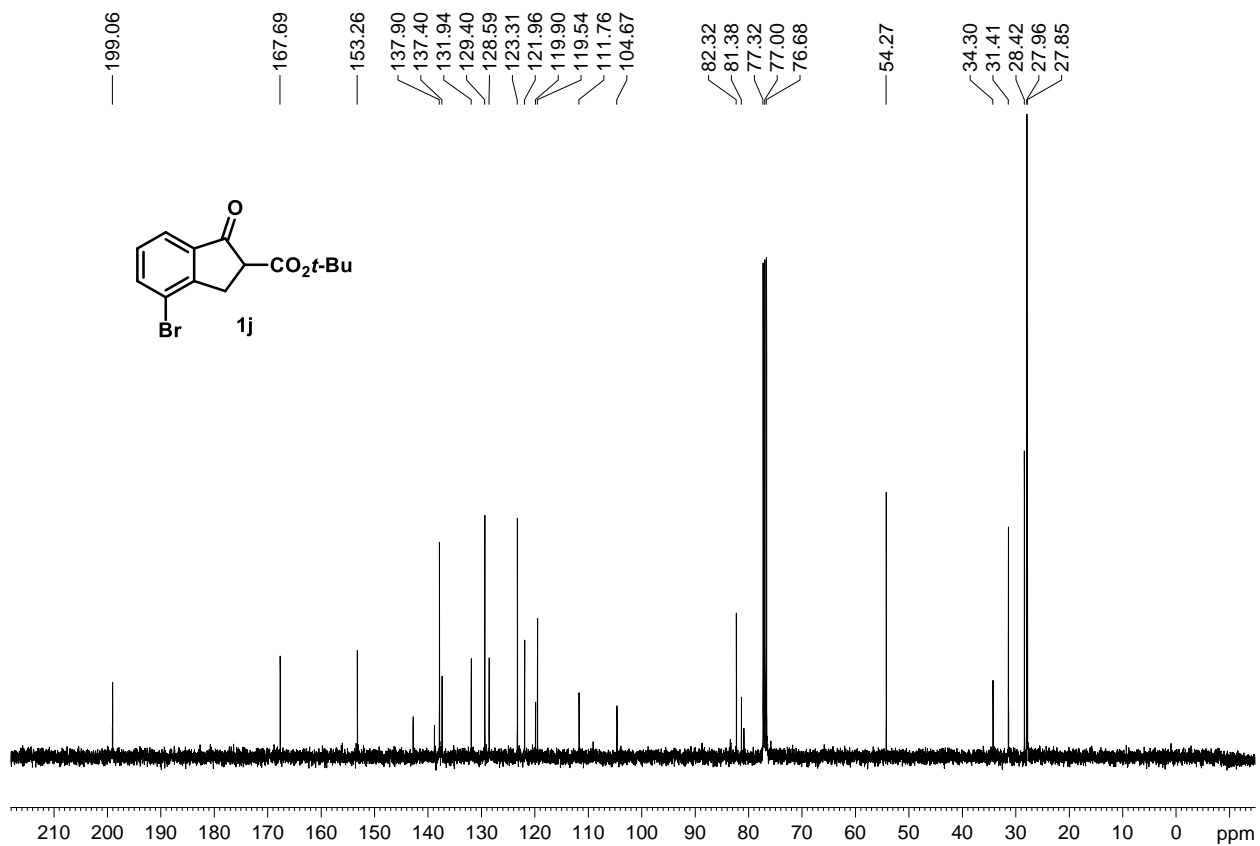
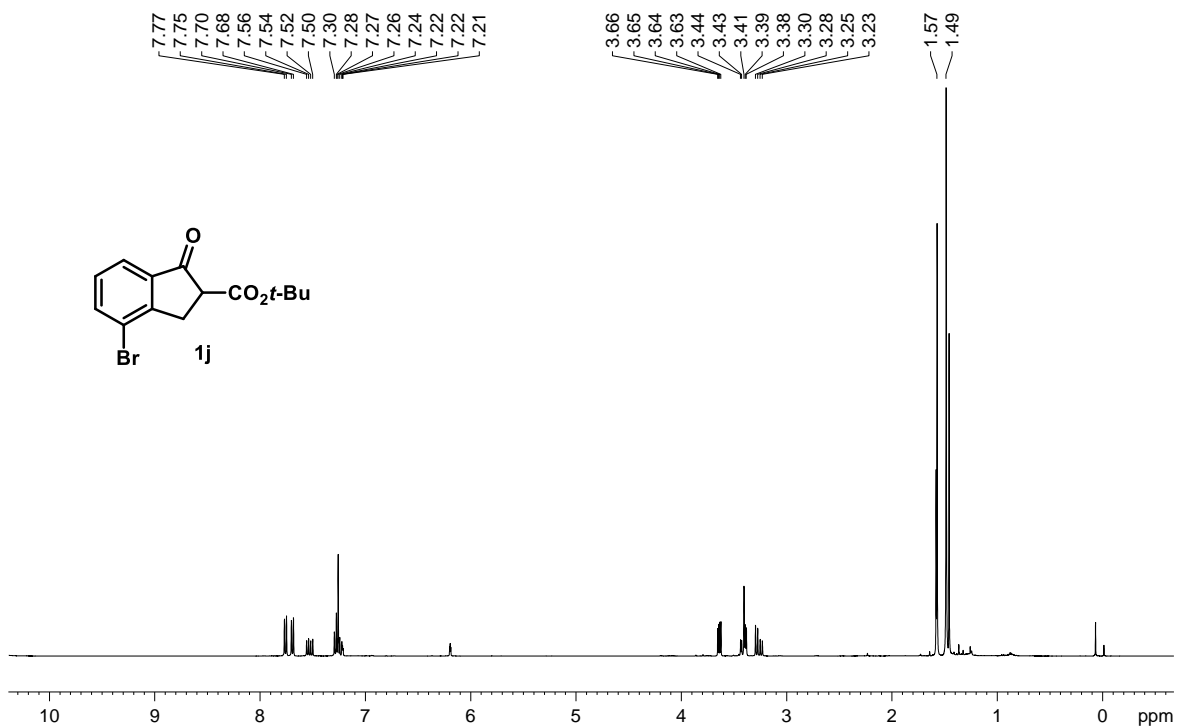


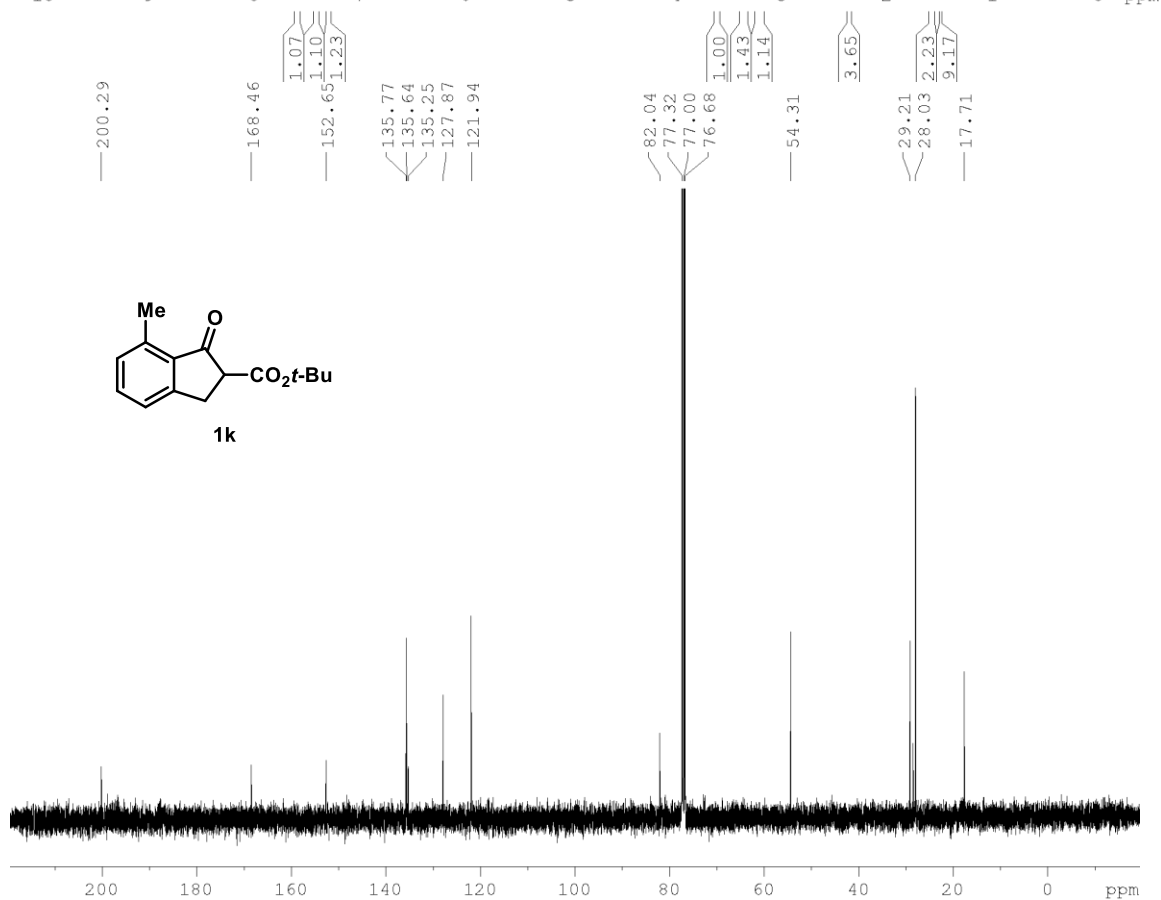
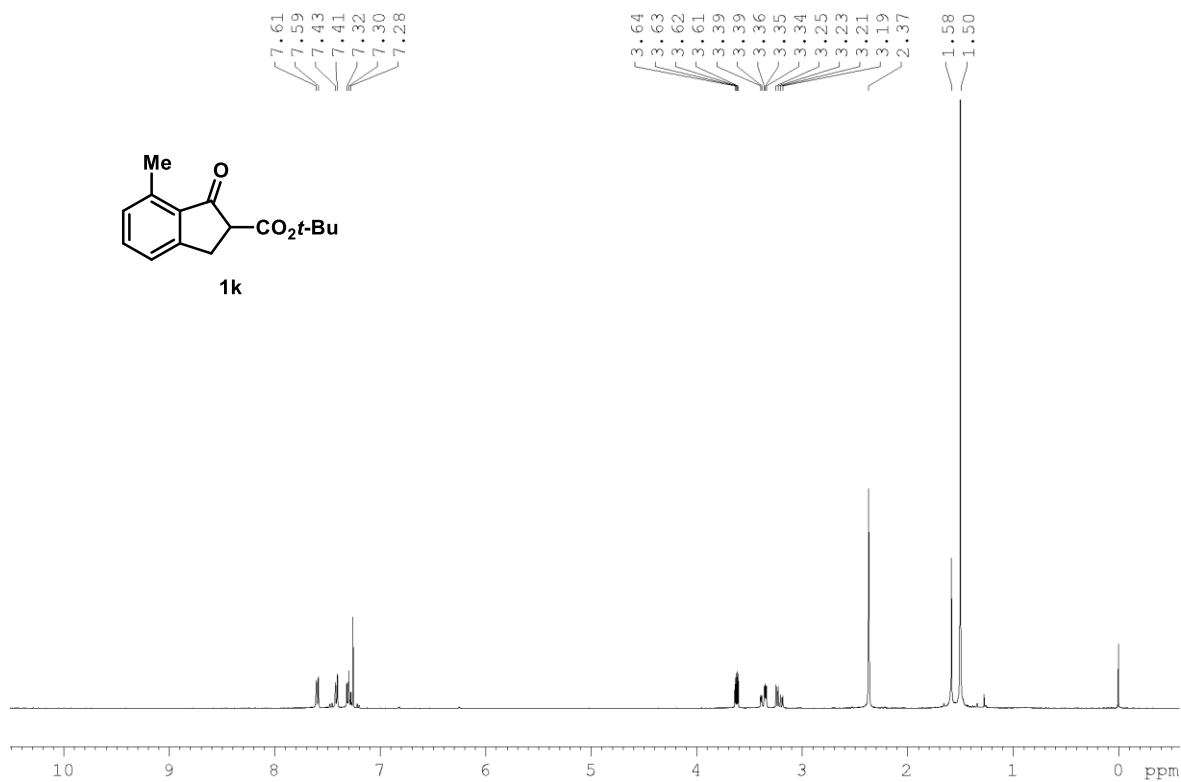


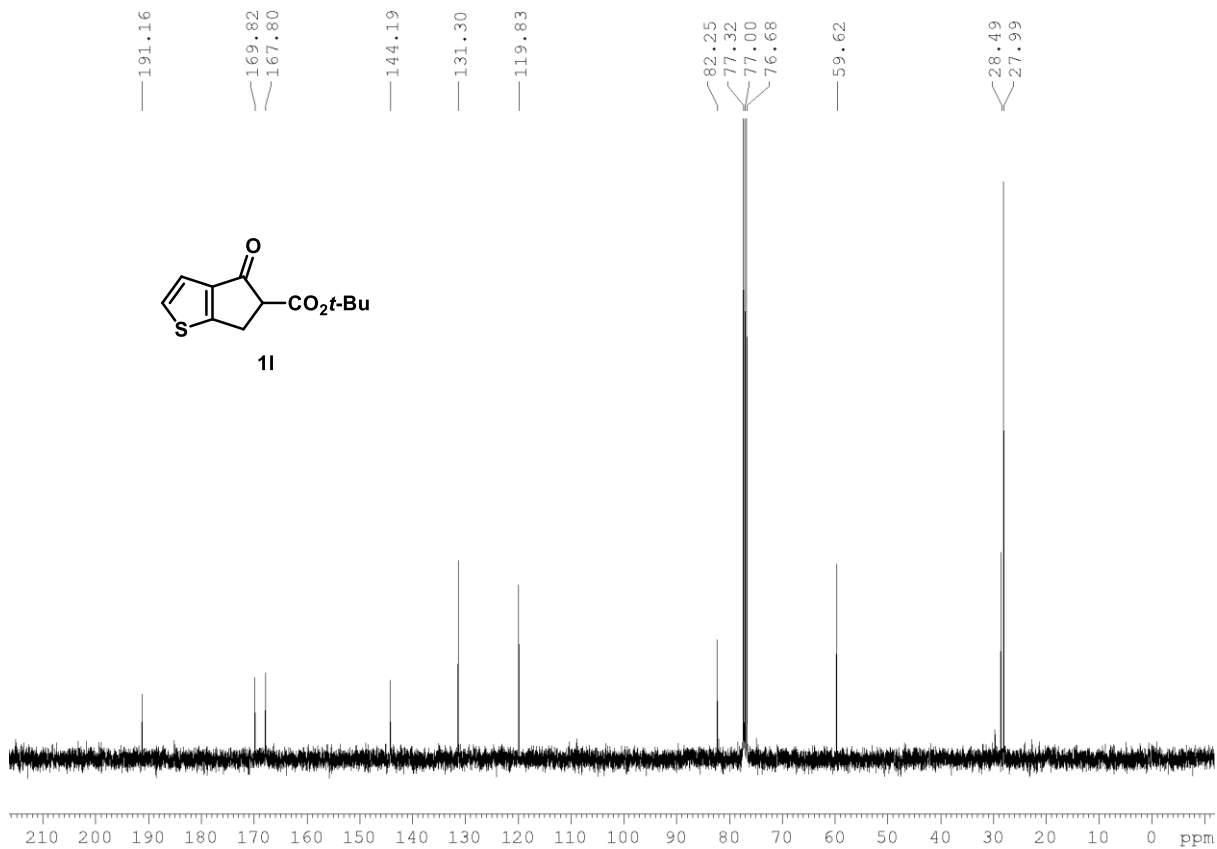
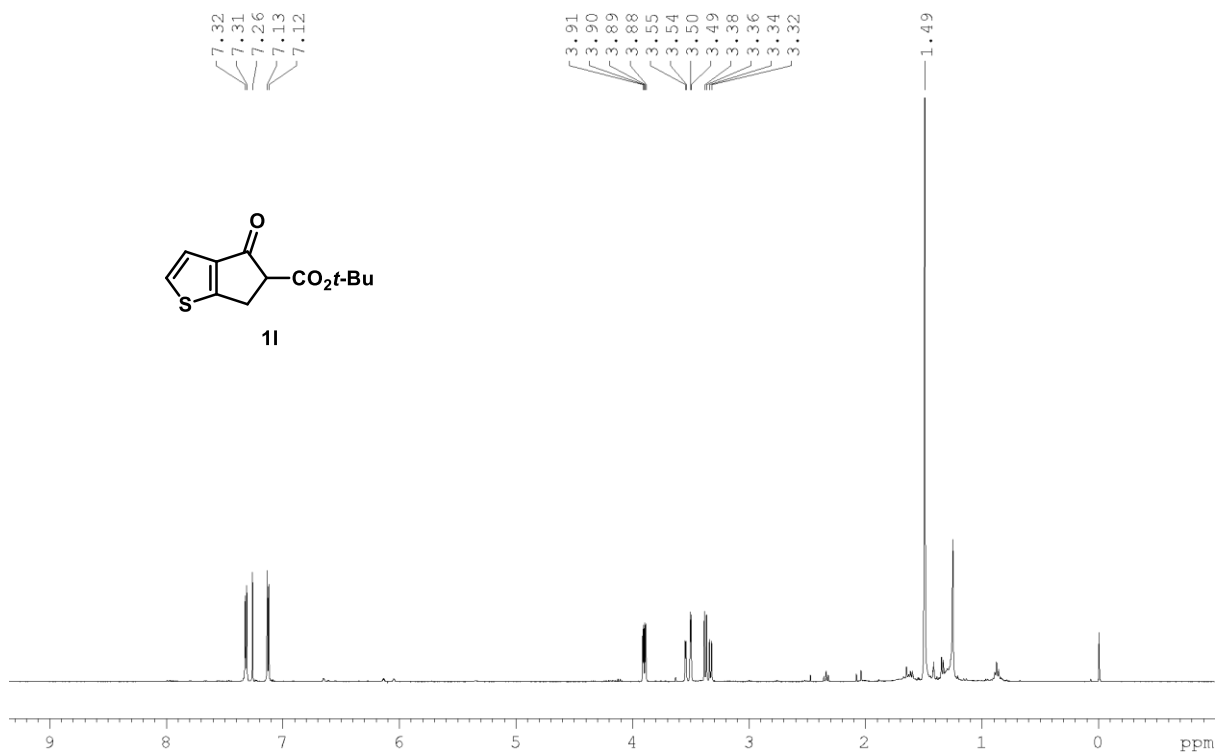


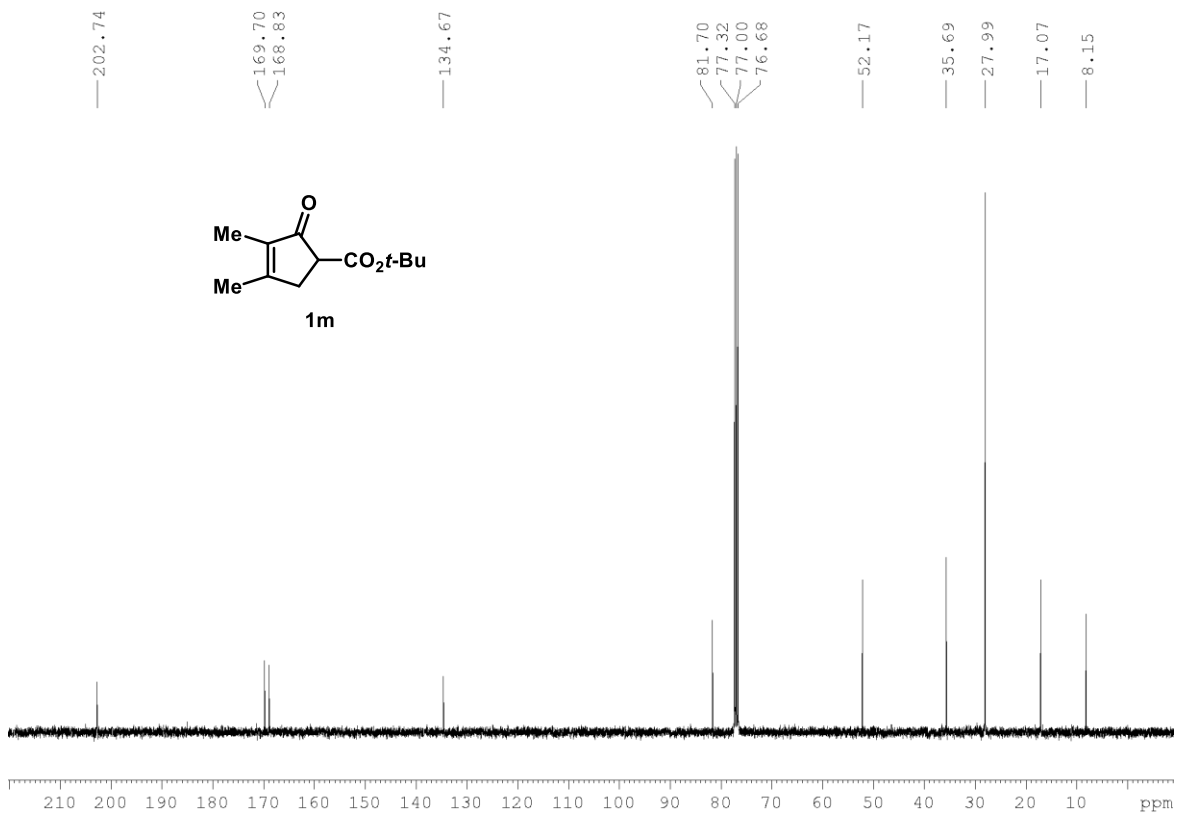
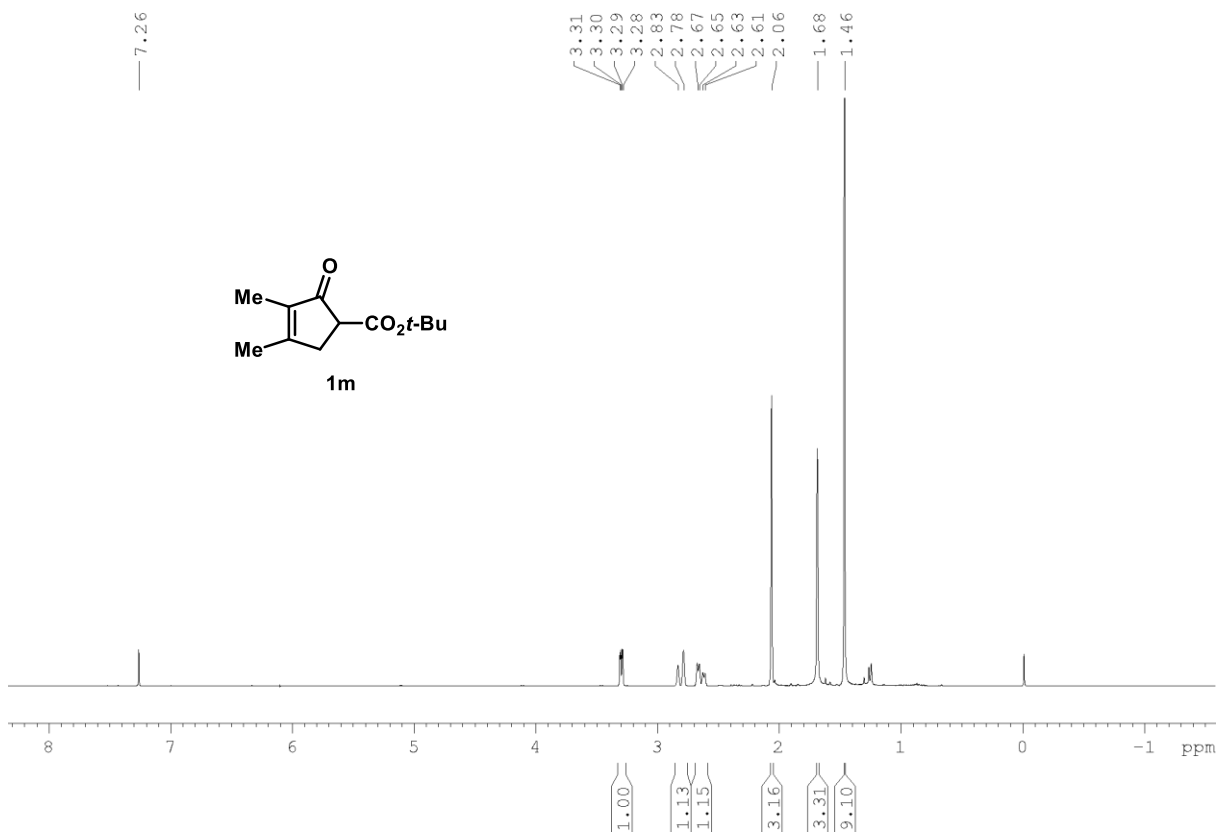


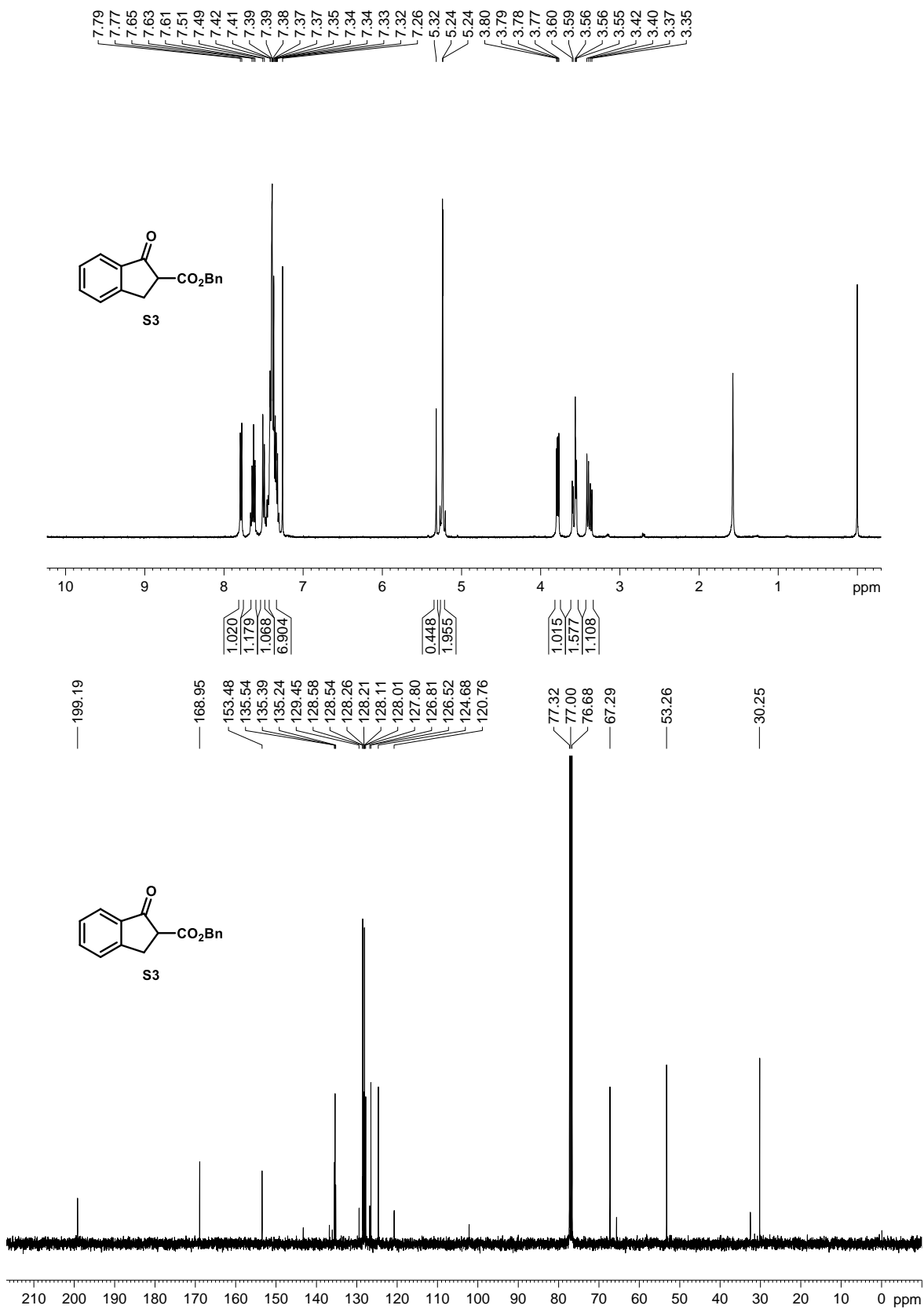


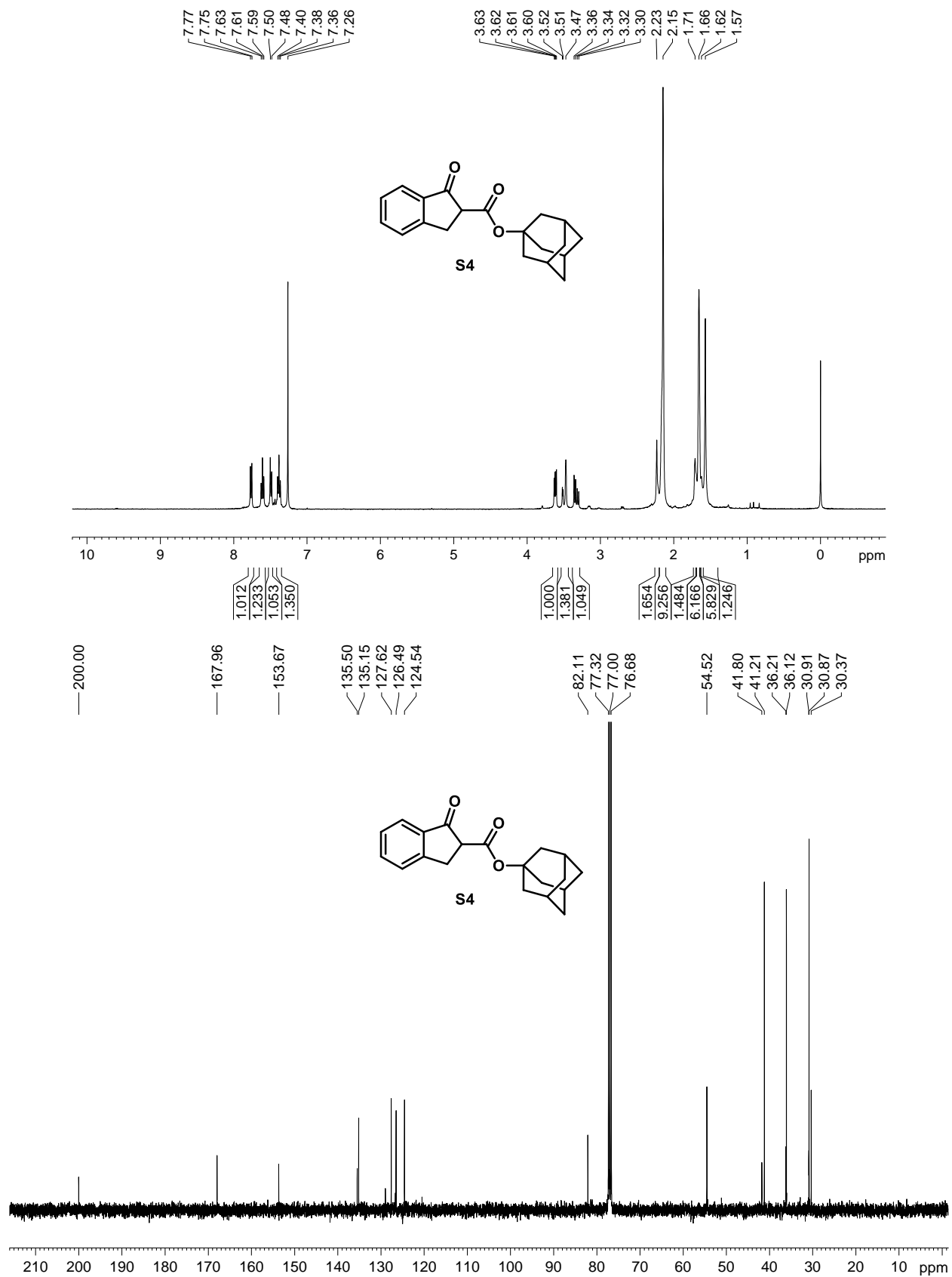


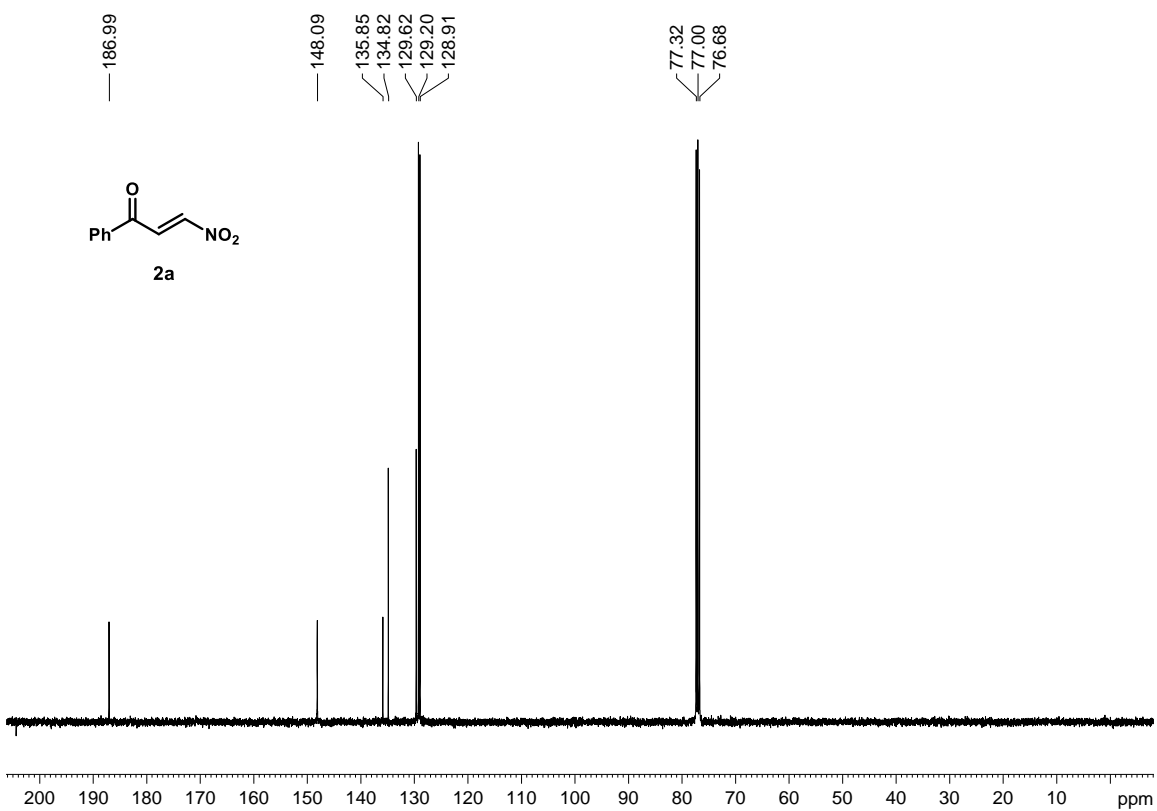
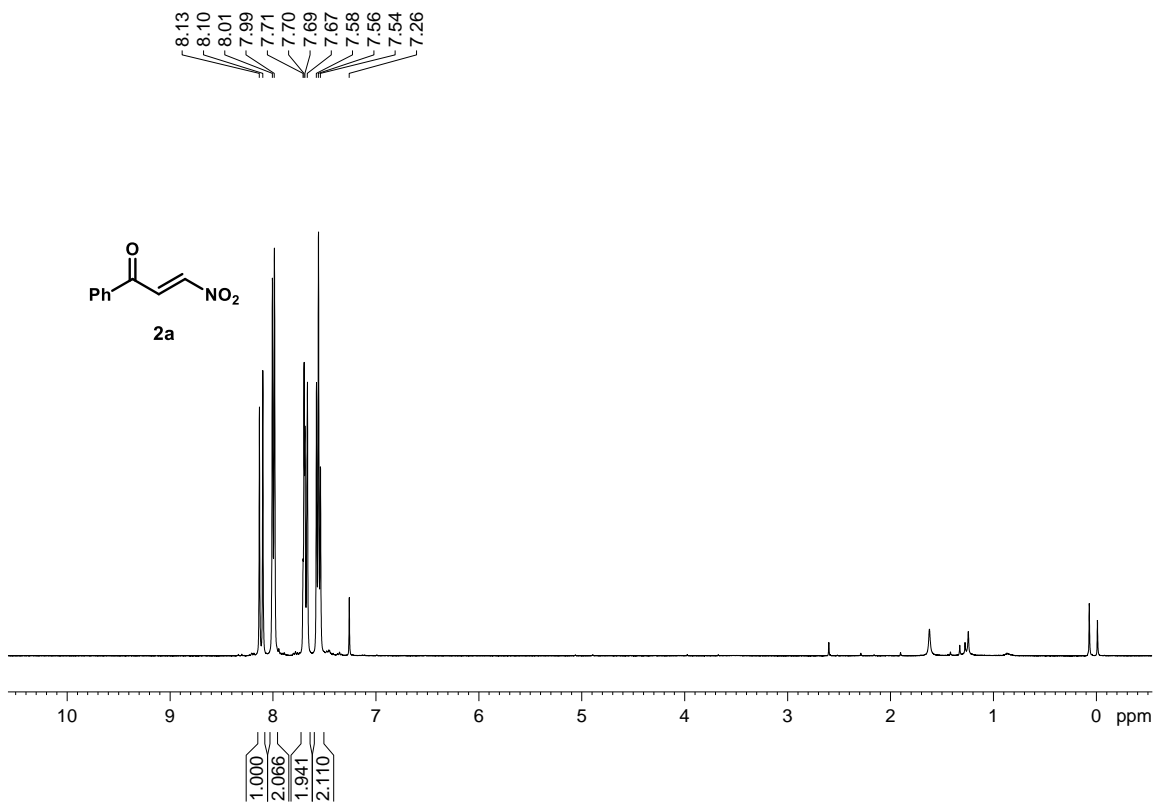


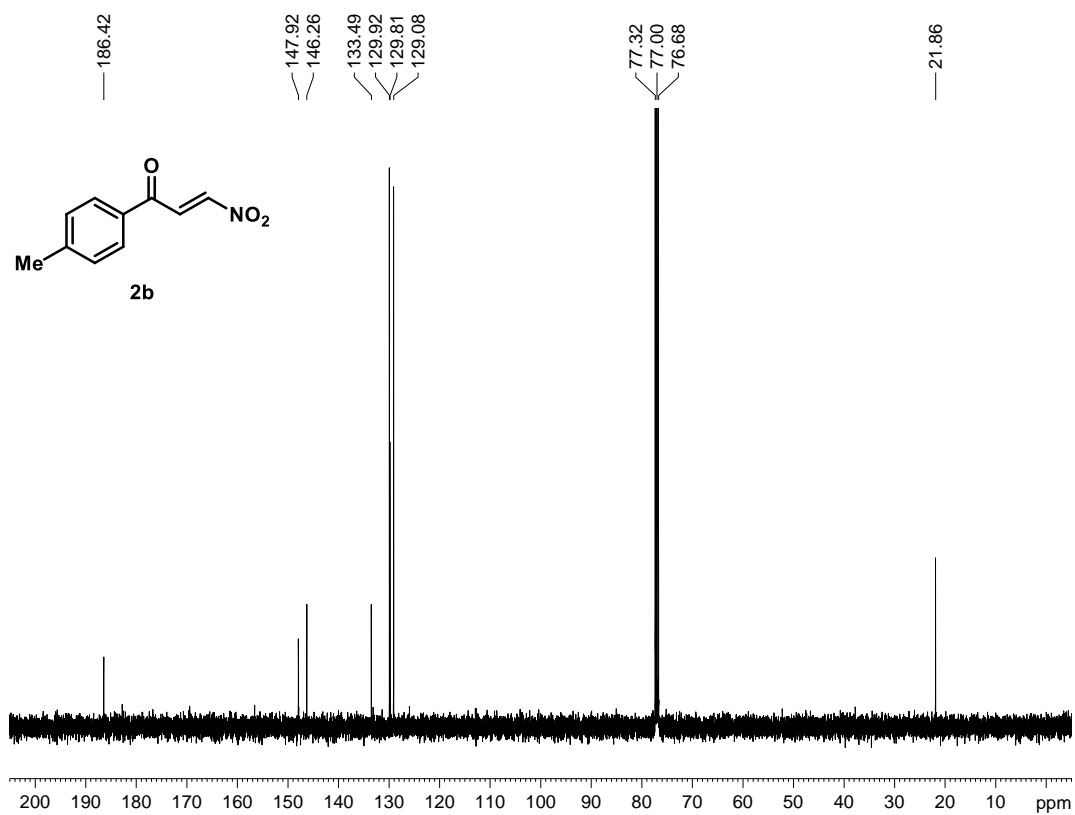
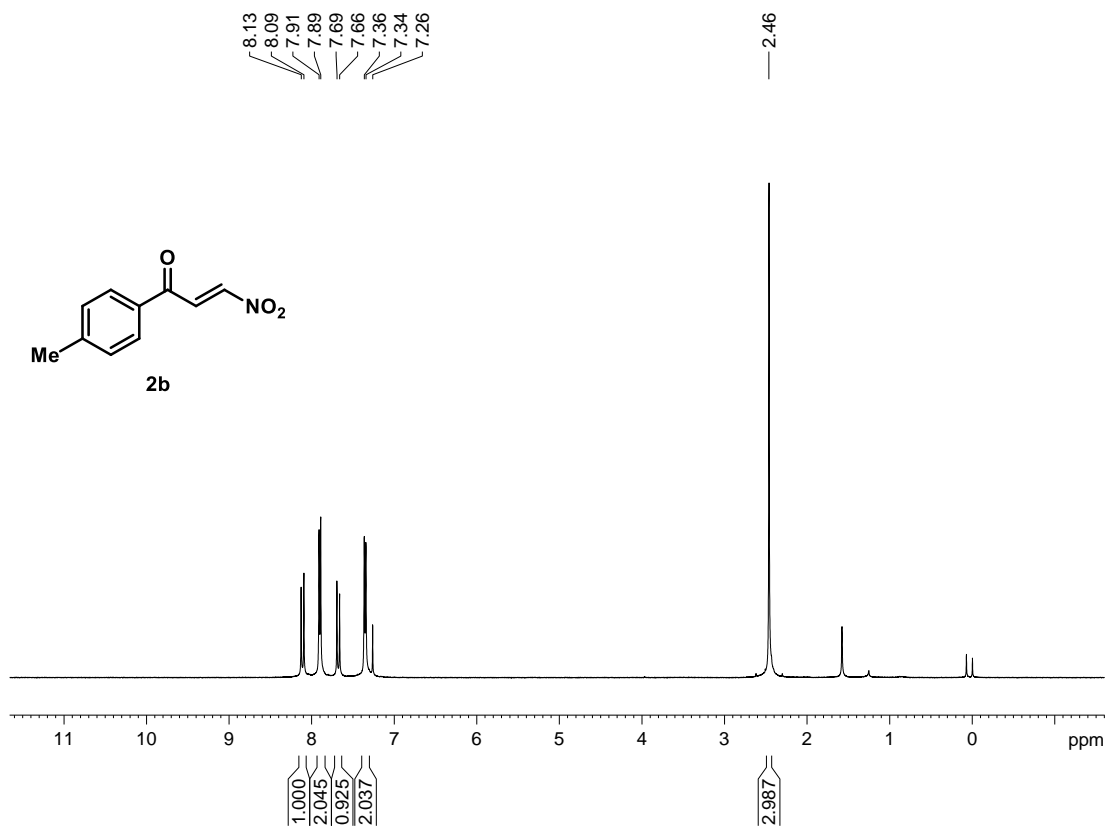


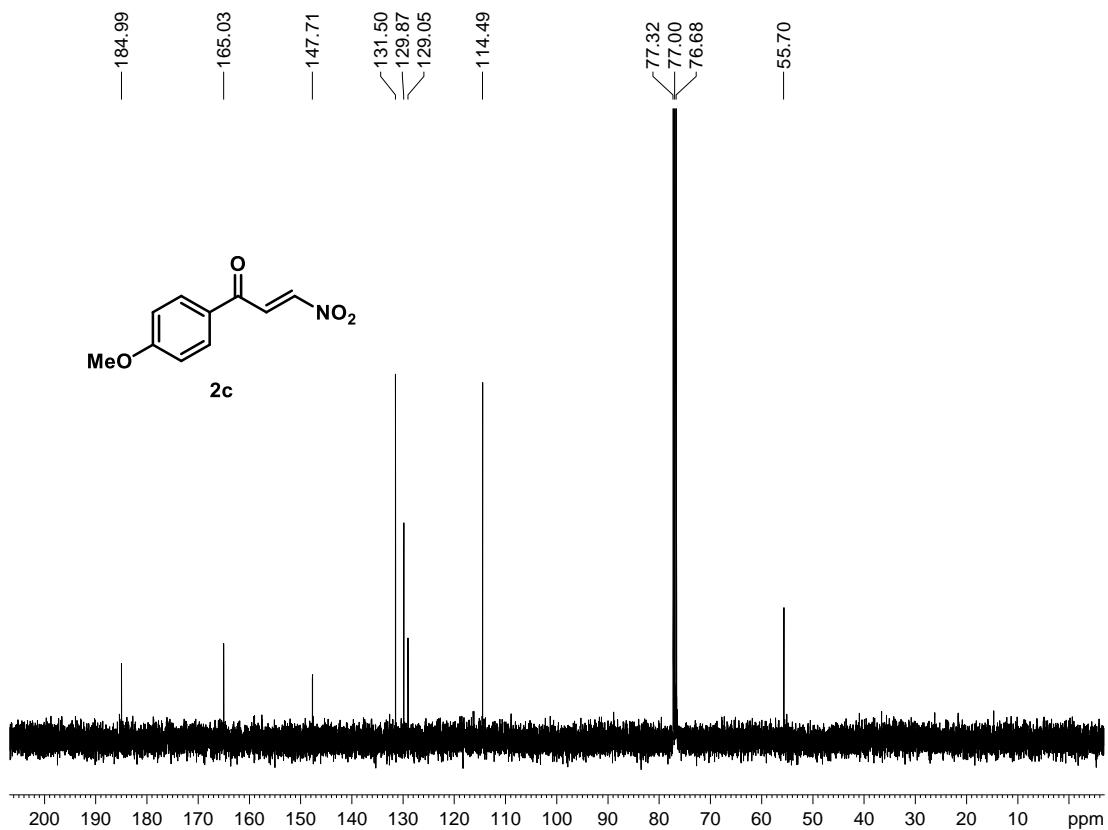
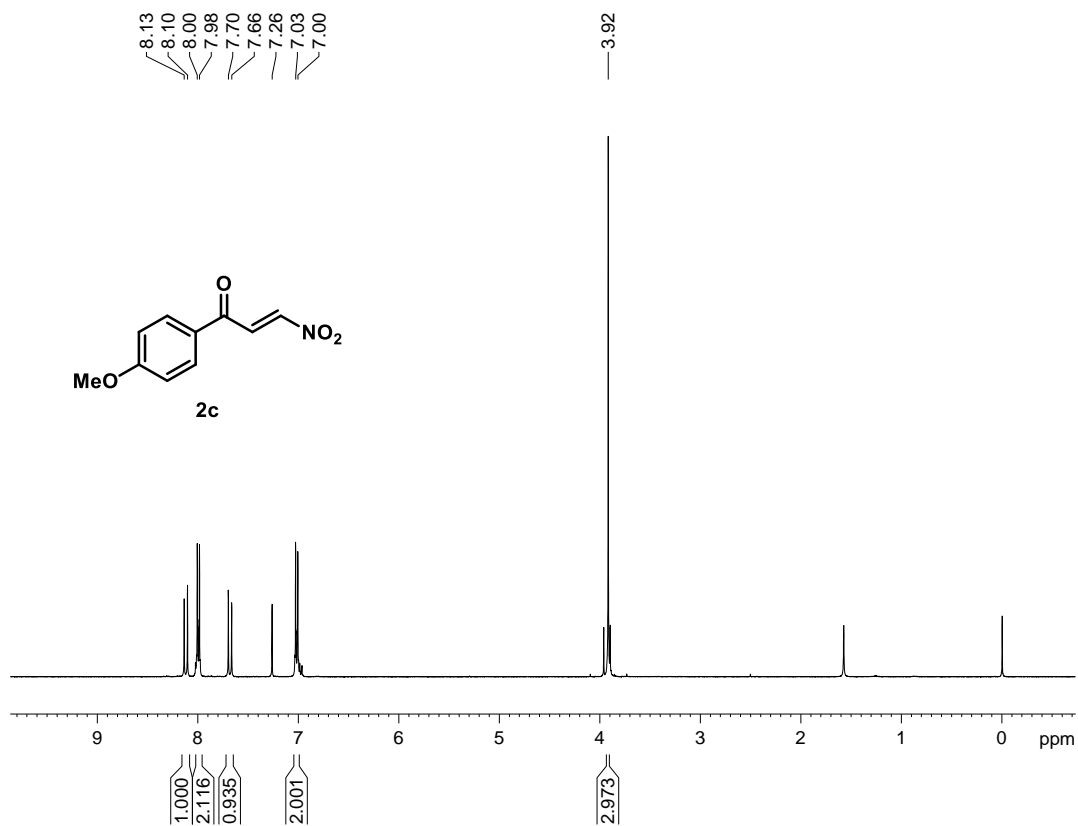


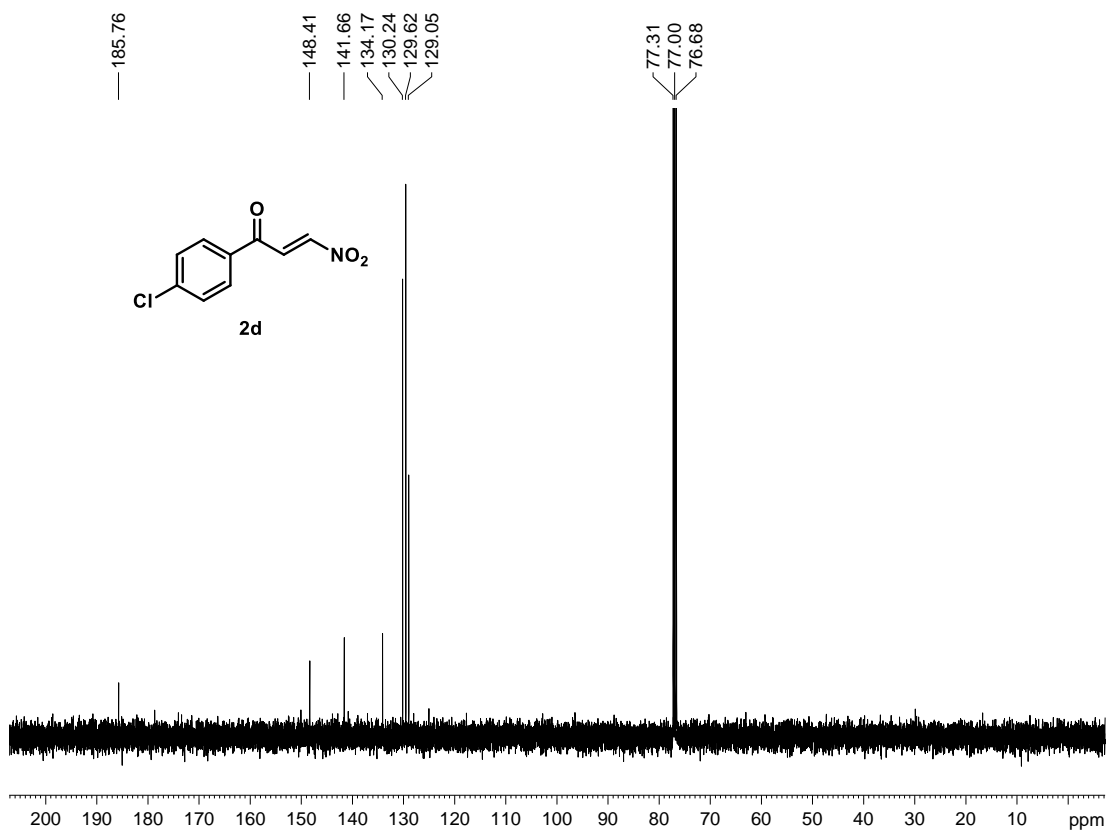
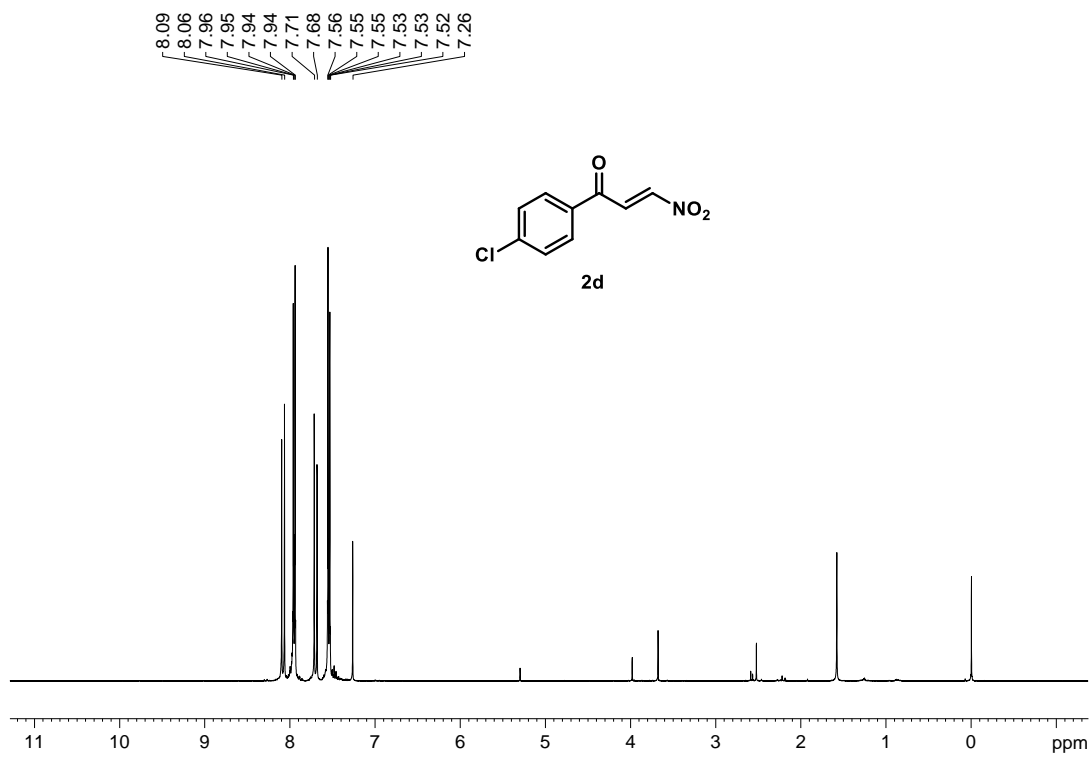


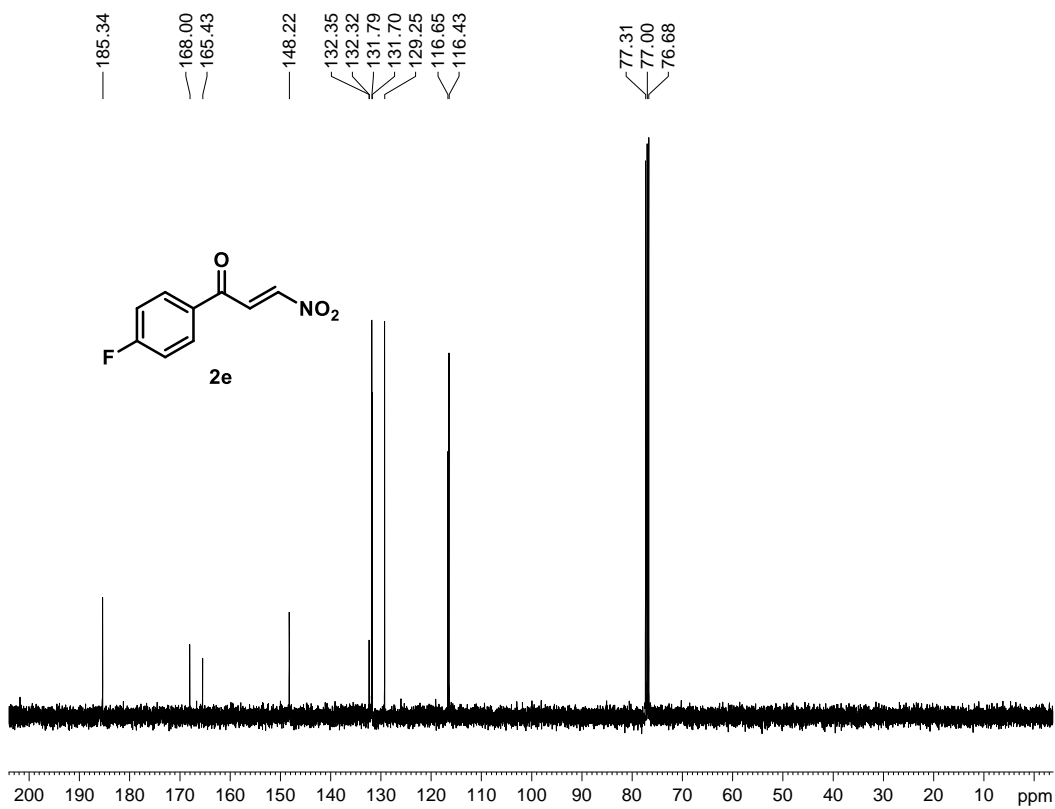
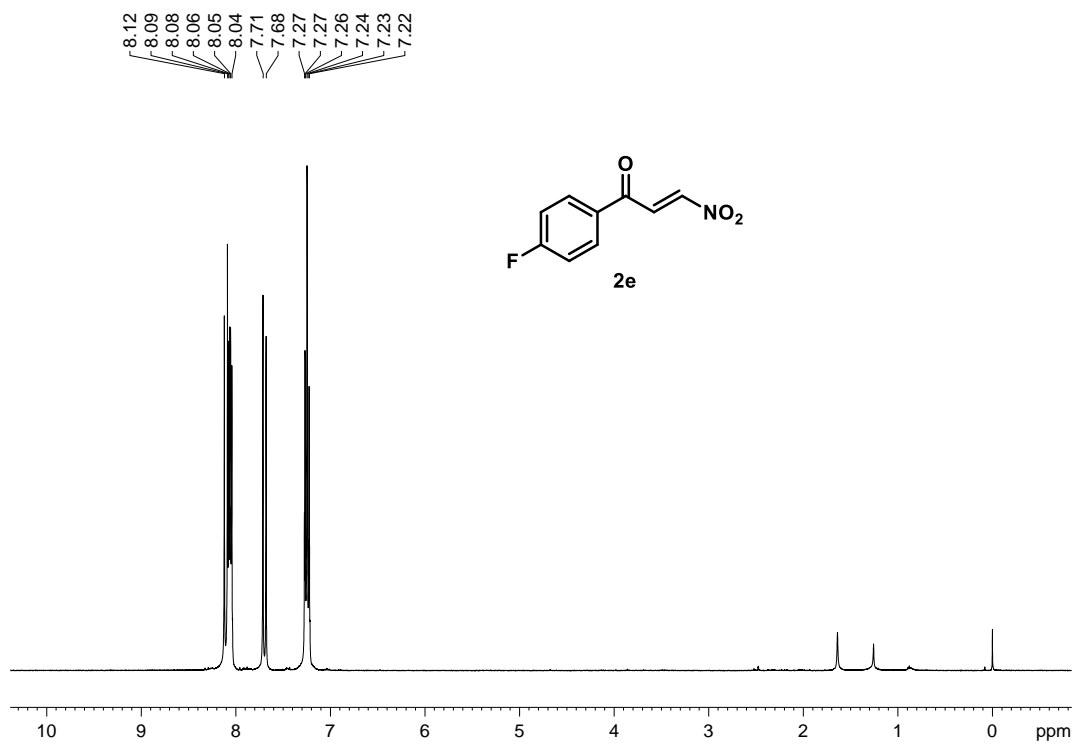


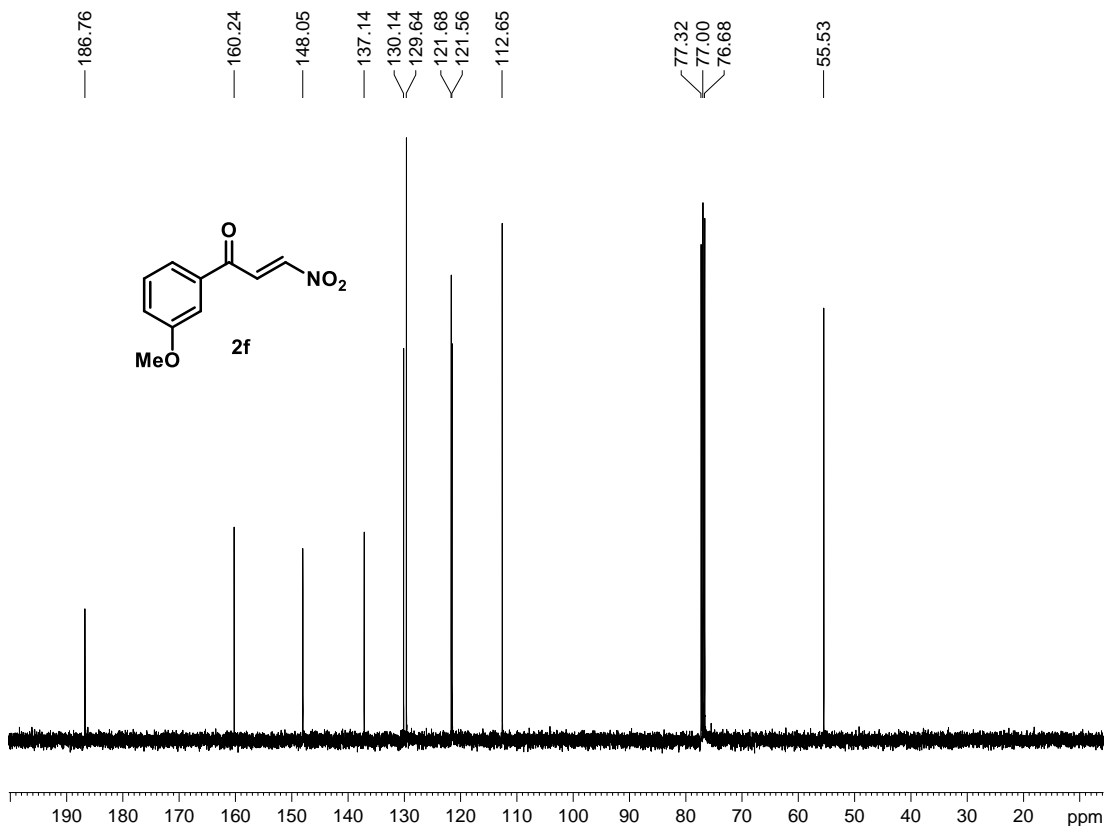
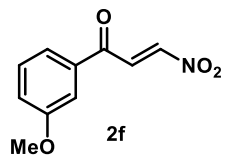
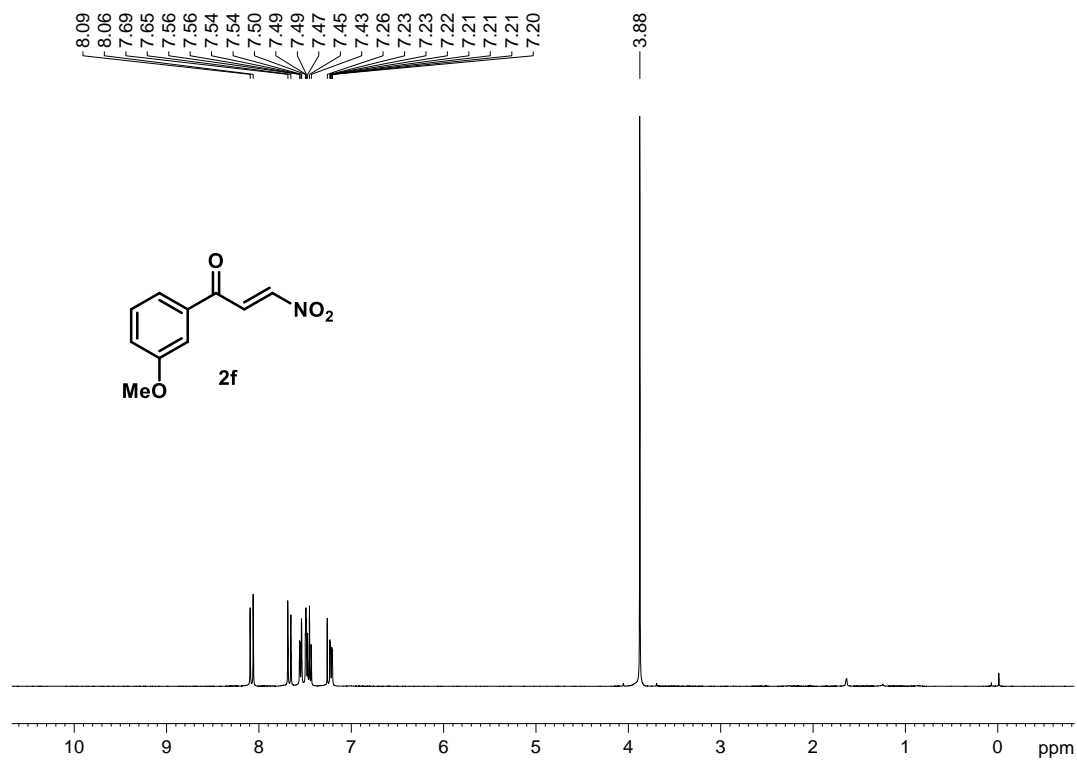


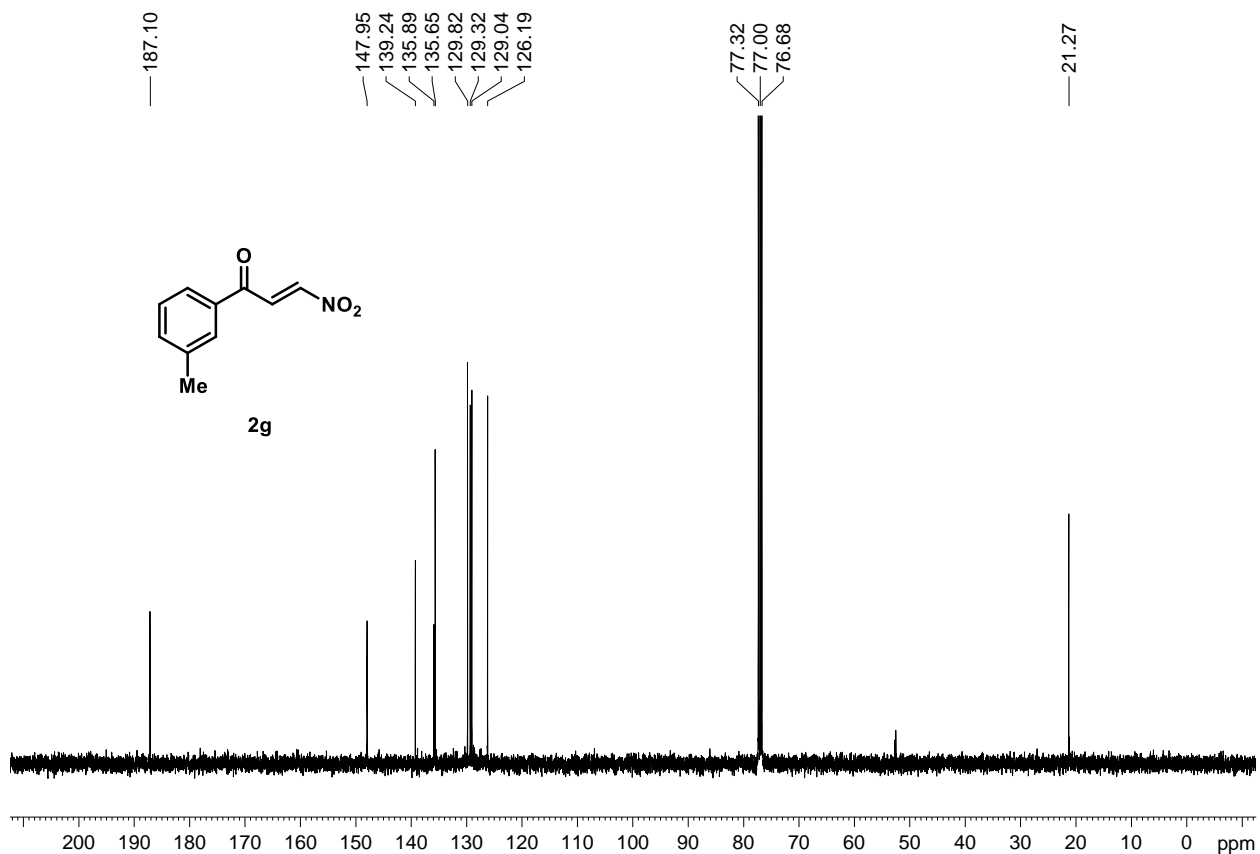
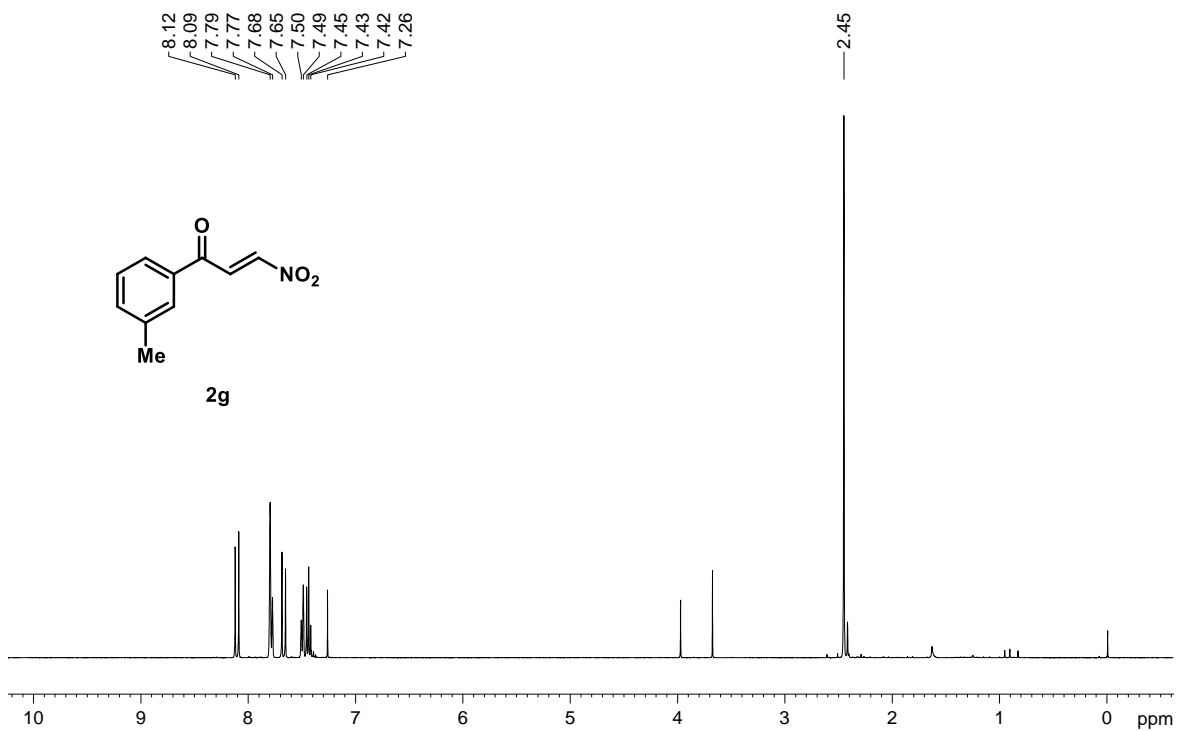


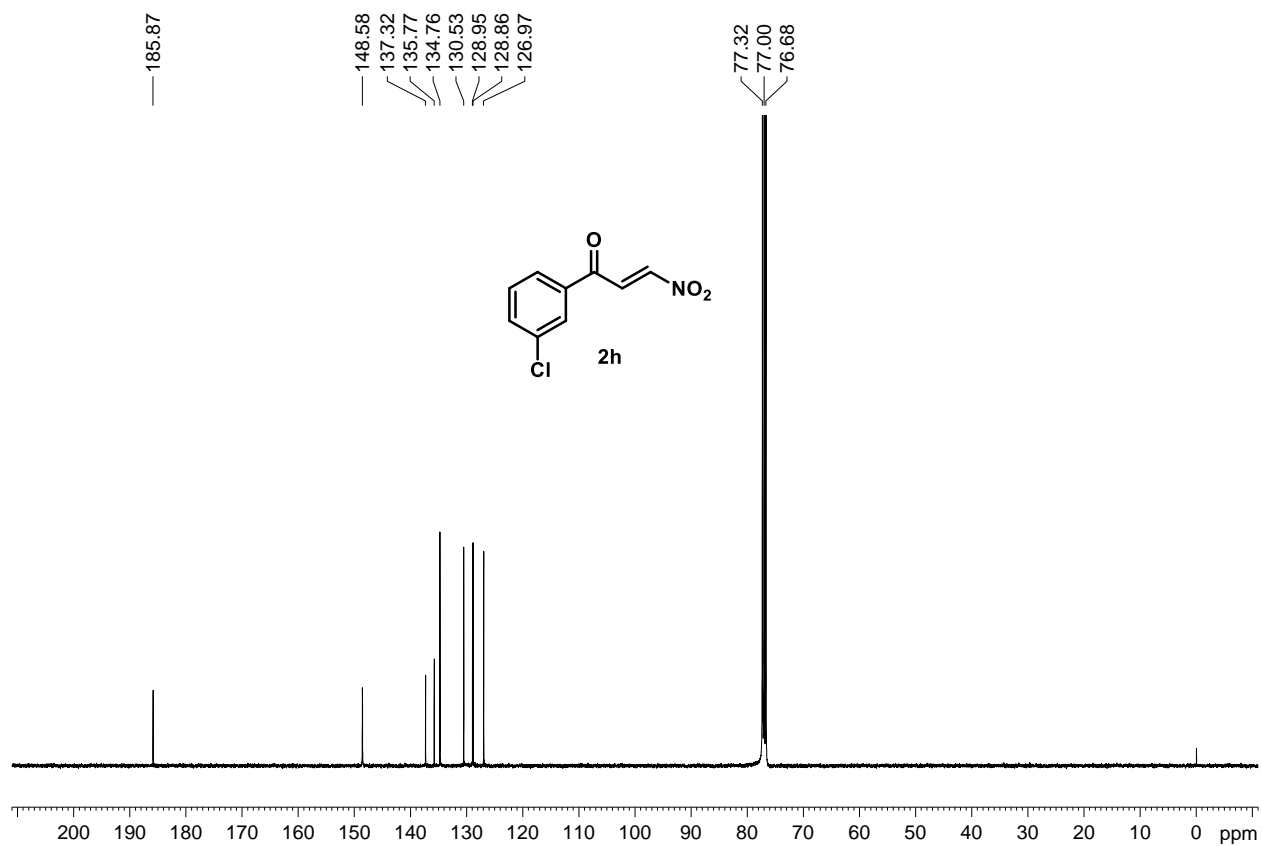
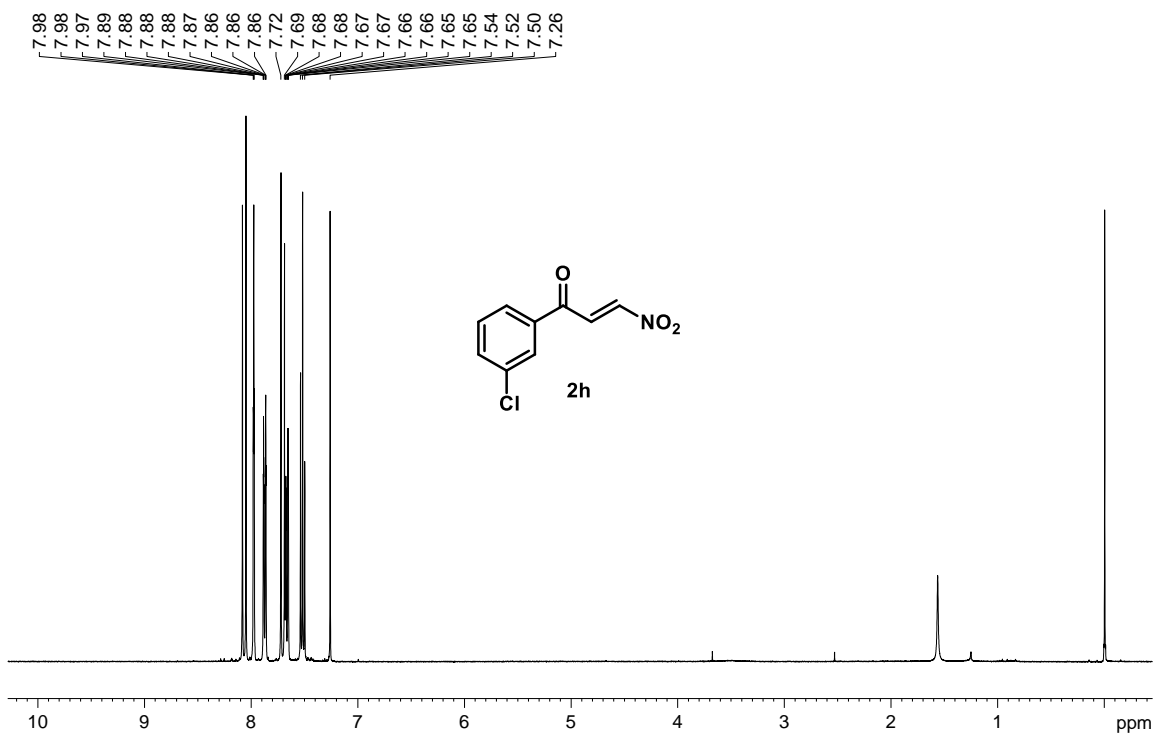


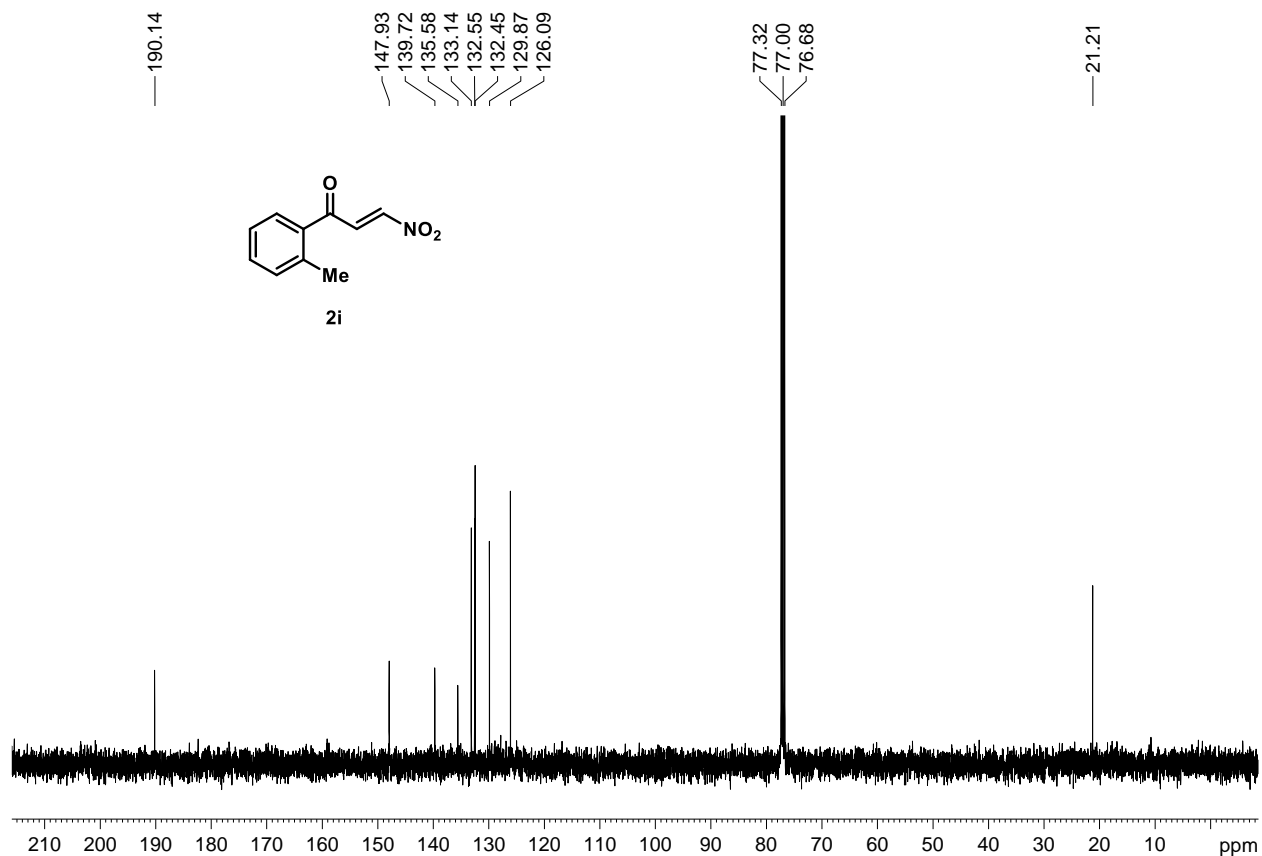
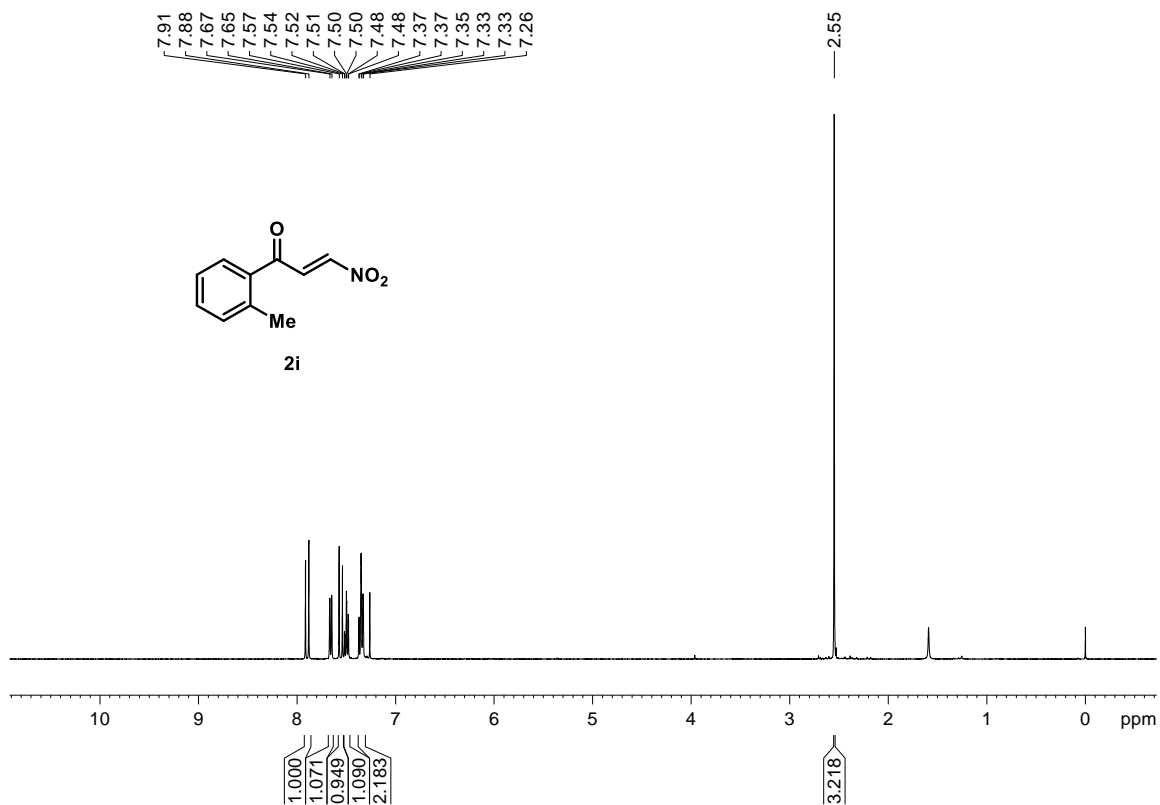


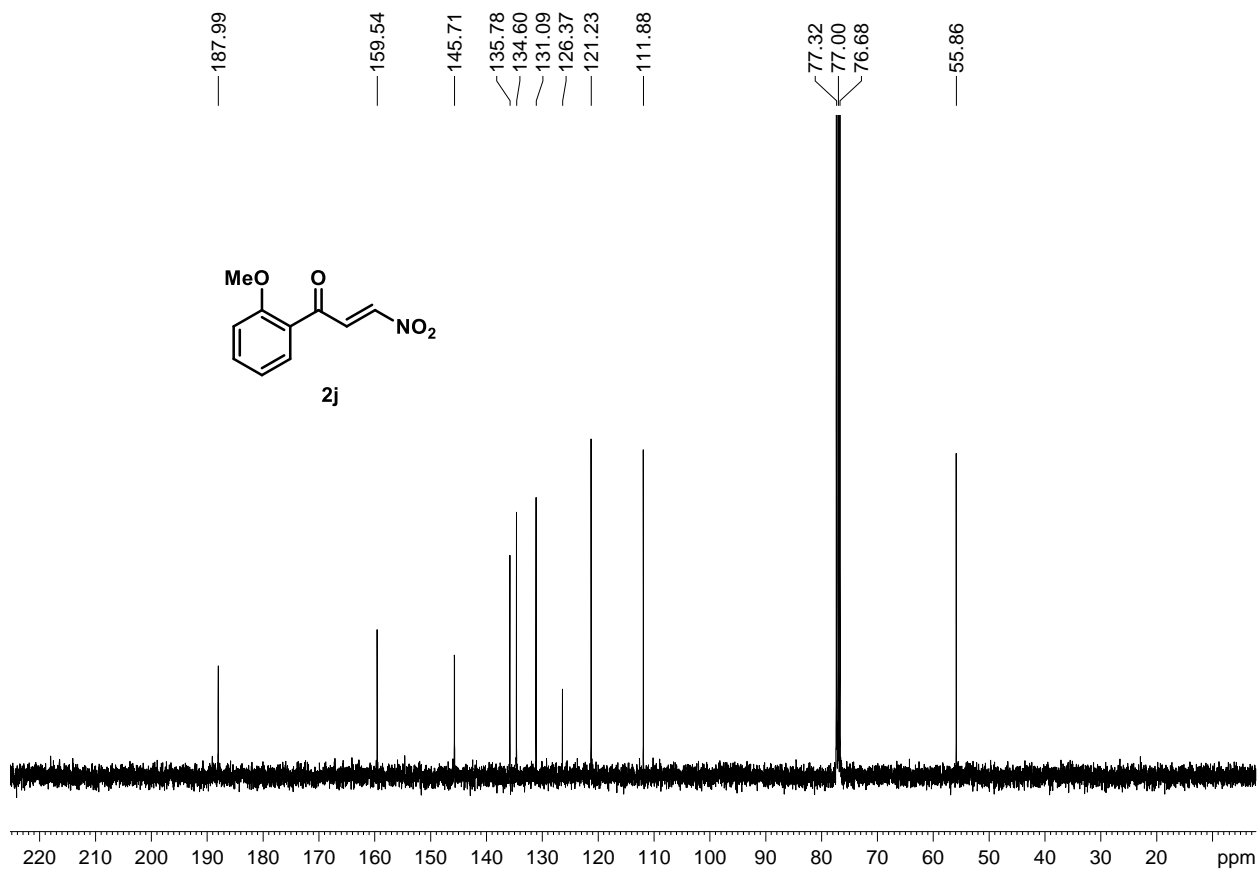
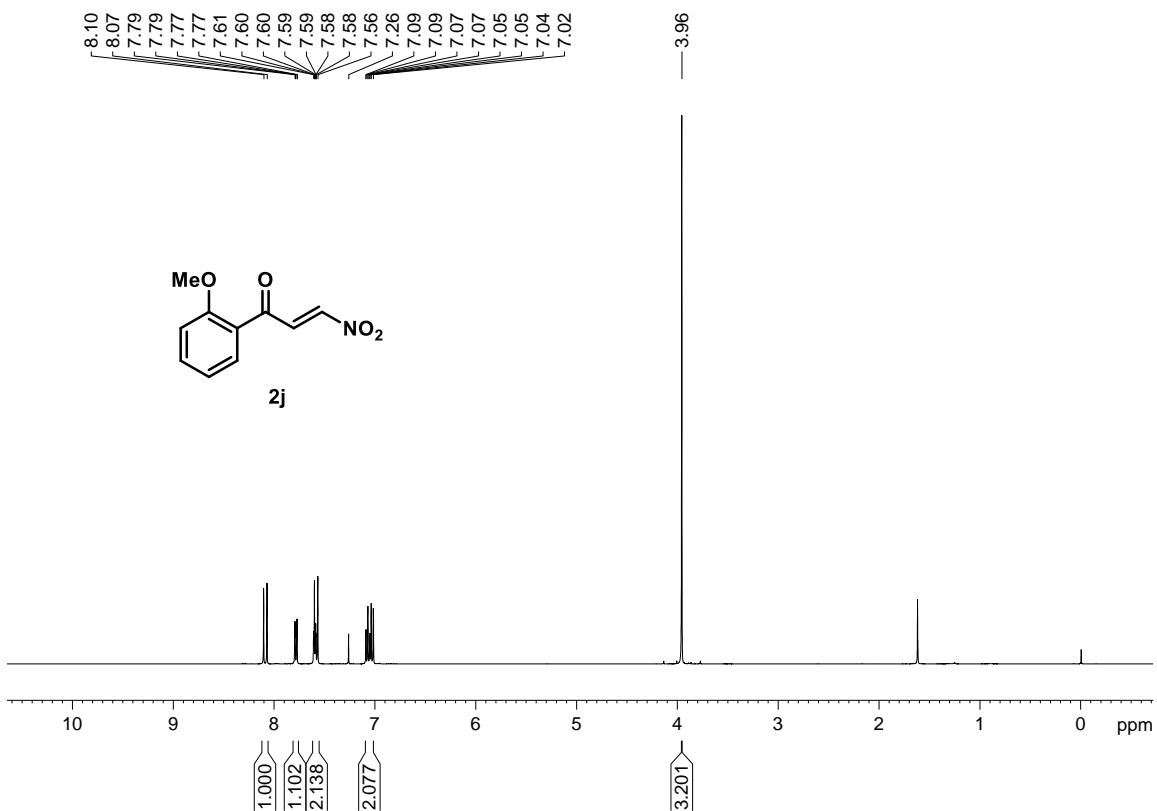


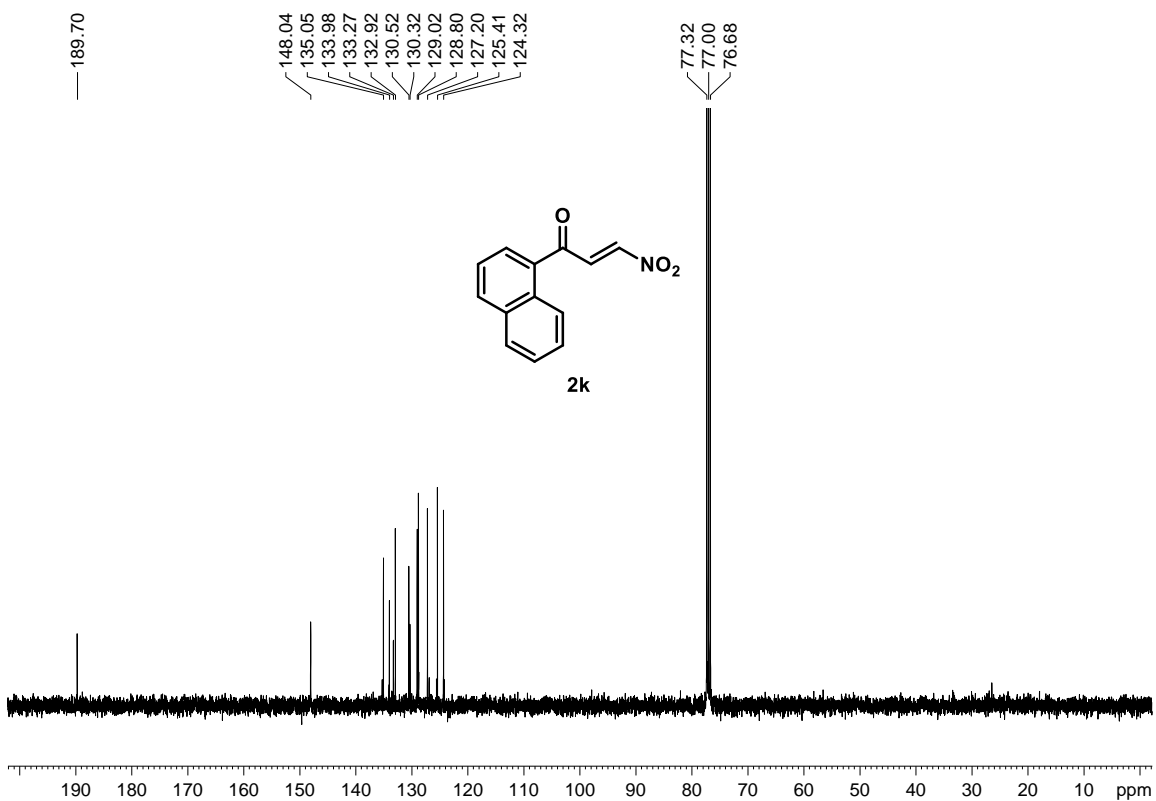
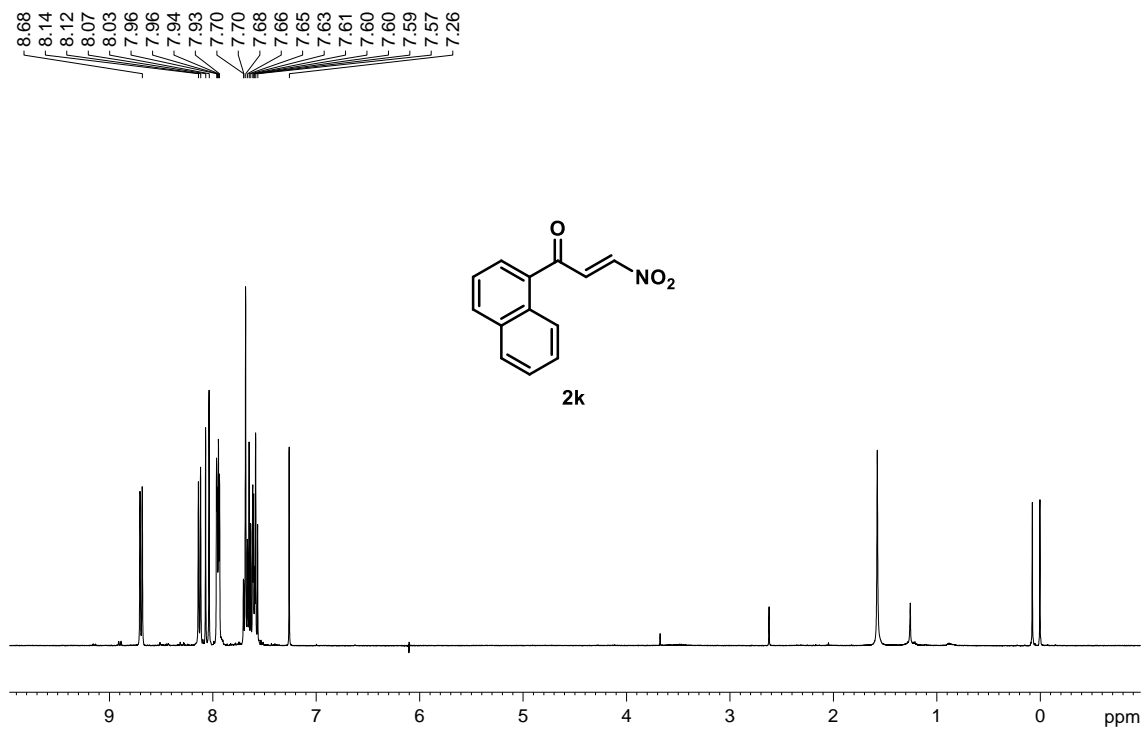


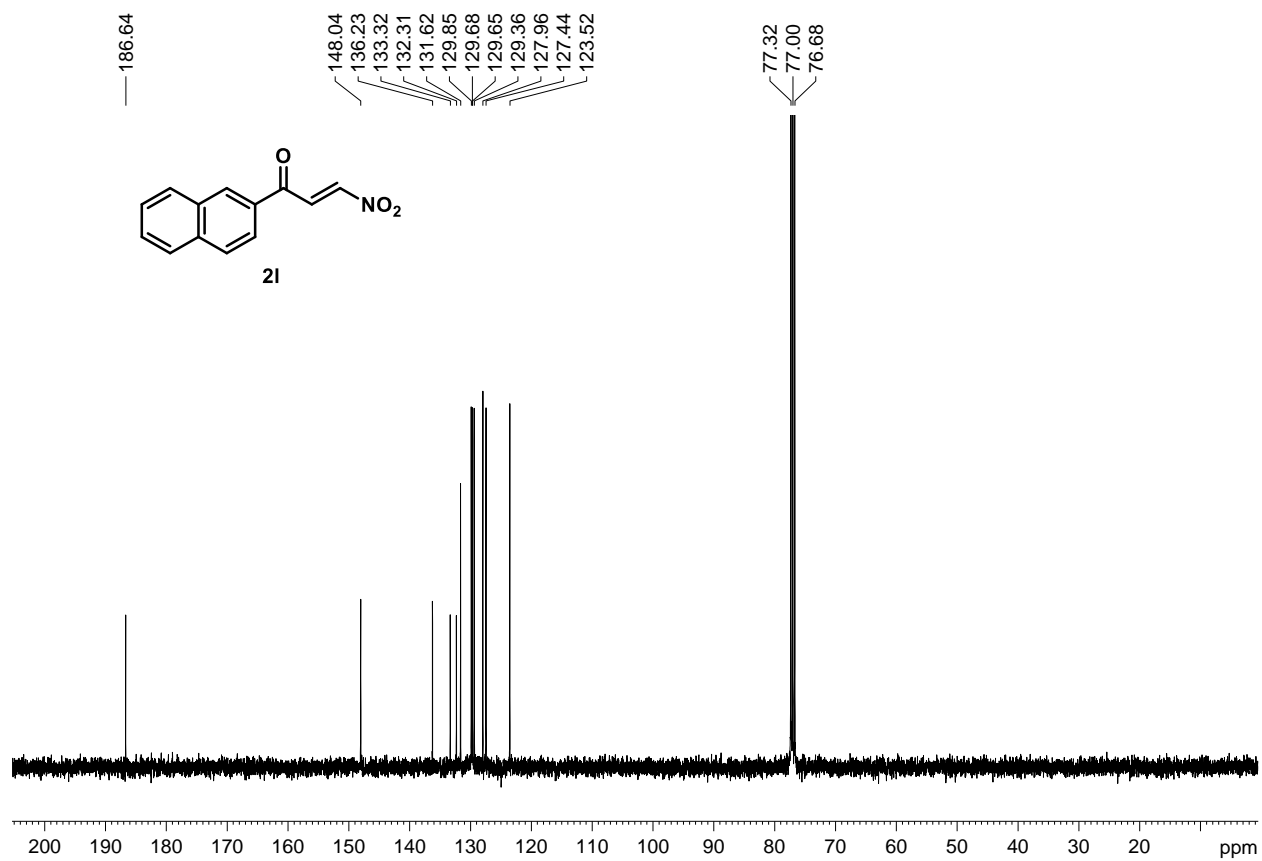
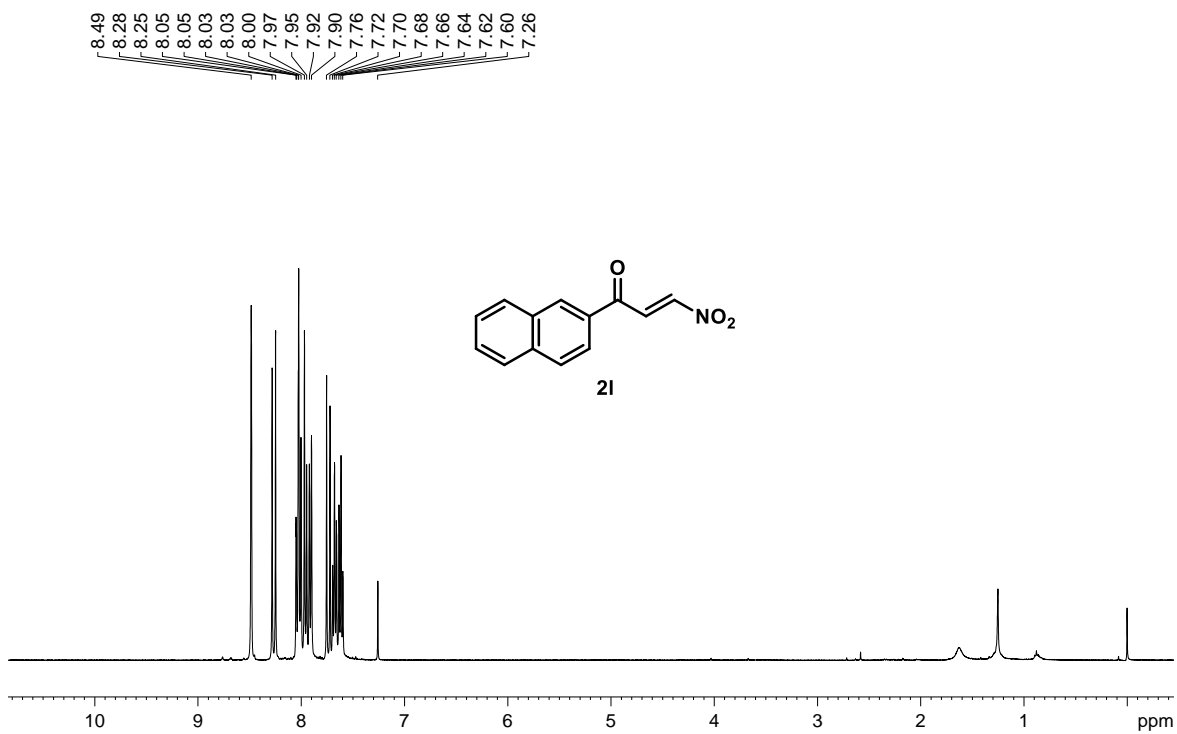


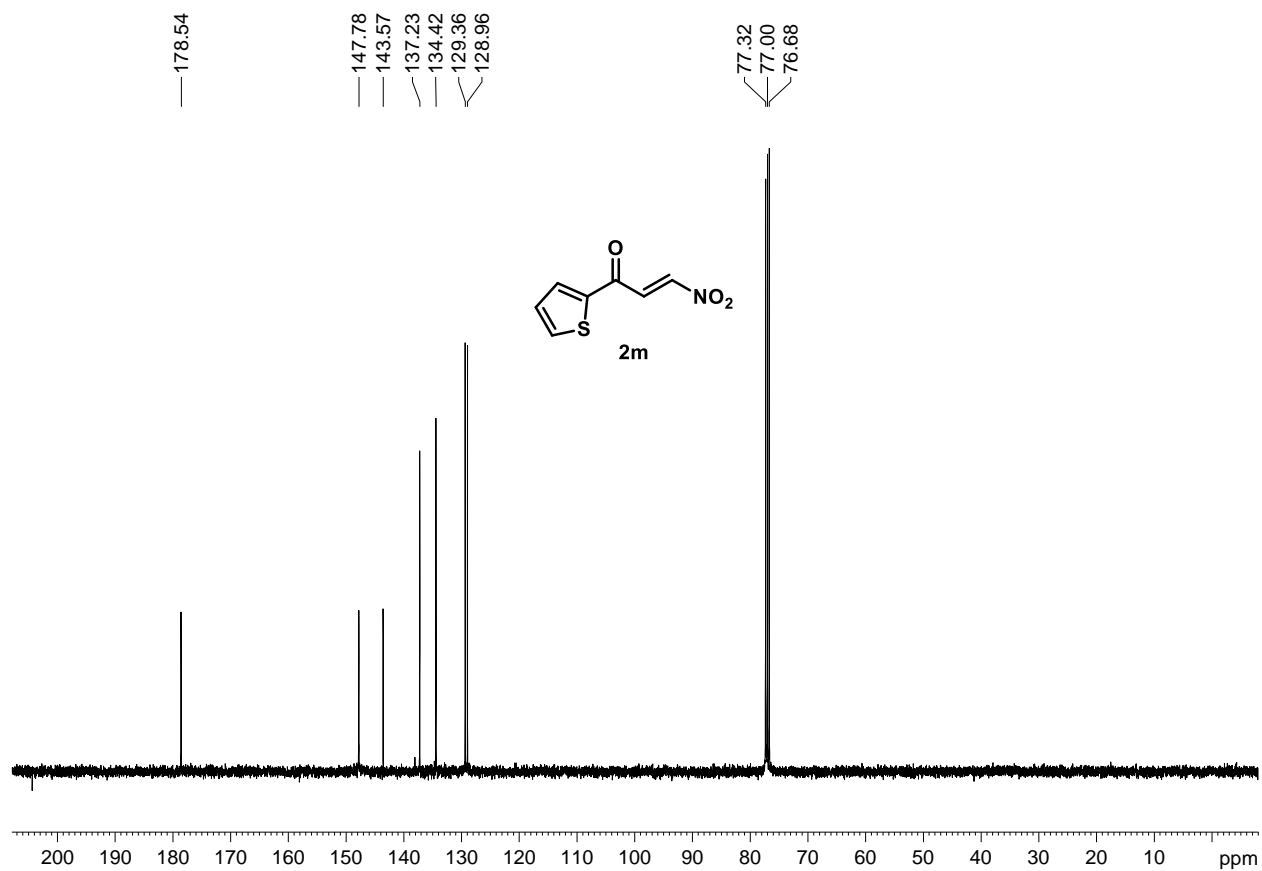
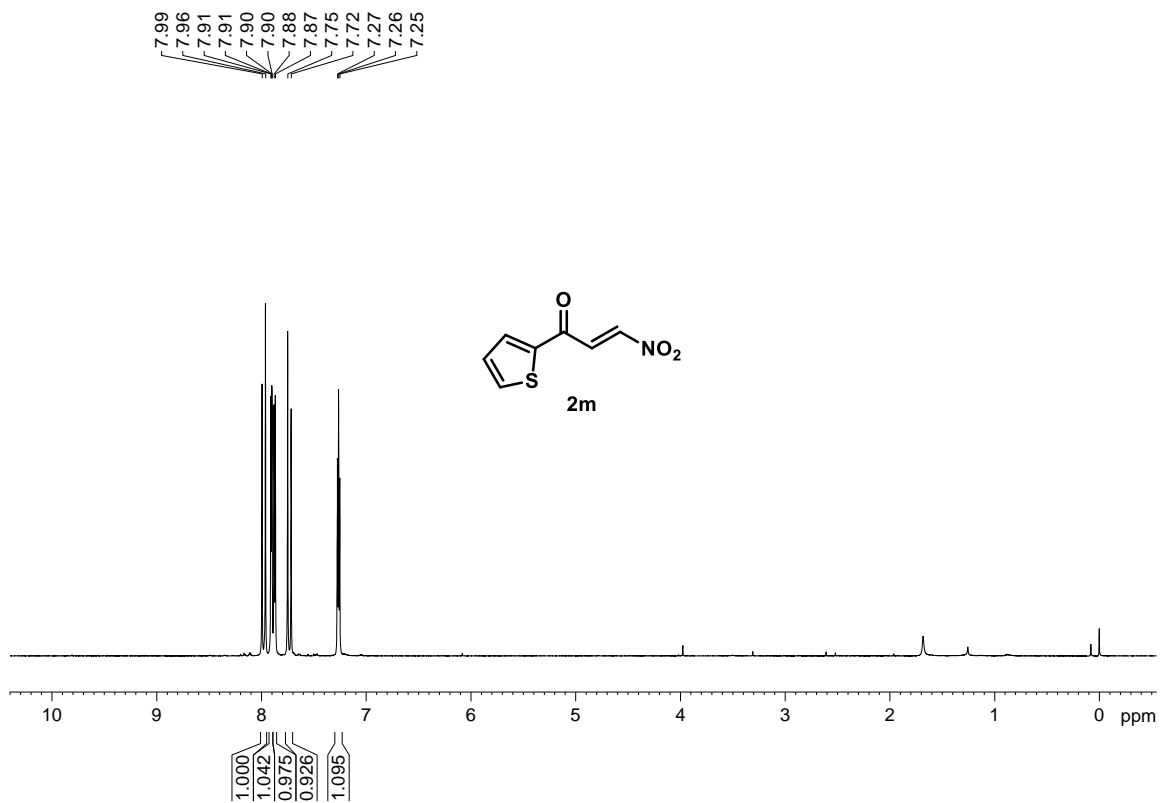


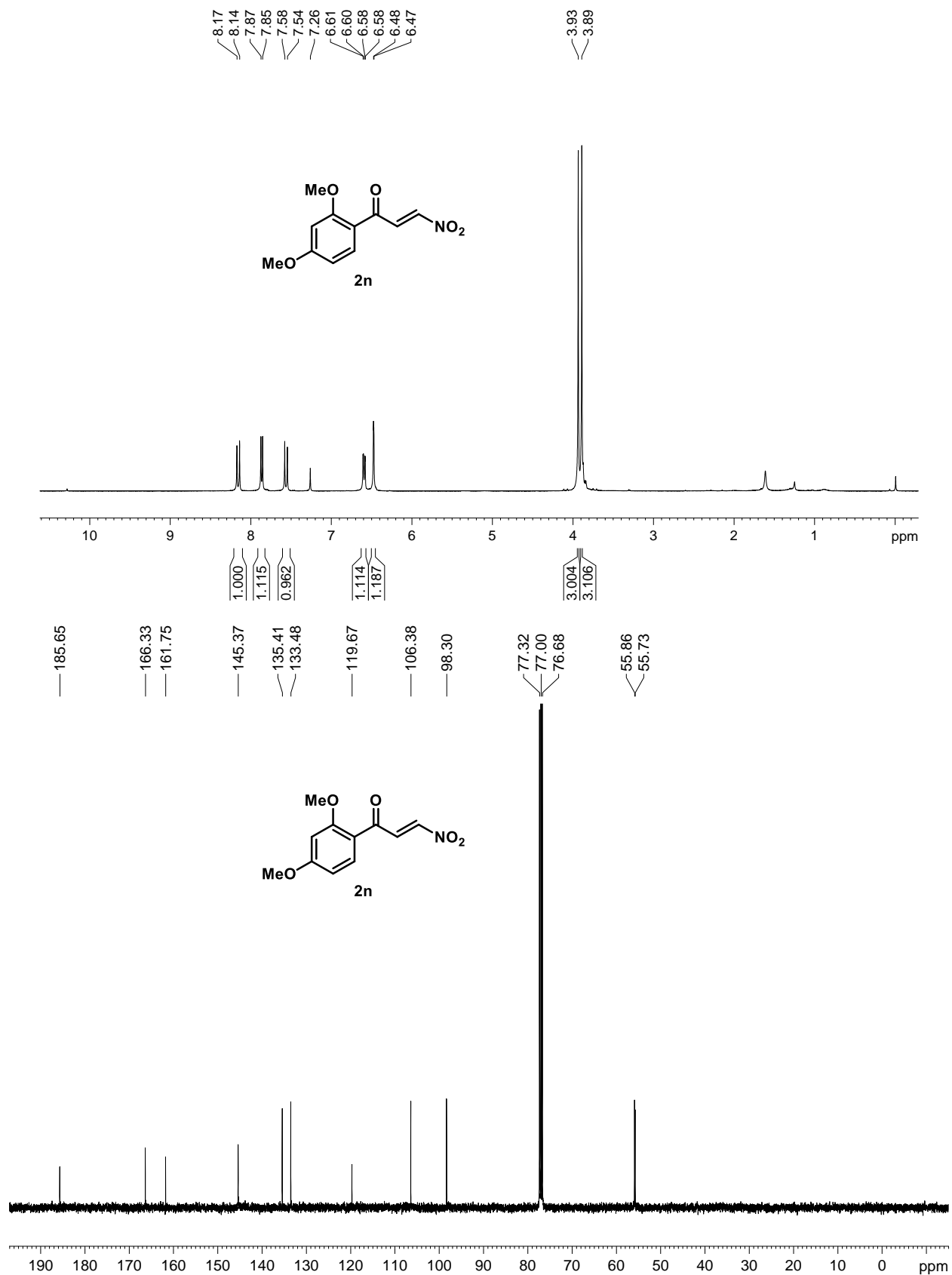


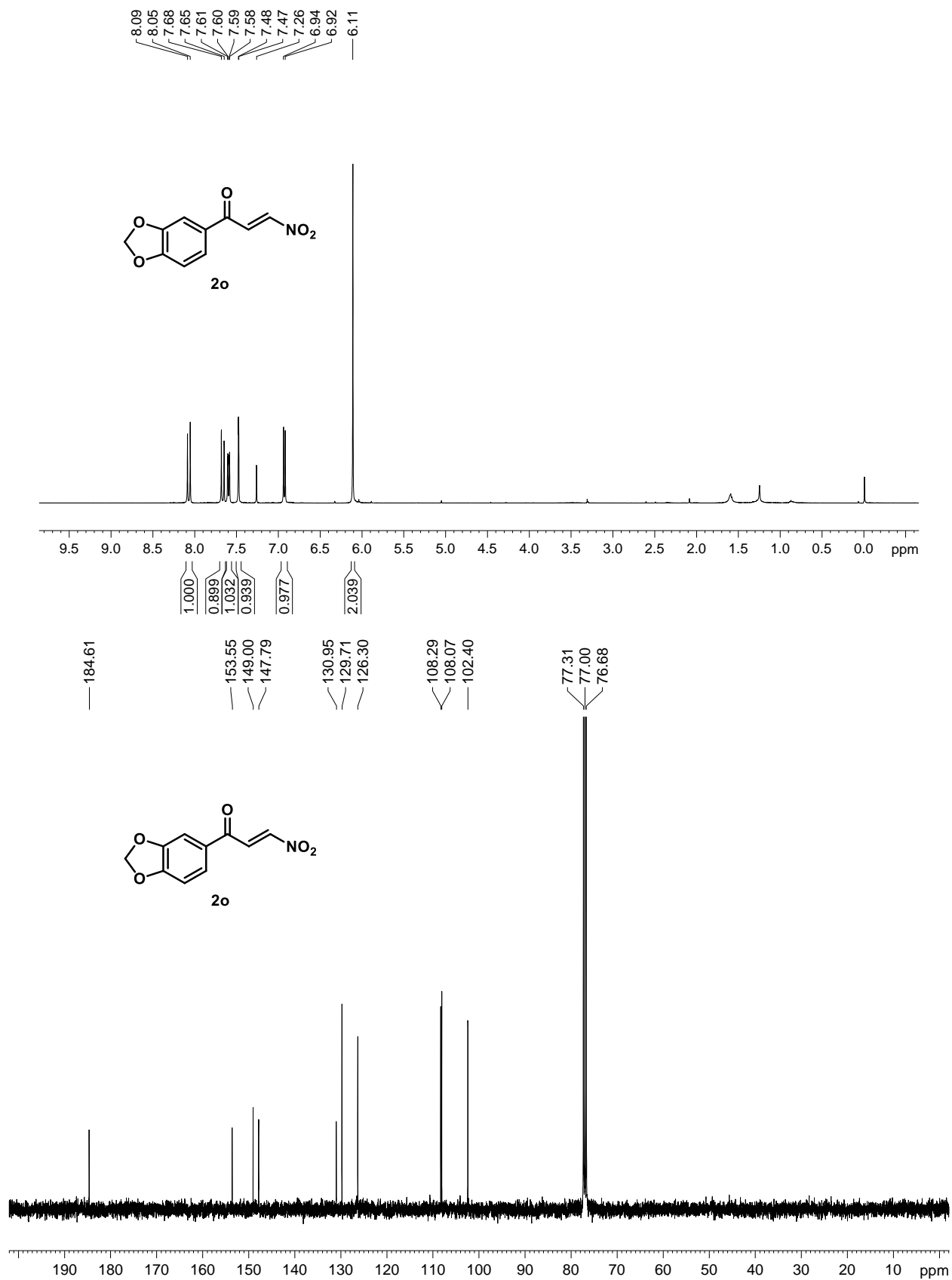


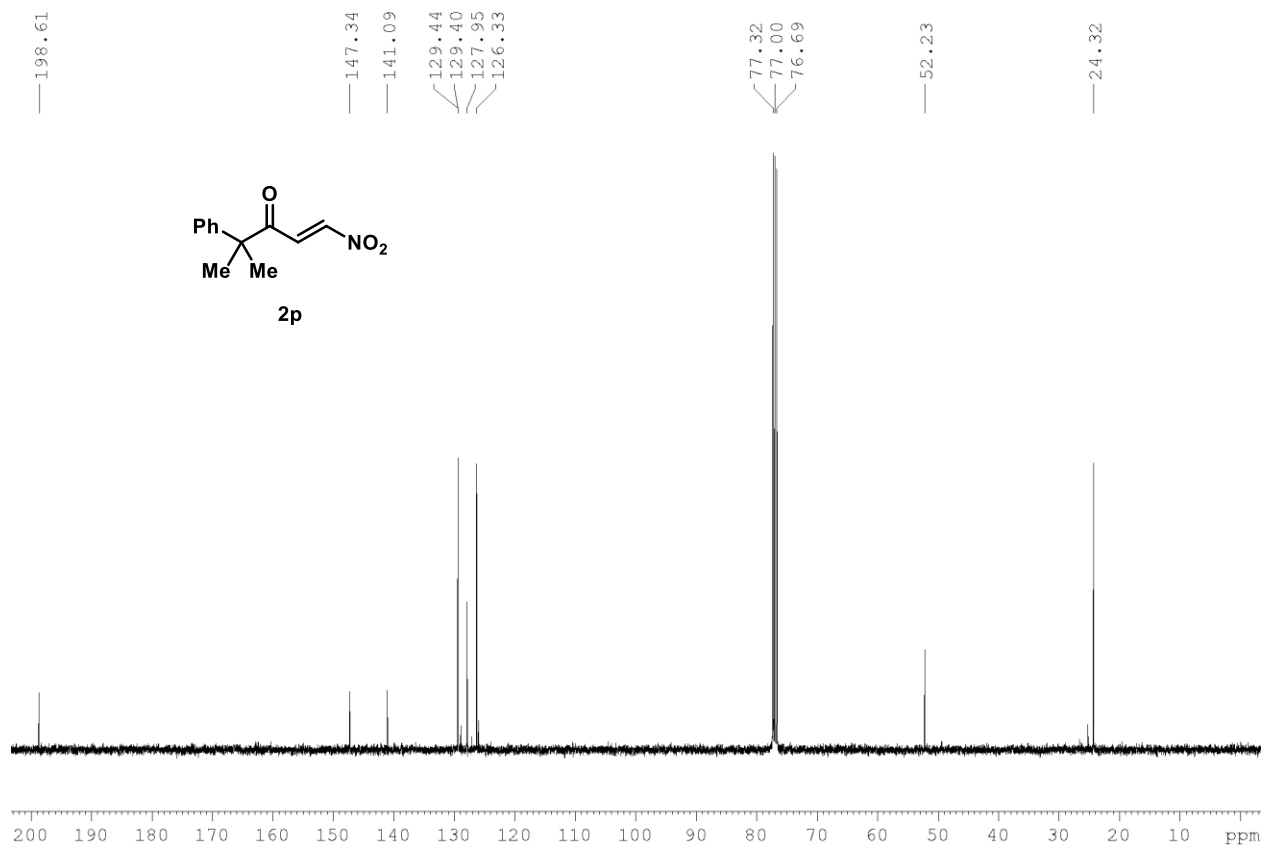
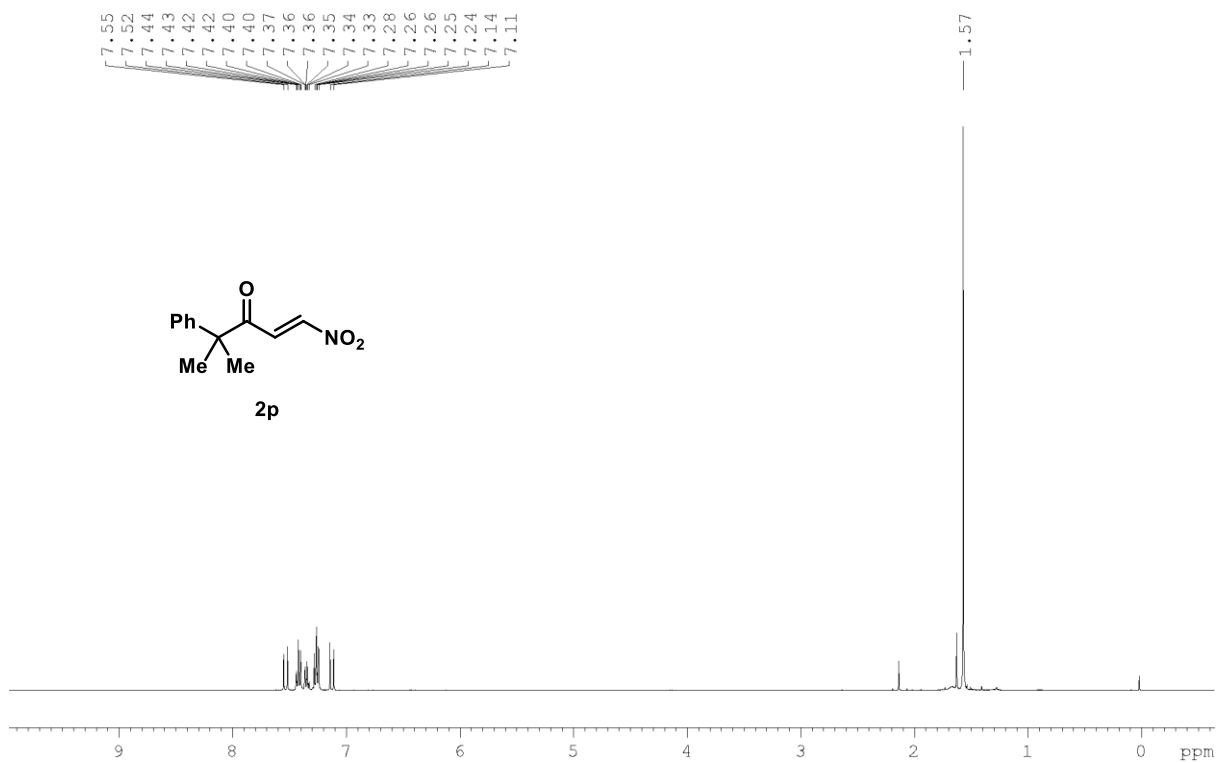


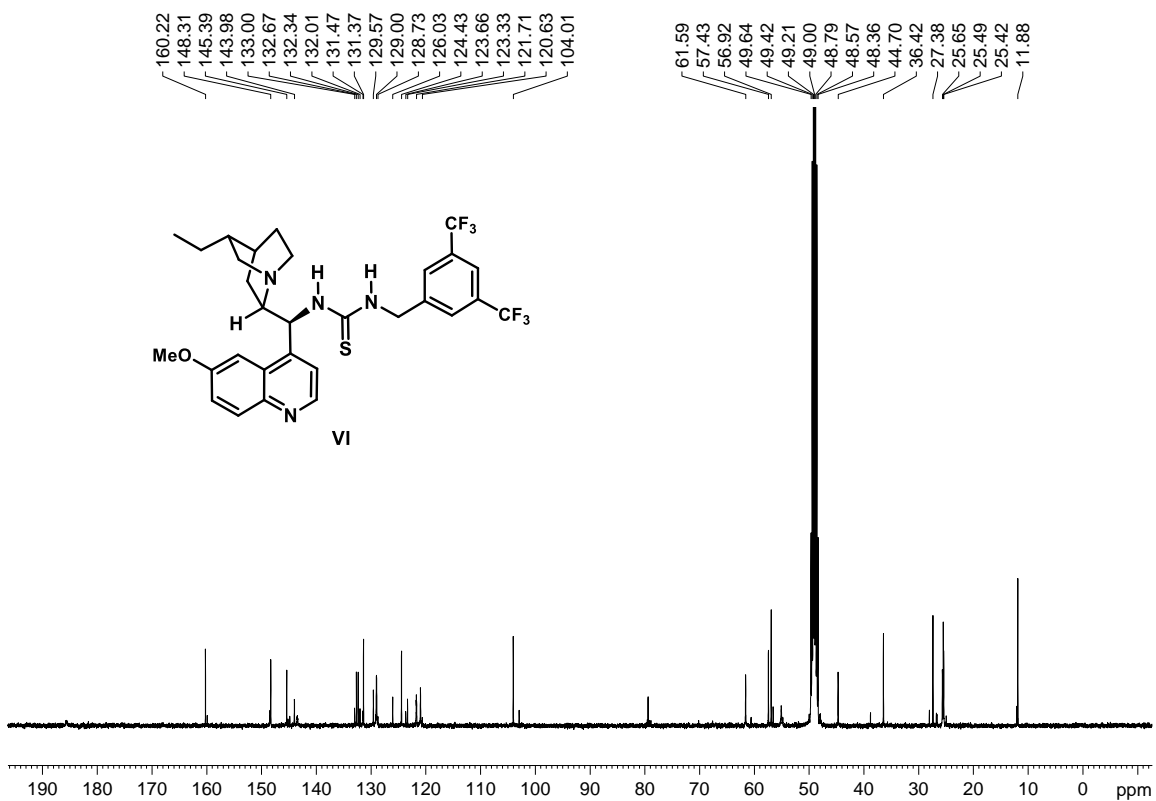
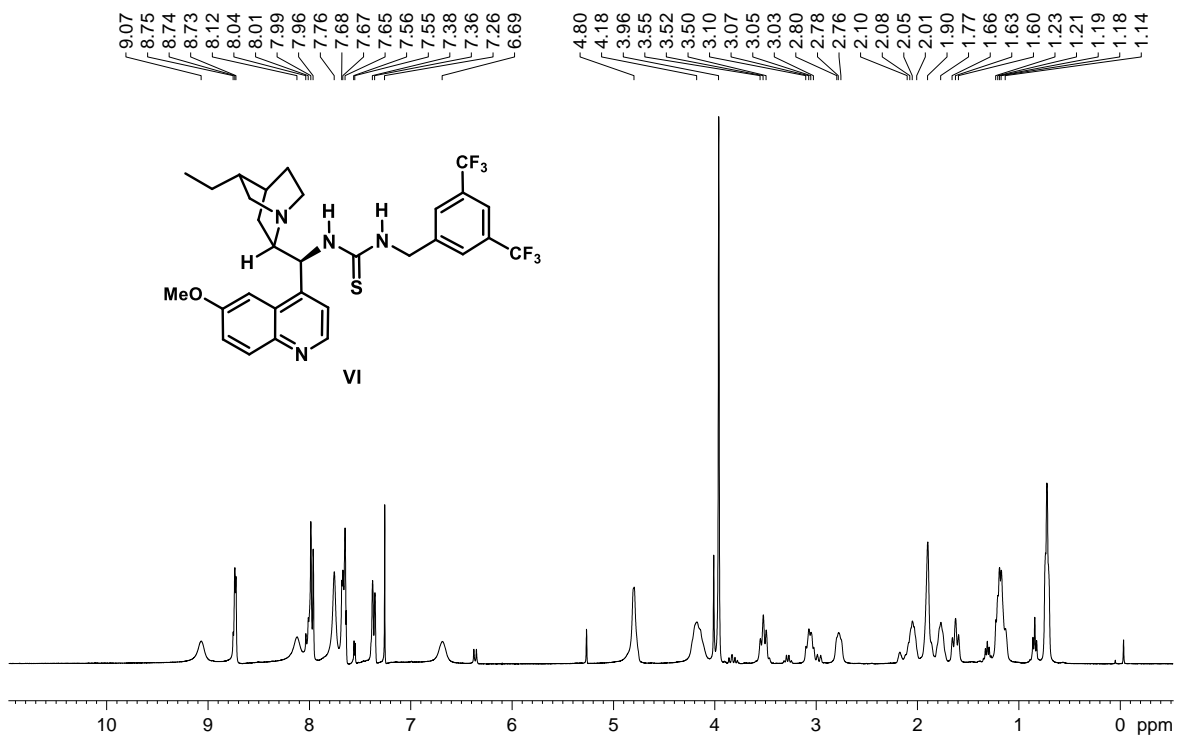


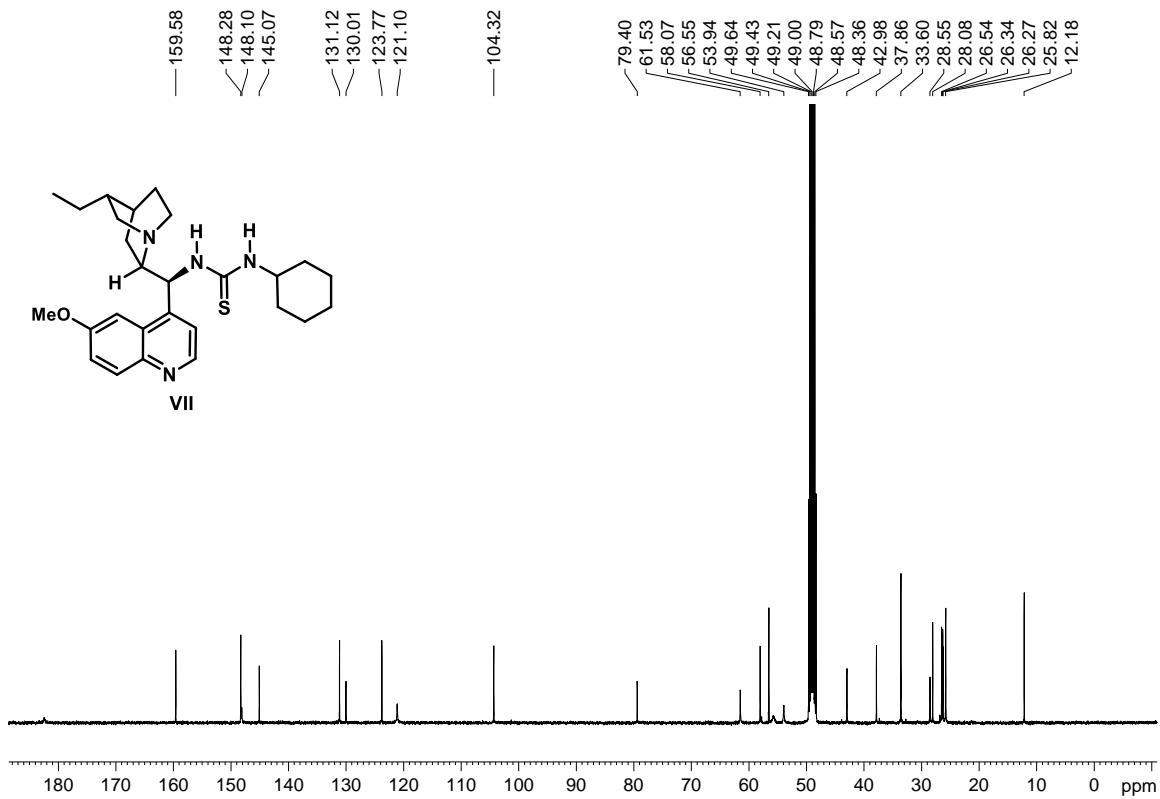
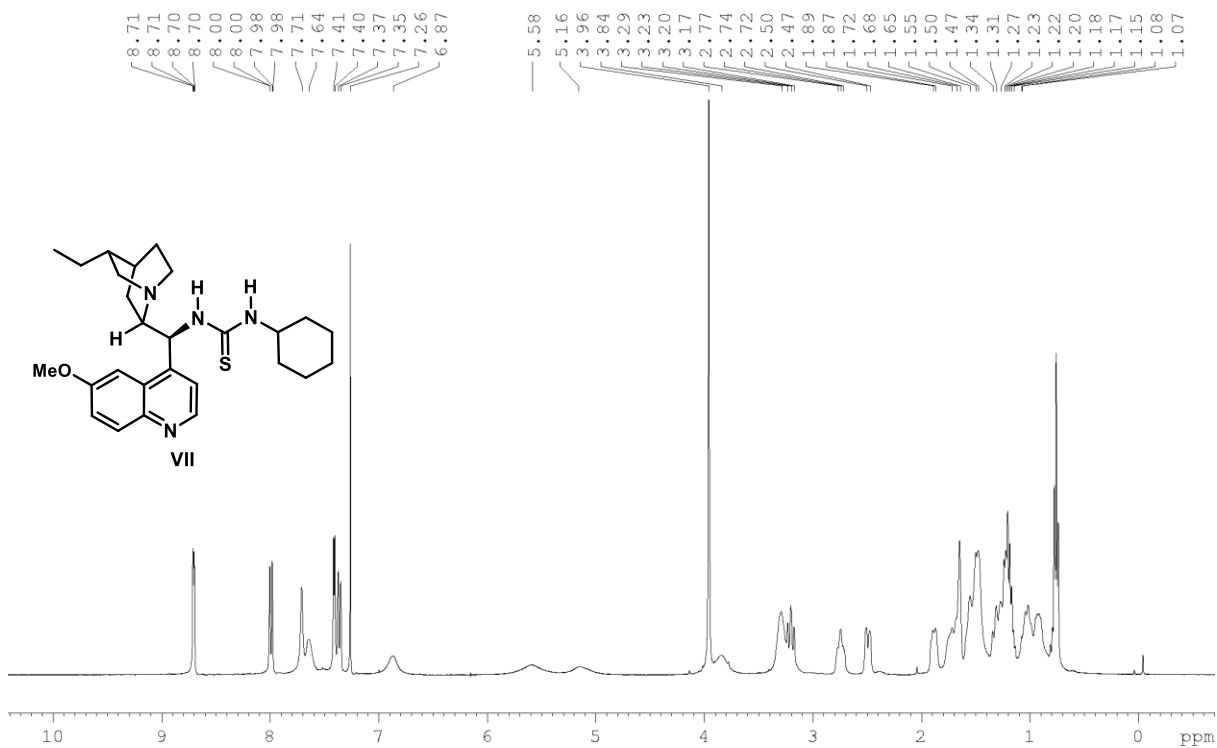


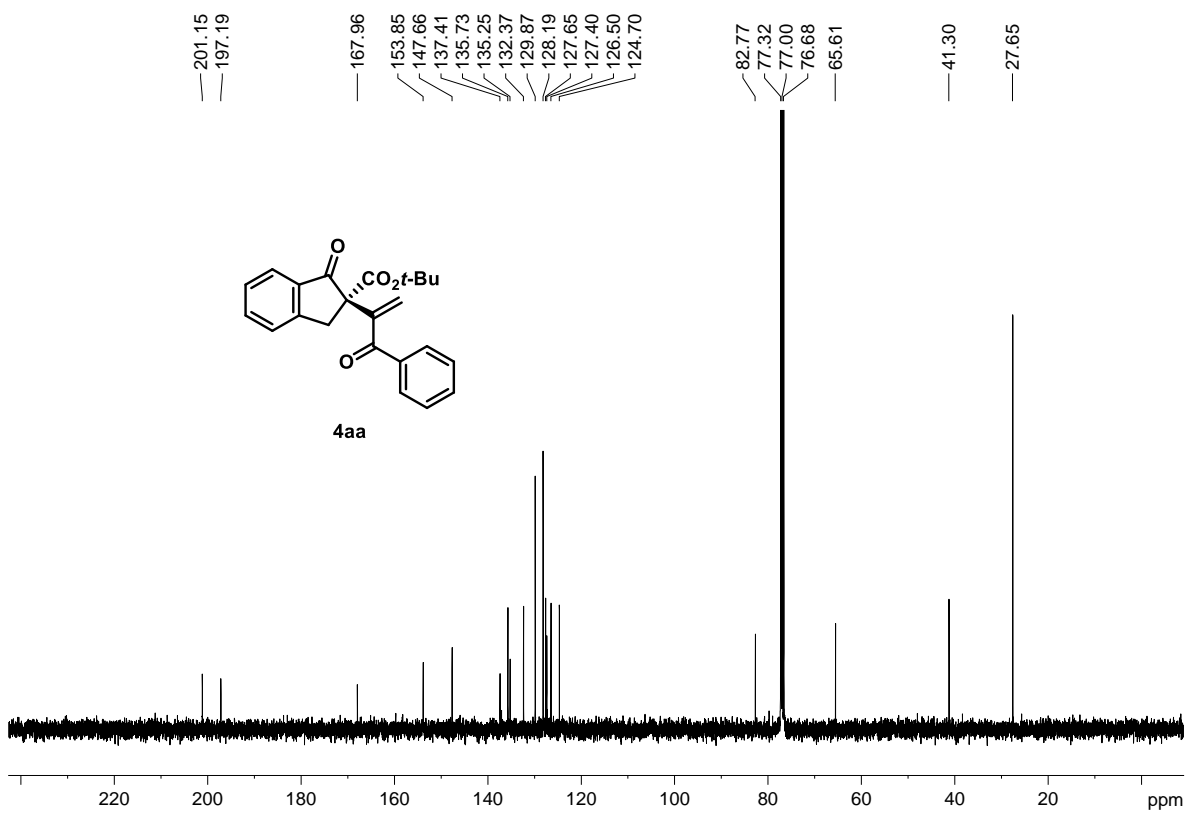
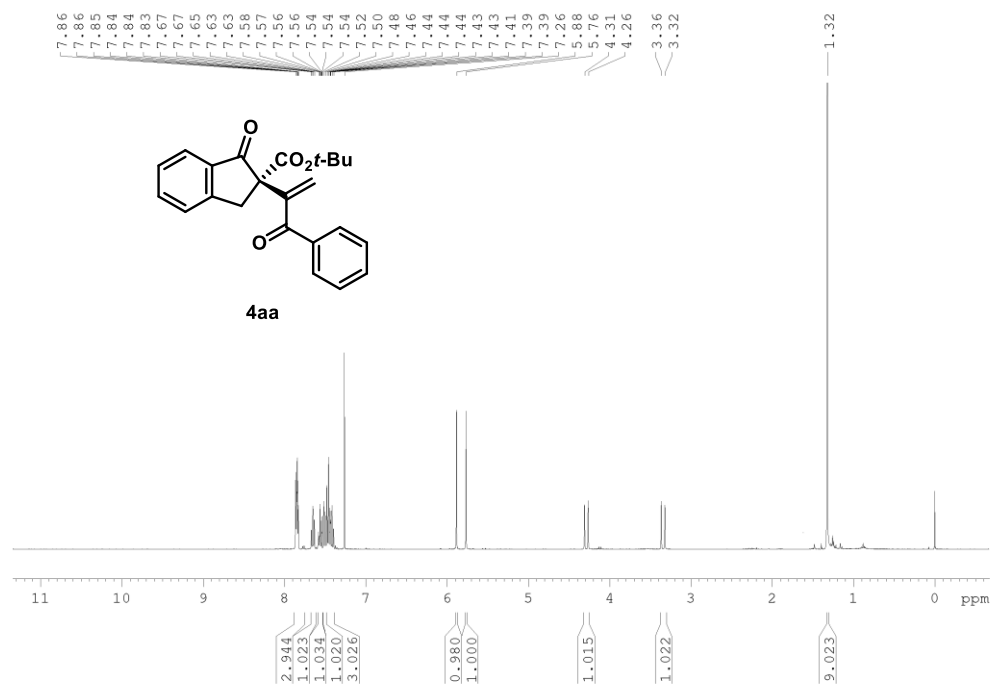


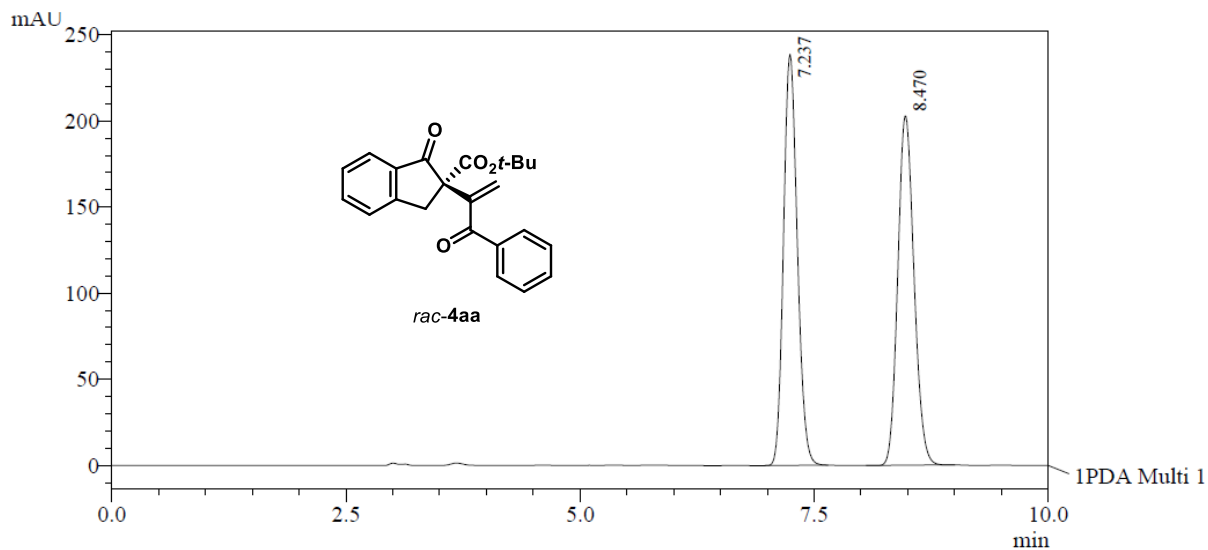












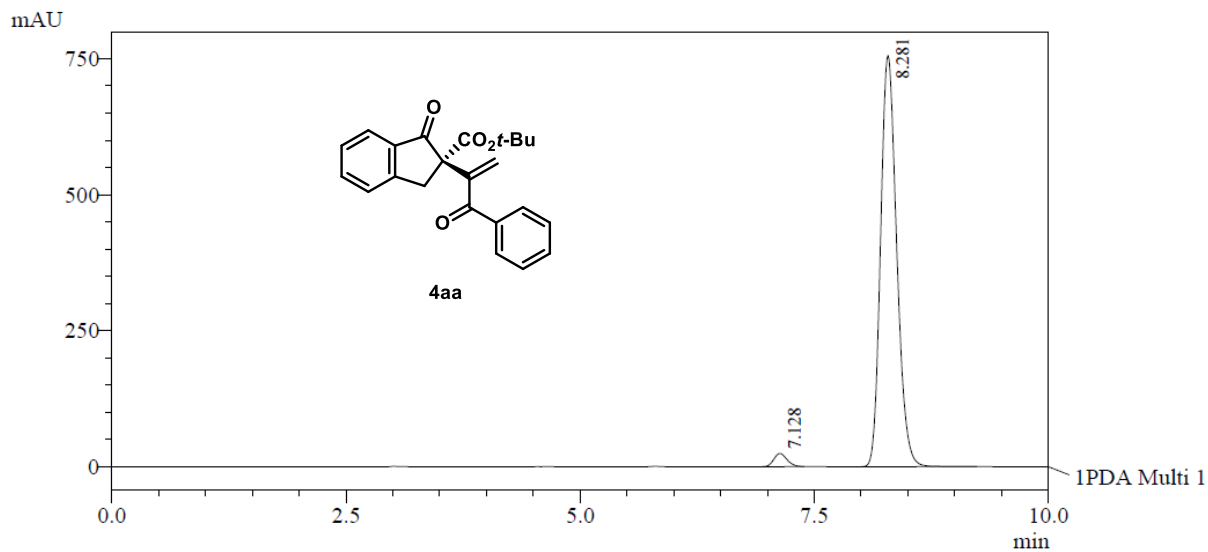
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	7.237	2446403	50.004
2	8.470	2446025	49.996
Total		4892428	100.000

Daicel Chiralpak AD-H column (*n*-Hexane/IPA = 90:10, 1.0 mL min⁻¹, 20 °C, 254 nm)

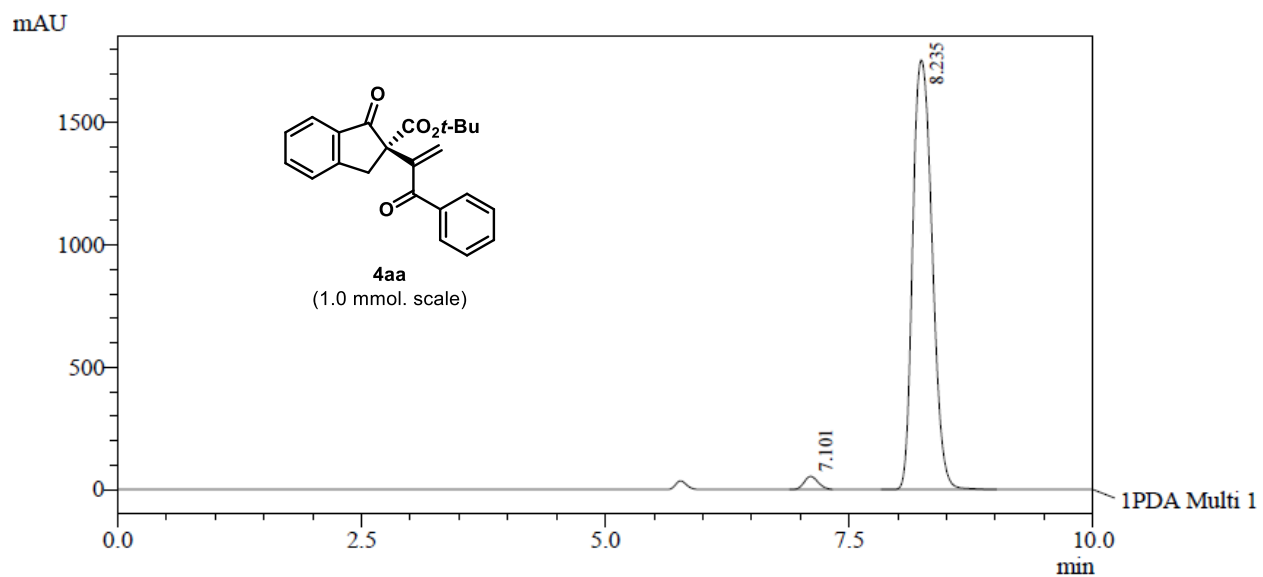


1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	7.128	236115	2.548
2	8.281	9030435	97.452
Total		9266550	100.000

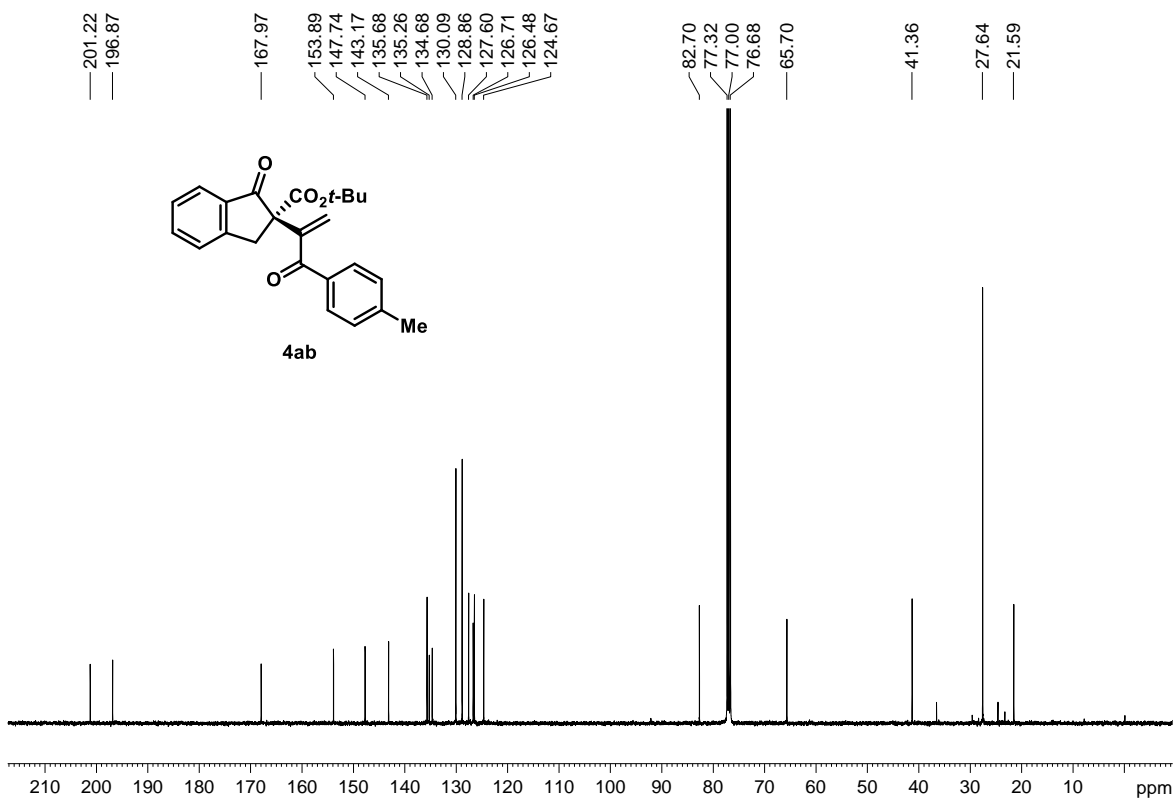
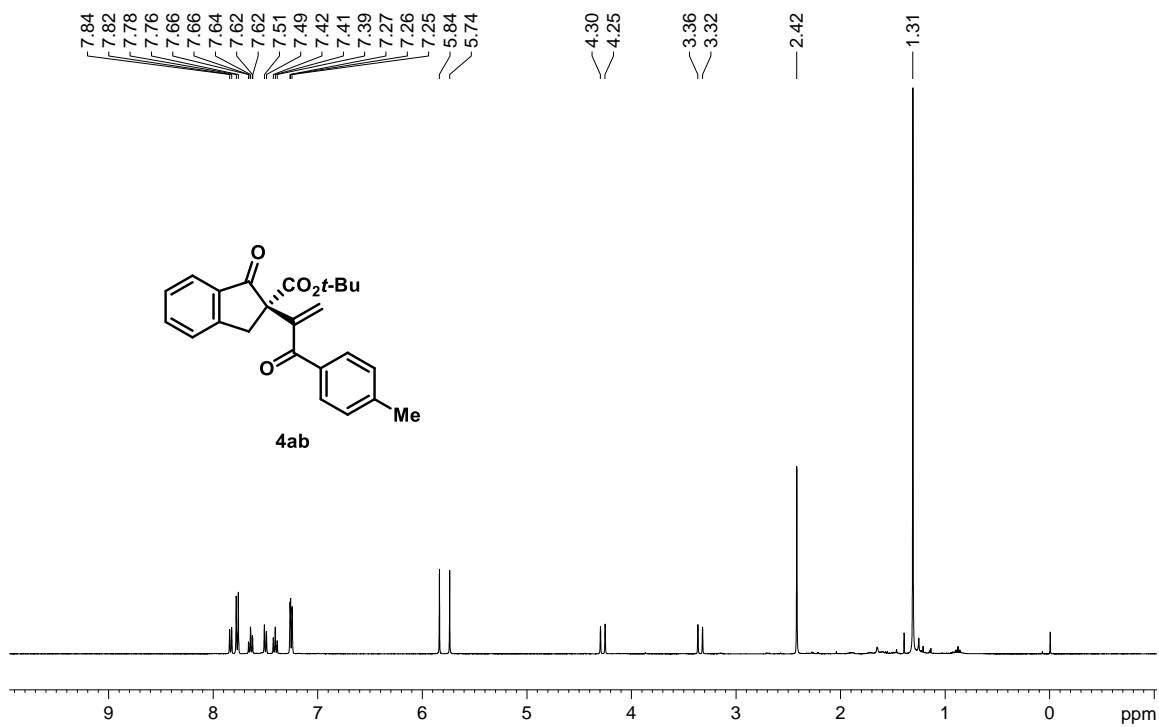


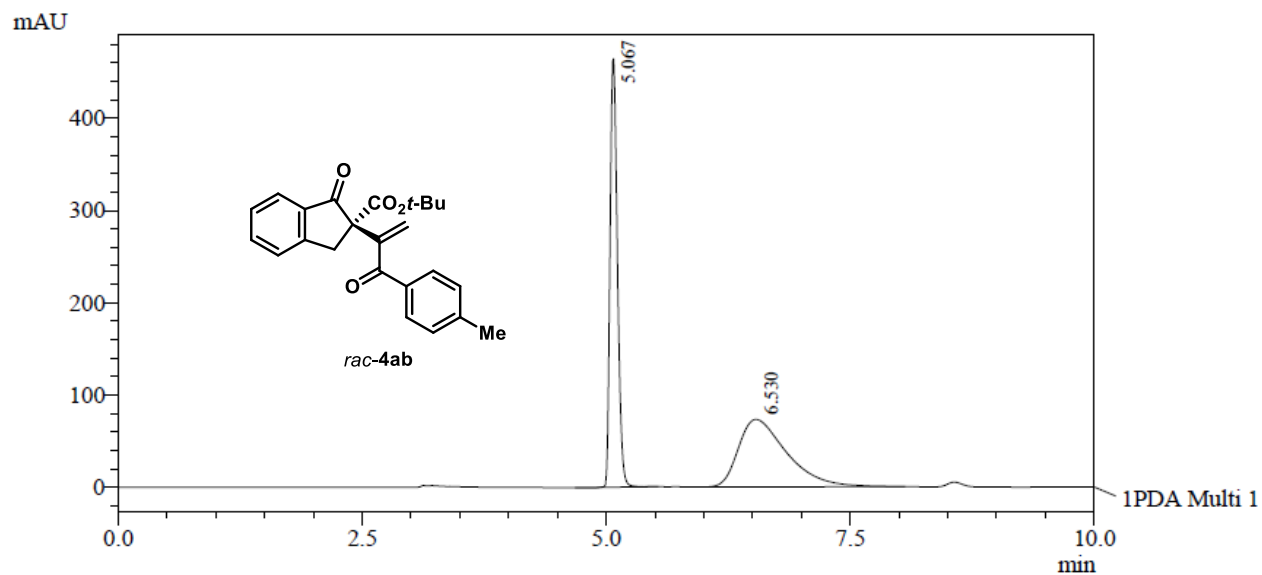
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	7.101	529228	2.129
2	8.235	24324376	97.871
Total		24853603	100.000





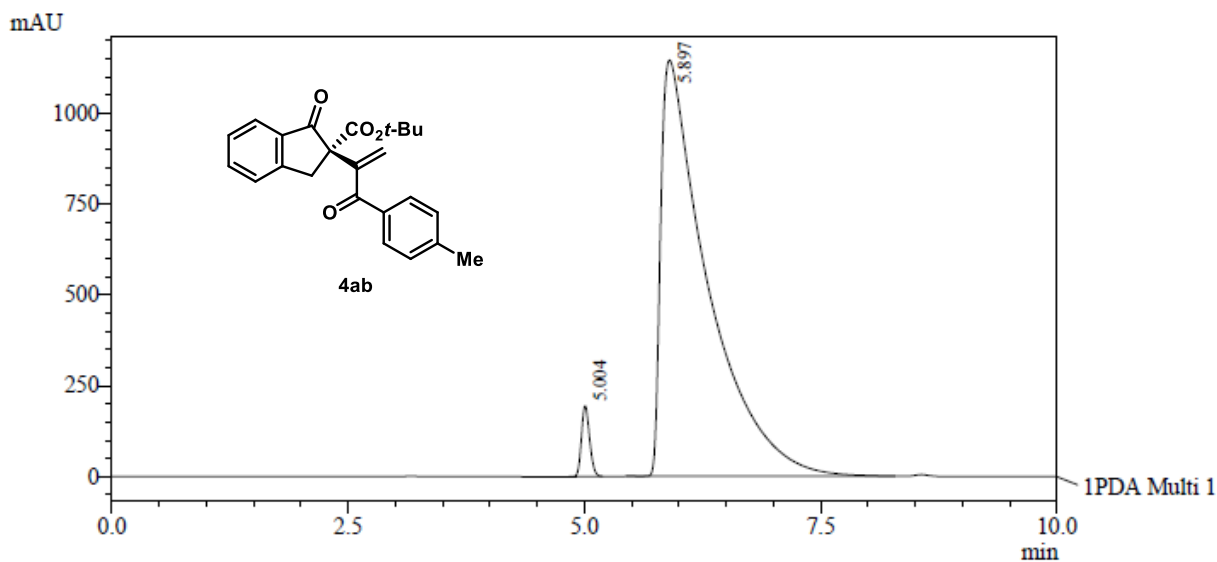
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.067	2438054	49.246
2	6.530	2512738	50.754
Total		4950792	100.000

Daicel Chiralpak AS-H column (*n*-Hexane/EtOH = 95:5, 1.0 mL min⁻¹, 20 °C, 254 nm)

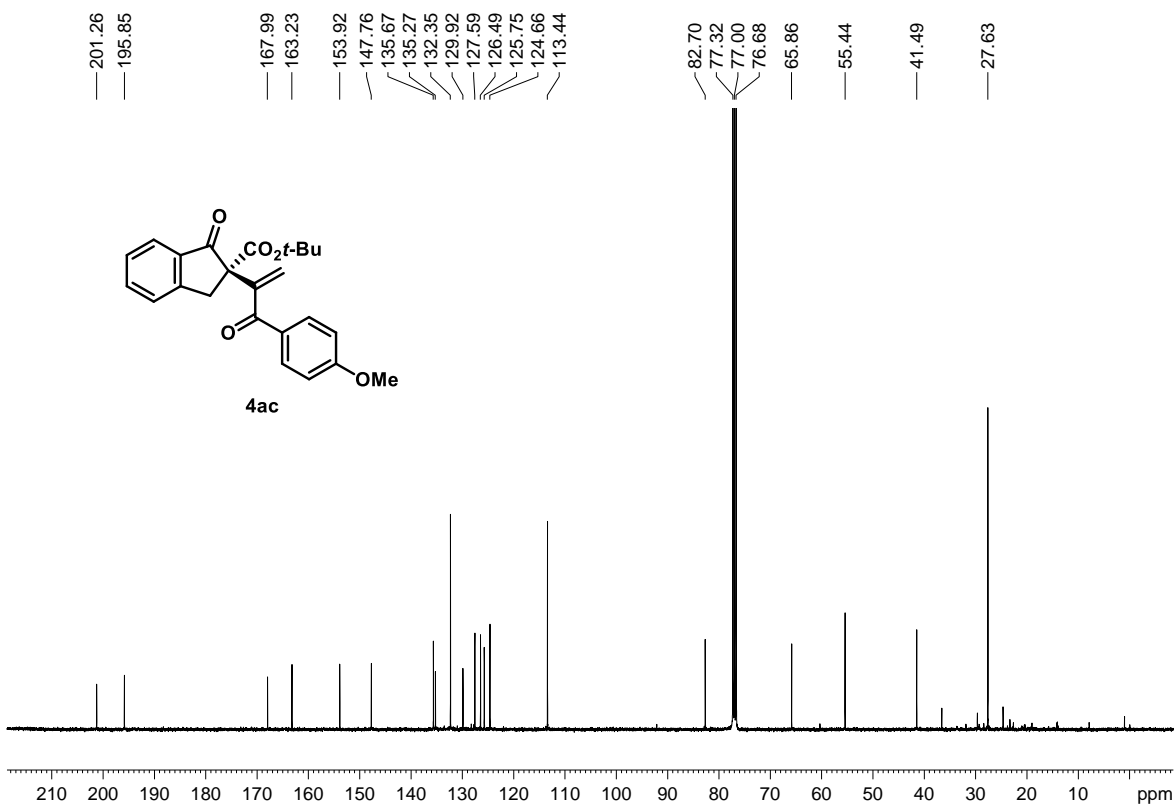
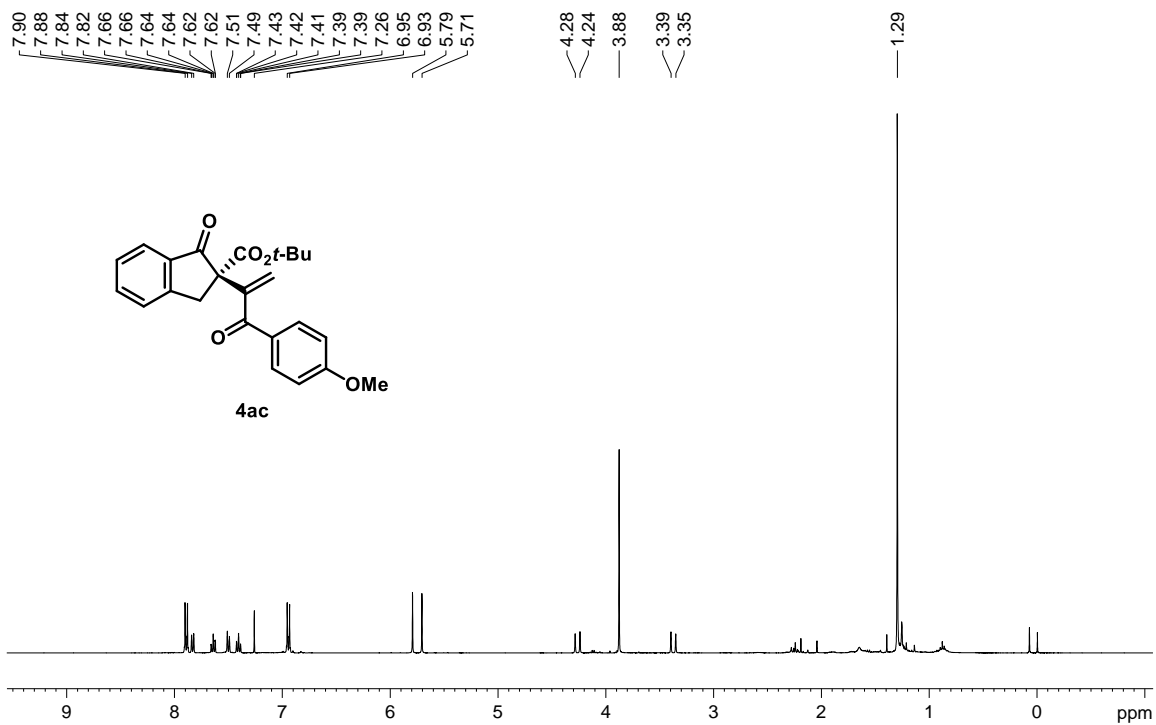


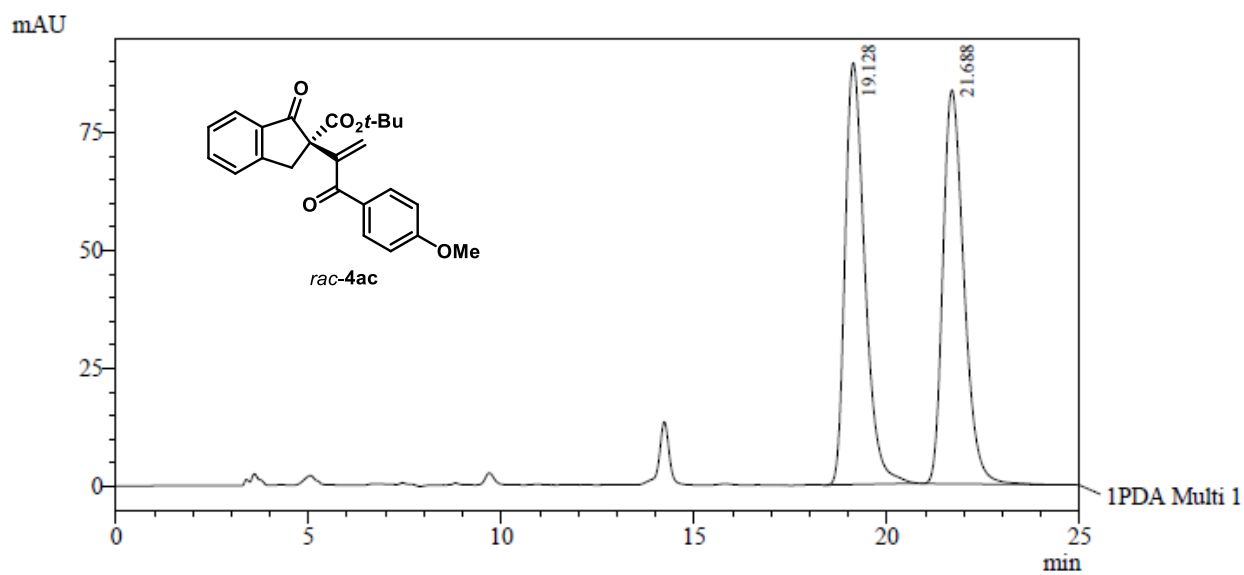
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.004	1167436	2.876
2	5.897	39421534	97.124
Total		40588970	100.000





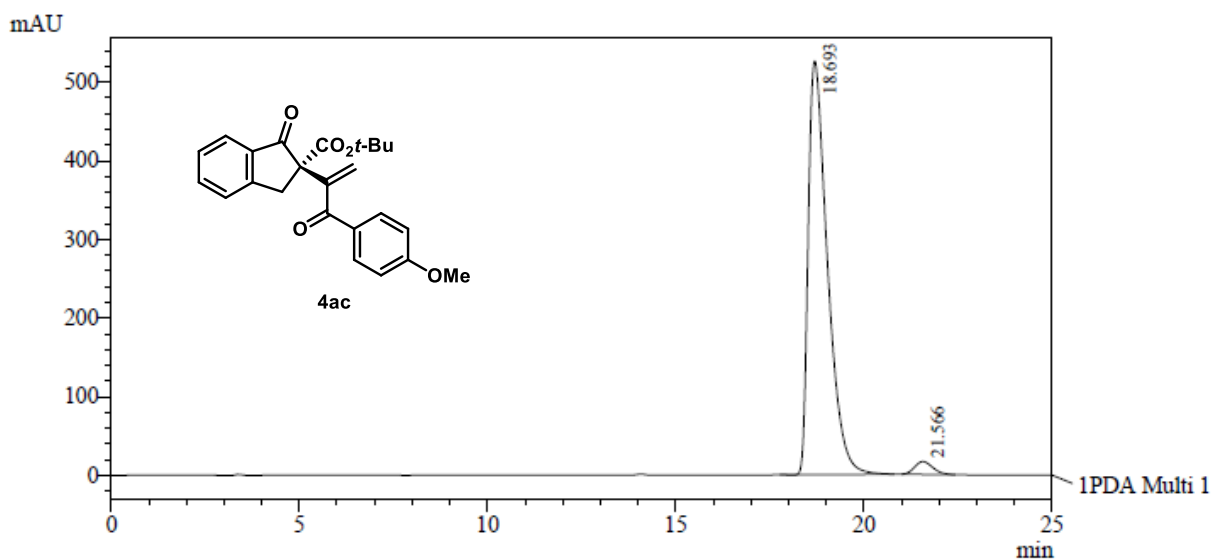
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	19.128	3182036	50.150
2	21.688	3162949	49.850
Total		6344985	100.000

Daicel Chiralpak ID column (*n*-Hexane/IPA = 90:10, 1.0 mL min⁻¹, 20 °C, 254 nm)

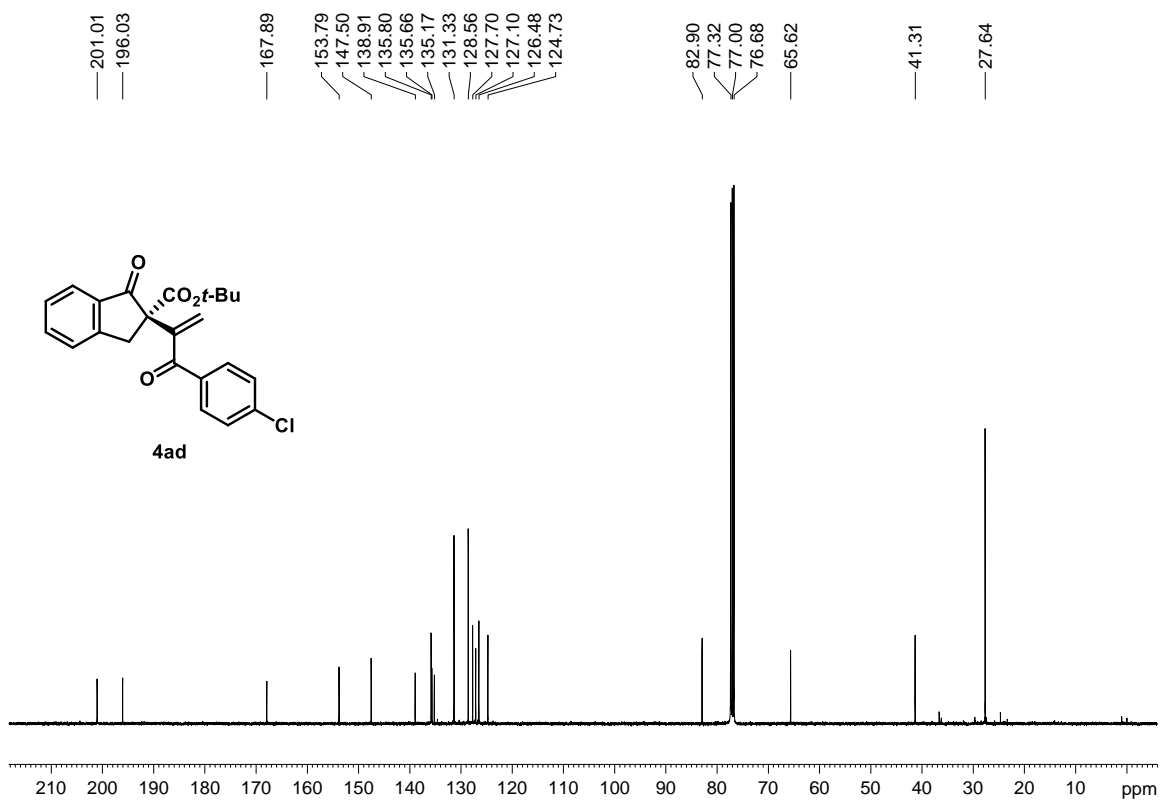
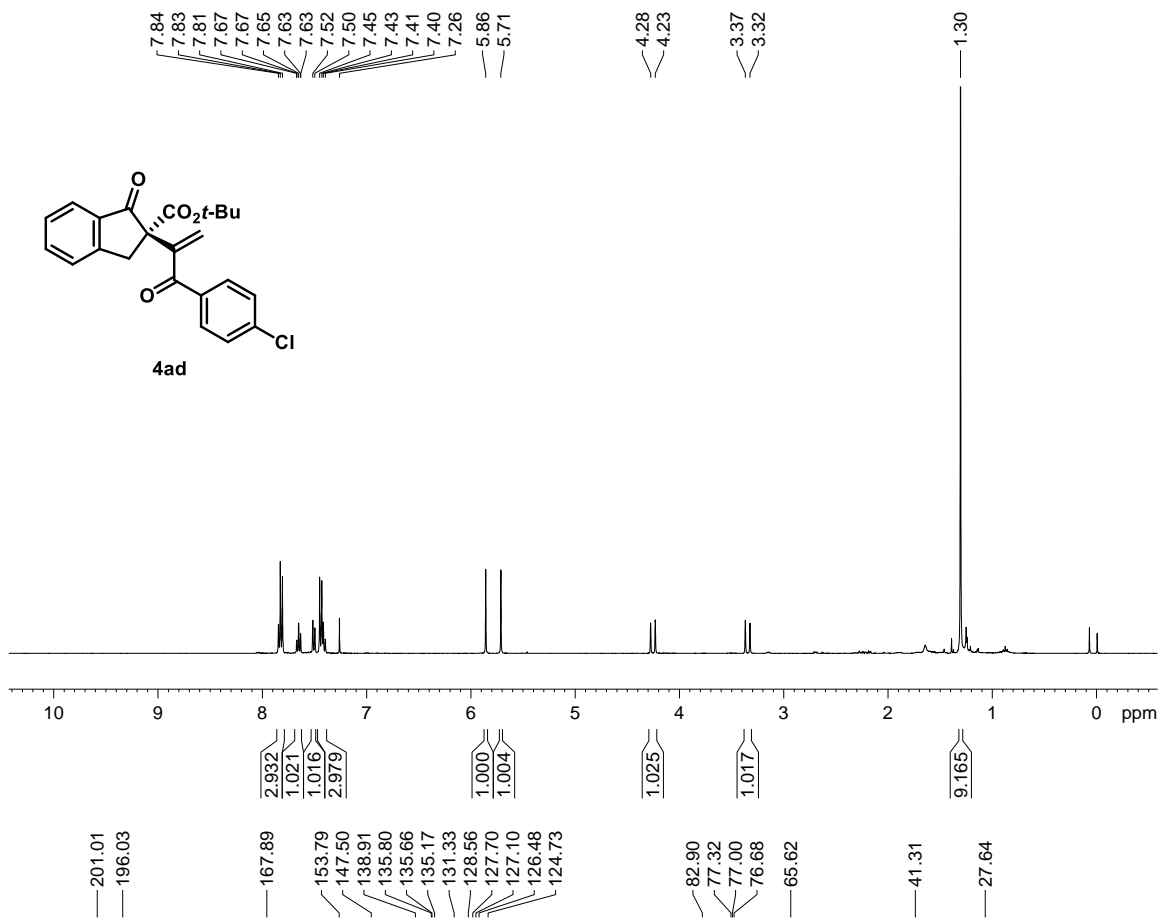


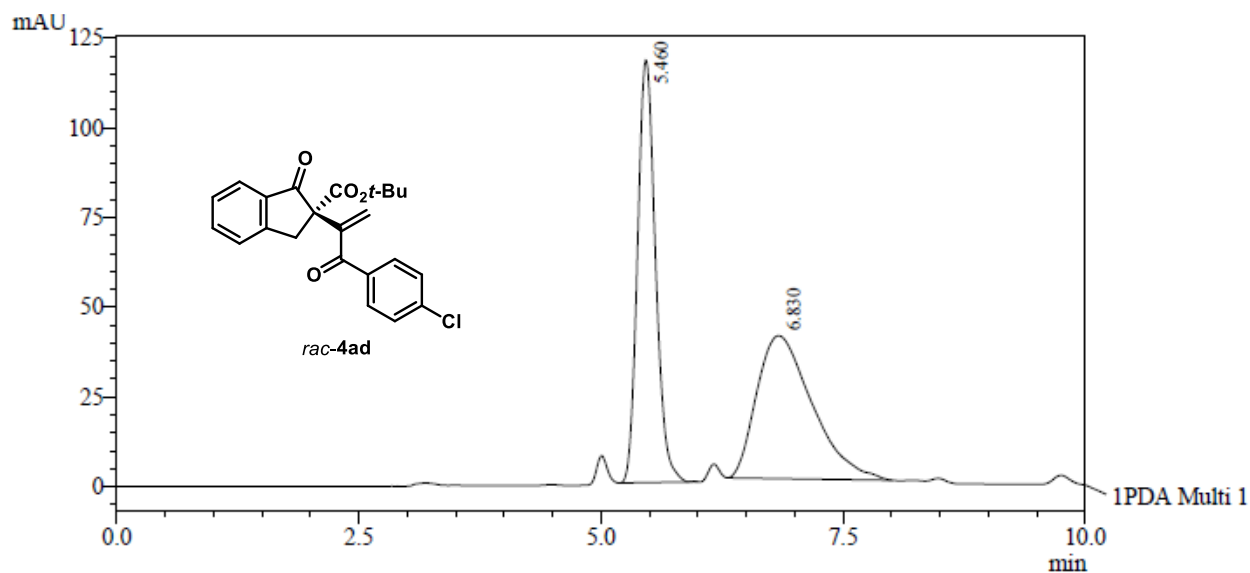
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	18.693	18662970	97.160
2	21.566	545576	2.840
Total		19208546	100.000





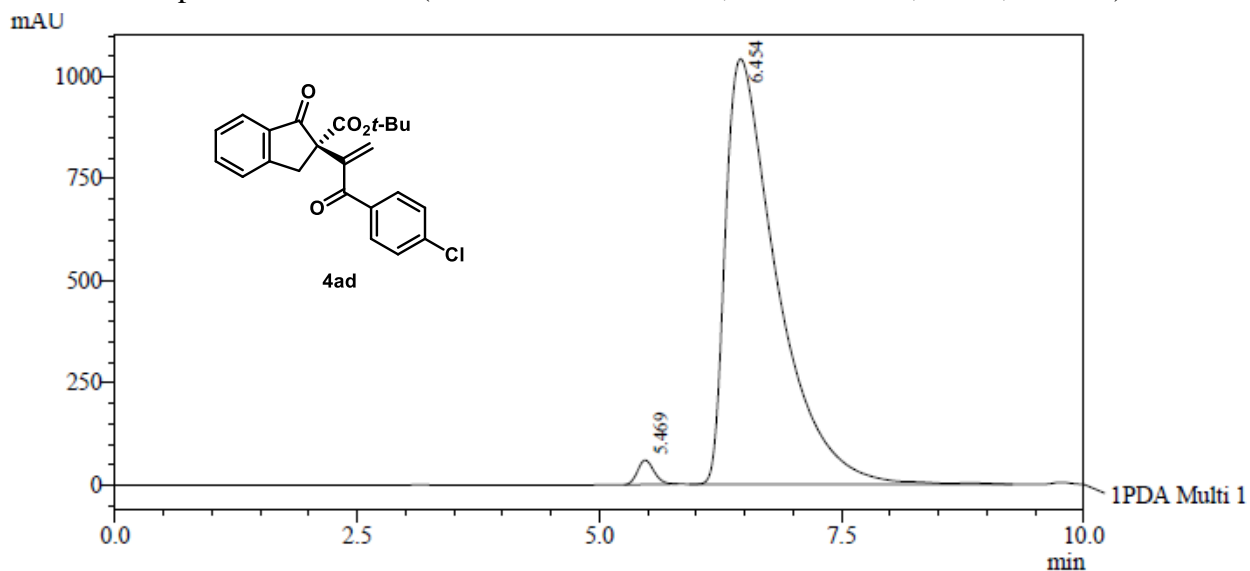
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.460	1521336	48.871
2	6.830	1591617	51.129
Total		3112953	100.000

Daicel Chiralpak AS-H column (*n*-Hexane/IPA = 90:10, 1.0 mL min⁻¹, 20 °C, 254 nm)

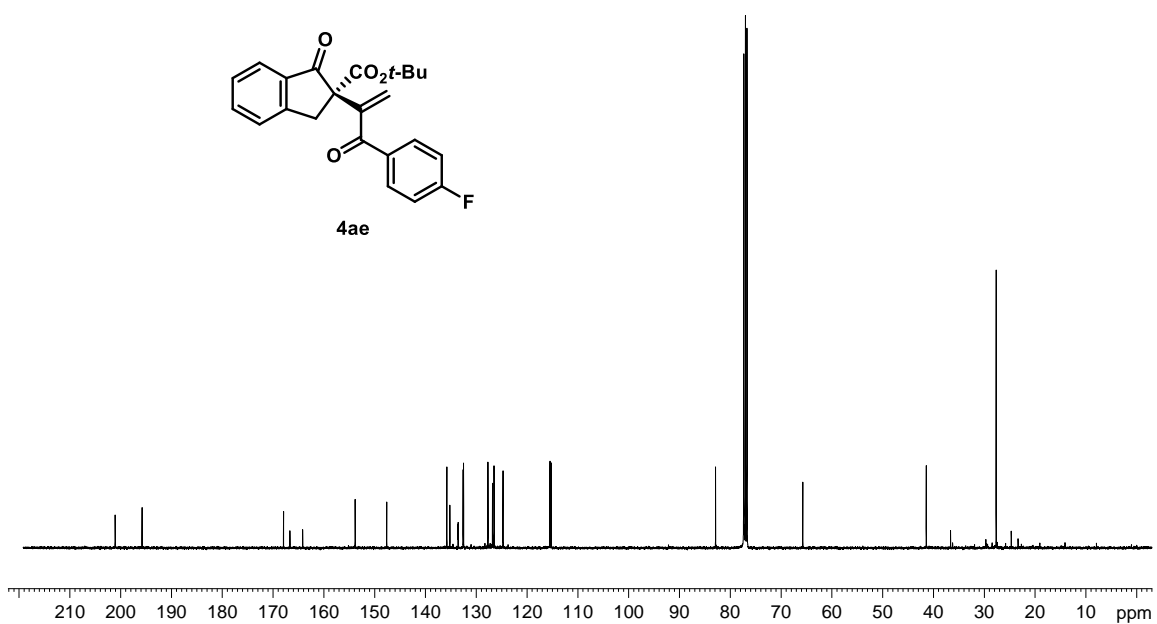
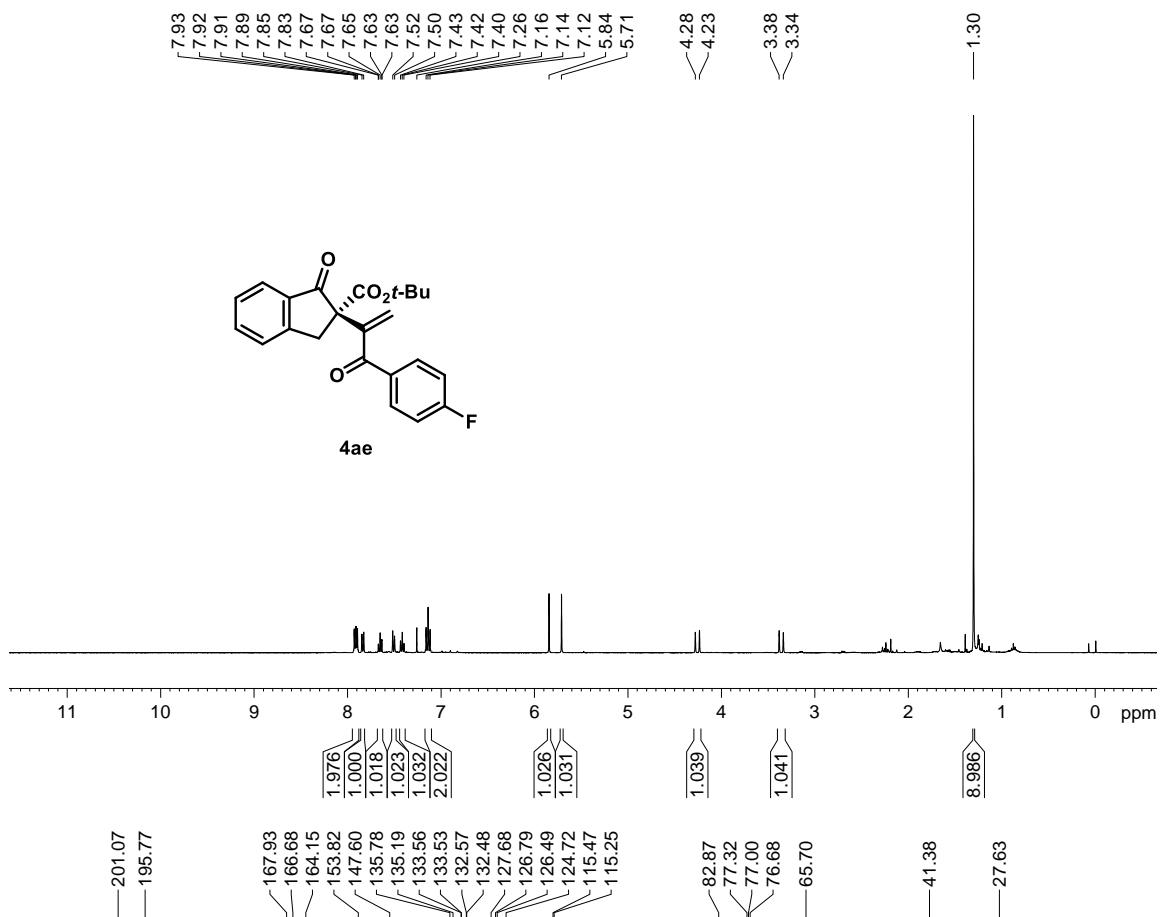


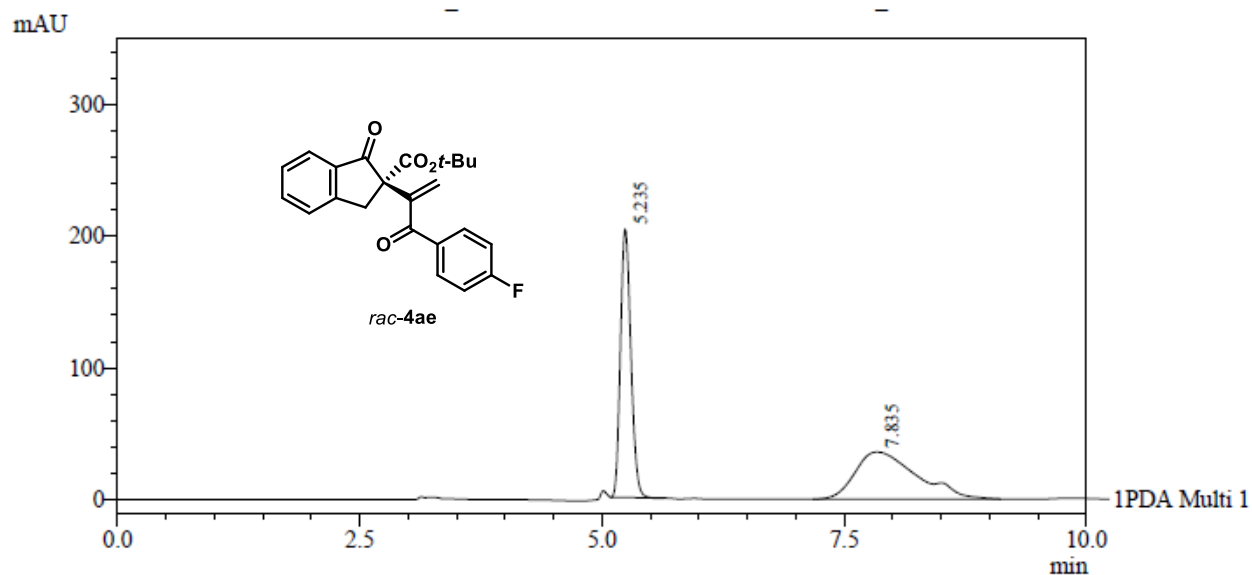
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.469	702583	1.791
2	6.454	38526749	98.209
Total		39229332	100.000





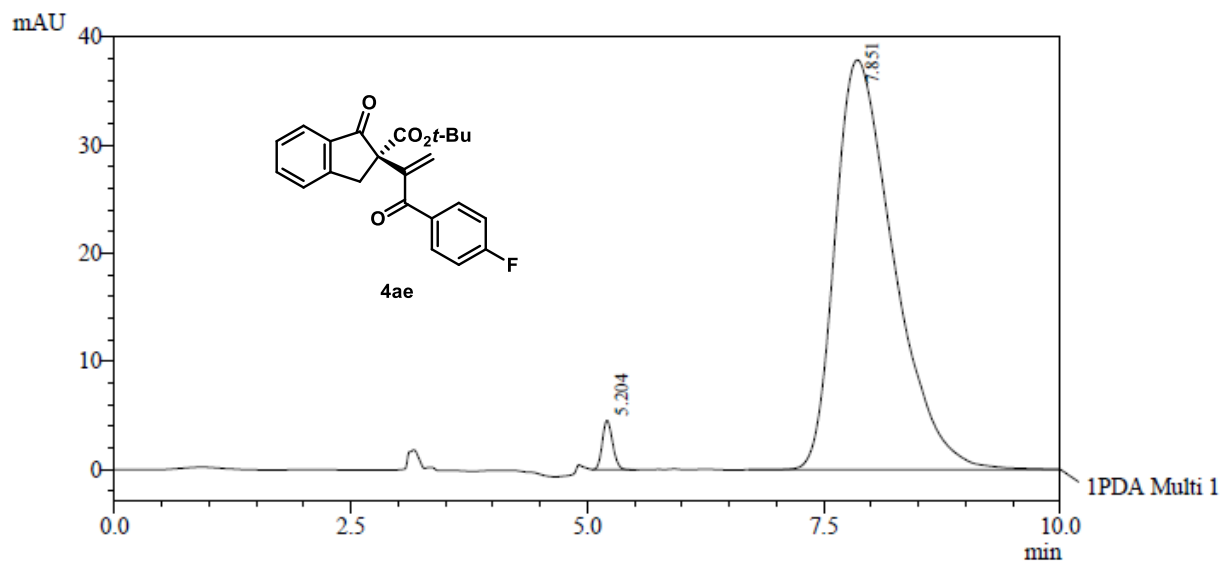
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.235	1524429	49.068
2	7.835	1582339	50.932
Total		3106769	100.000

Daicel Chiralpak AS-H column (*n*-Hexane/EtOH = 95:5, 1.0 mL min⁻¹, 20 °C, 254 nm)

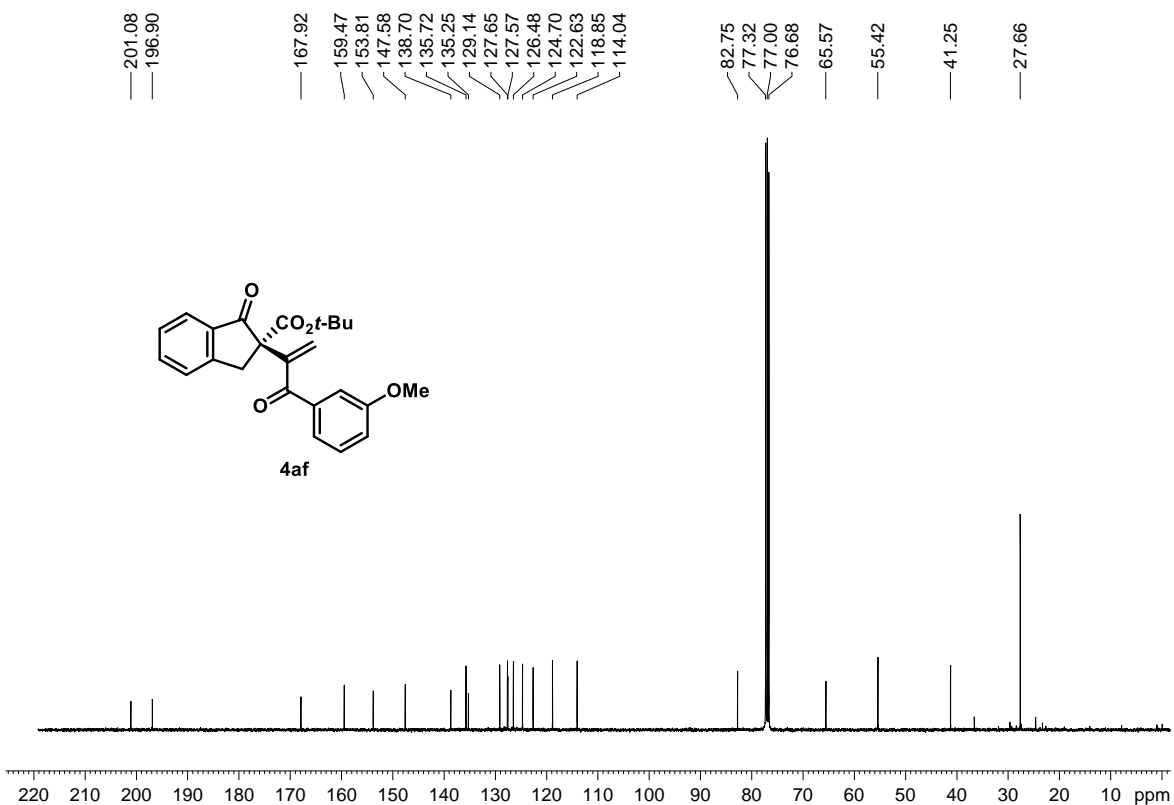
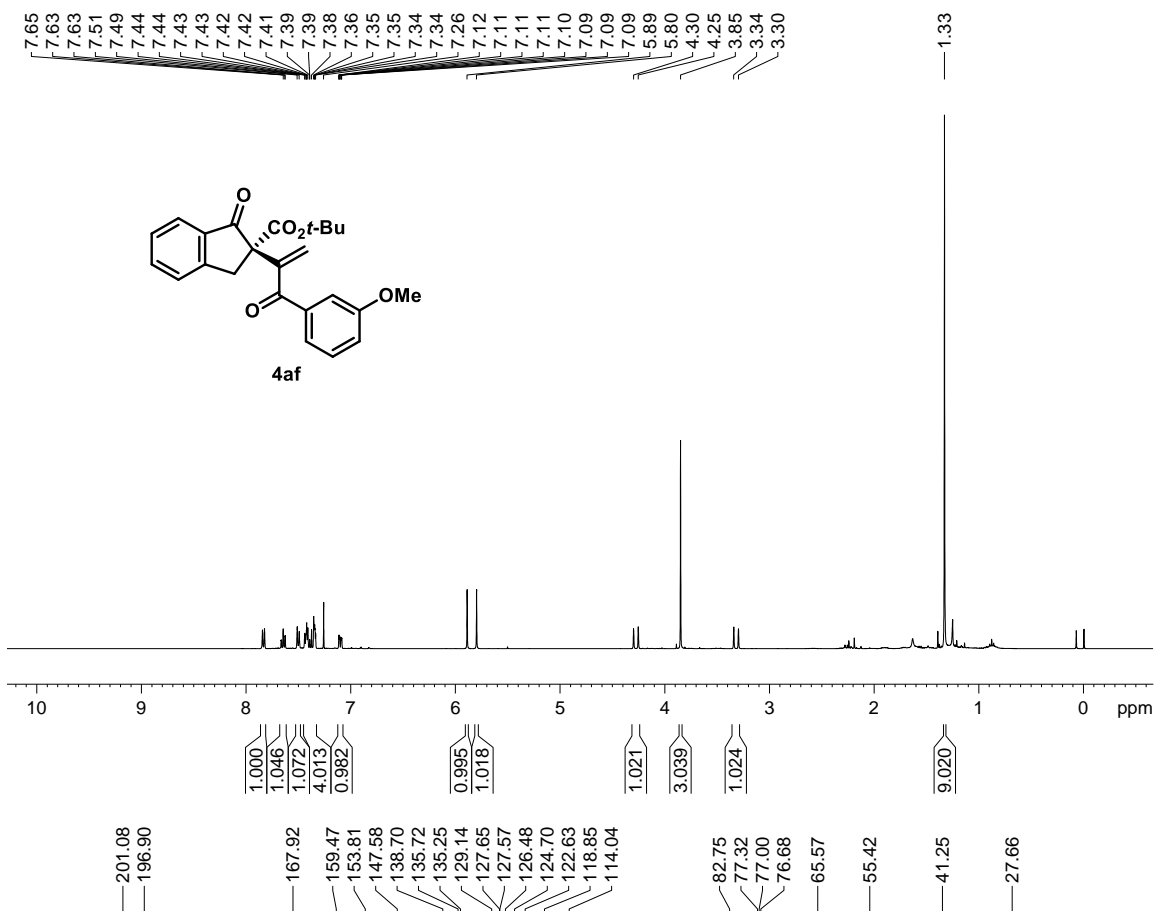


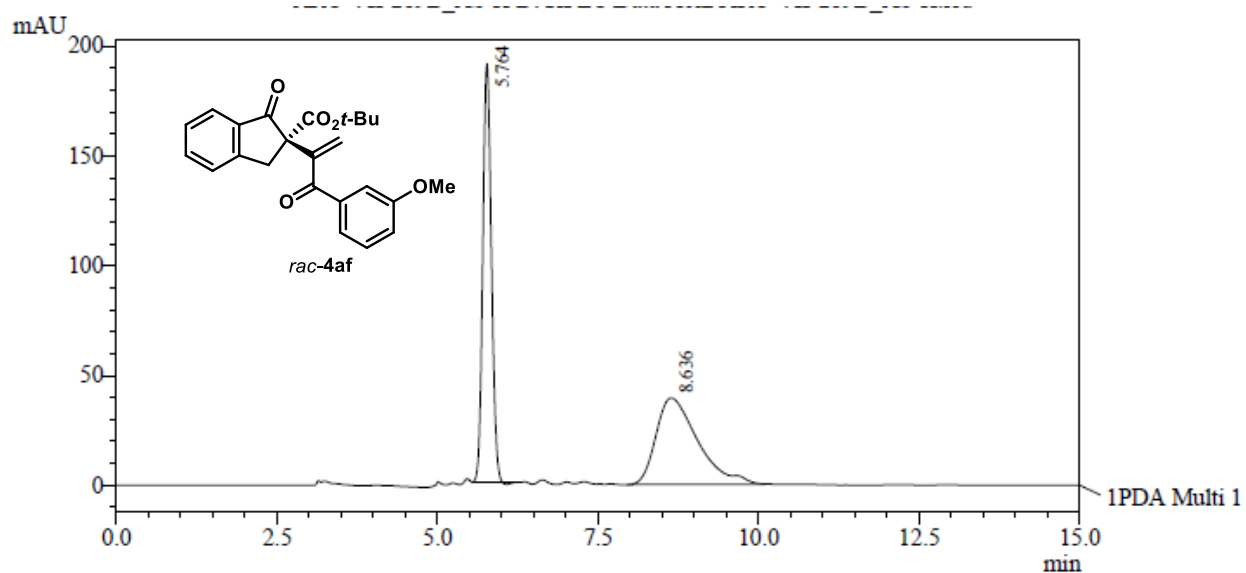
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.204	34509	2.068
2	7.851	1634251	97.932
Total		1668761	100.000





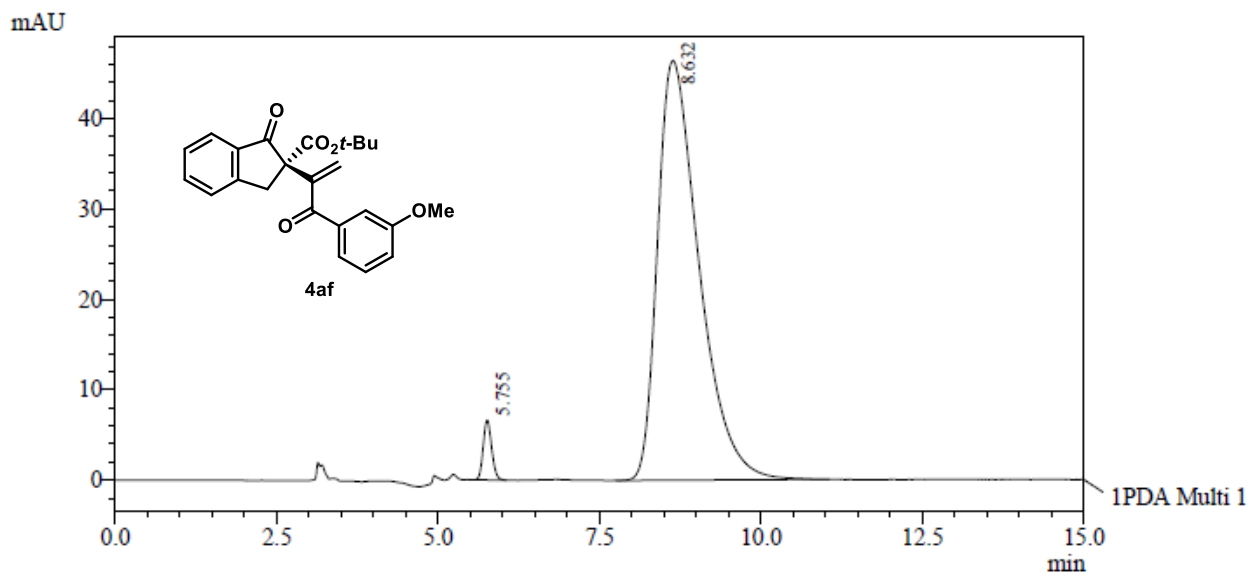
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.764	1765094	49.733
2	8.636	1784073	50.267
Total		3549167	100.000

Daicel Chiralpak AS-H column (*n*-Hexane/EtOH = 95:5, 1.0 mL min⁻¹, 20 °C, 254 nm)

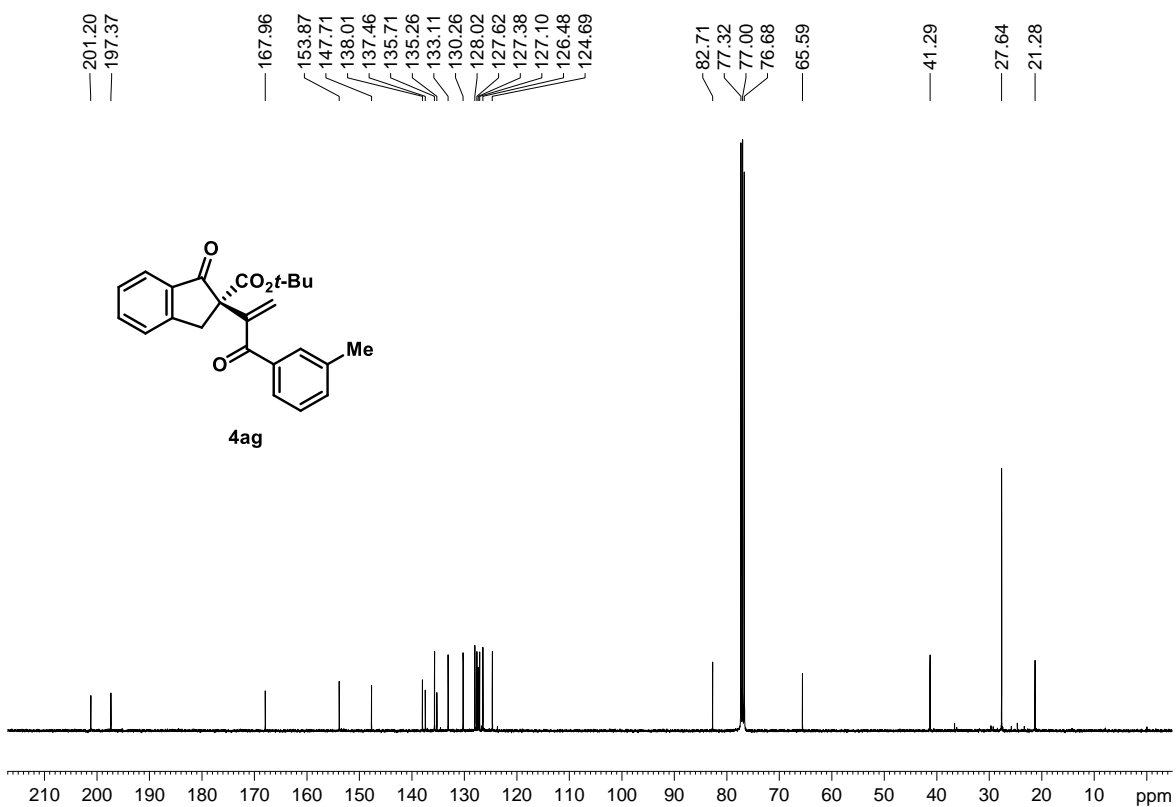
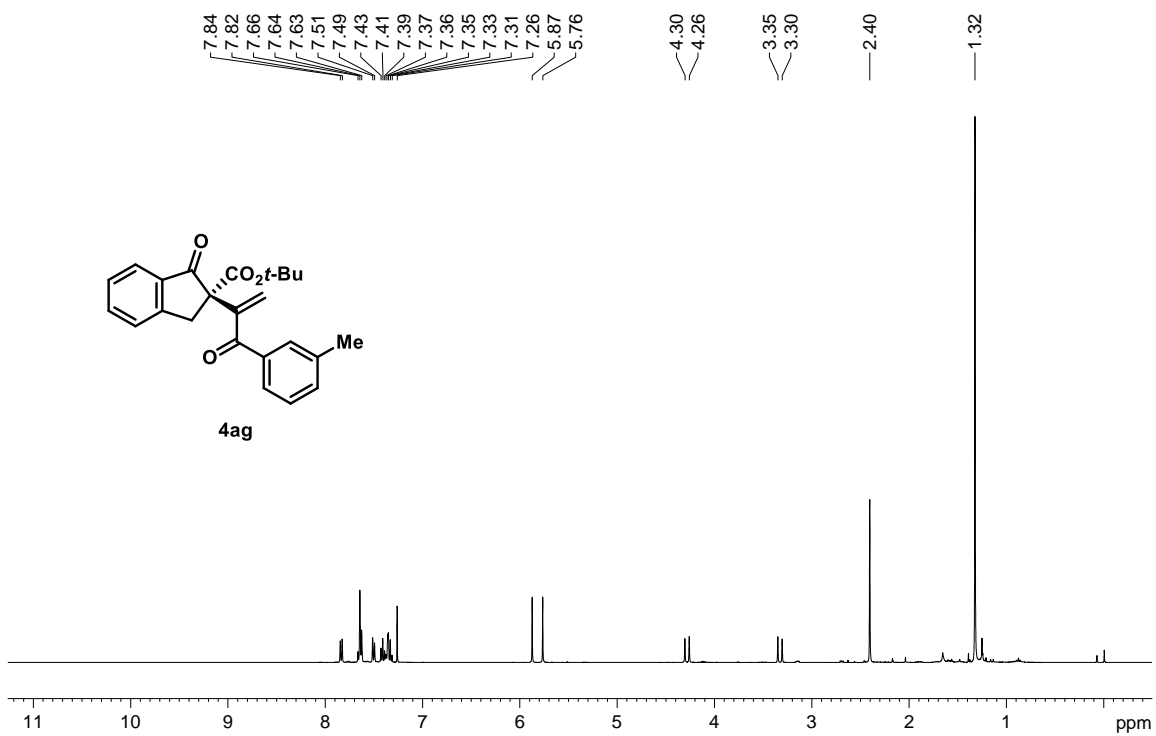


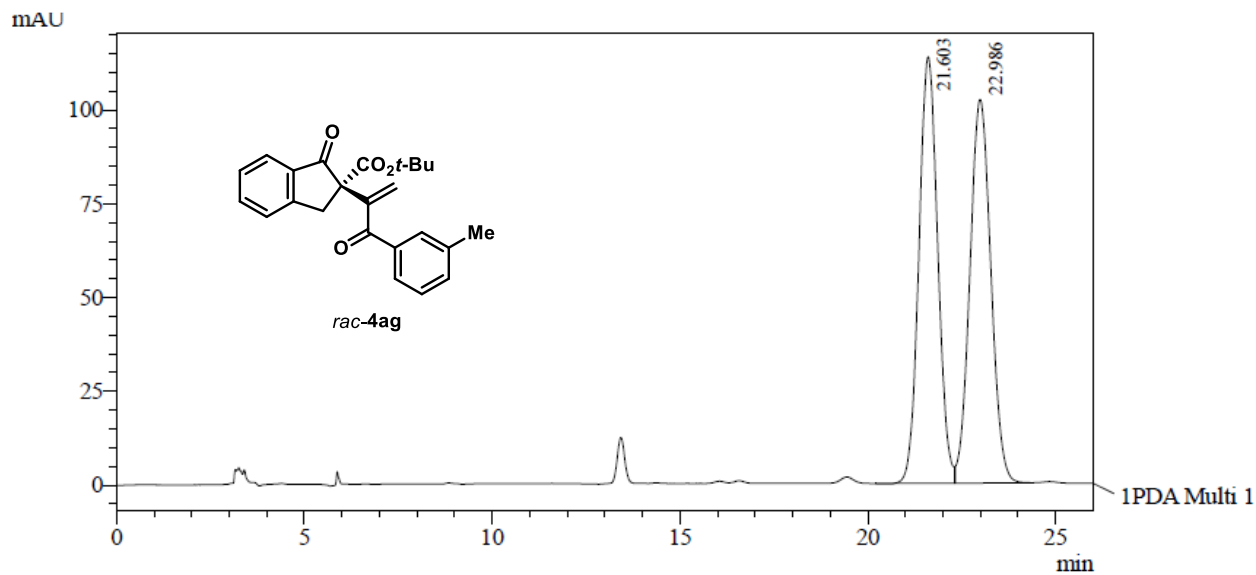
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.755	60357	2.824
2	8.632	2077175	97.176
Total		2137532	100.000





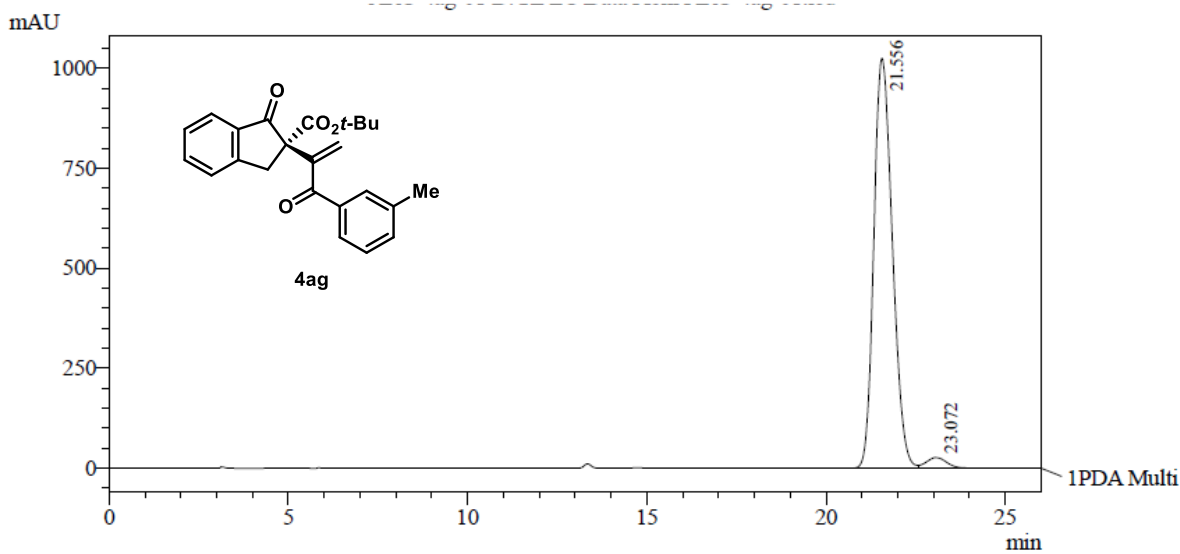
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	21.603	3957952	49.905
2	22.986	3973055	50.095
Total		7931007	100.000

Daicel Chiralpak IG column (*n*-Hexane/EtOH = 95:5, 1.0 mL min⁻¹, 20 °C, 254



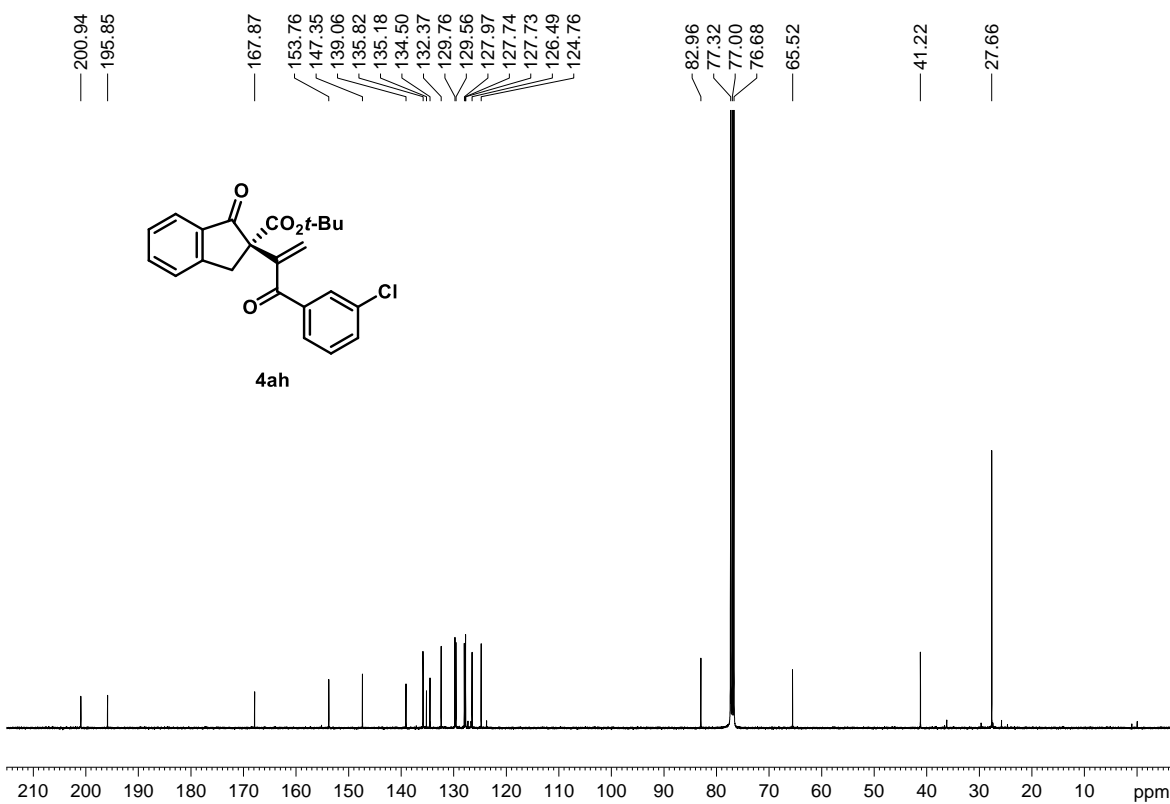
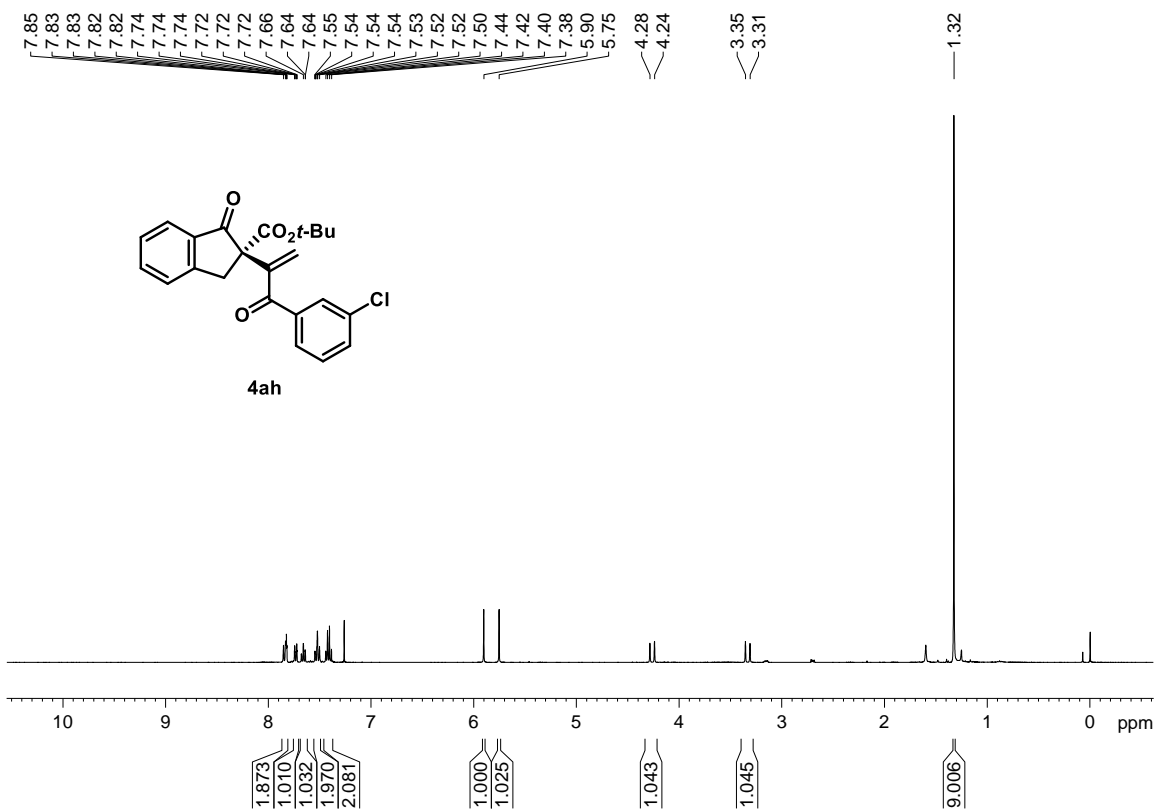
1 PDA Multi 1 / 254nm 4nm

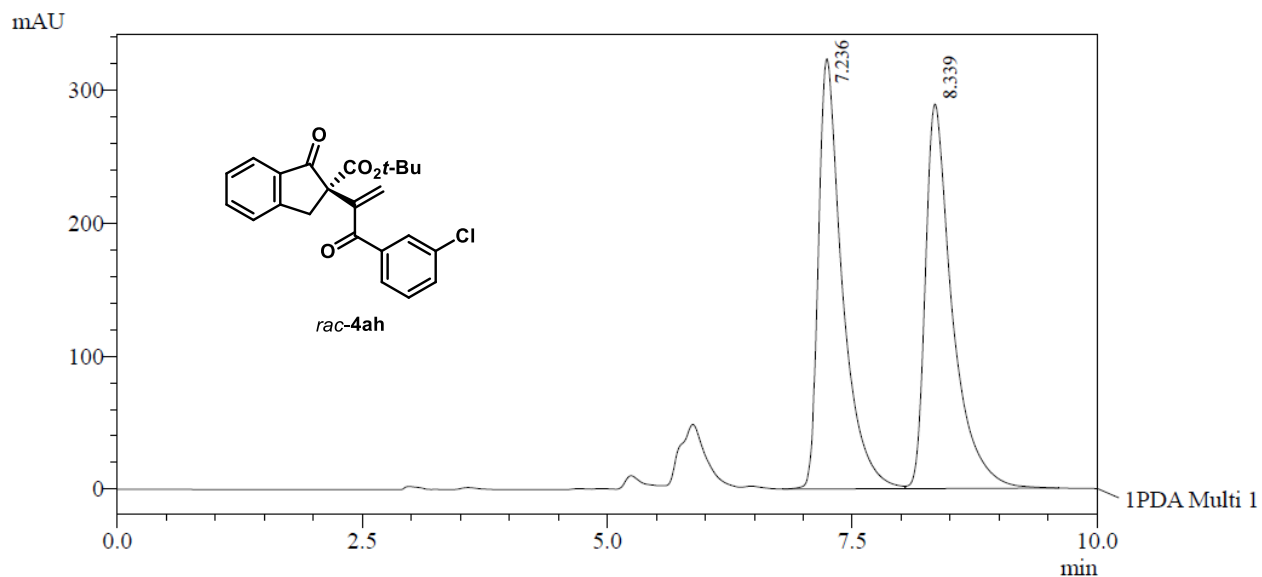
PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	21.556	36870630	97.227
2	23.072	1051770	2.773
Total		37922400	100.000

nm)





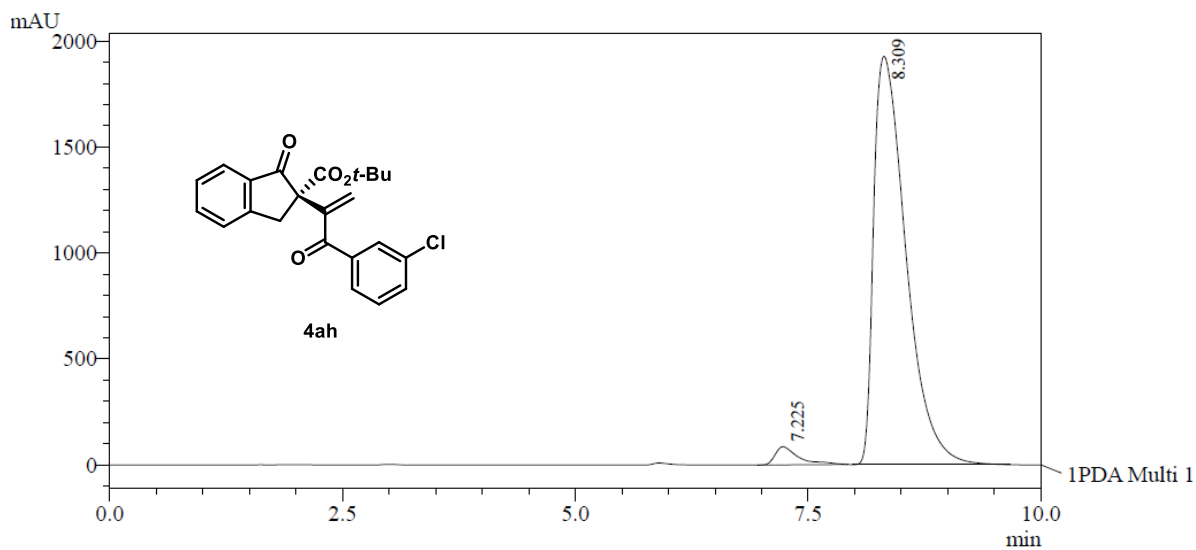
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	7.236	5508303	49.937
2	8.339	5522214	50.063
Total		11030517	100.000

Daicel Chiralpak IG column (*n*-Hexane/IPA = 90:10, 1.0 mL min⁻¹, 20 °C, 254 nm)

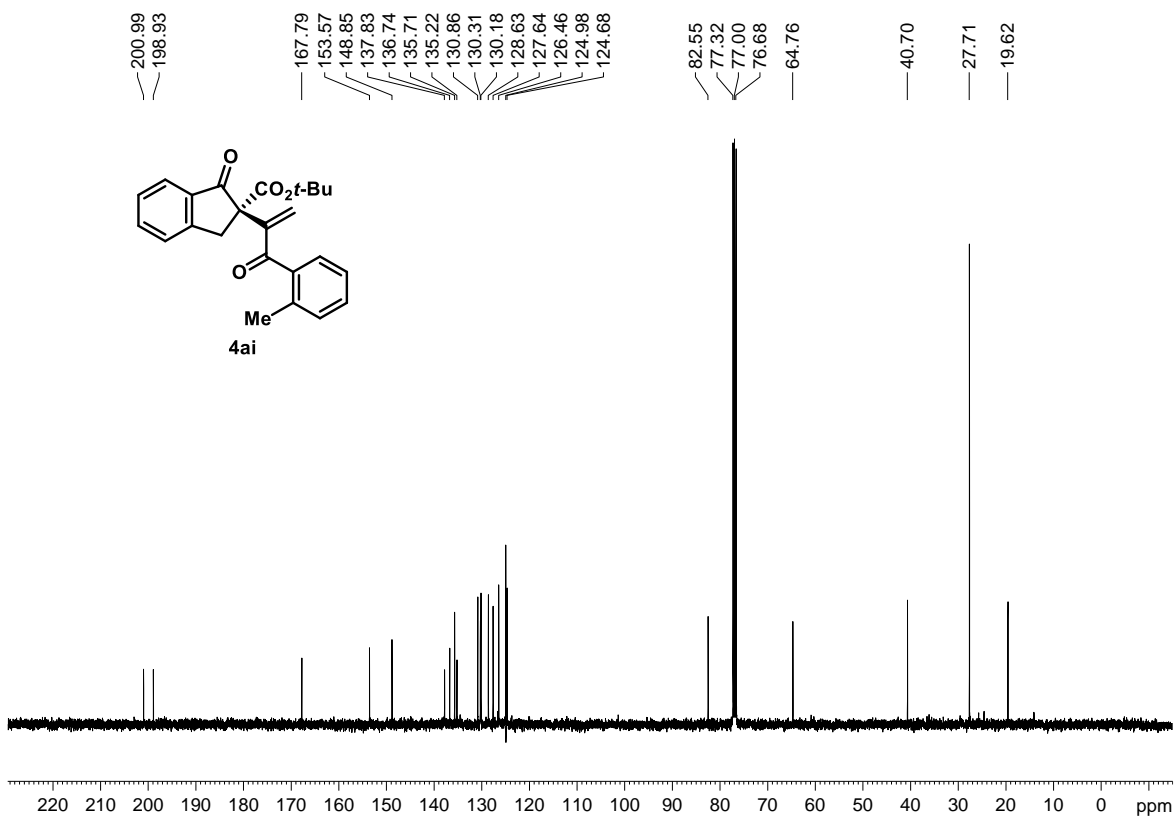
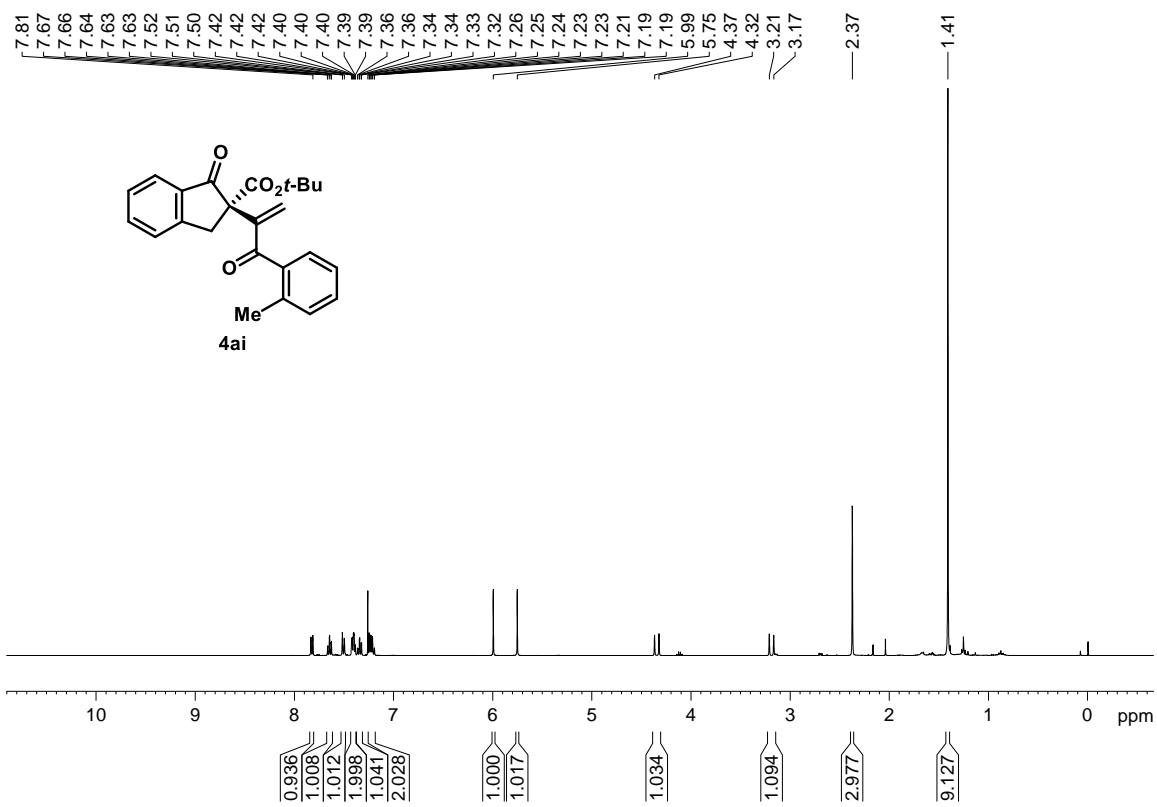


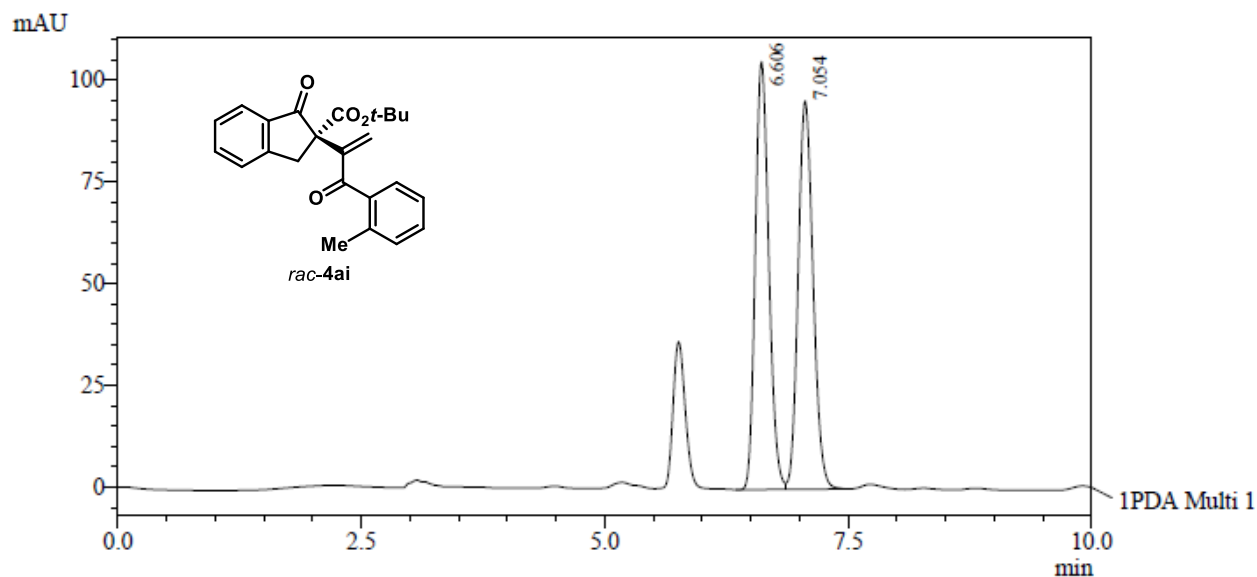
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	7.225	1508143	3.144
2	8.309	46457758	96.856
Total		47965901	100.000





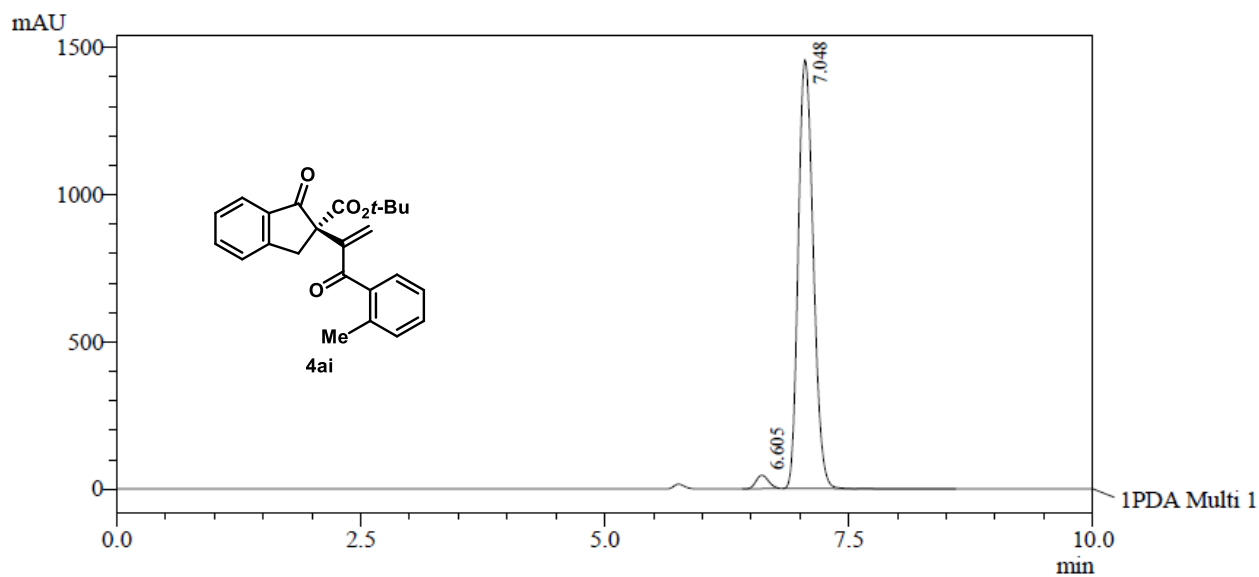
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	6.606	1015388	49.877
2	7.054	1020416	50.123
Total		2035804	100.000

Daicel Chiralpak AD-H column (*n*-Hexane/IPA = 90:10, 1.0 mL min⁻¹, 20 °C, 254 nm)

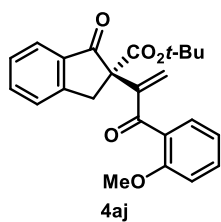
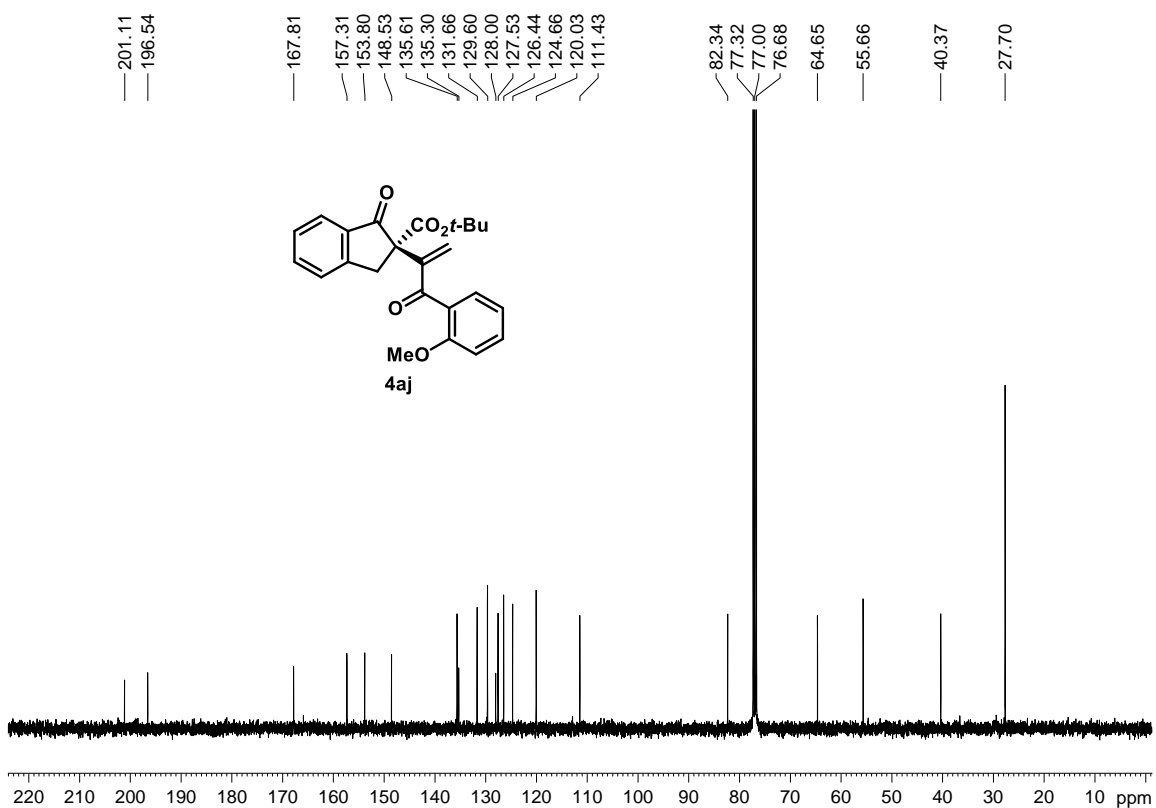
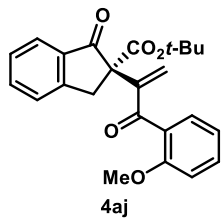
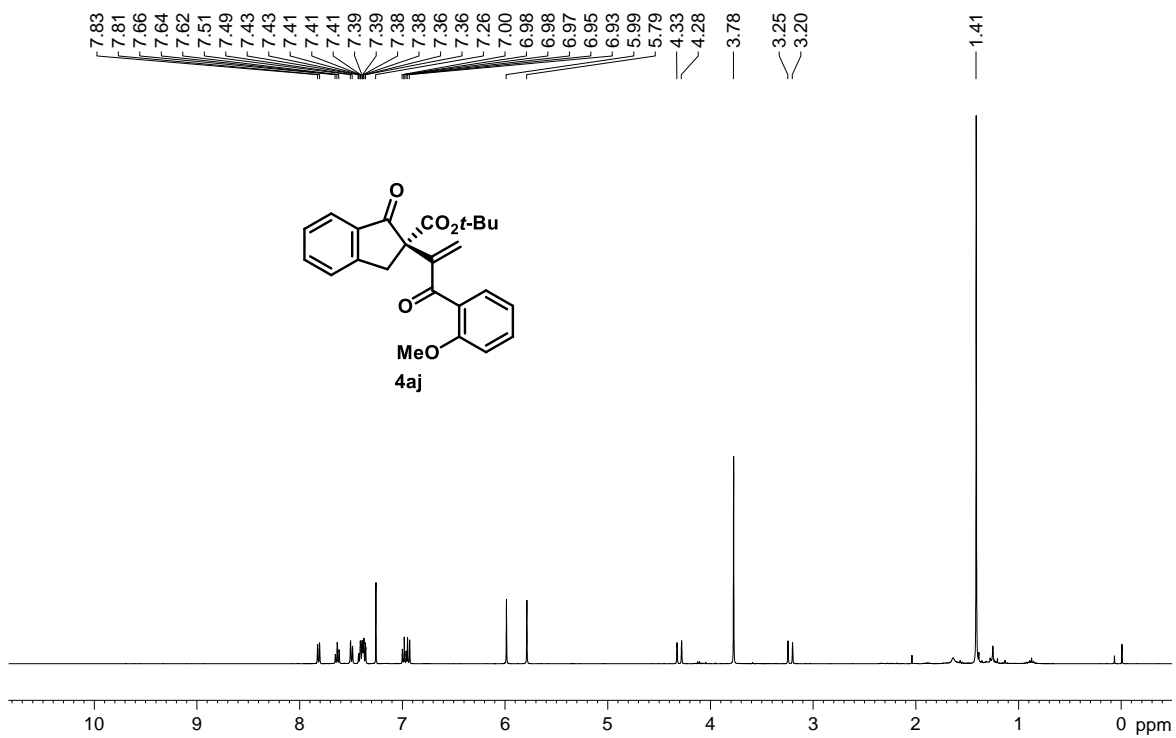


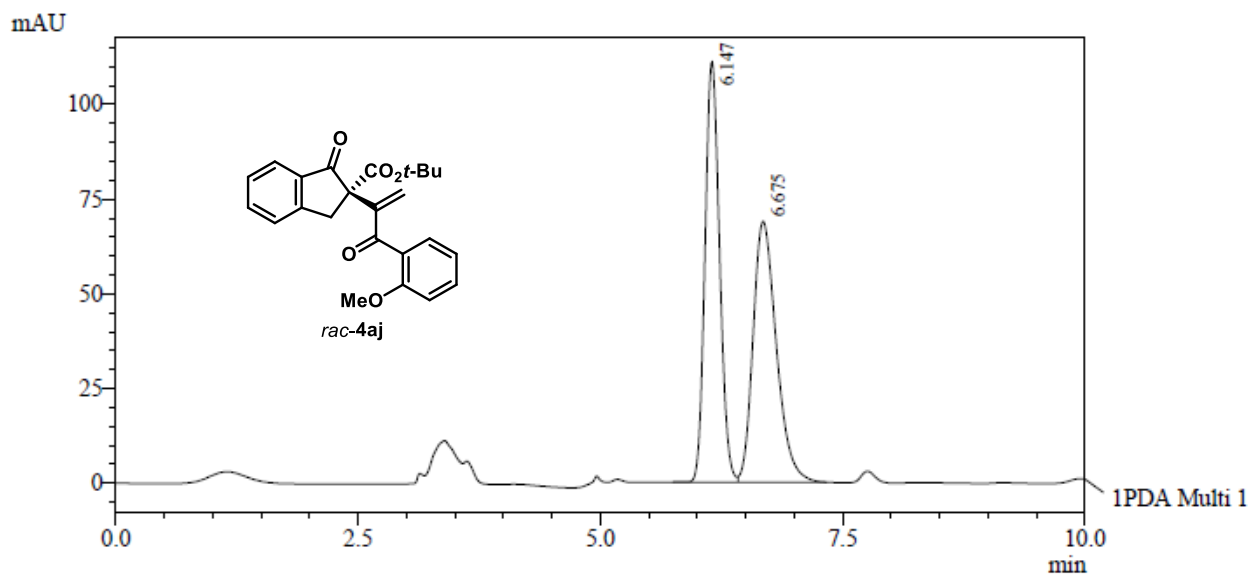
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	6.605	408127	2.540
2	7.048	15659442	97.460
Total		16067569	100.000





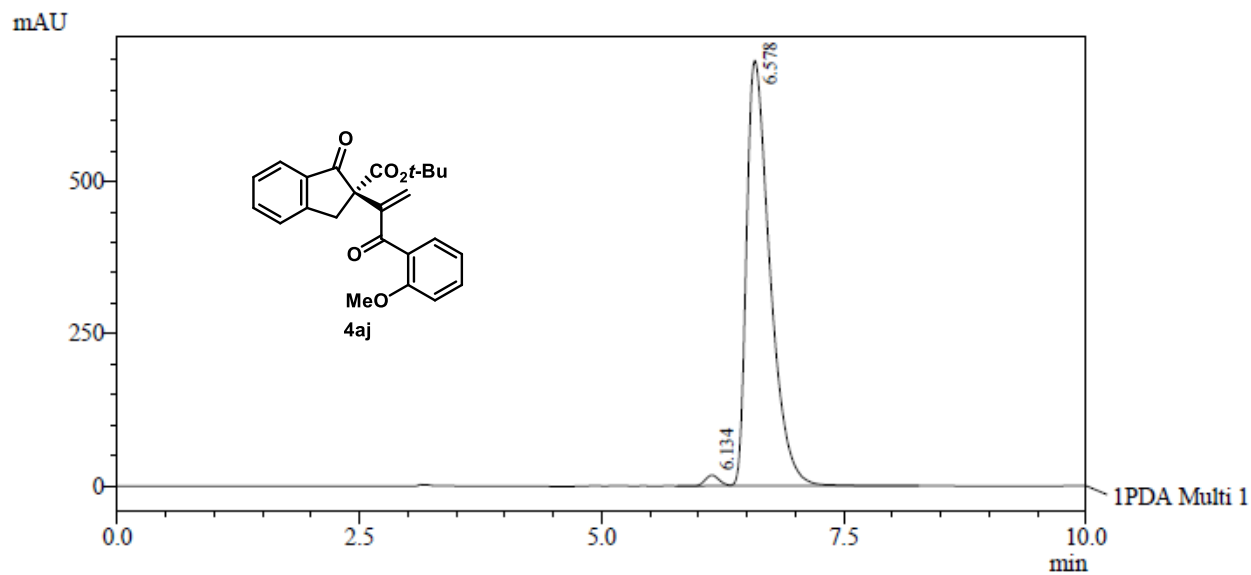
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	6.147	1161038	50.227
2	6.675	1150541	49.773
Total		2311579	100.000

Daicel Chiralpak AS-H column (n-Hexane/EtOH = 95:5, 1.0 mL min⁻¹, 20 °C, 254 nm)

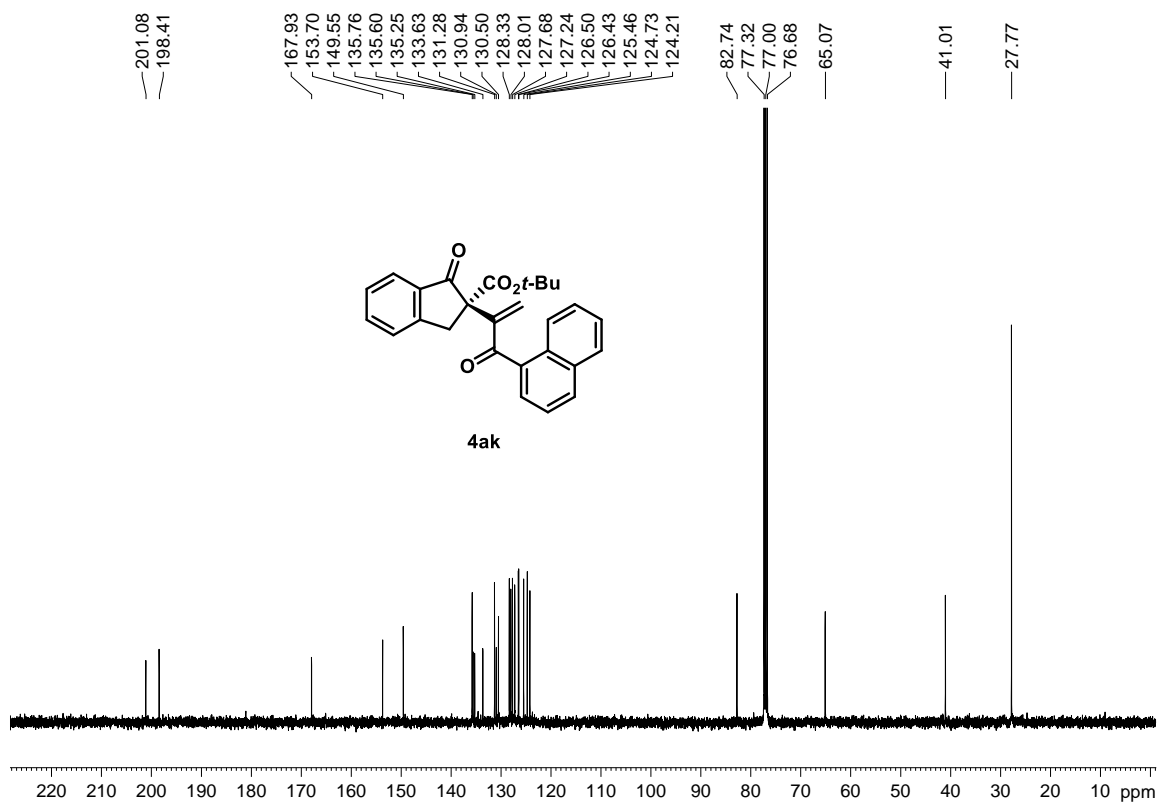
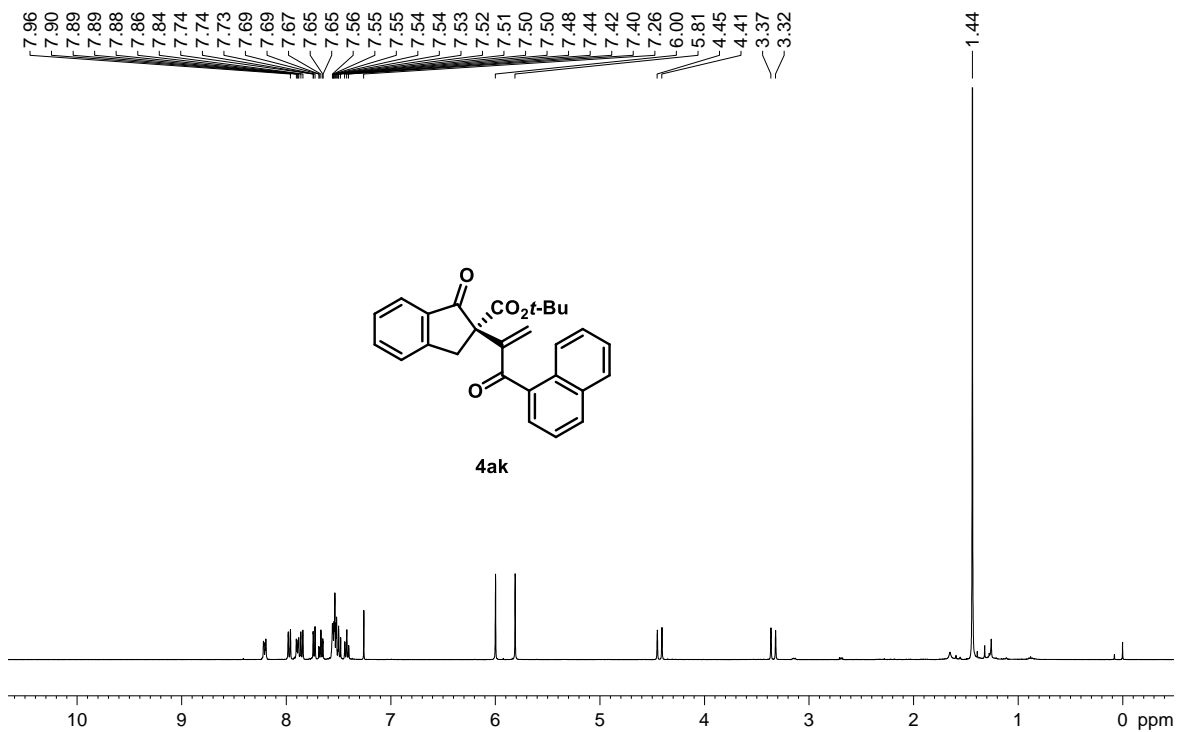


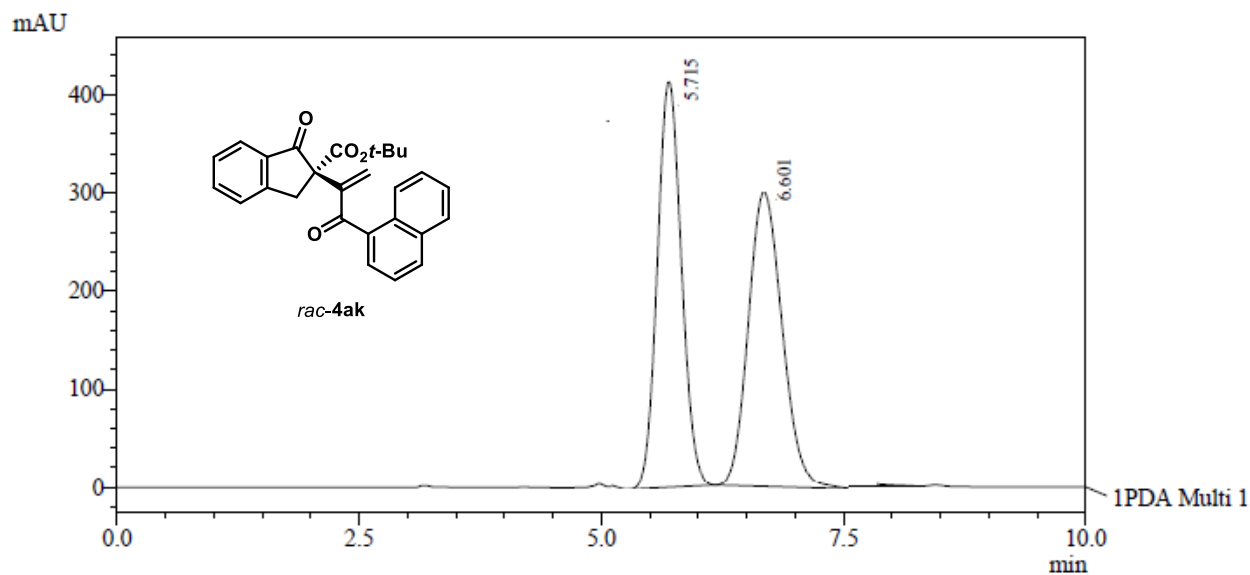
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	6.134	178517	1.500
2	6.578	11723617	98.500
Total		11902134	100.000





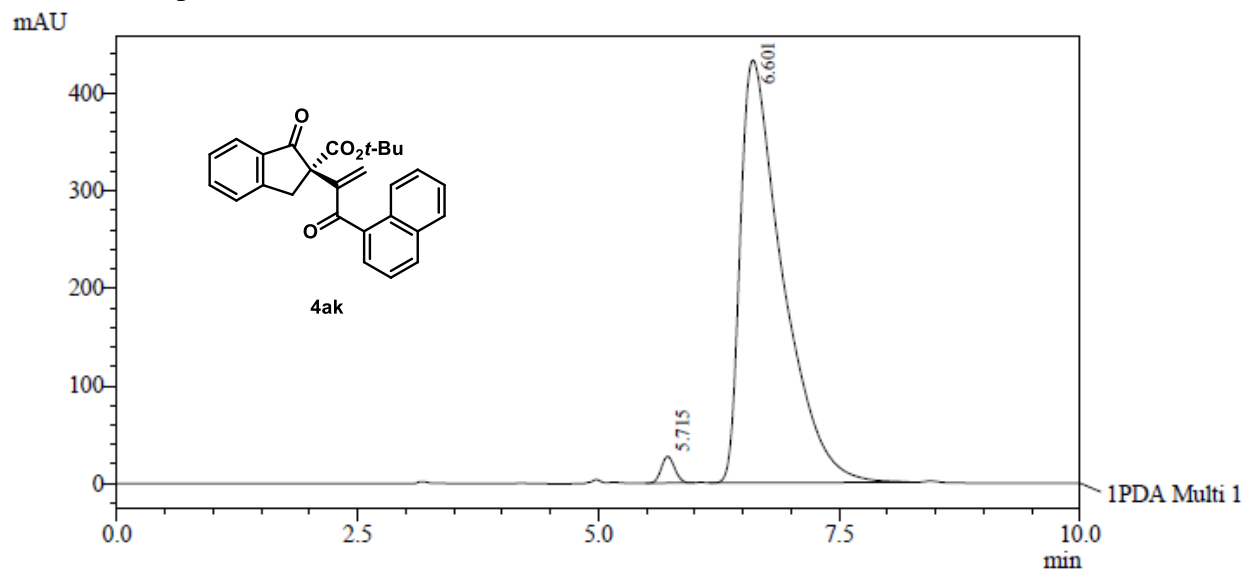
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.715	836145	49.586
2	6.601	850102	50.414
Total		1686248	100.000

Daicel Chiralpak AS-H column (*n*-Hexane/EtOH = 95:5, 1.0 mL min⁻¹, 20 °C, 254 nm)

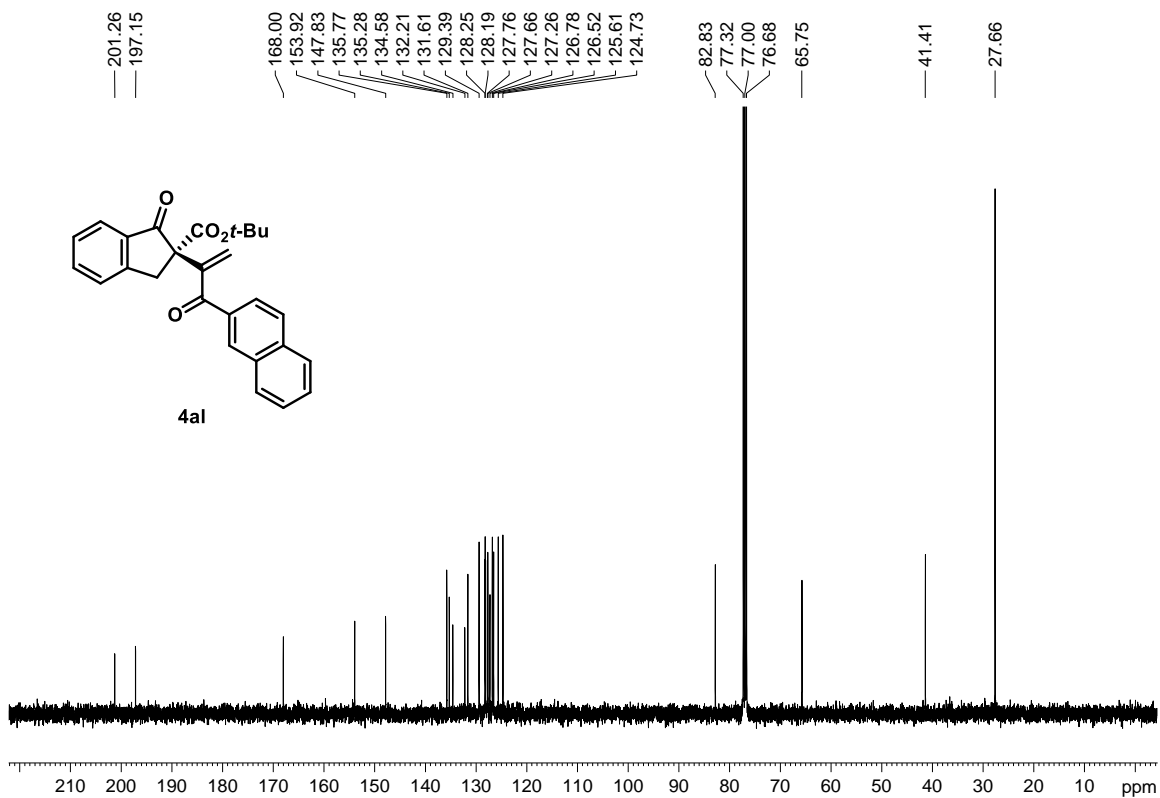
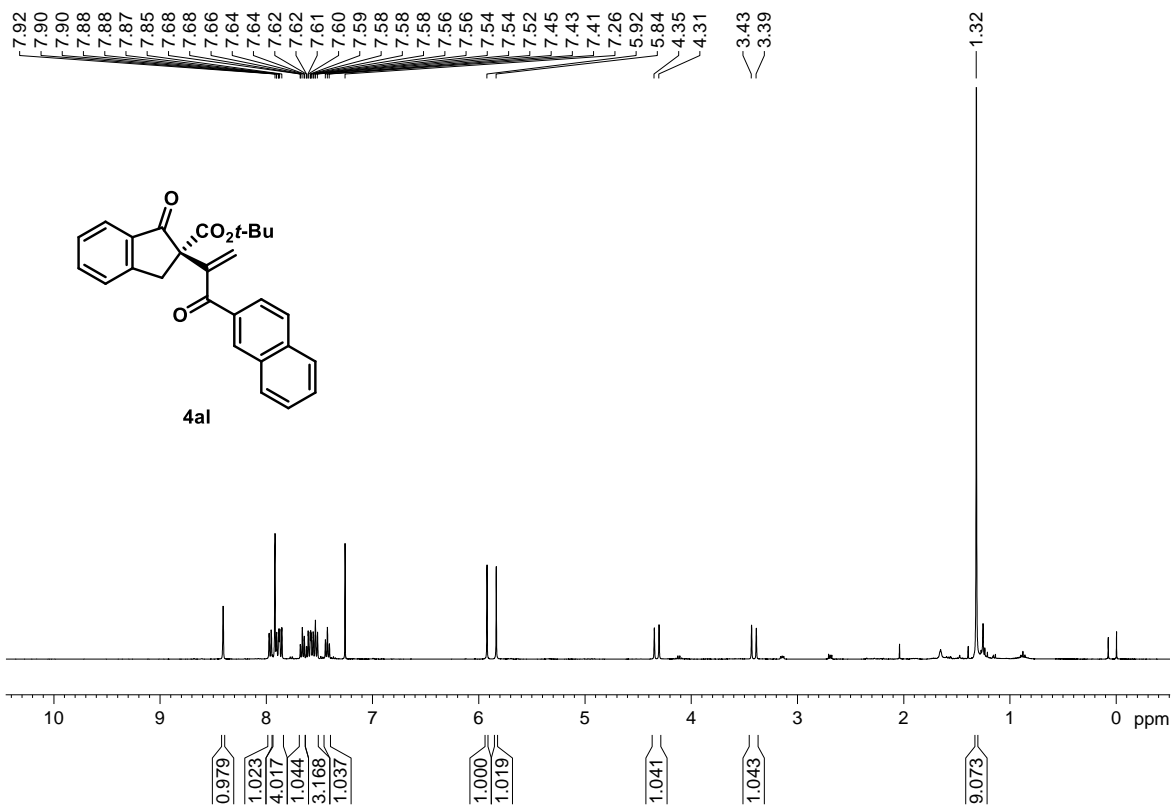


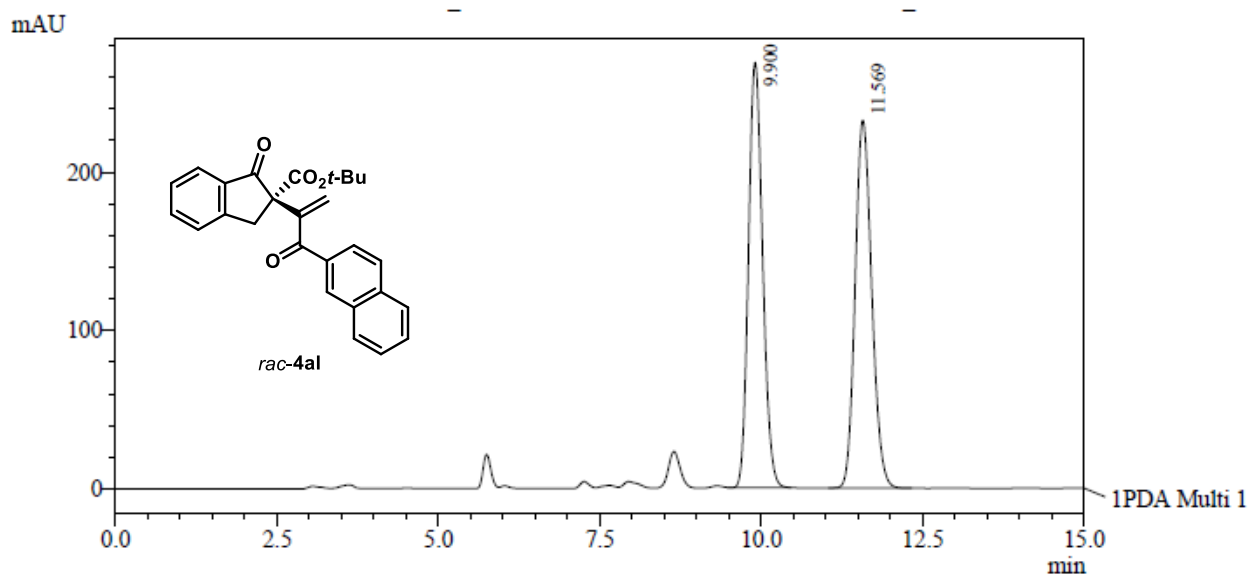
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.715	261275	1.941
2	6.601	13198951	98.059
Total		13460226	100.000





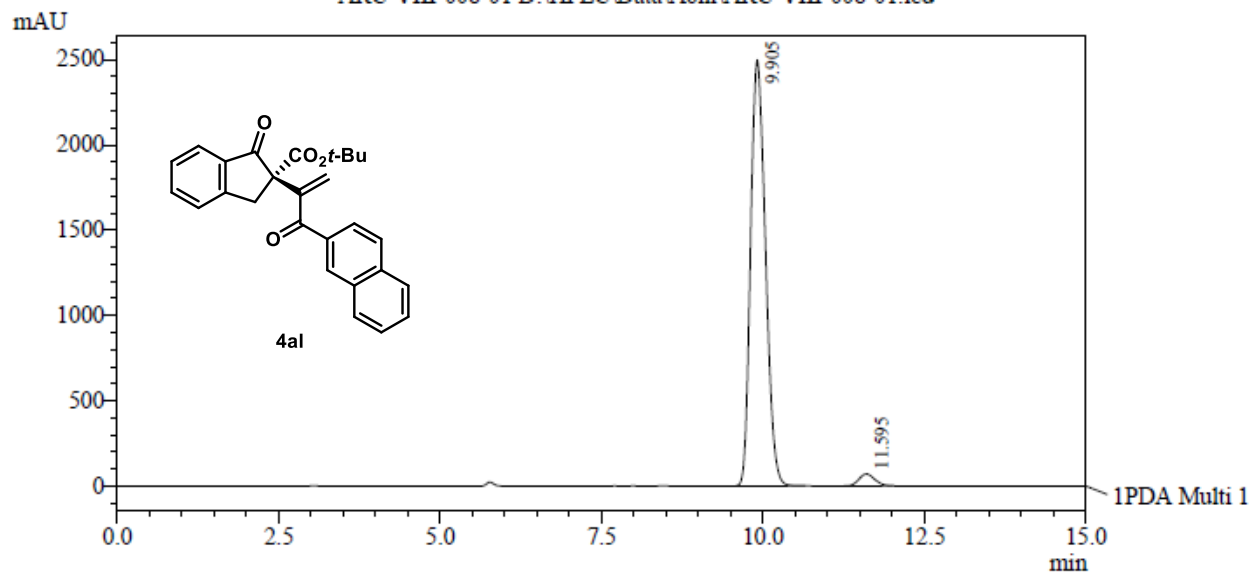
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	9.900	4097008	49.666
2	11.569	4152104	50.334
Total		8249112	100.000

Daicel Chiralpak AD-H column (*n*-Hexane/IPA = 90:10, 1.0 mL min⁻¹, 20 °C, 254 nm)

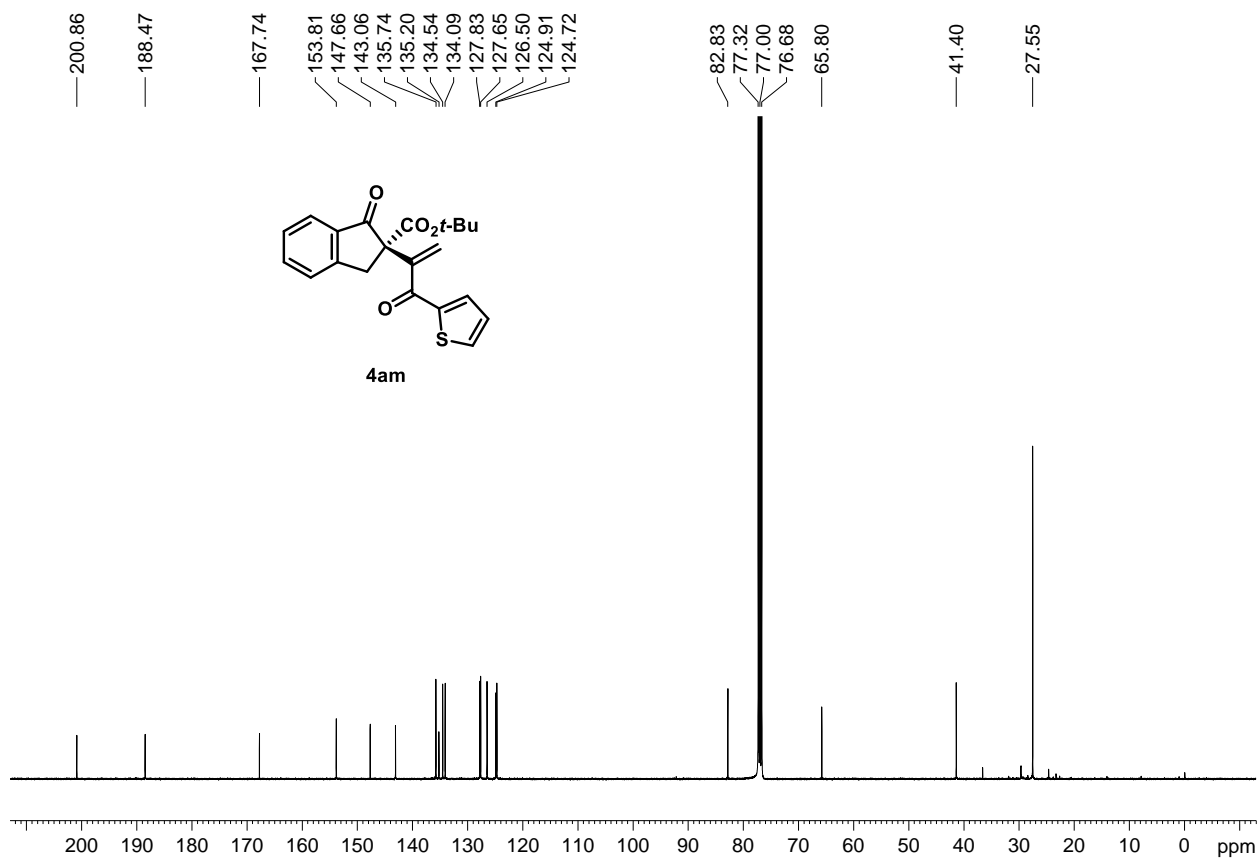
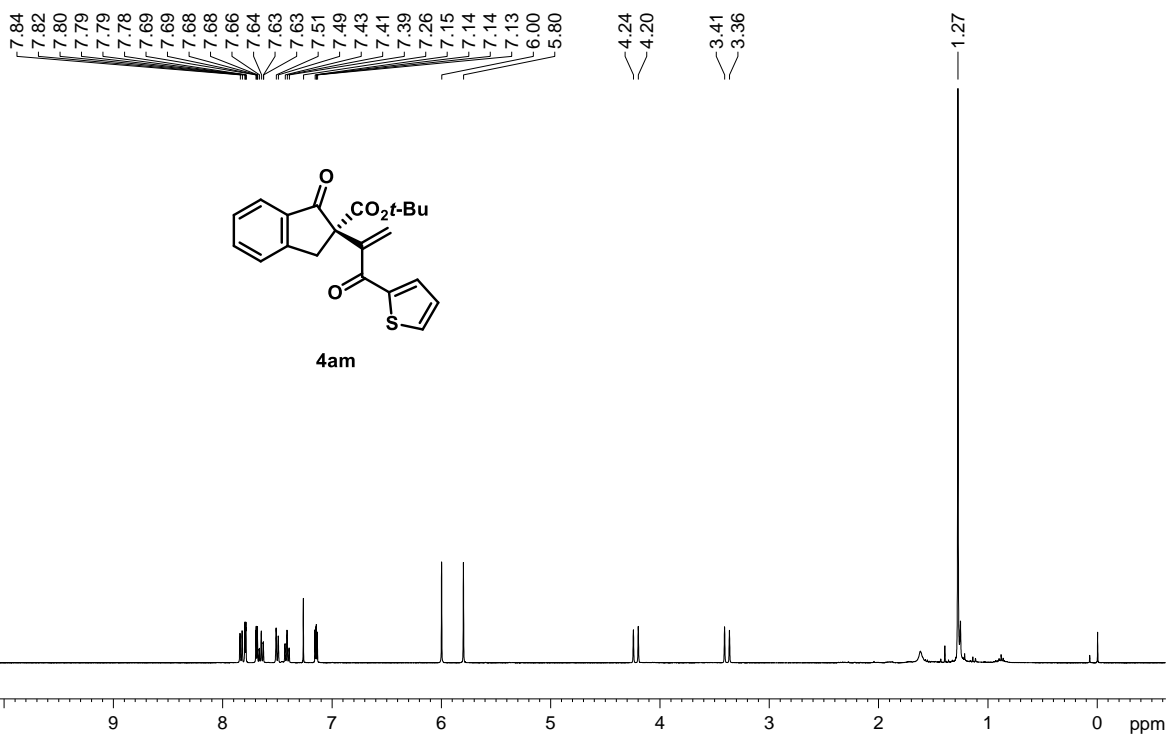


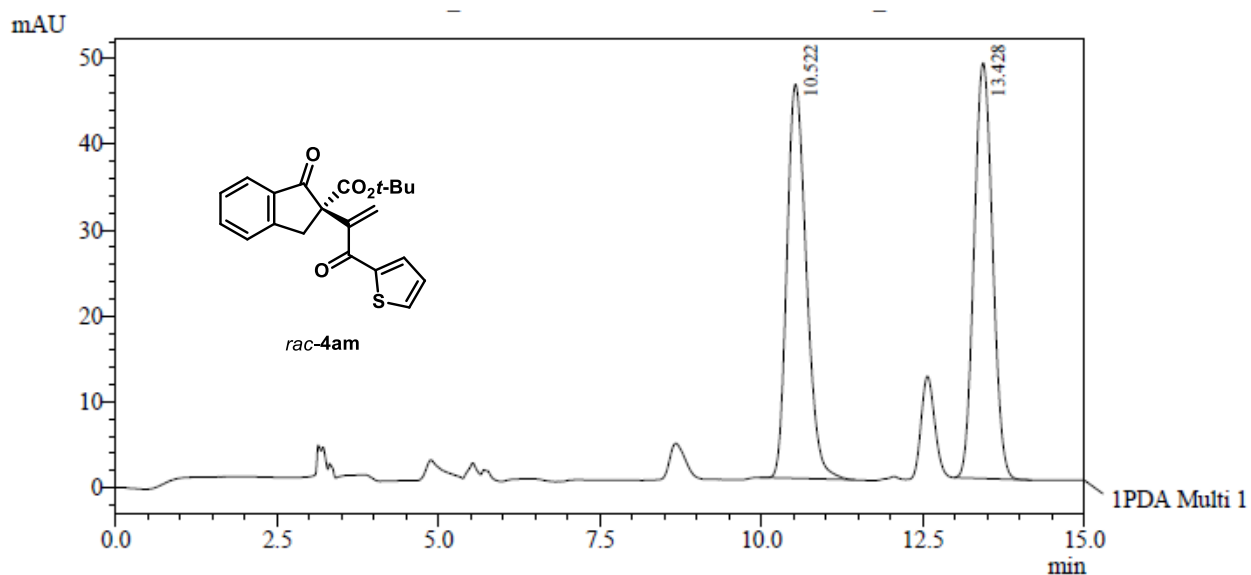
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	9.905	40029105	97.075
2	11.595	1206070	2.925
Total		41235176	100.000





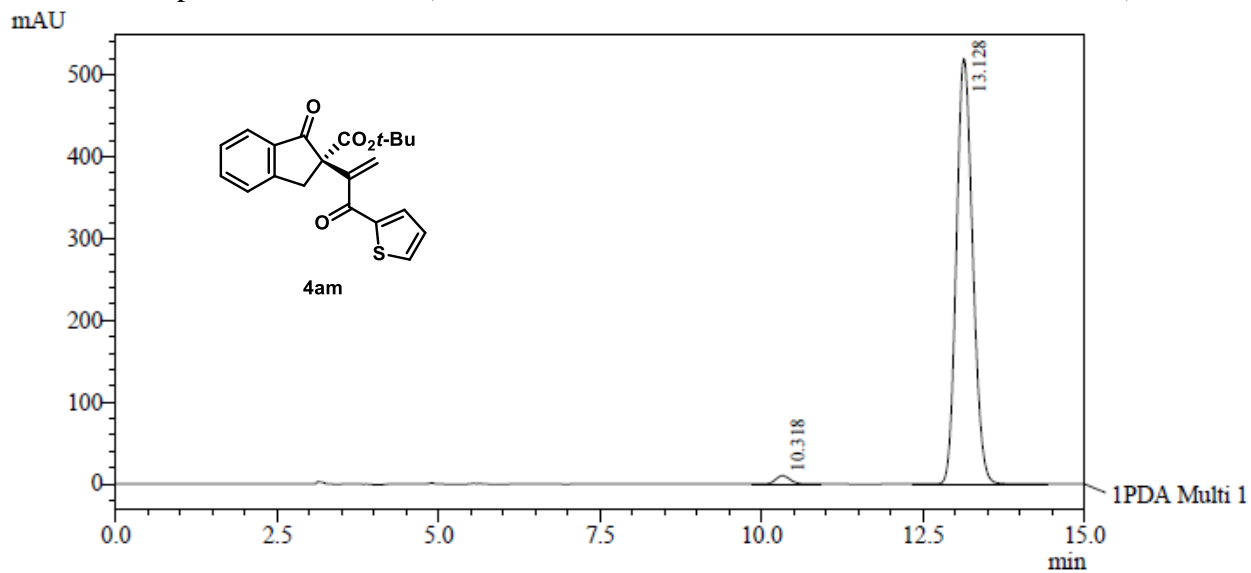
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	10.522	962969	49.970
2	13.428	964121	50.030
Total		1927089	100.000

Daicel Chiralpak AD-H column (*n*-Hexane/EtOH = 95:5, 1.0 mL min⁻¹, 20 °C, 254 nm)

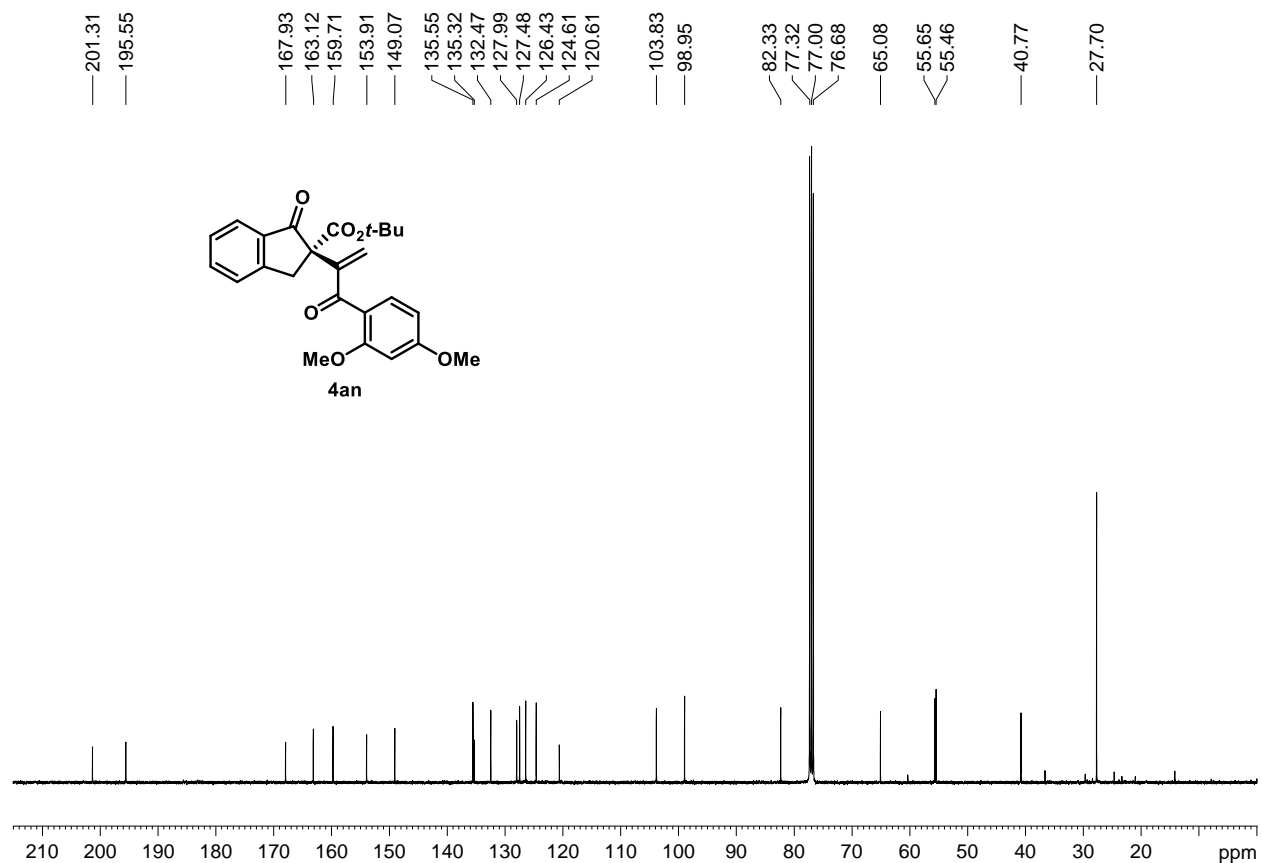
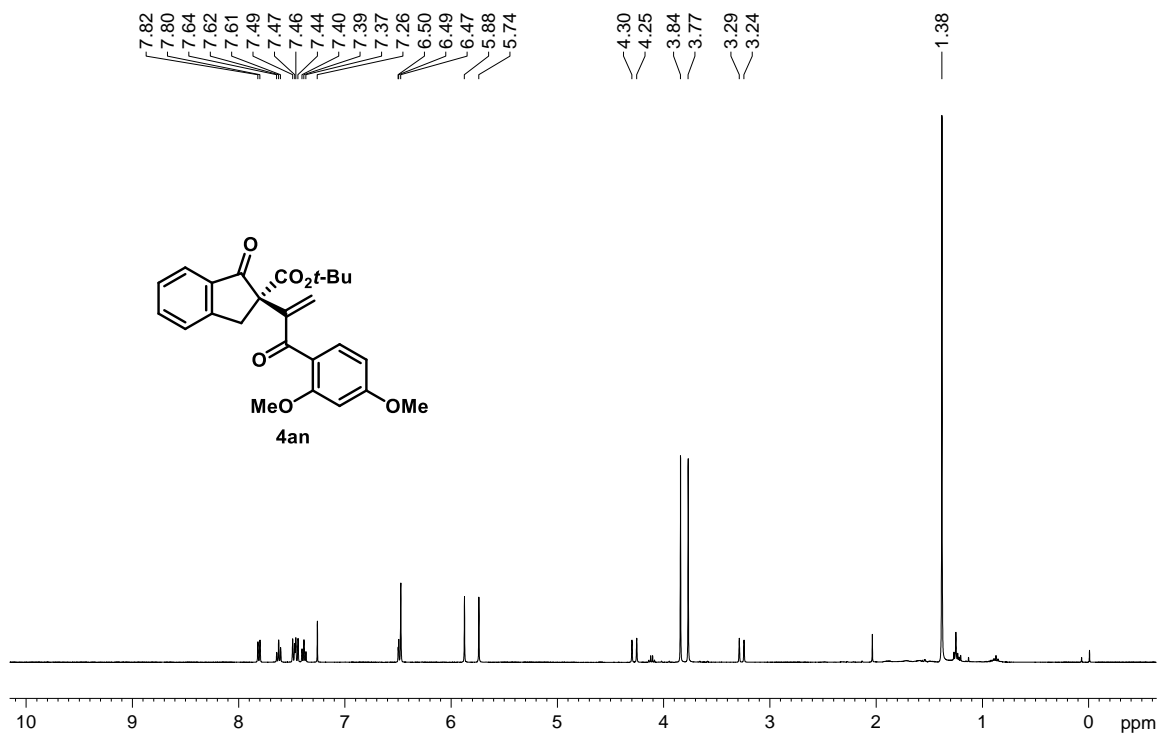


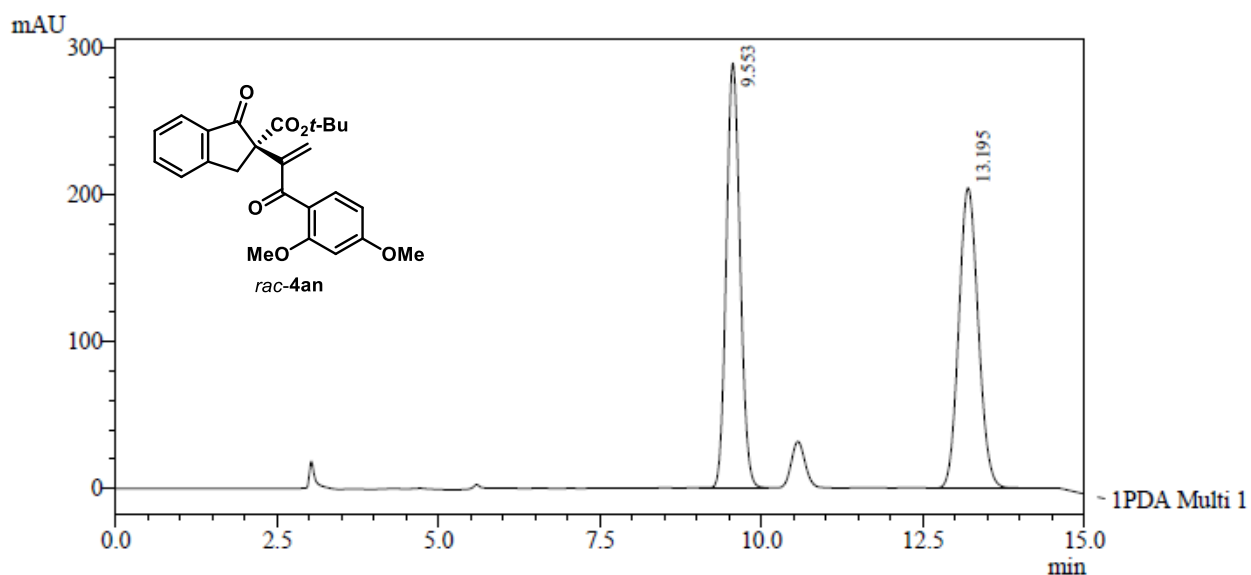
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	10.318	158092	1.699
2	13.128	9144511	98.301
Total		9302603	100.000





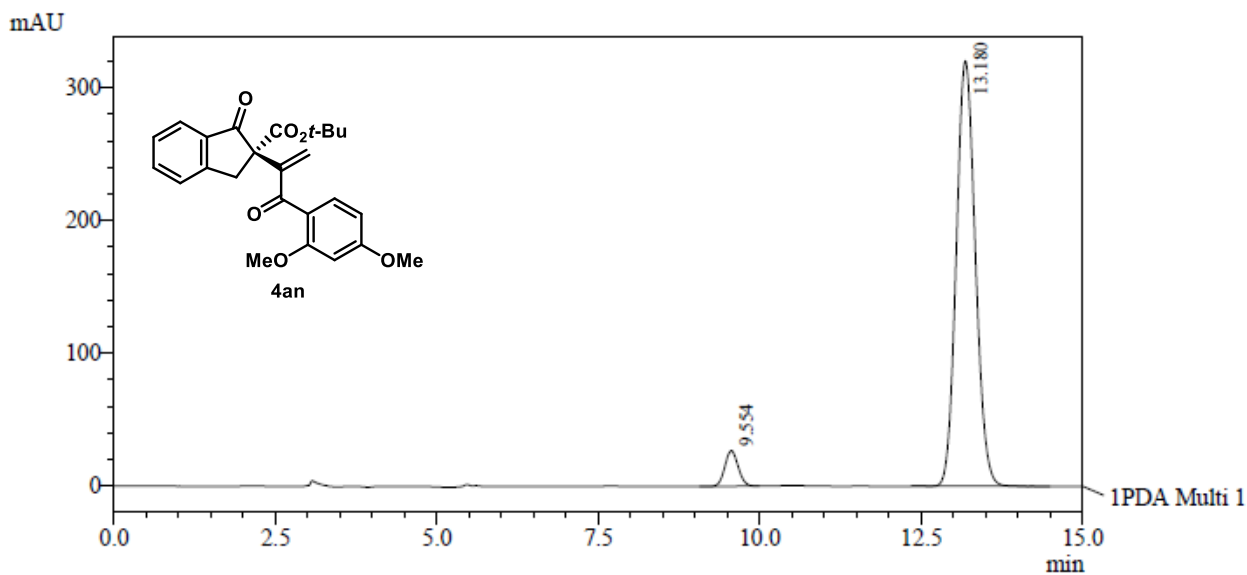
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	9.553	4281621	50.004
2	13.195	4280856	49.996
Total		8562477	100.000

Phenomenex C-1 column (*n*-Hexane/EtOH = 95:5, 1.0 mL min⁻¹, 20 °C, 254 nm)

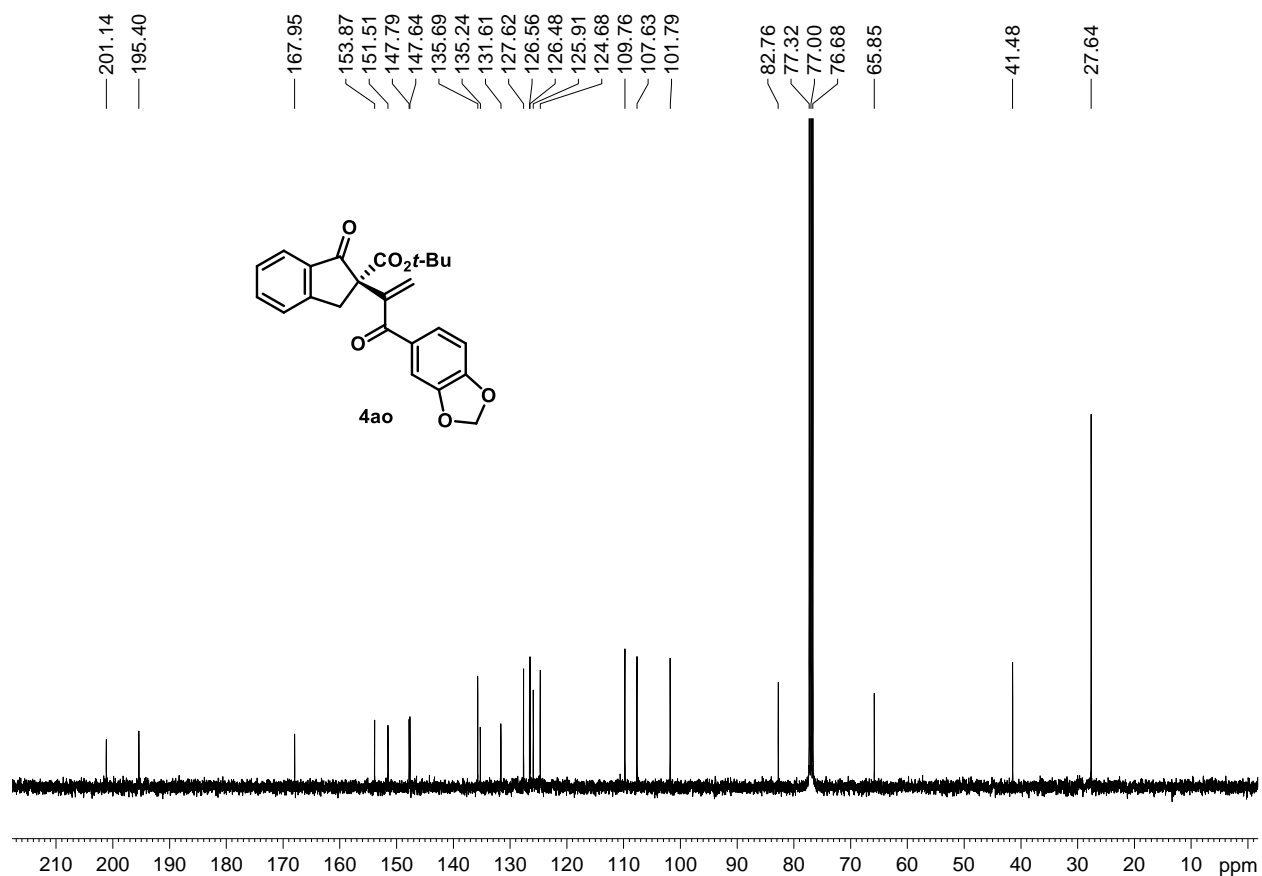
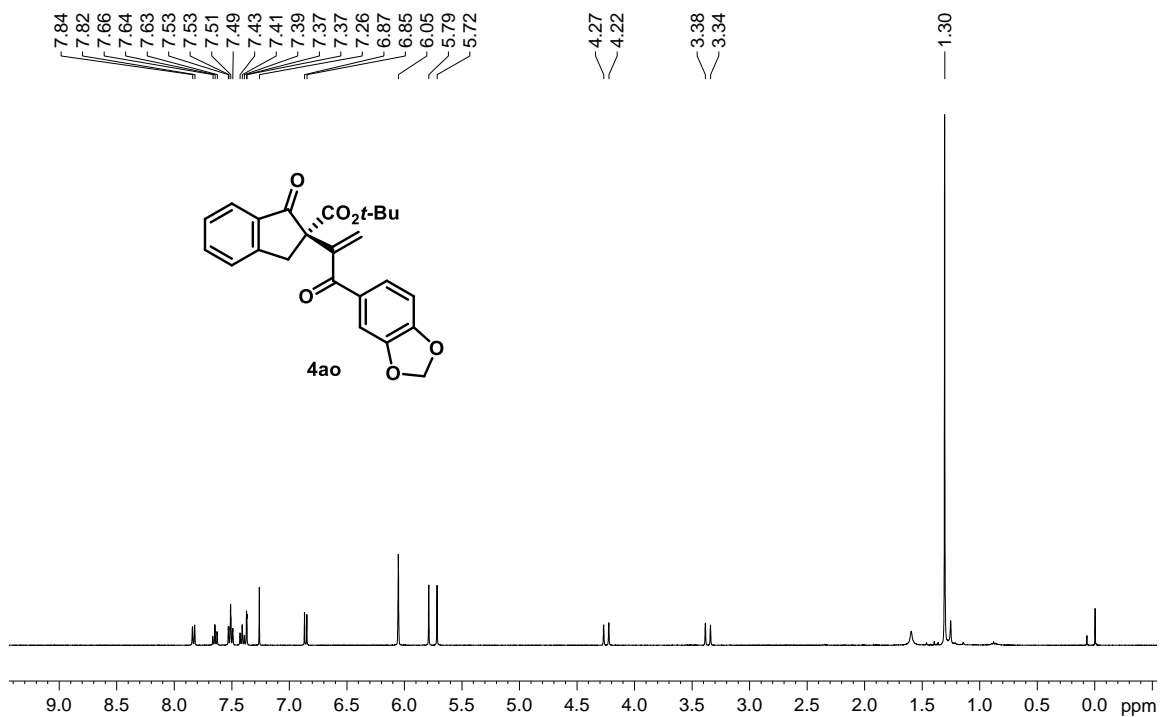


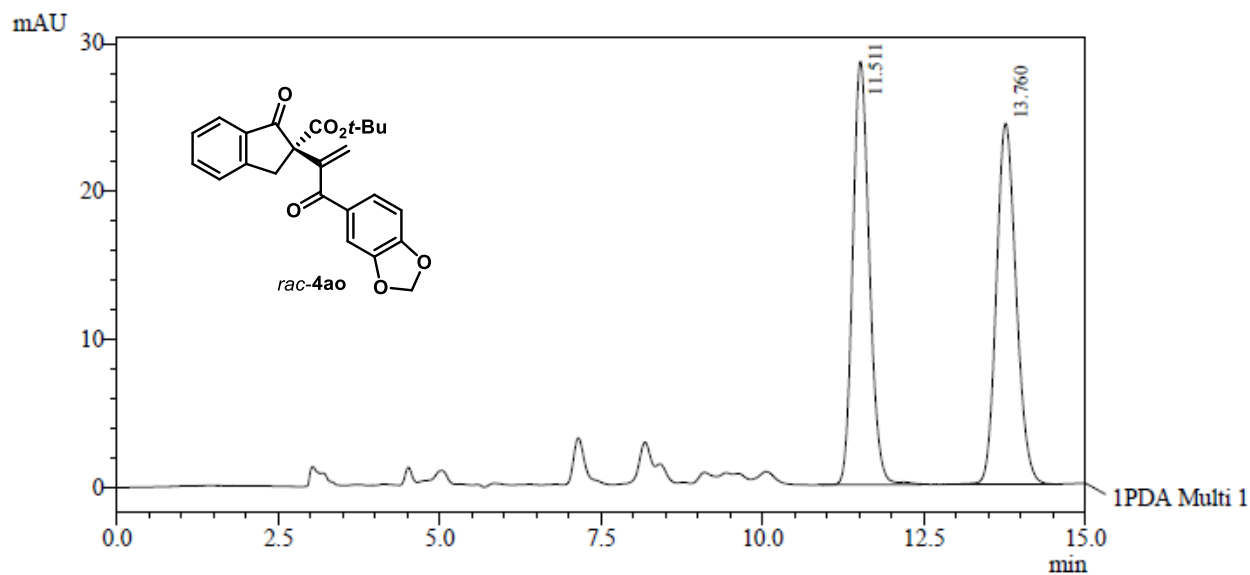
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	9.554	382952	5.492
2	13.180	6589838	94.508
Total		6972790	100.000





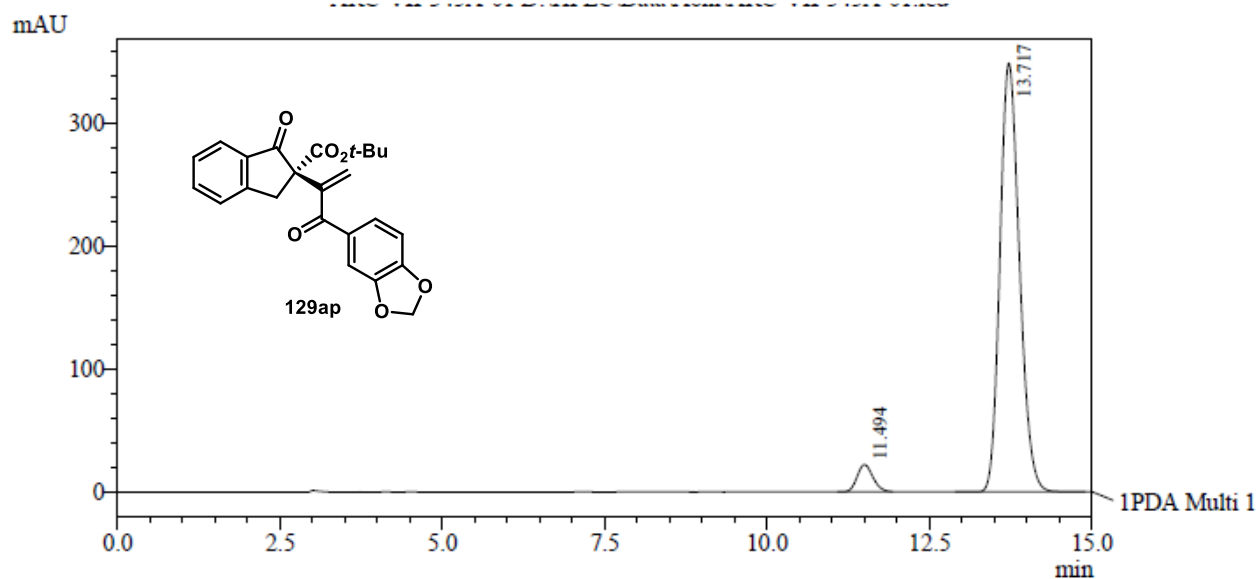
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	11.511	510522	49.588
2	13.760	518998	50.412
Total		1029520	100.000

Daicel Chiralpak AD-H column (*n*-Hexane/IPA = 90:10, 1.0 mL min⁻¹, 20 °C, 254 nm)

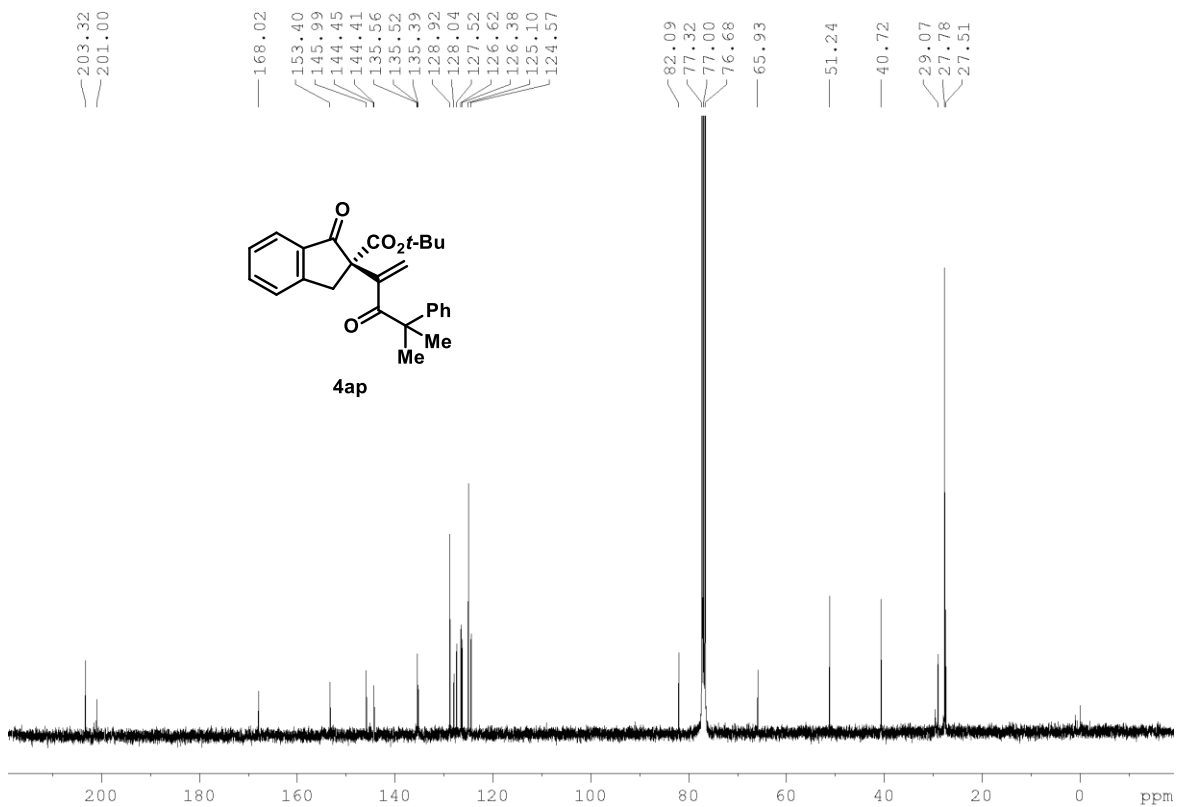
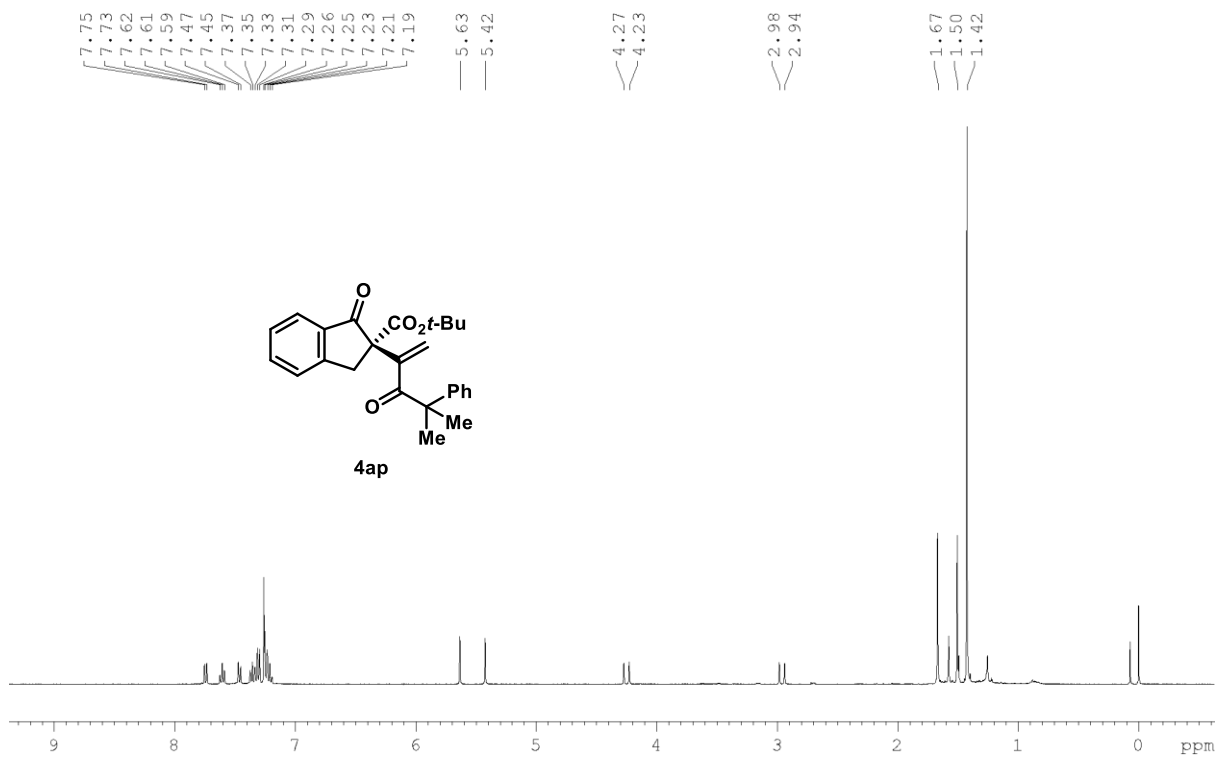


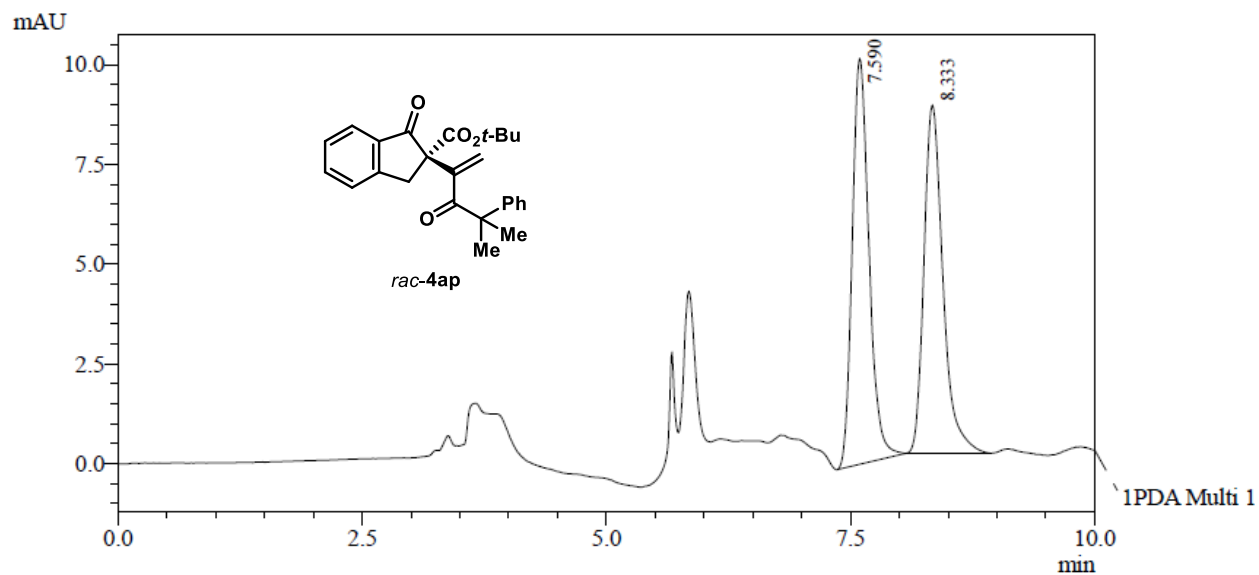
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	11.494	373385	4.858
2	13.717	7311850	95.142
Total		7685236	100.000





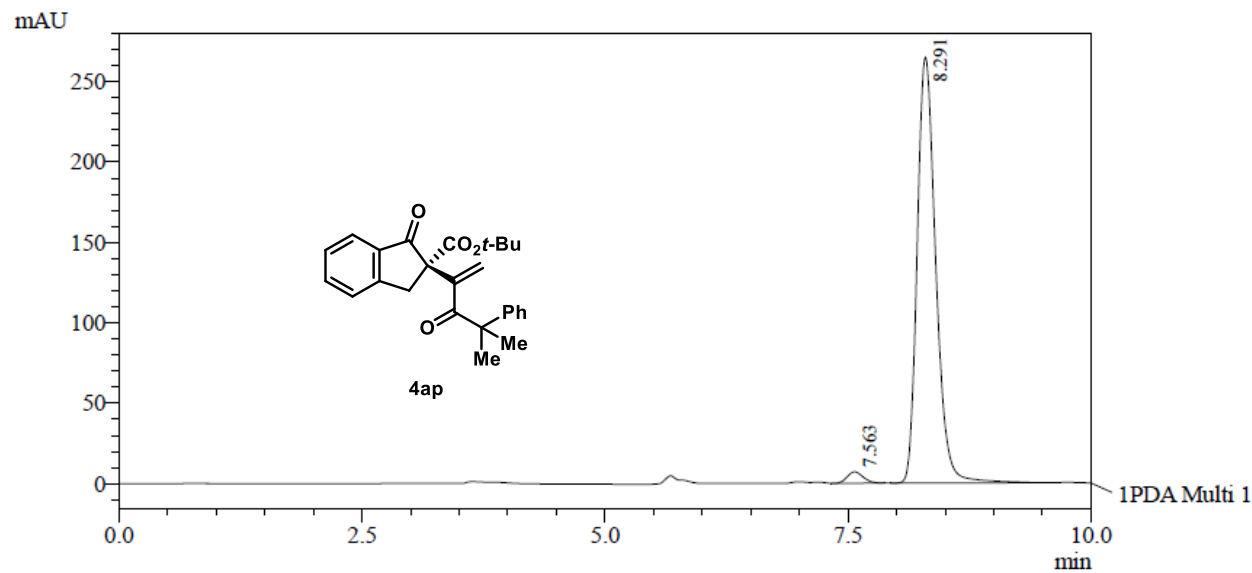
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	7.590	121248	50.658
2	8.333	118097	49.342
Total		239346	100.000

Daicel Chiralpak IE column (*n*-Hexane/EtOH = 95:5, 1.0 mL min⁻¹, 20 °C, 254 nm)

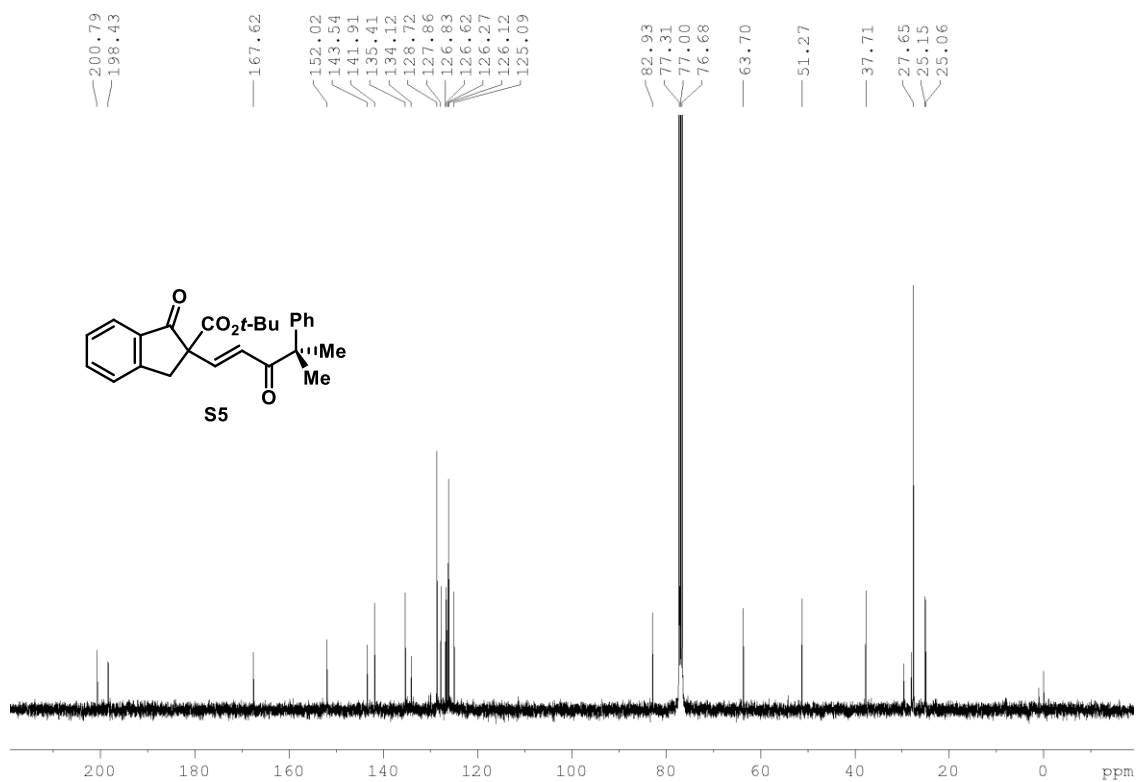
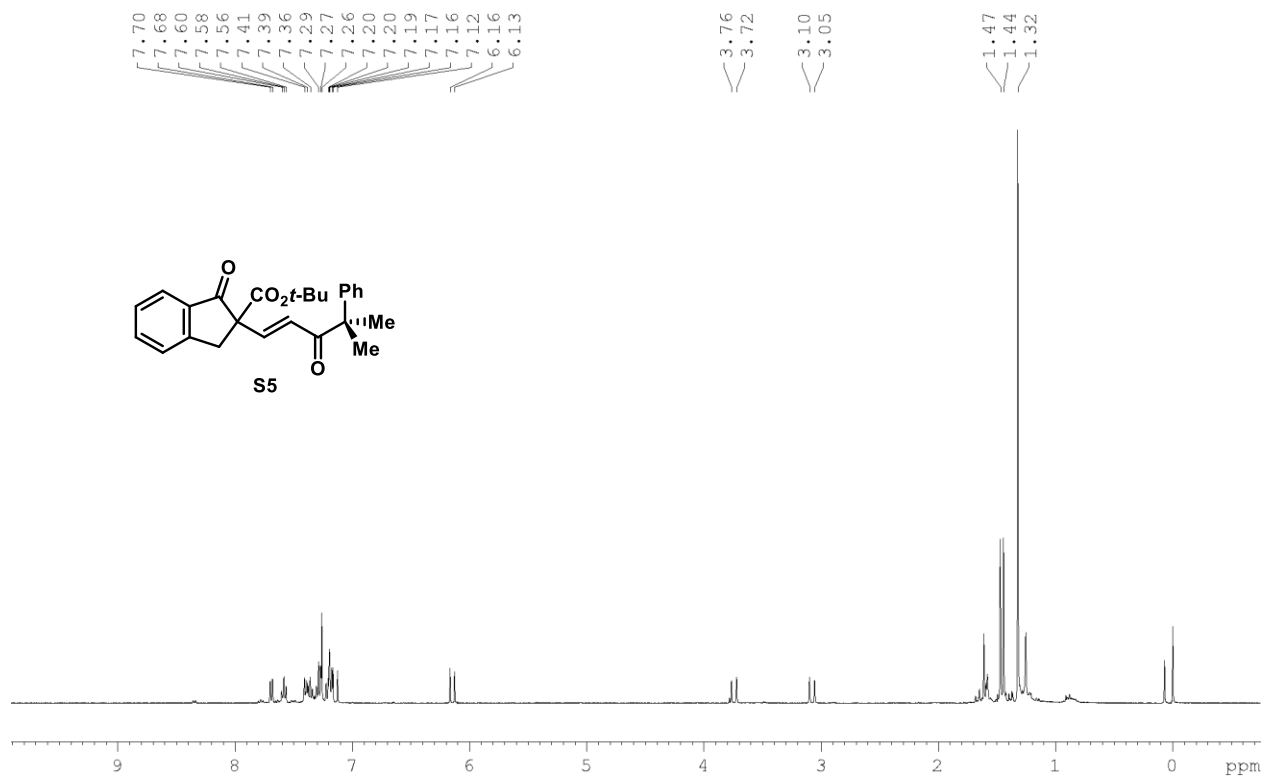


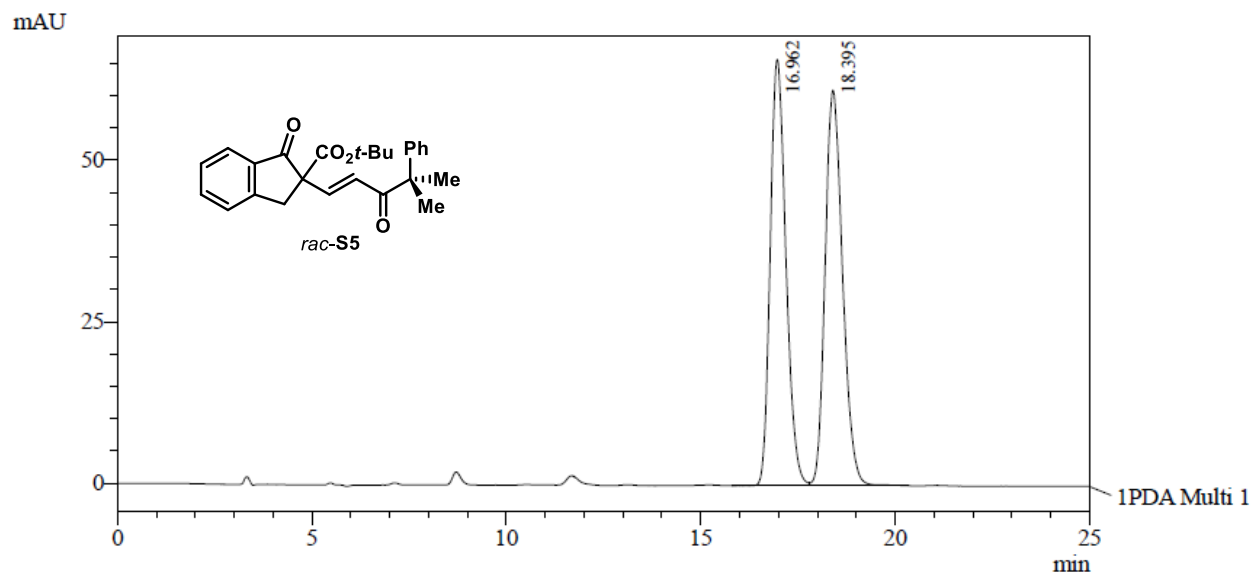
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	7.563	80982	2.250
2	8.291	3517655	97.750
Total		3598636	100.000





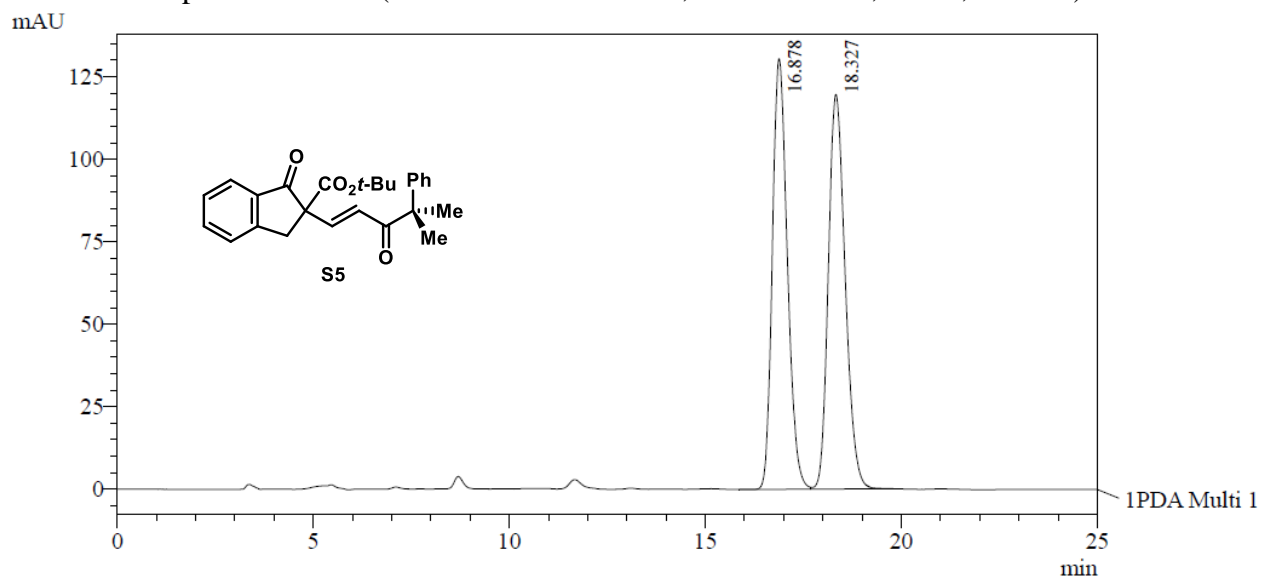
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	16.962	1851722	49.150
2	18.395	1915808	50.850
Total		3767530	100.000

Daicel Chiralpak IE column (*n*-Hexane/IPA = 90:10, 1.0 mL min⁻¹, 20 °C, 254 nm)

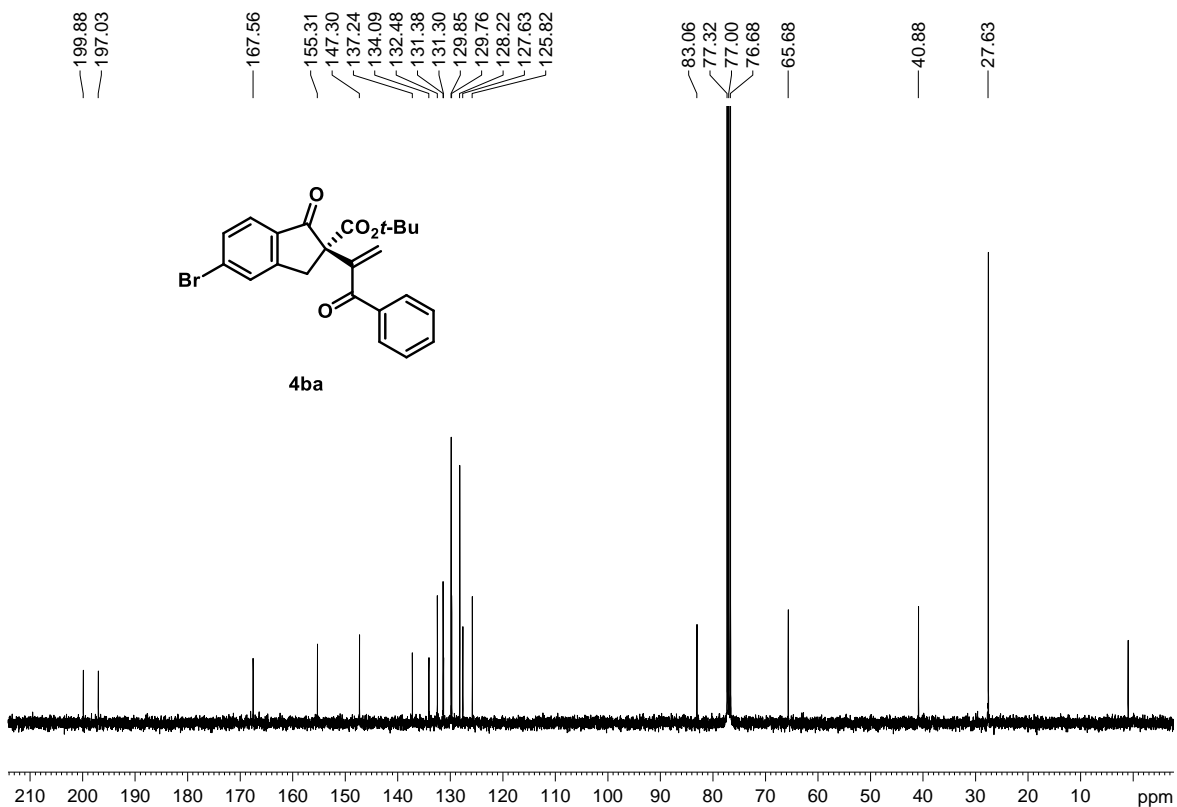
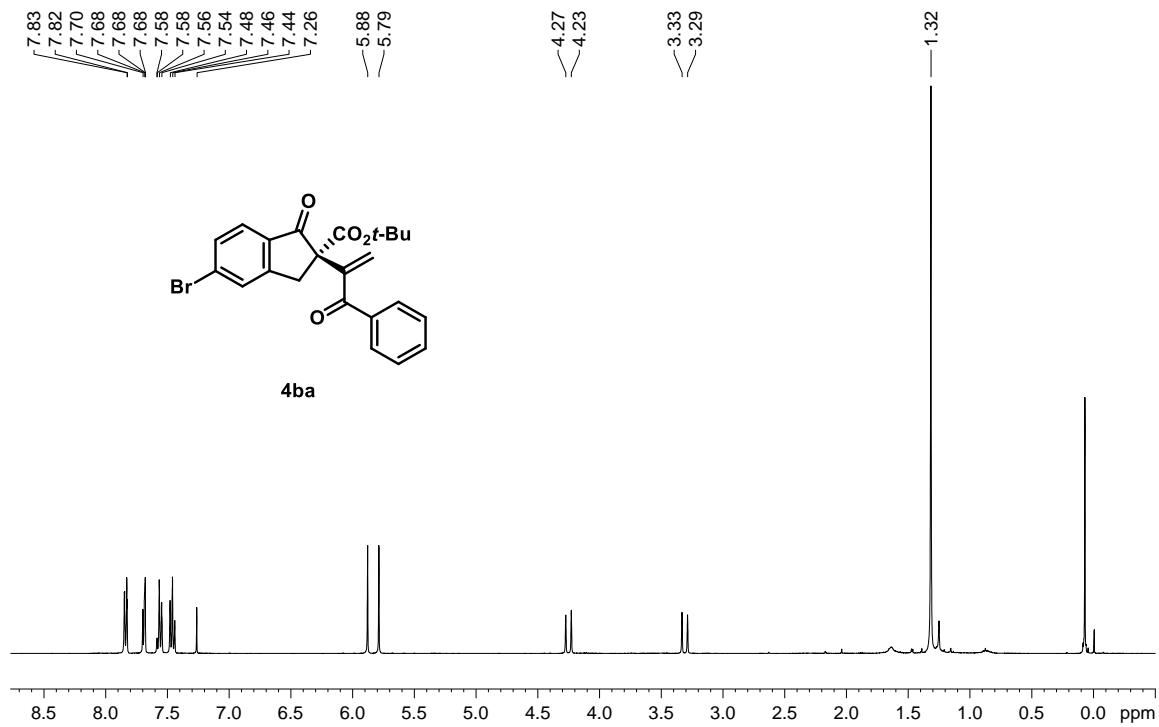


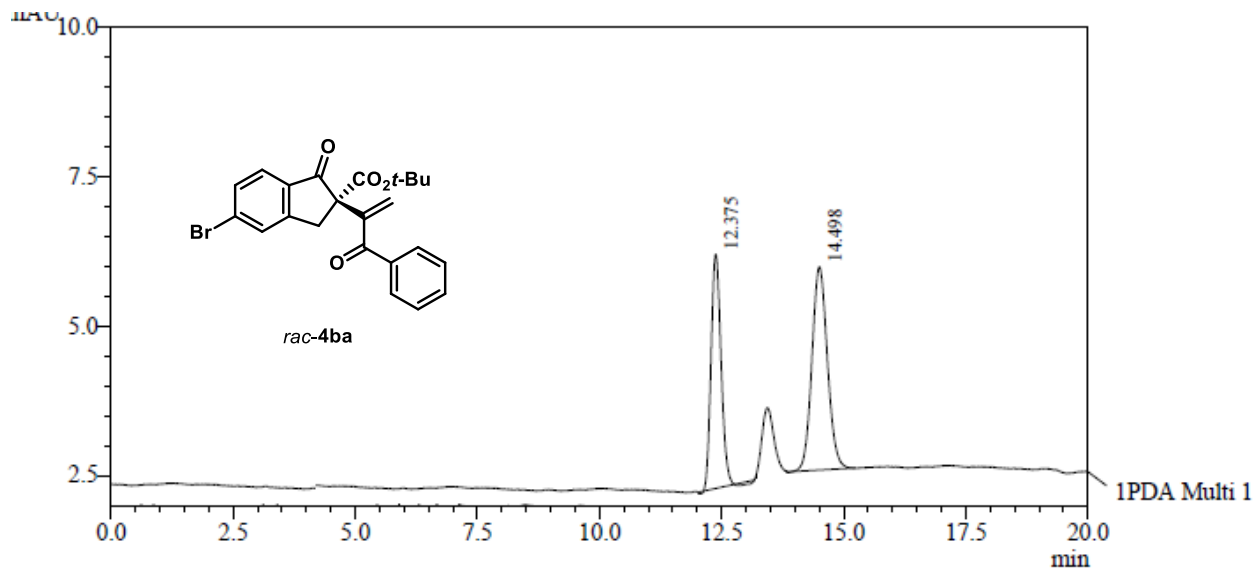
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	16.878	3470845	49.229
2	18.327	3579552	50.771
Total		7050398	100.000





1 PDA Multi 1 / 254nm 4nm

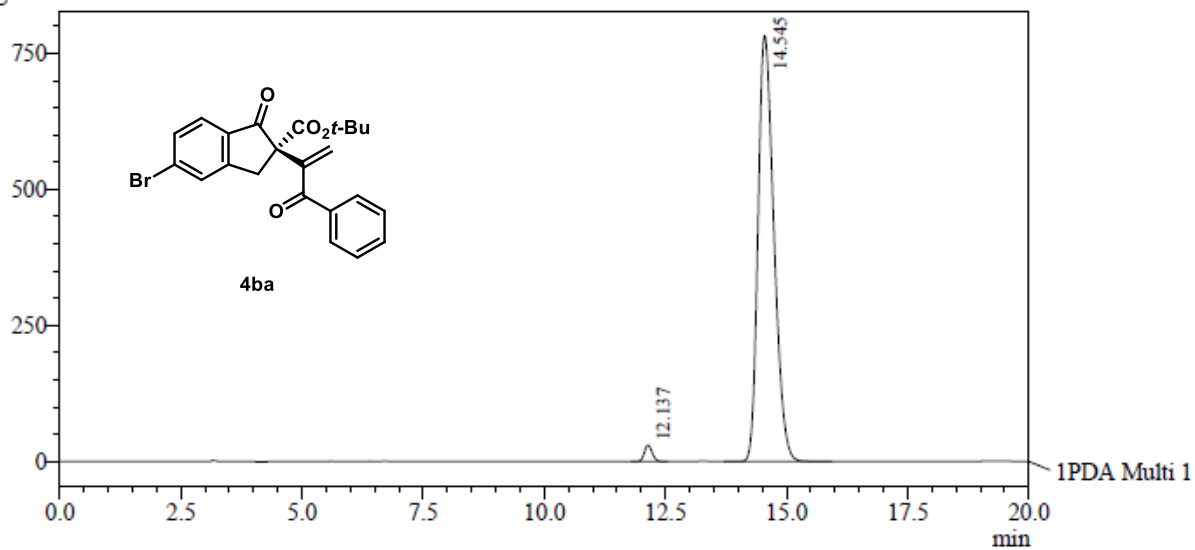
PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	12.375	75403	50.113
2	14.498	75063	49.887
Total		150466	100.000

Daicel Chiralpak AD-H column (*n*-Hexane/EtOH = 95:5, 1.0 mL min⁻¹, 20 °C, 254 nm)

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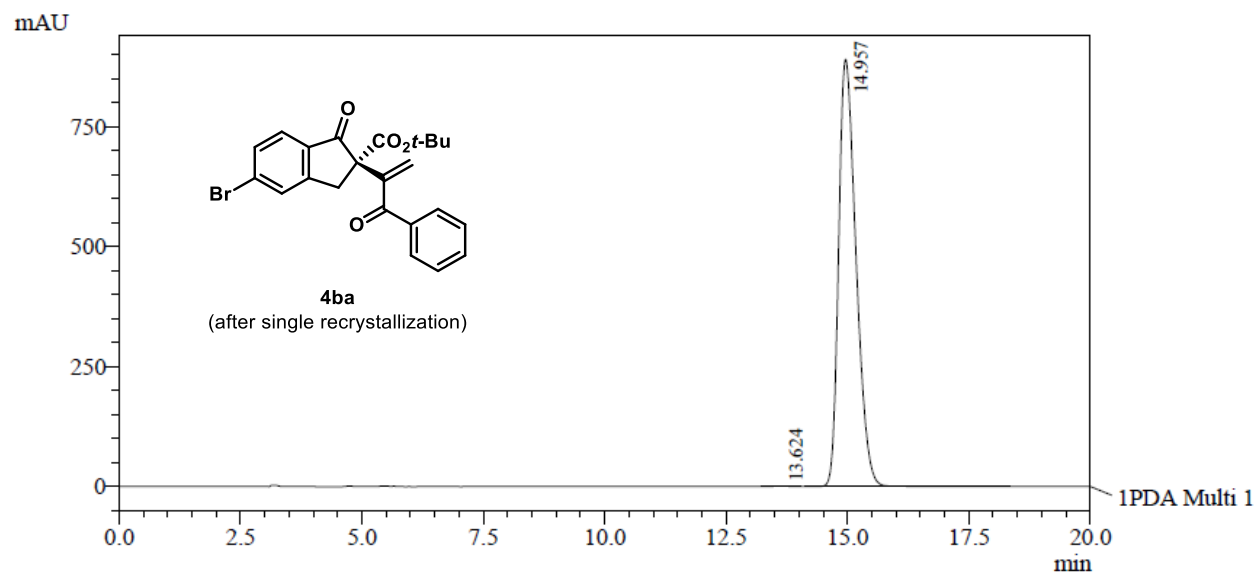


1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	12.137	341963	1.882
2	14.545	17827076	98.118
Total		18169039	100.000

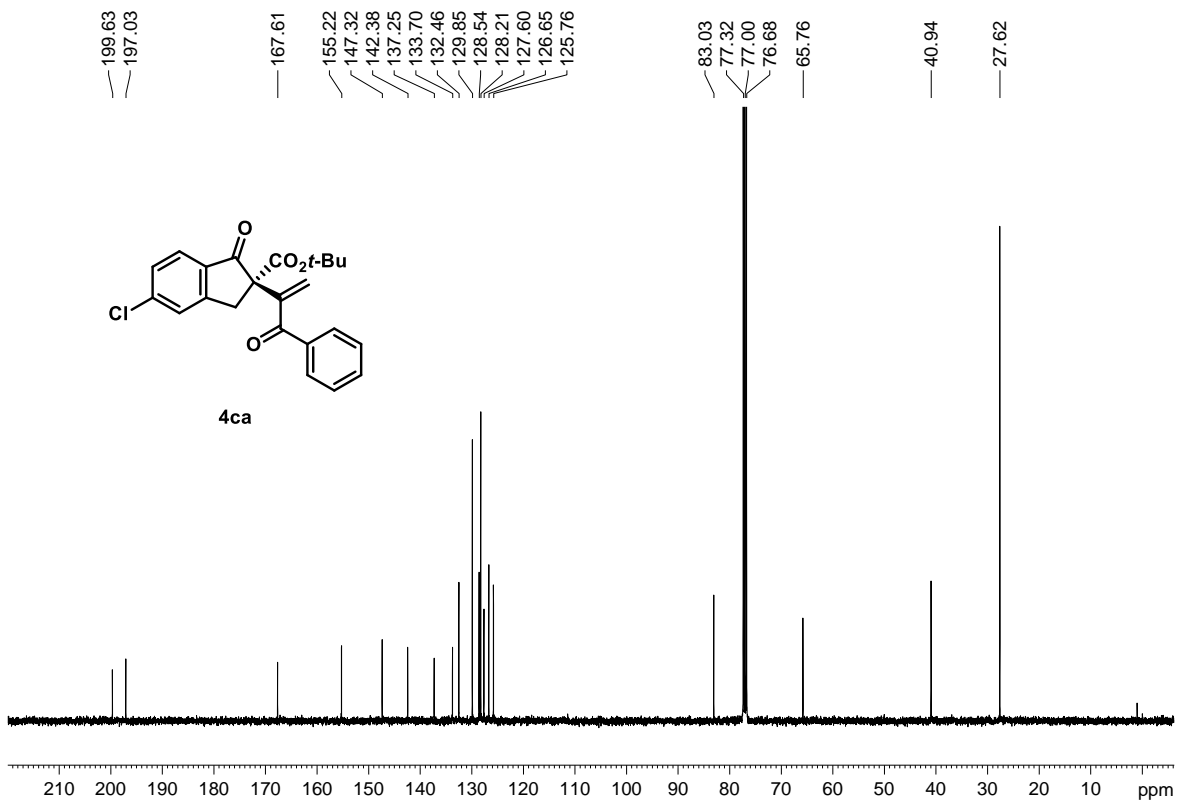
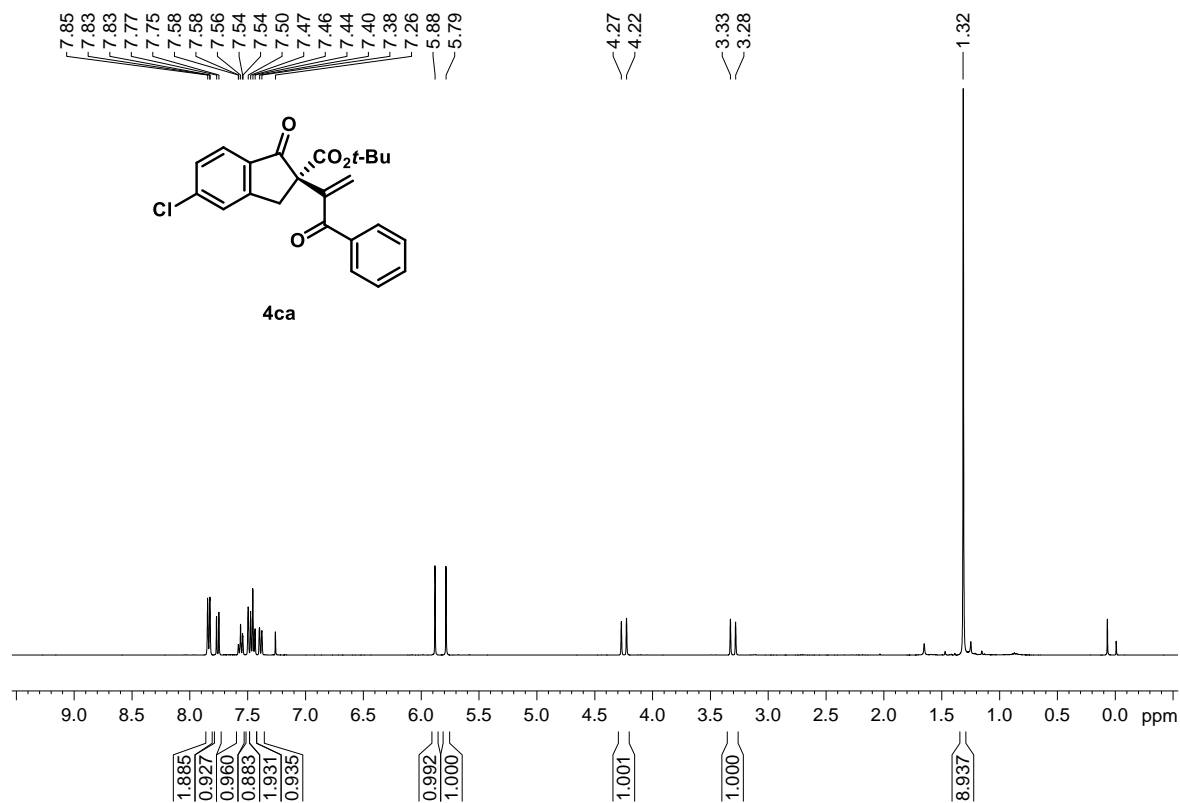


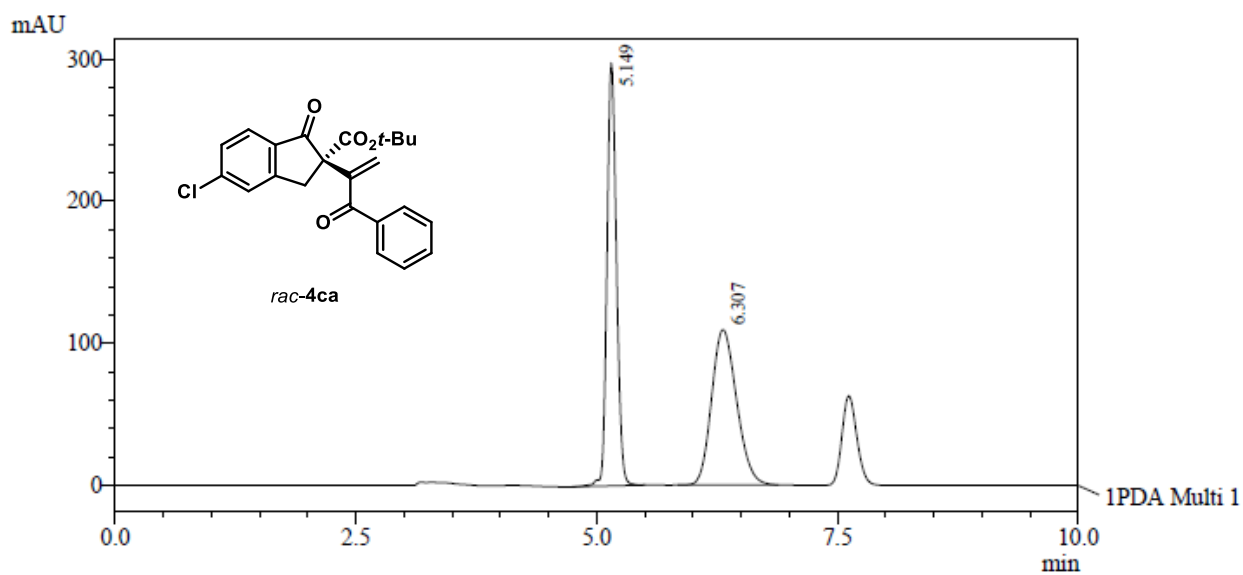
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	13.624	17545	0.079
2	14.957	22132168	99.921
Total		22149713	100.000





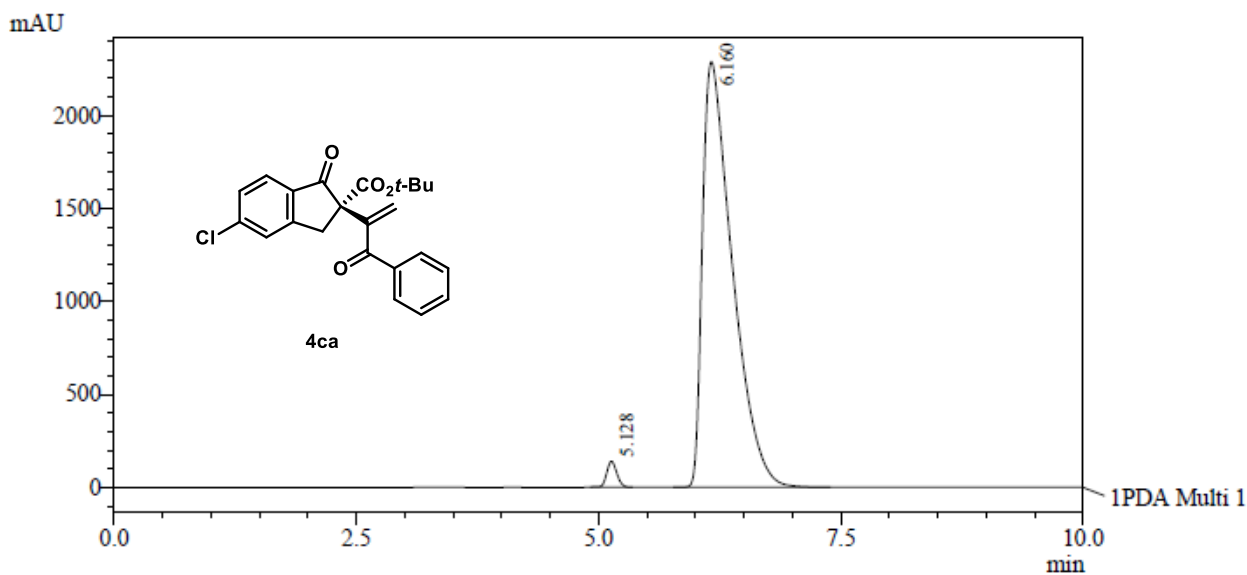
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.149	2040003	50.811
2	6.307	1974901	49.189
Total		4014904	100.000

Daicel Chiralpak AS-H column (*n*-Hexane/EtOH = 95:5, 1.0 mL min⁻¹, 20 °C, 254 nm)

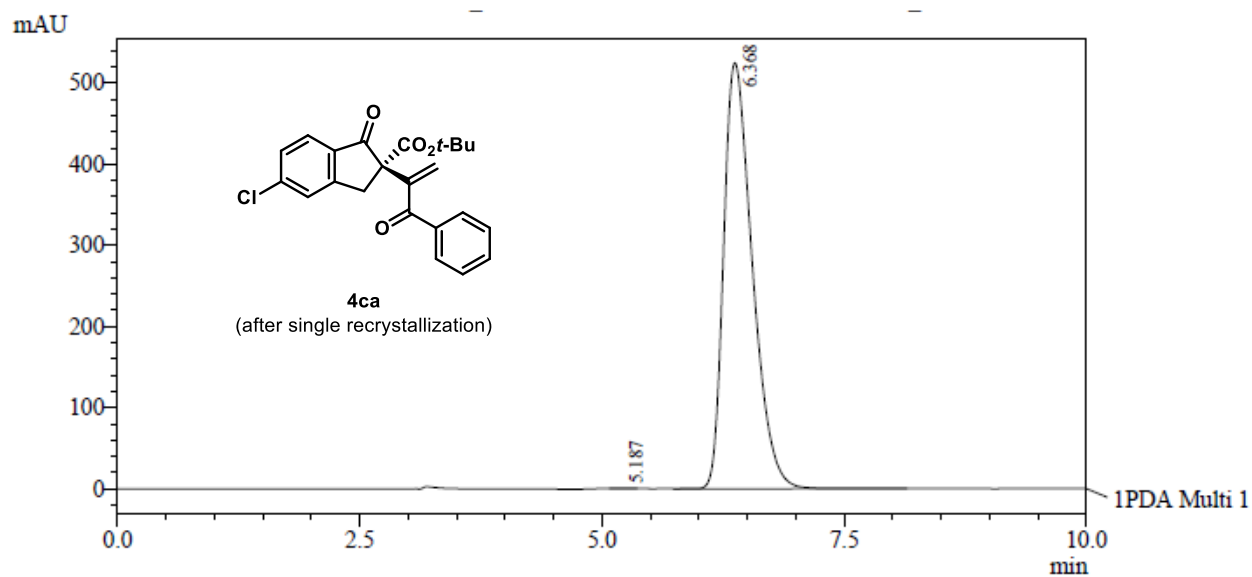


1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

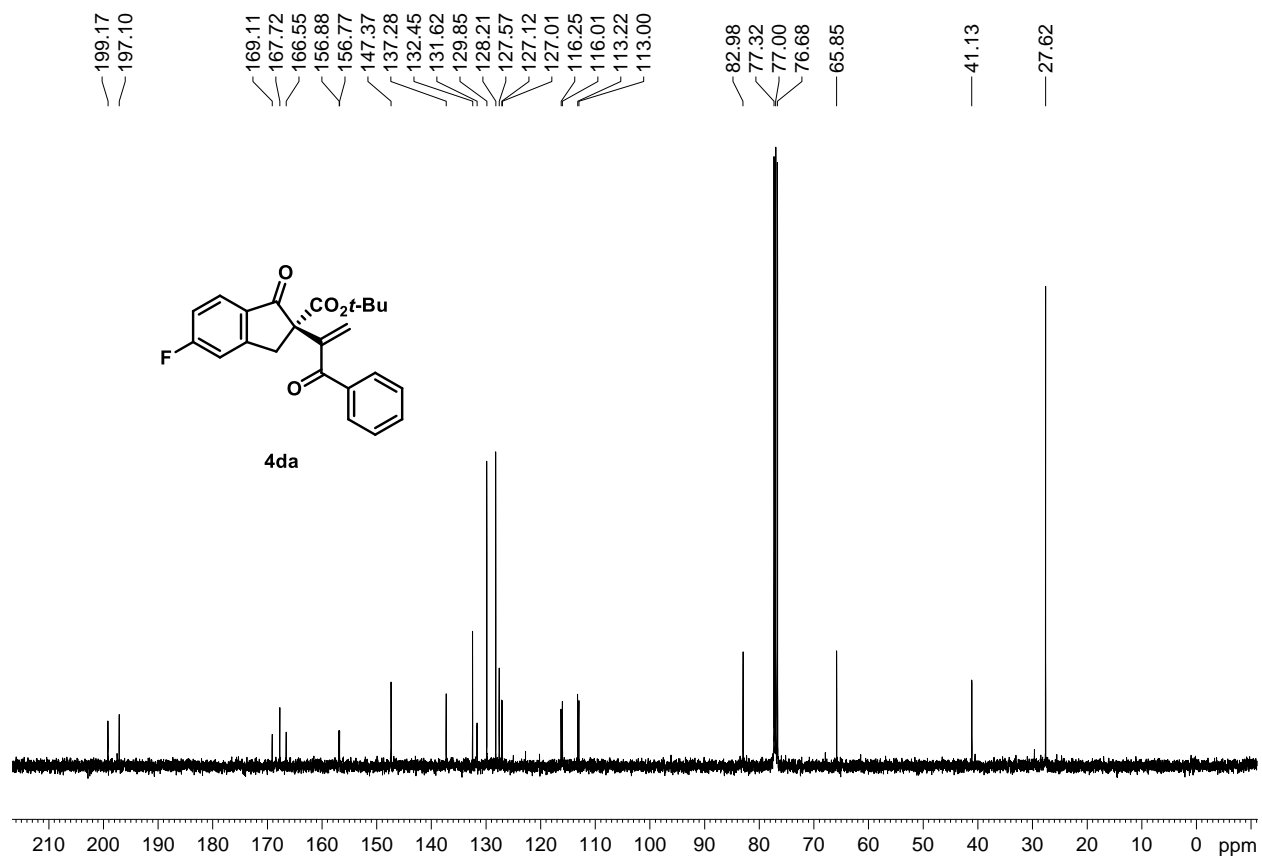
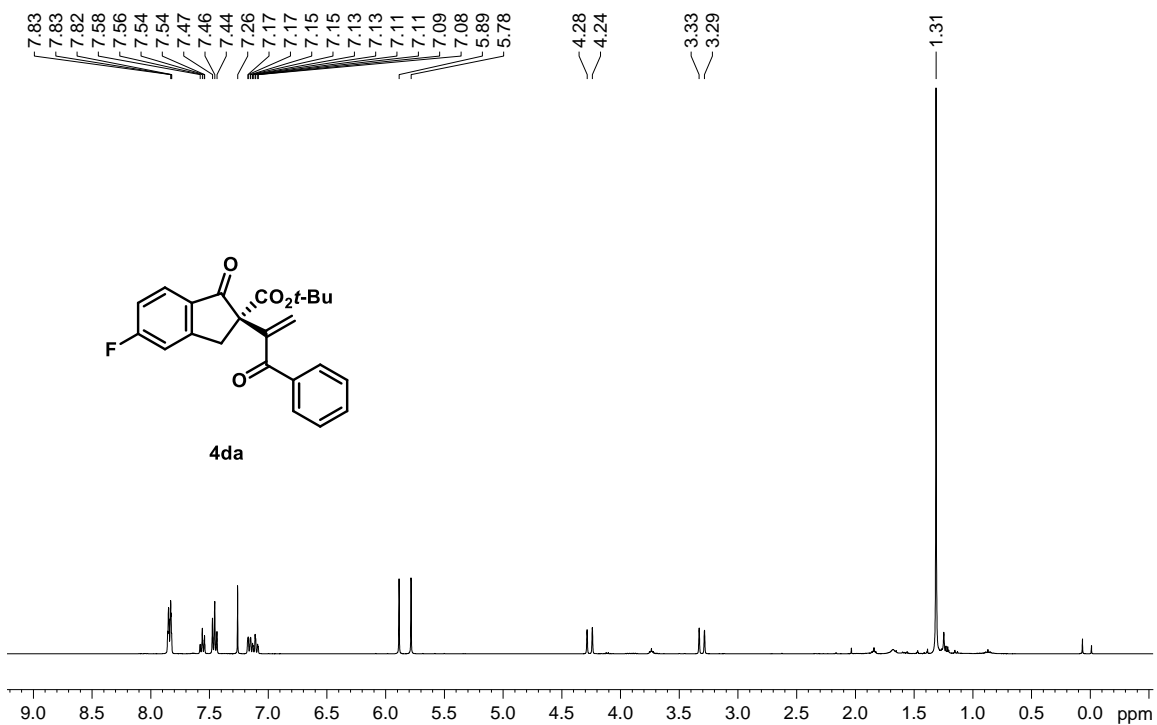
Peak#	Ret. Time	Area	Area %
1	5.128	1006629	2.006
2	6.160	49174146	97.994
Total		50180775	100.000

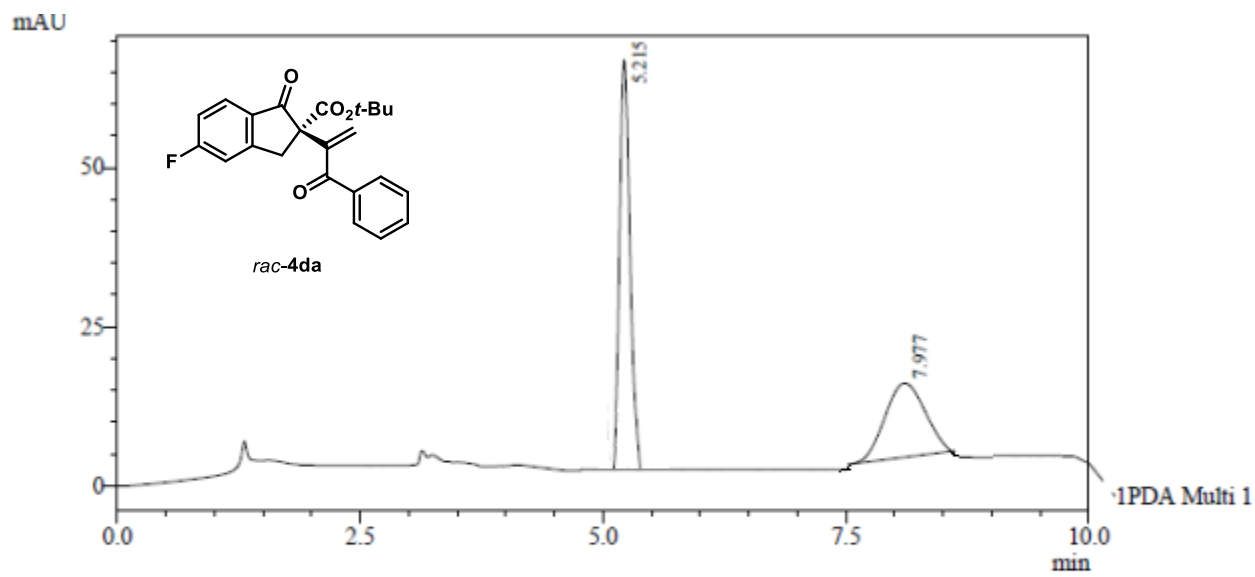


PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.187	3023	0.028
2	6.368	10781915	99.972
Total		10784938	100.000





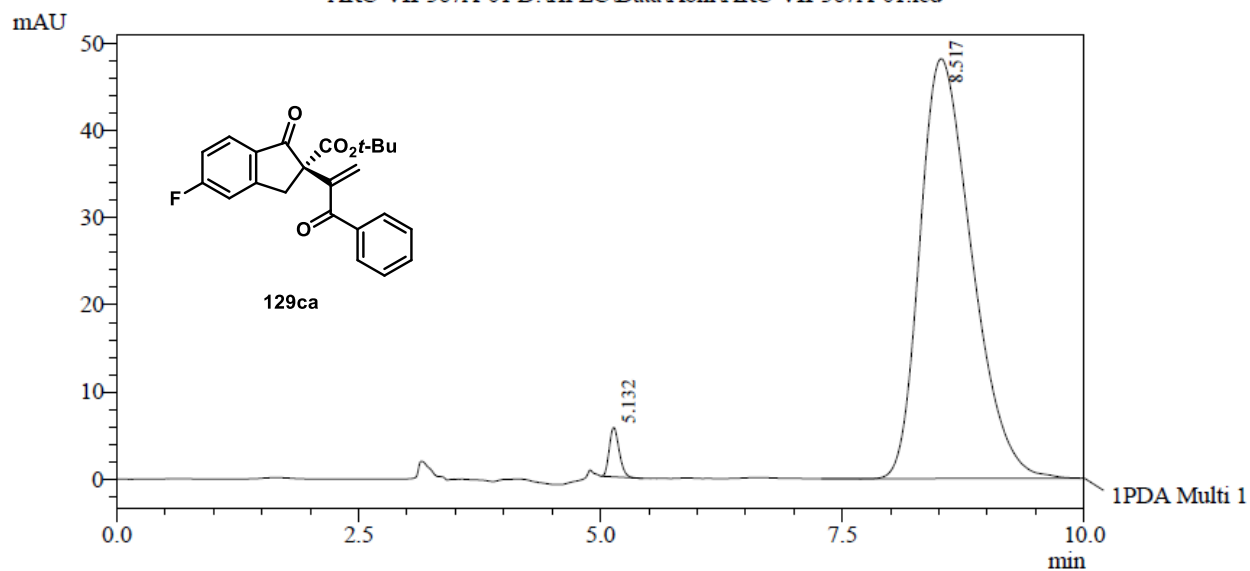
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.215	370735	52.609
2	7.977	333961	47.391
Total		704696	100.000

Daicel Chiralpak AS-H column (*n*-Hexane/EtOH = 95:5, 1.0 mL min⁻¹, 20 °C, 254 nm)

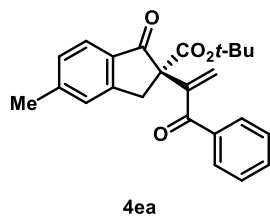
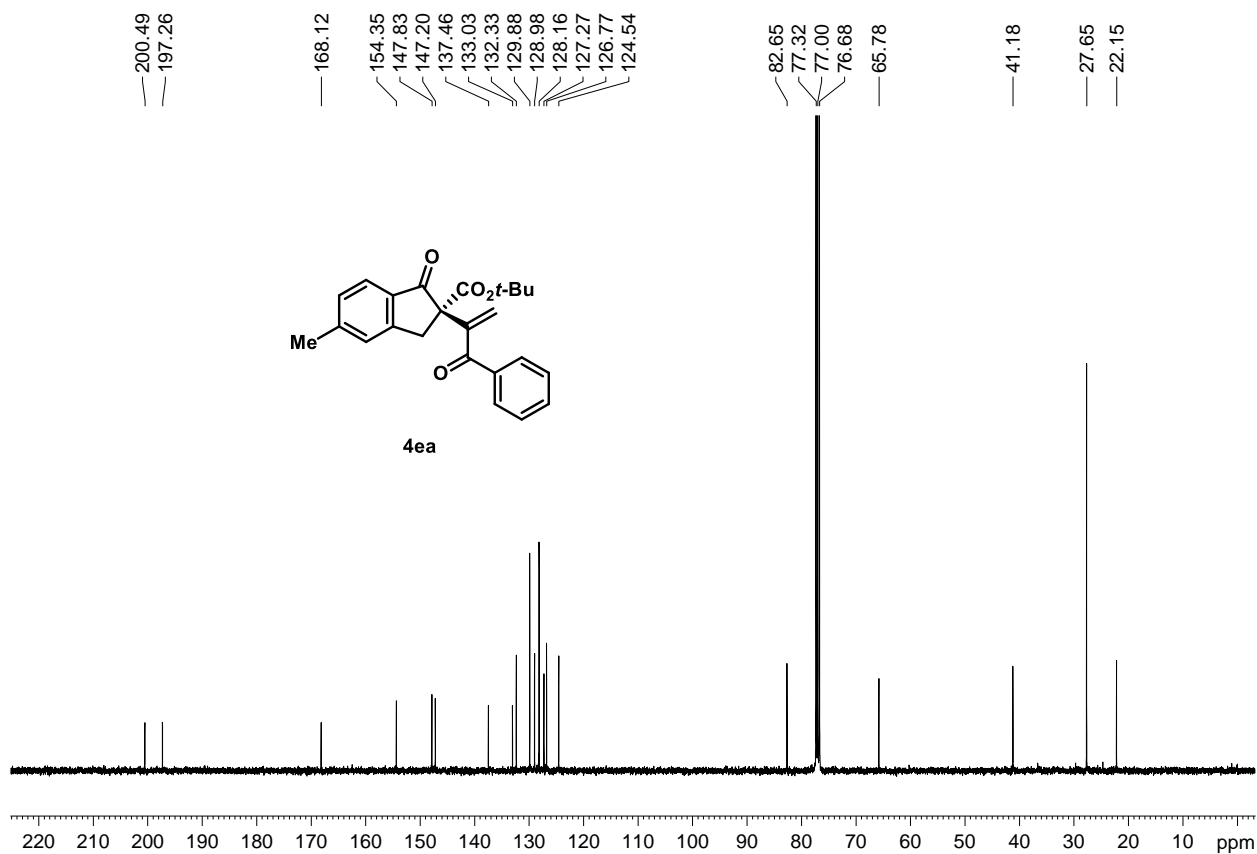
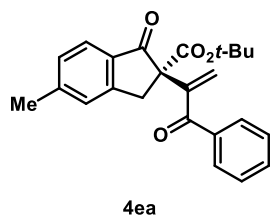
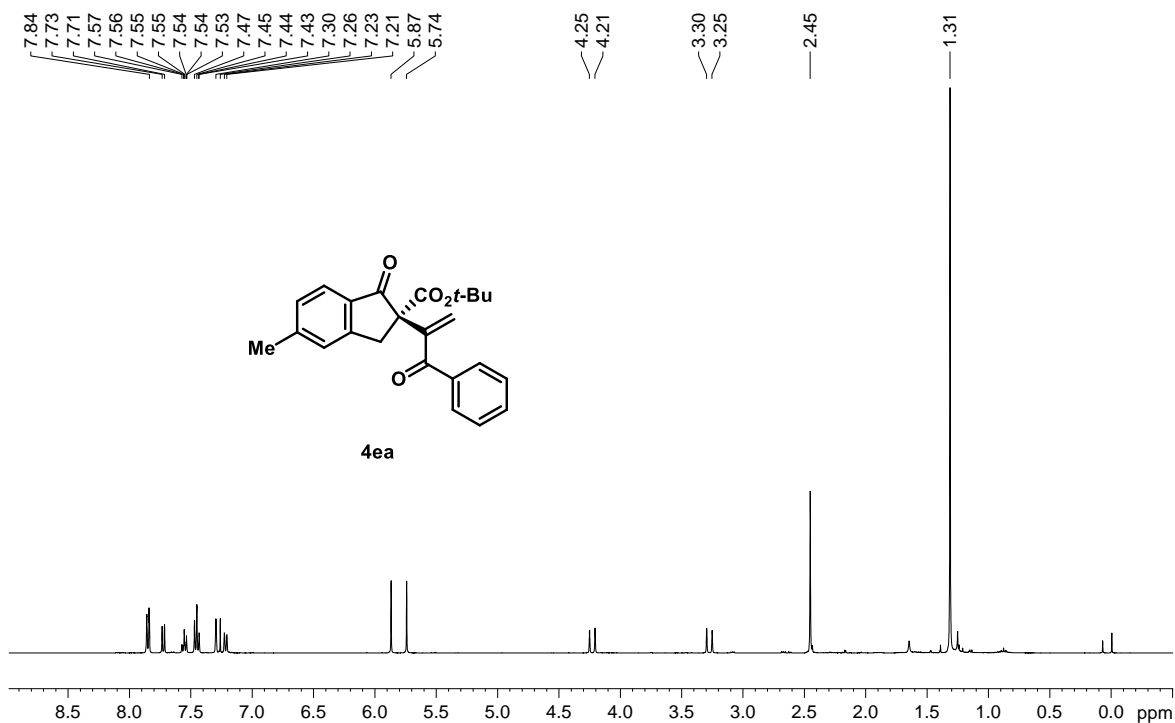


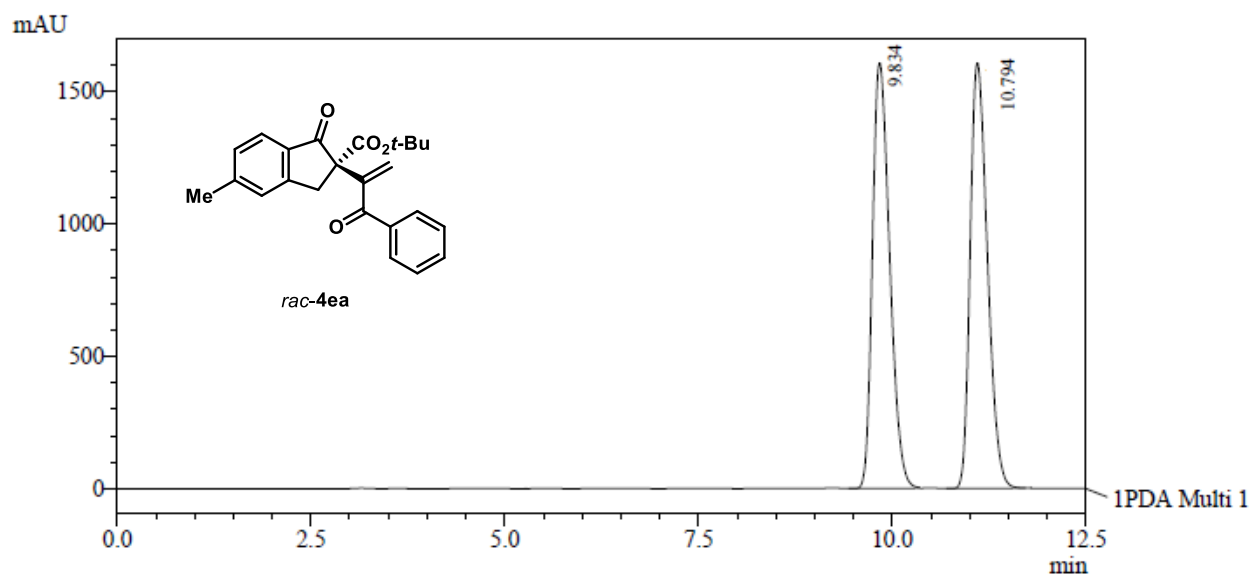
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.132	40430	2.204
2	8.517	1794205	97.796
Total		1834635	100.000





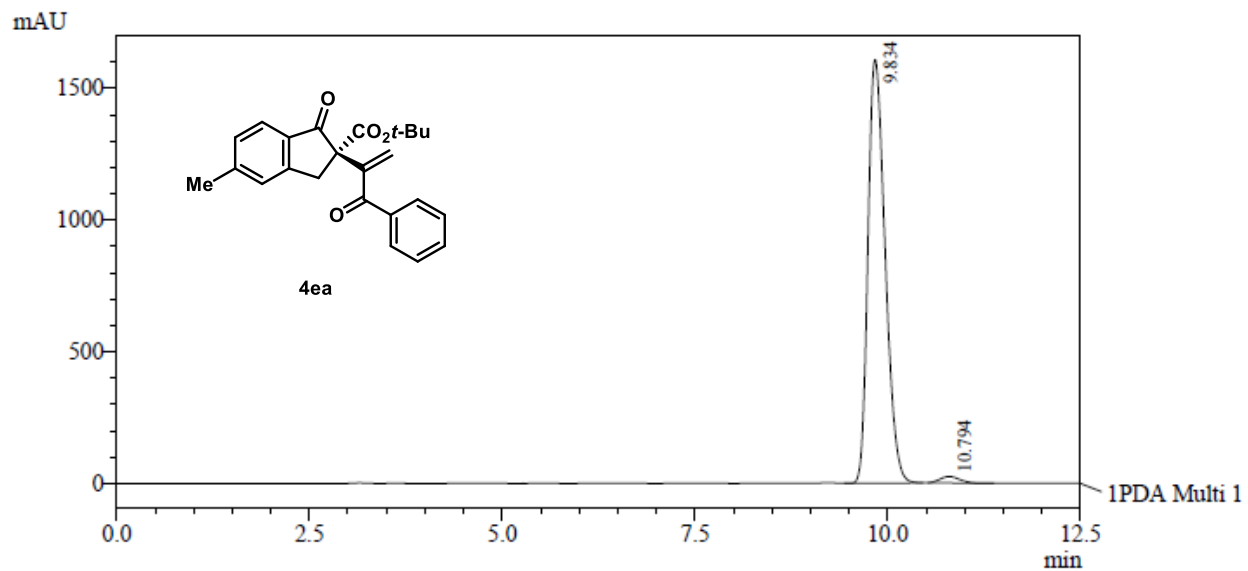
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	9.834	1540045	50.911
2	10.794	1484926	49.089
Total		3024971	100.000

Daicel Chiralpak AD-H column (*n*-Hexane/EtOH = 95:5, 1.0 mL min⁻¹, 20 °C, 254 nm)

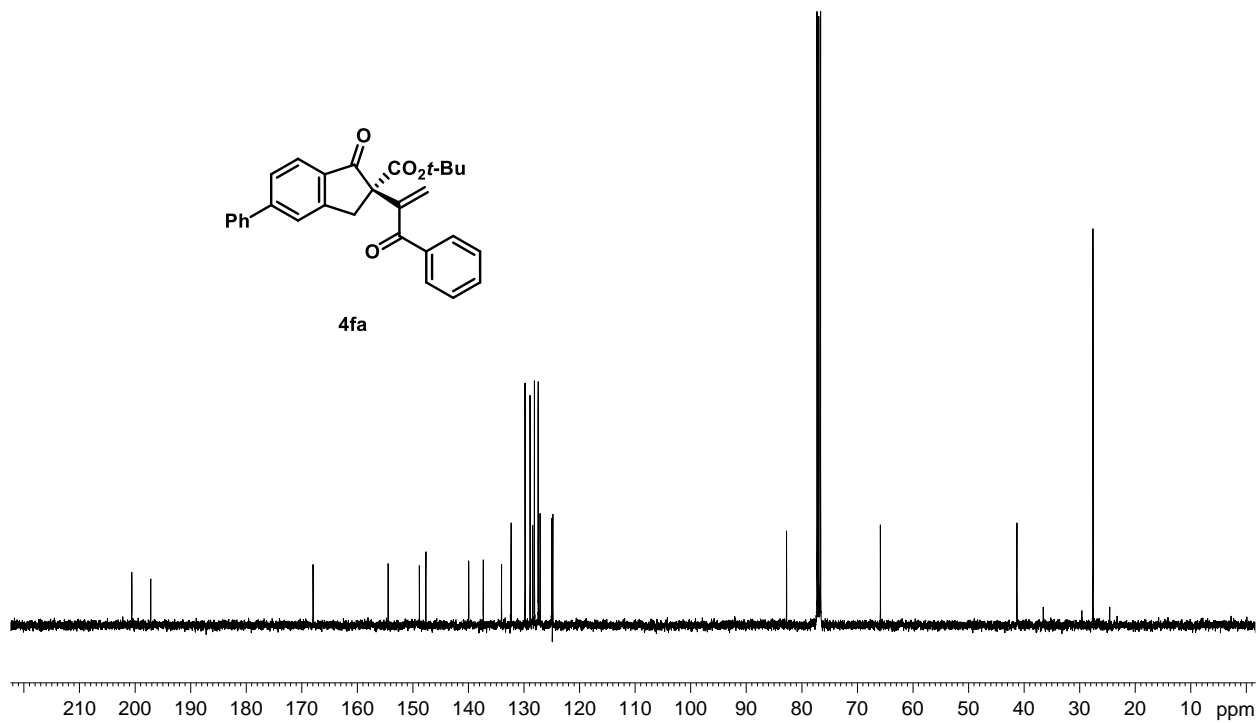
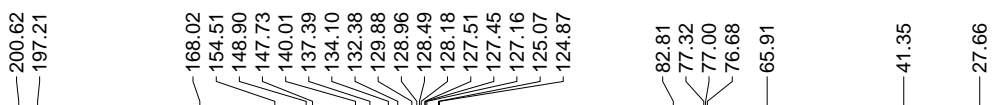
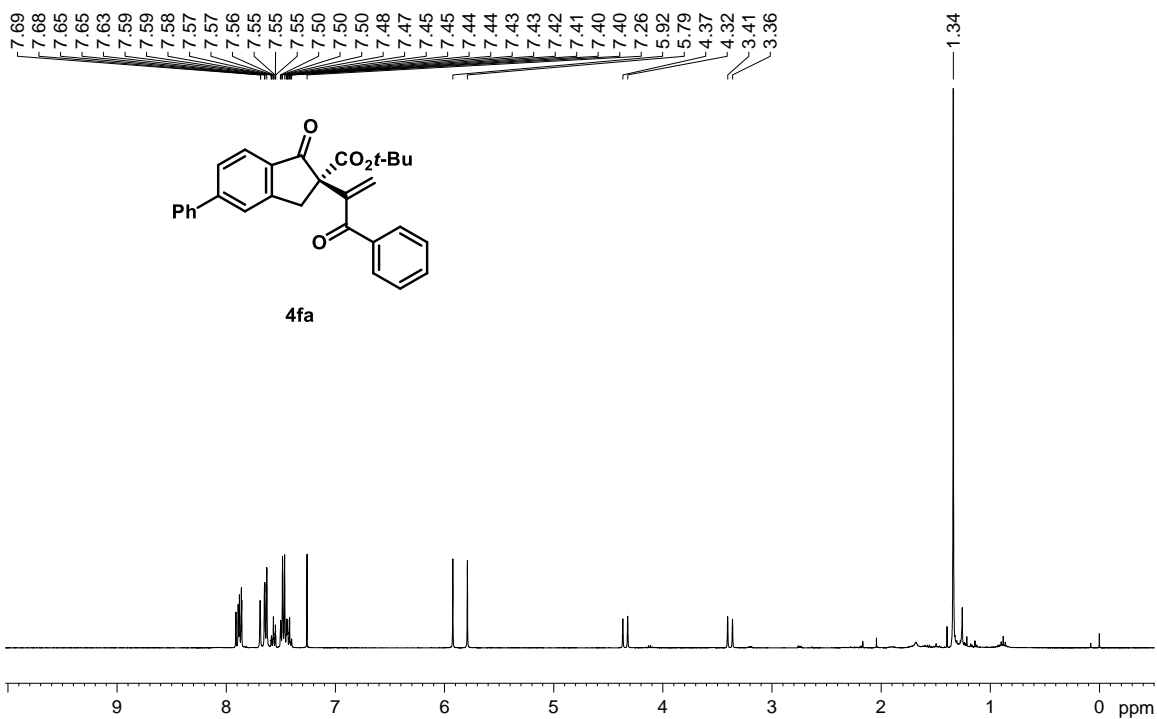


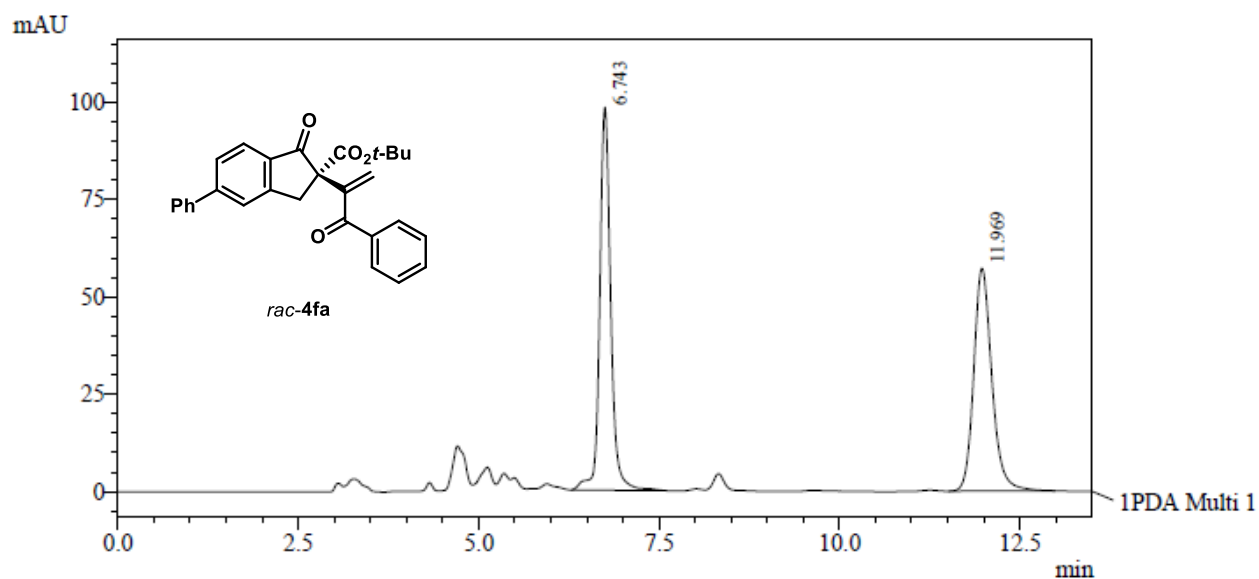
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	9.834	24879281	98.306
2	10.794	428661	1.694
Total		25307942	100.000





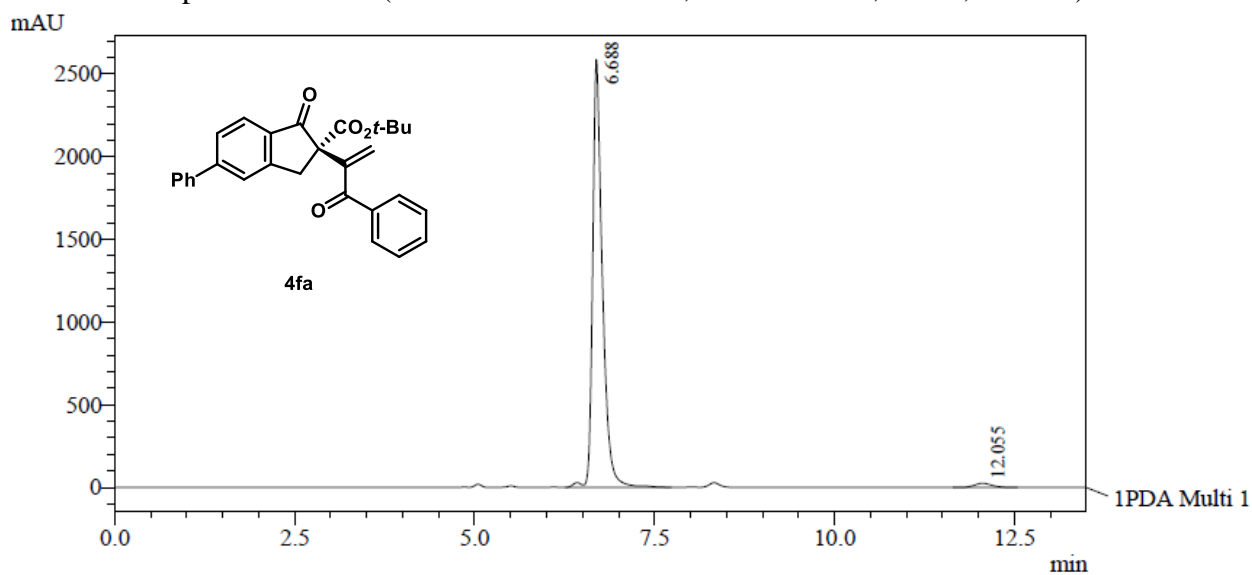
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	6.743	1042853	51.017
2	11.969	1001294	48.983
Total		2044147	100.000

Daicel Chiralpak IB column (*n*-Hexane/IPA = 90:10, 1.0 mL min⁻¹, 20 °C, 254 nm)

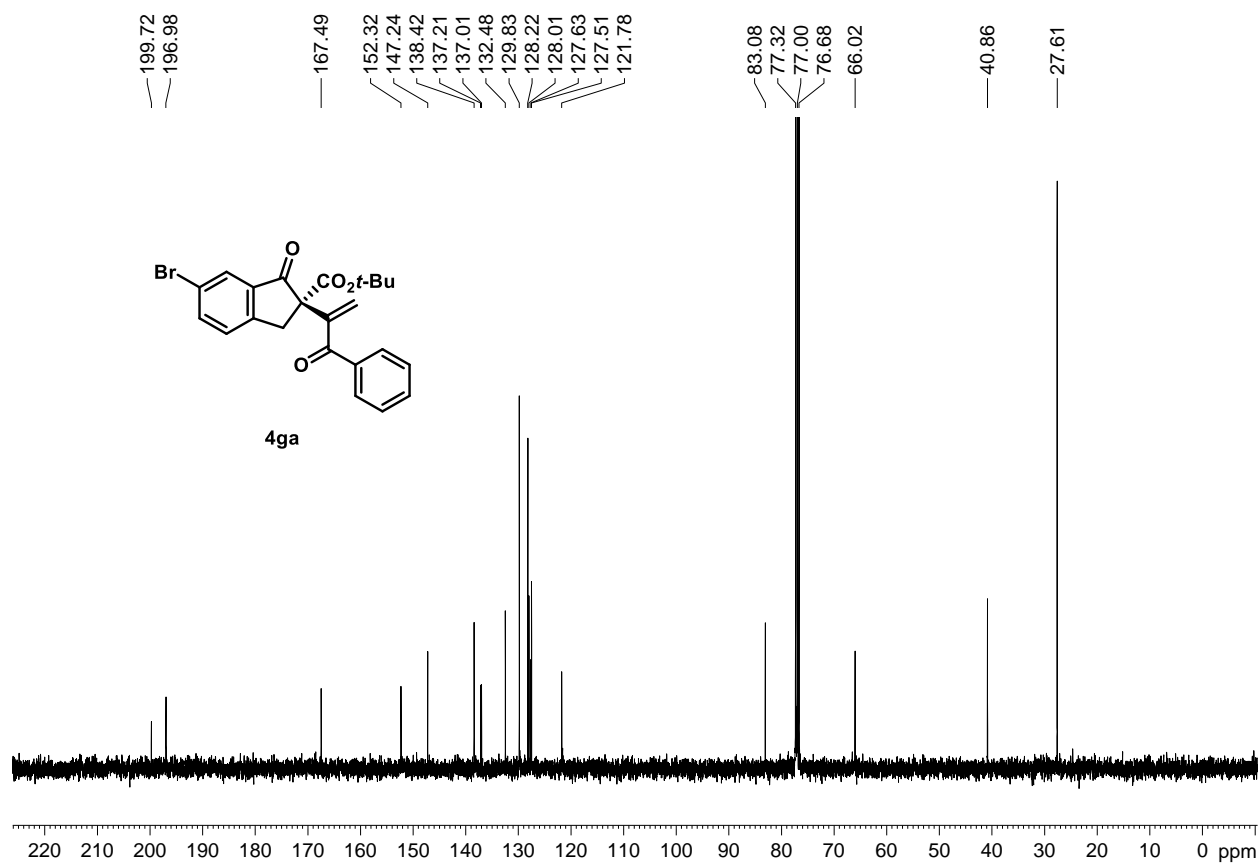
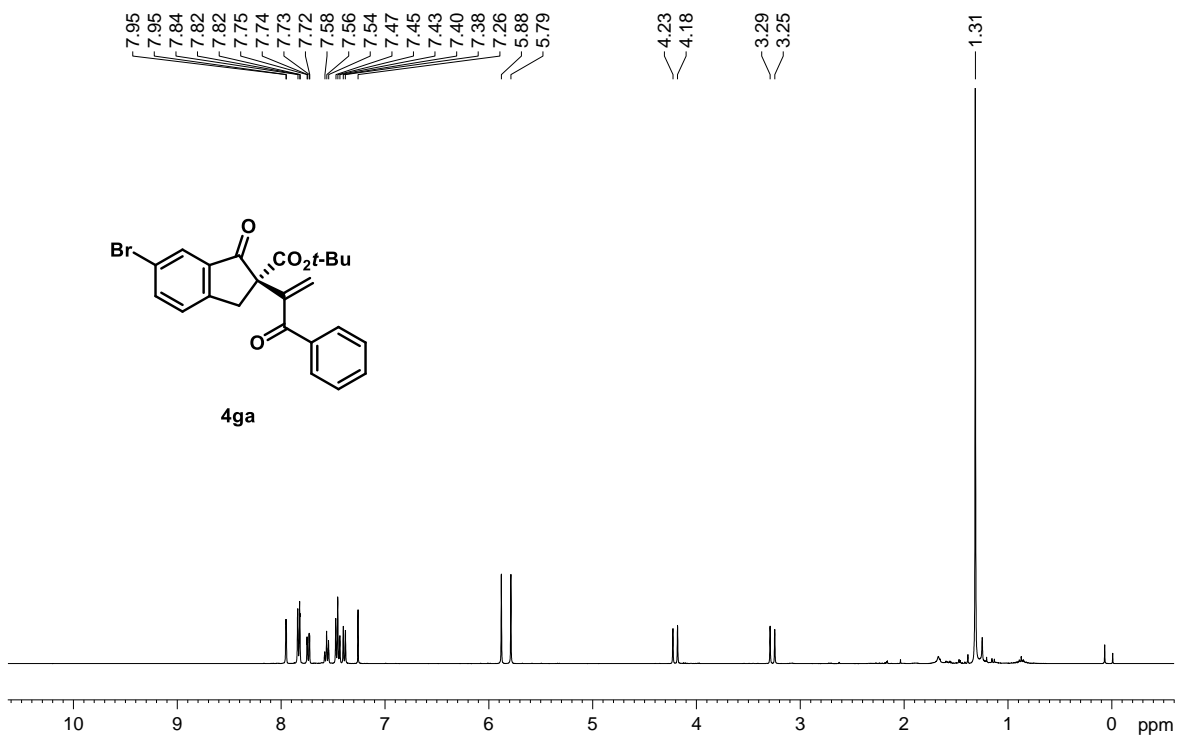


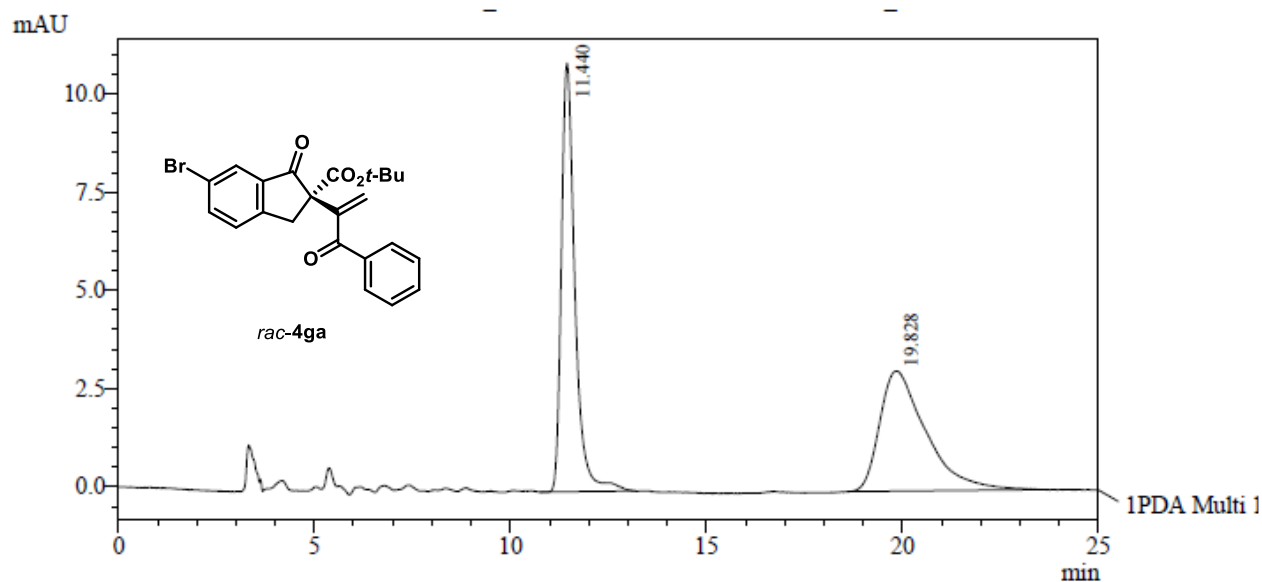
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	6.688	24367322	98.252
2	12.055	433585	1.748
Total		24800907	100.000





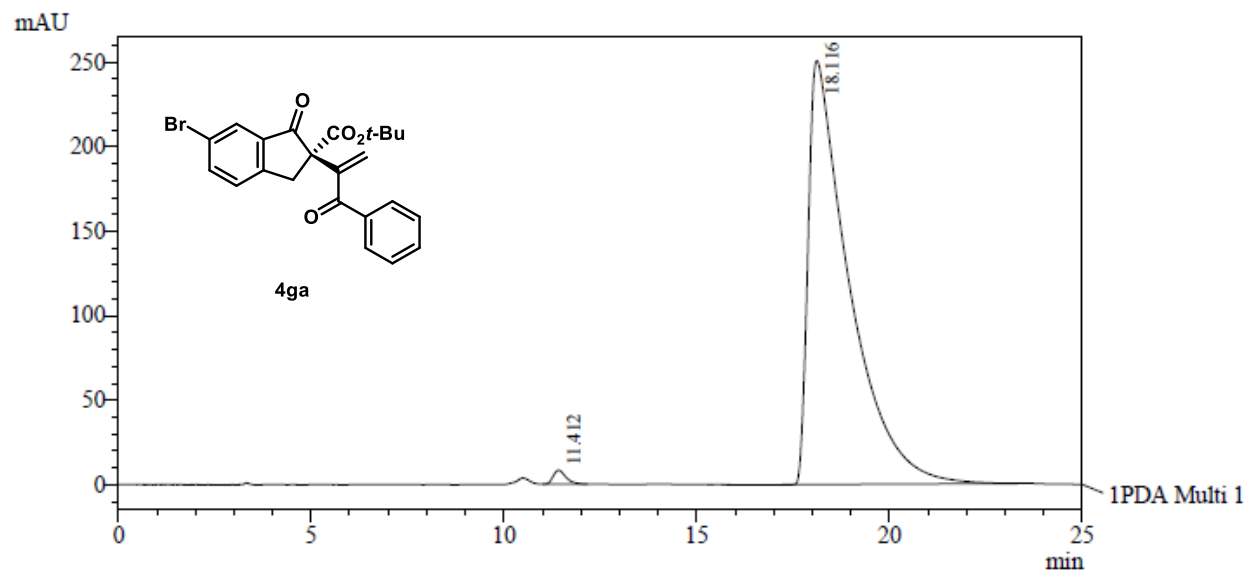
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	11.440	262086	51.166
2	19.828	250137	48.834
Total		512224	100.000

Daicel Chiralpak IE column (*n*-Hexane/IPA = 90:10, 1.0 mL min⁻¹, 20 °C, 254 nm)

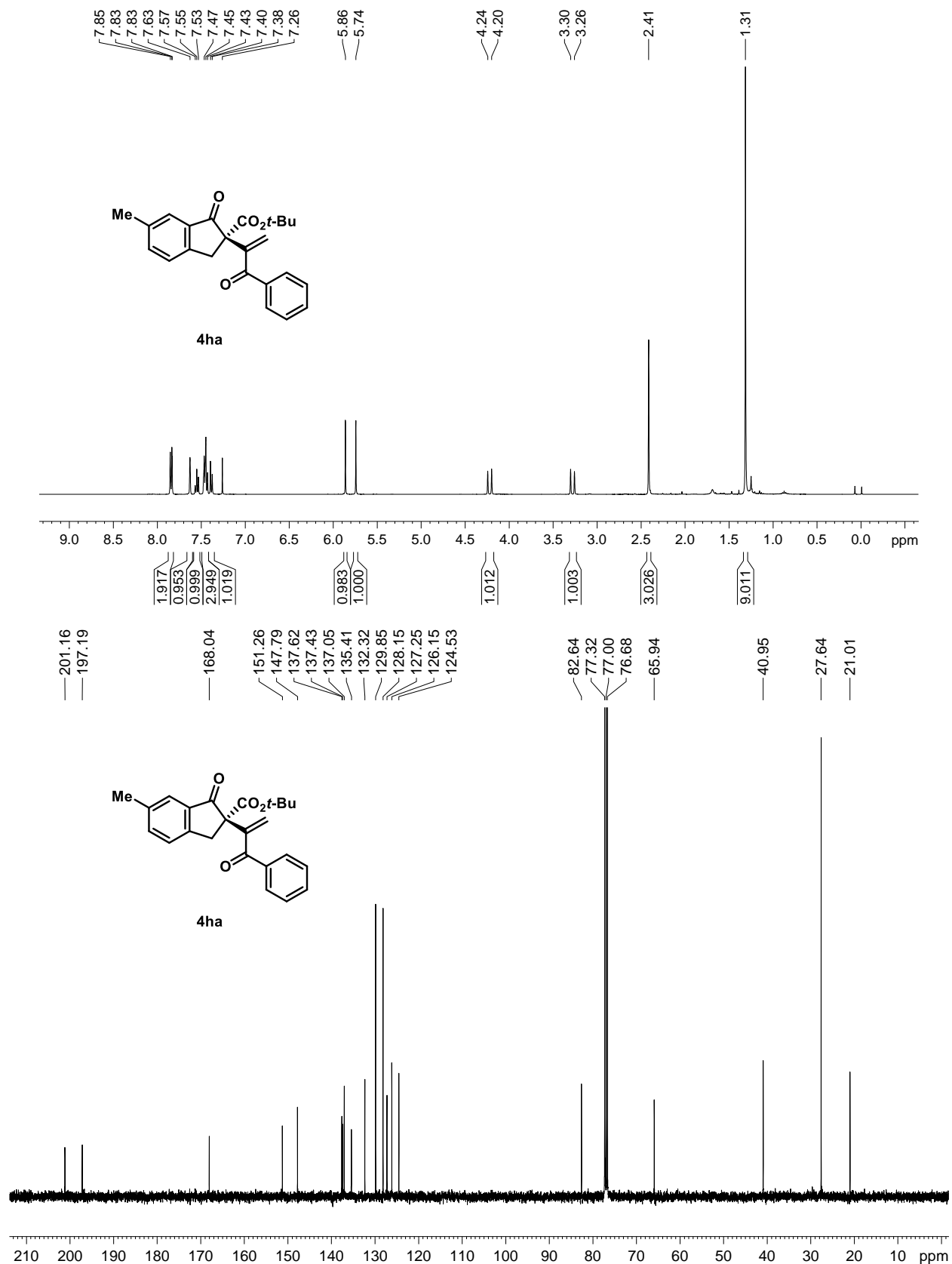


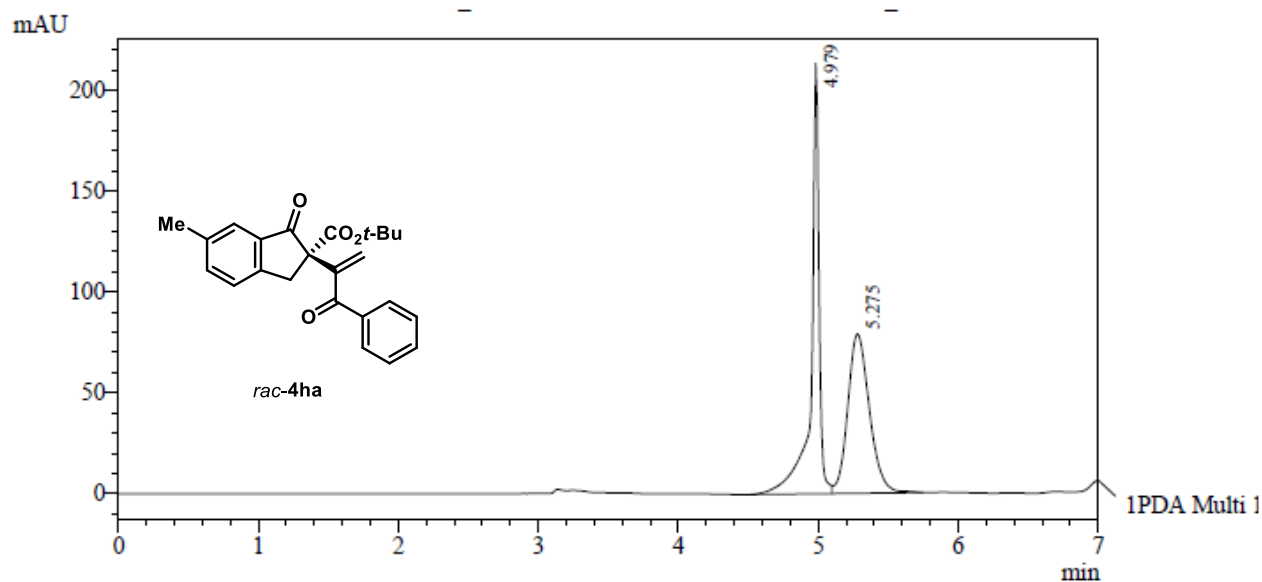
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	11.412	187942	1.006
2	18.116	18485113	98.994
Total		18673055	100.000





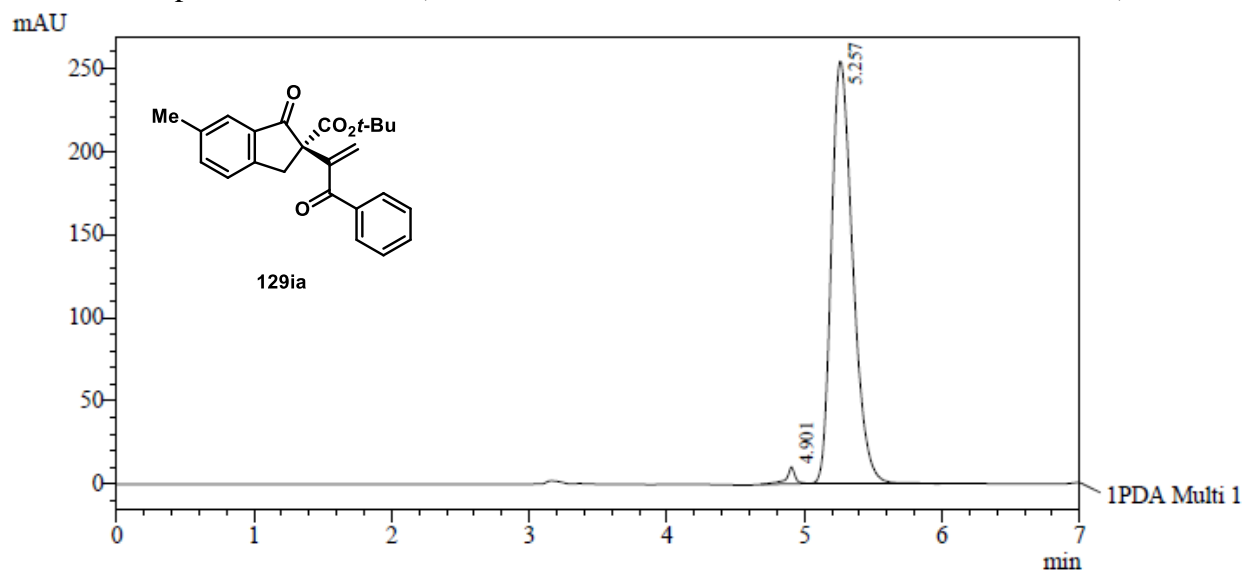
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	4.979	830728	49.407
2	5.275	850675	50.593
Total		1681404	100.000

Daicel Chiralpak AS-H column (*n*-Hexane/EtOH = 95:5, 1.0 mL min⁻¹, 20 °C, 254 nm)

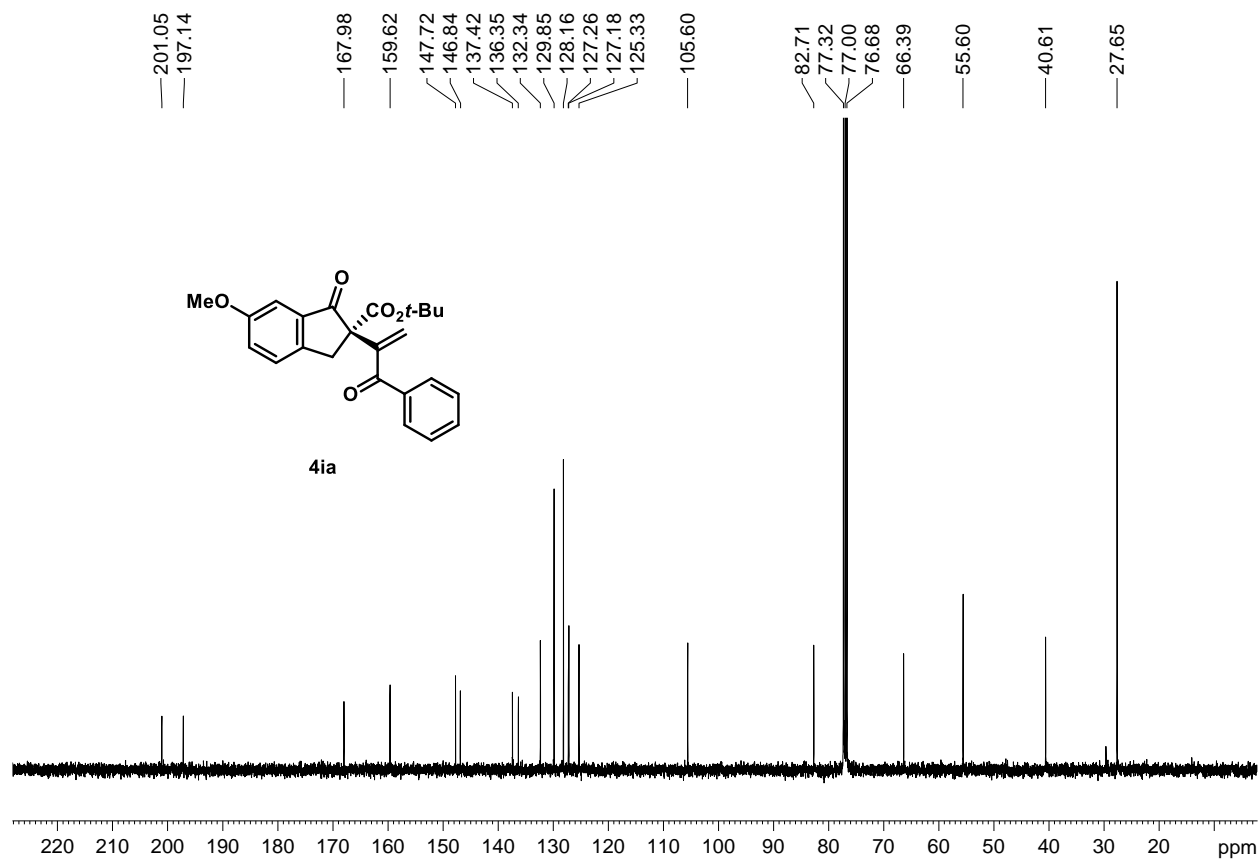
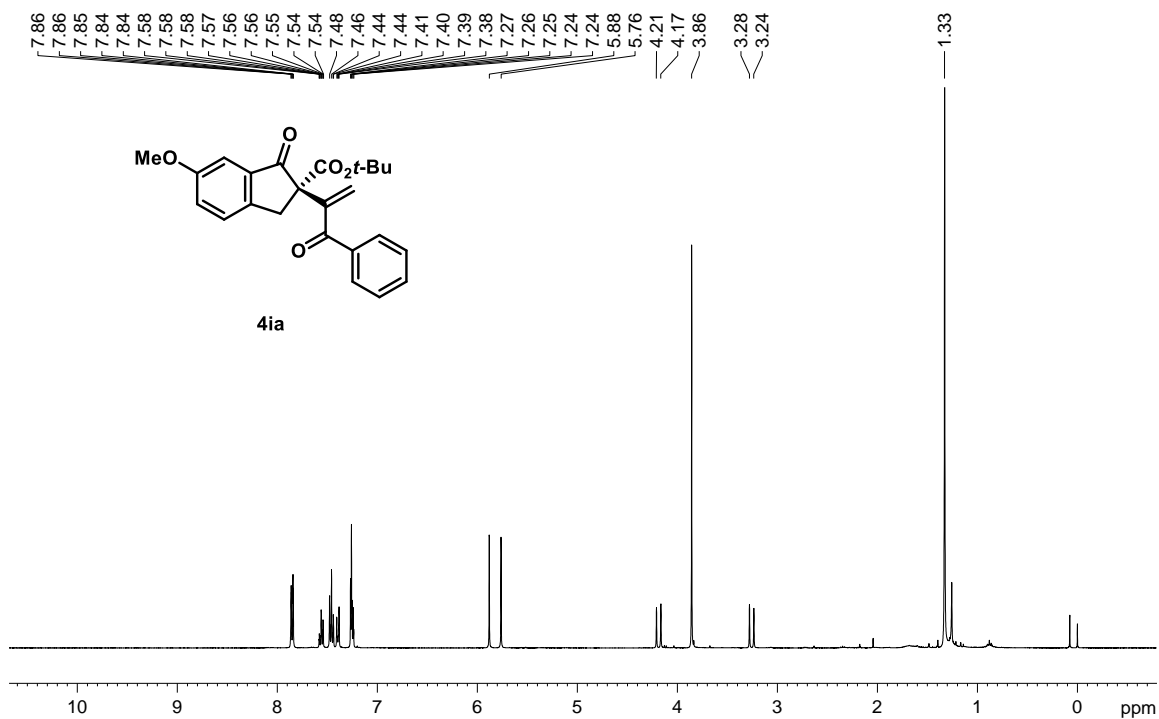


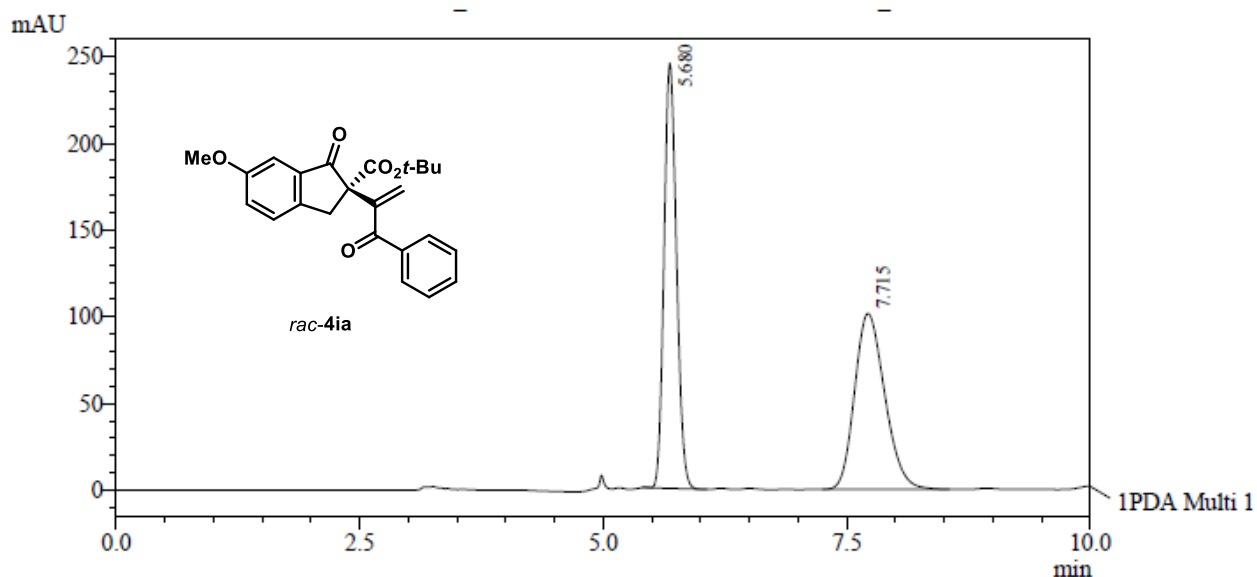
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	4.901	43839	1.577
2	5.257	2736220	98.423
Total		2780059	100.000





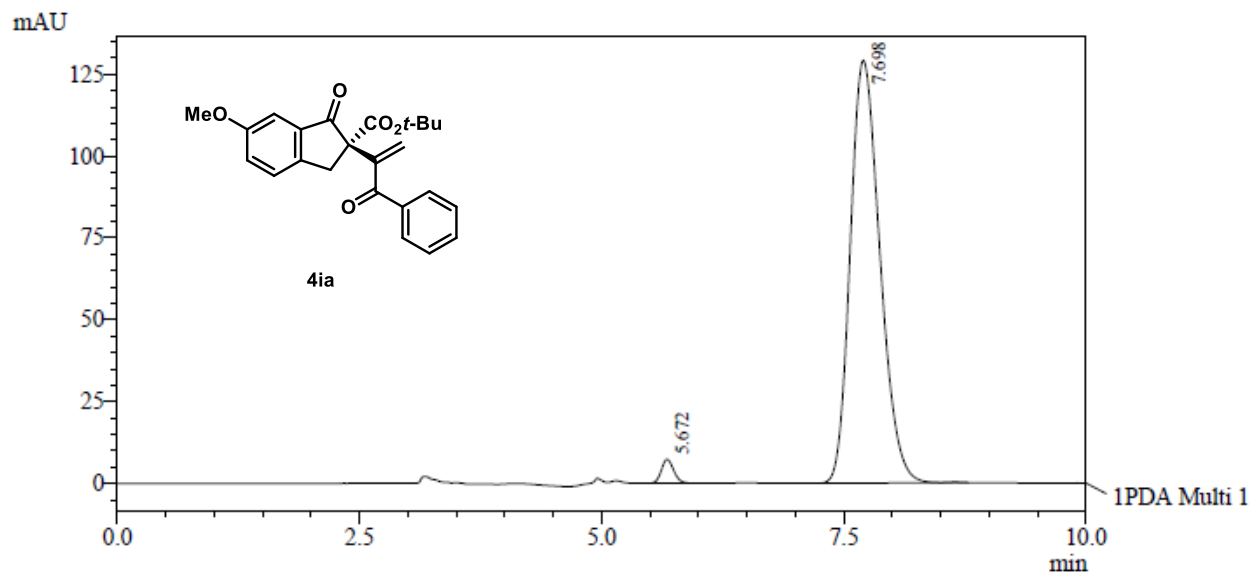
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.680	2182074	49.971
2	7.715	2184618	50.029
Total		4366692	100.000

Daicel Chiralpak AS-H column (*n*-Hexane/EtOH = 95:5, 1.0 mL min⁻¹, 20 °C, 254 nm)

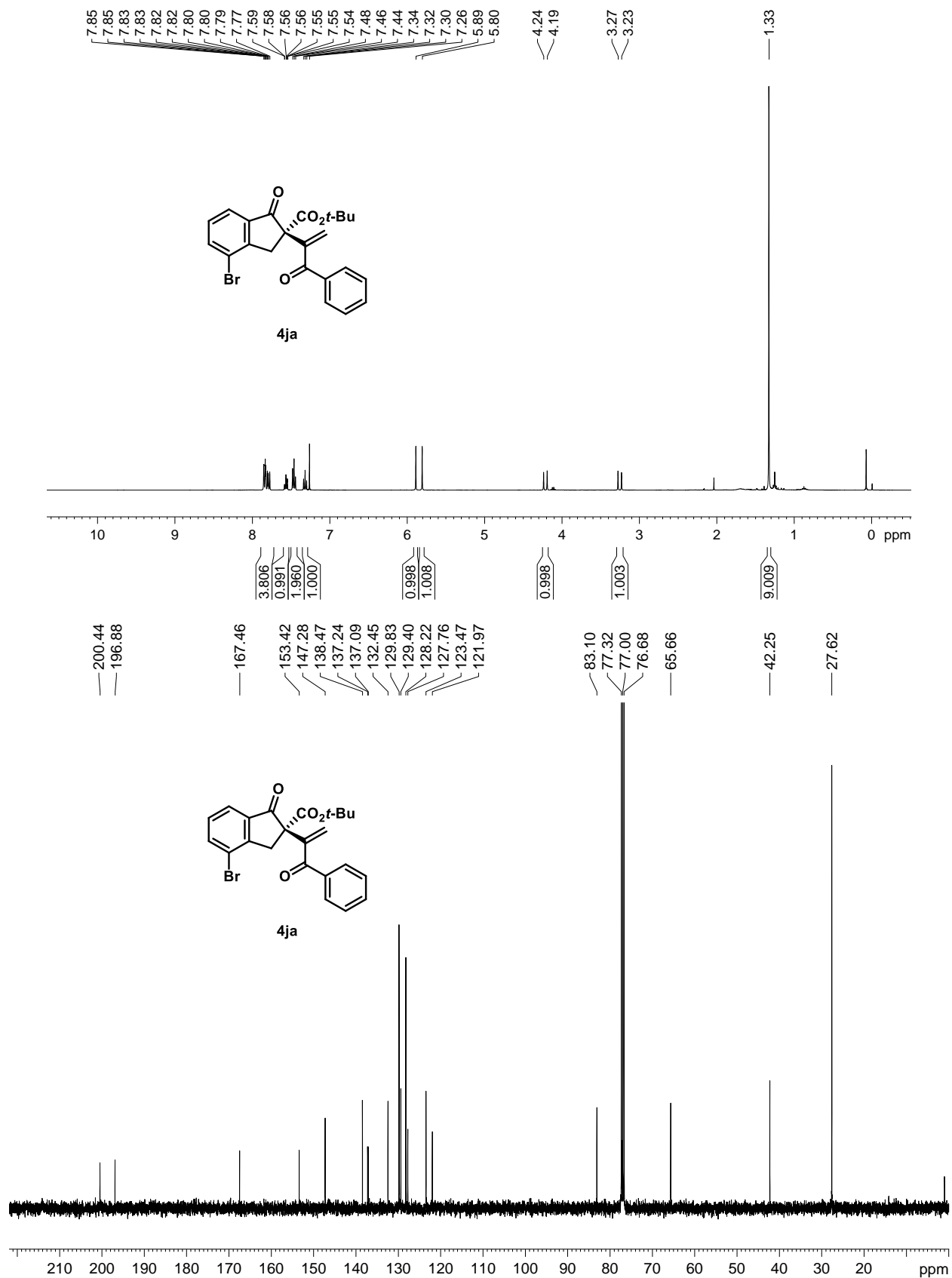


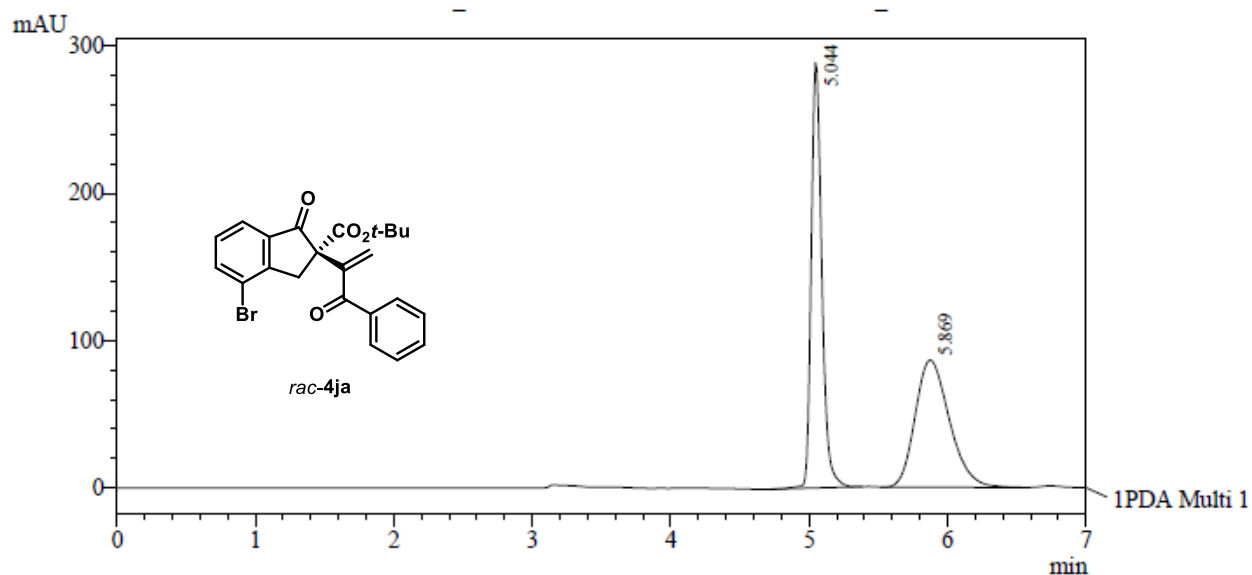
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.672	64327	2.284
2	7.698	2752598	97.716
Total		2816925	100.000





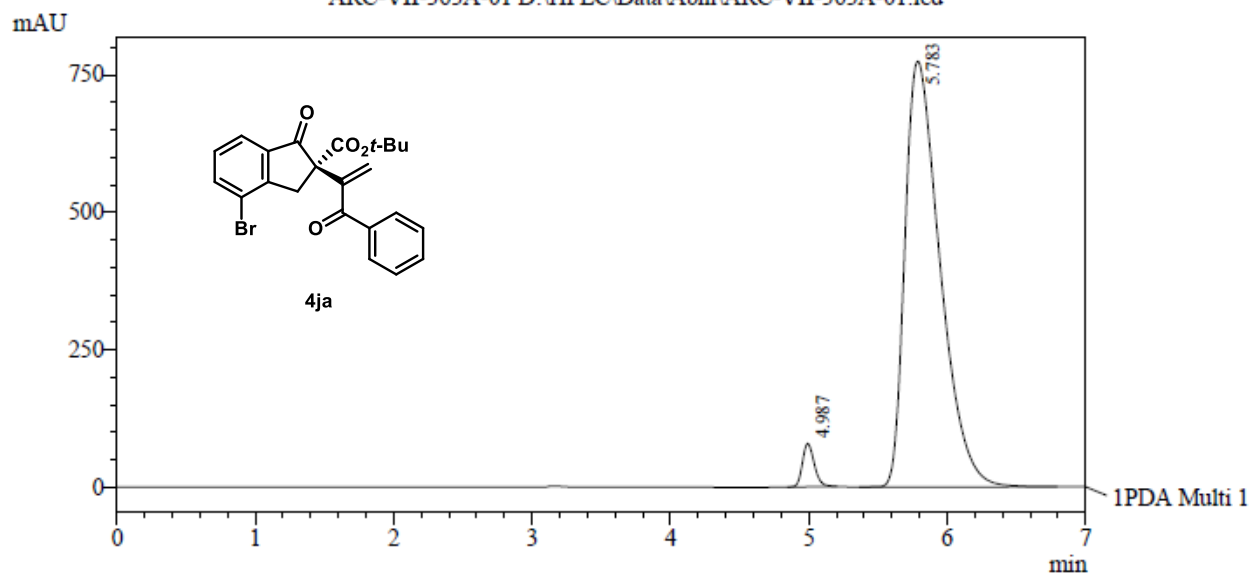
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.044	1540045	50.911
2	5.869	1484926	49.089
Total		3024971	100.000

Daicel Chiralpak AS-H column (*n*-Hexane/EtOH = 95:5, 1.0 mL min⁻¹, 20 °C, 254 nm)

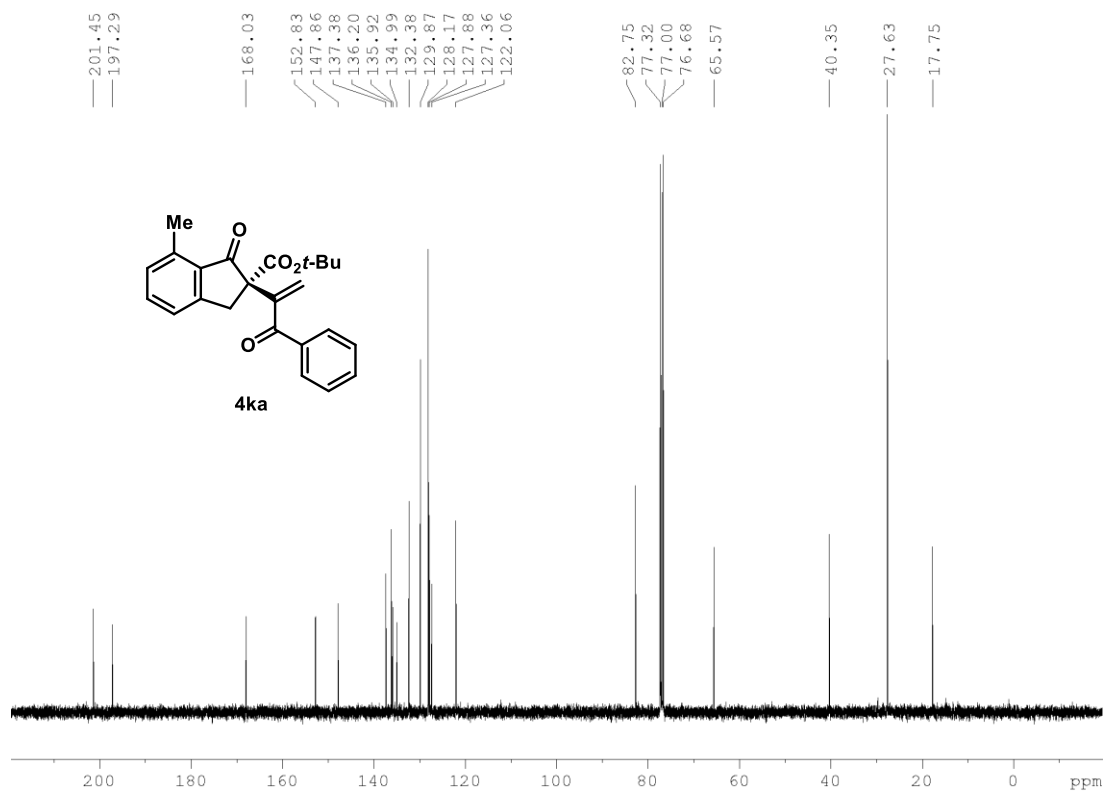
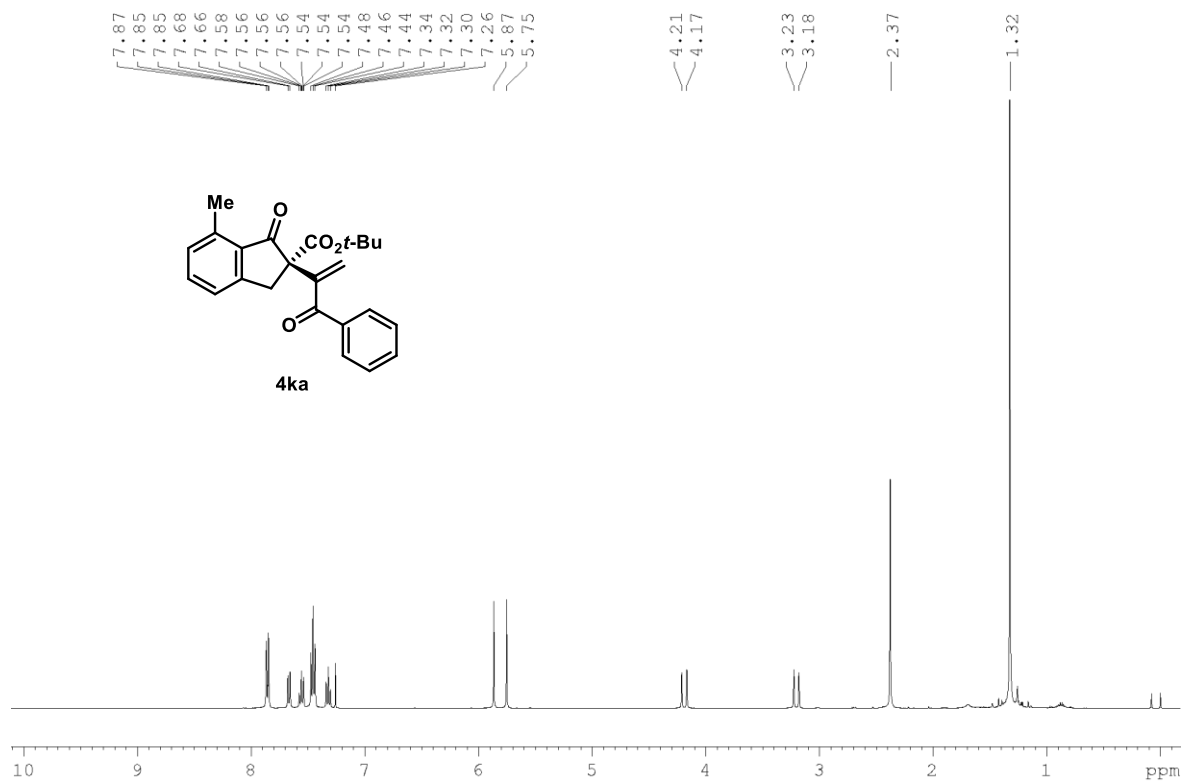


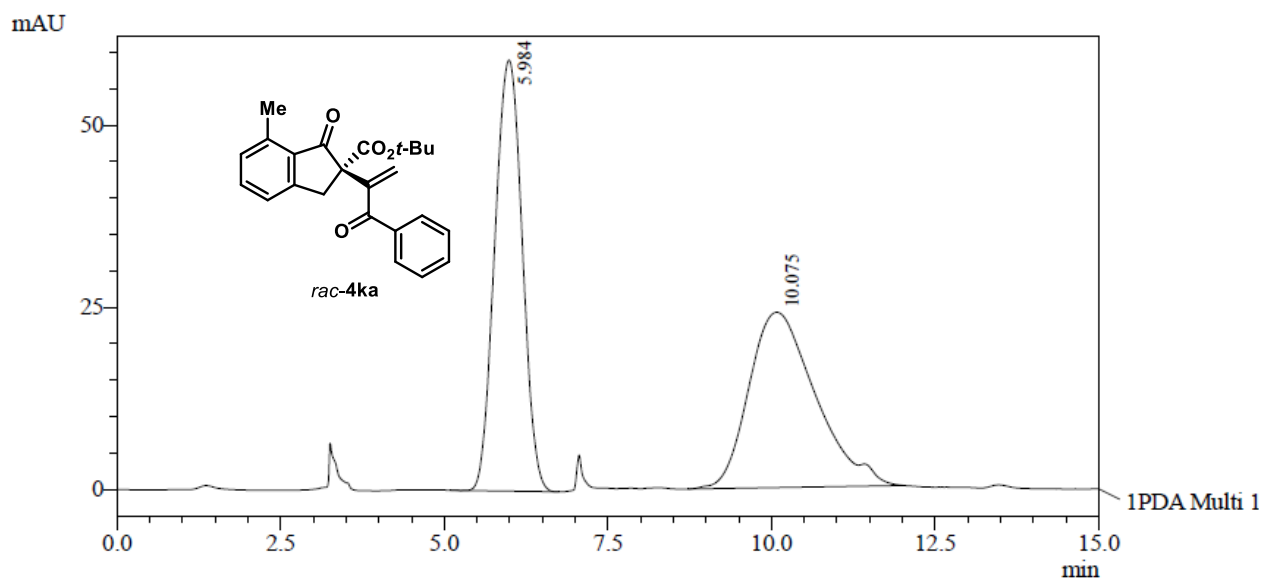
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	4.987	471970	3.340
2	5.783	13659276	96.660
Total		14131246	100.000





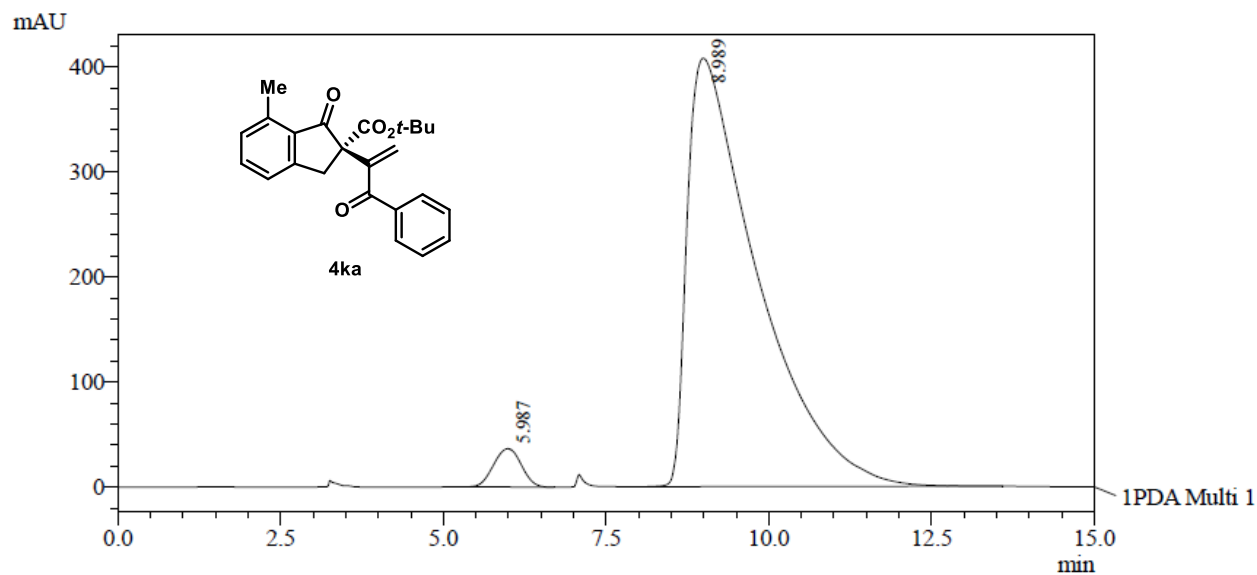
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.984	1730760	50.309
2	10.075	1709510	49.691
Total		3440270	100.000

Daicel Chiralpak AS-H column (*n*-Hexane/EtOH = 98:2, 1.0 mL min⁻¹, 20 °C, 254 nm)

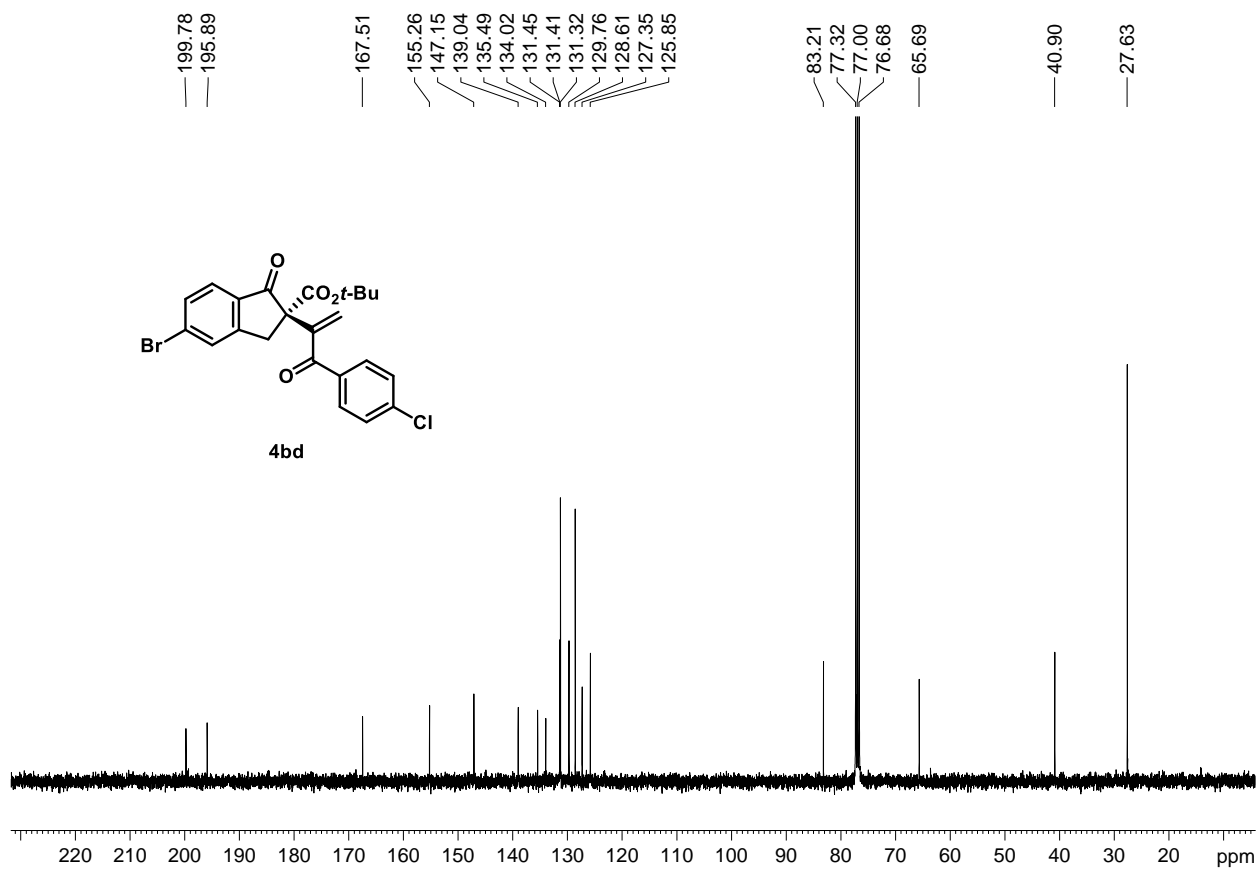
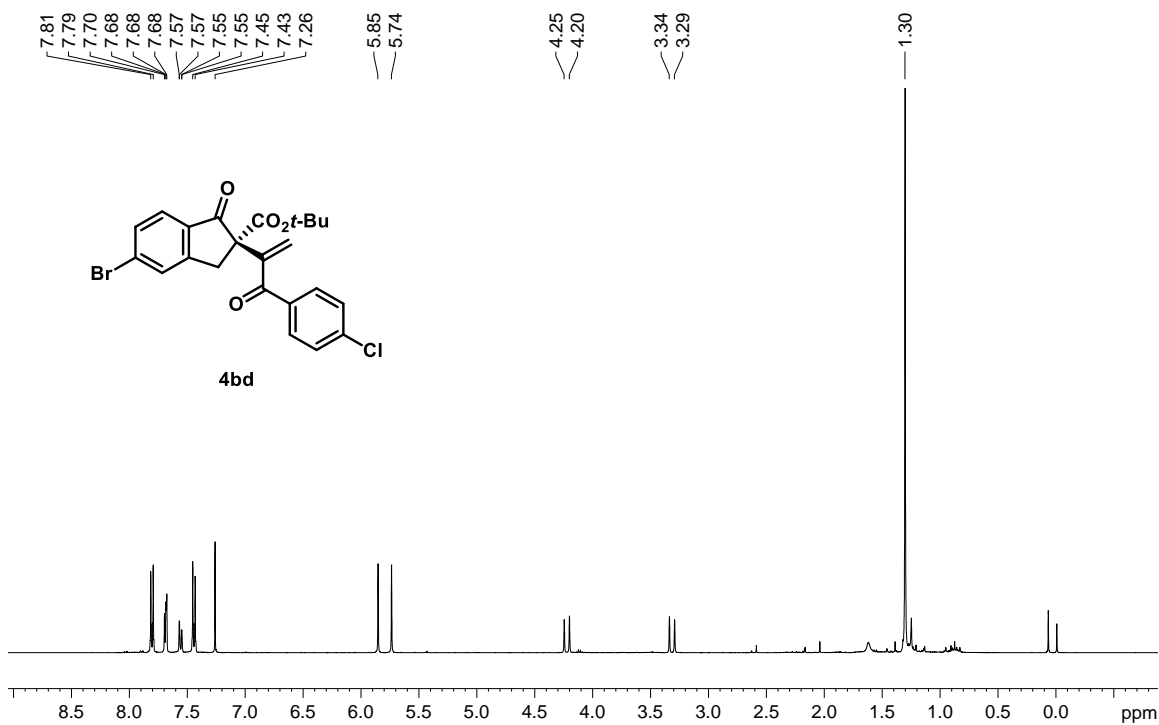


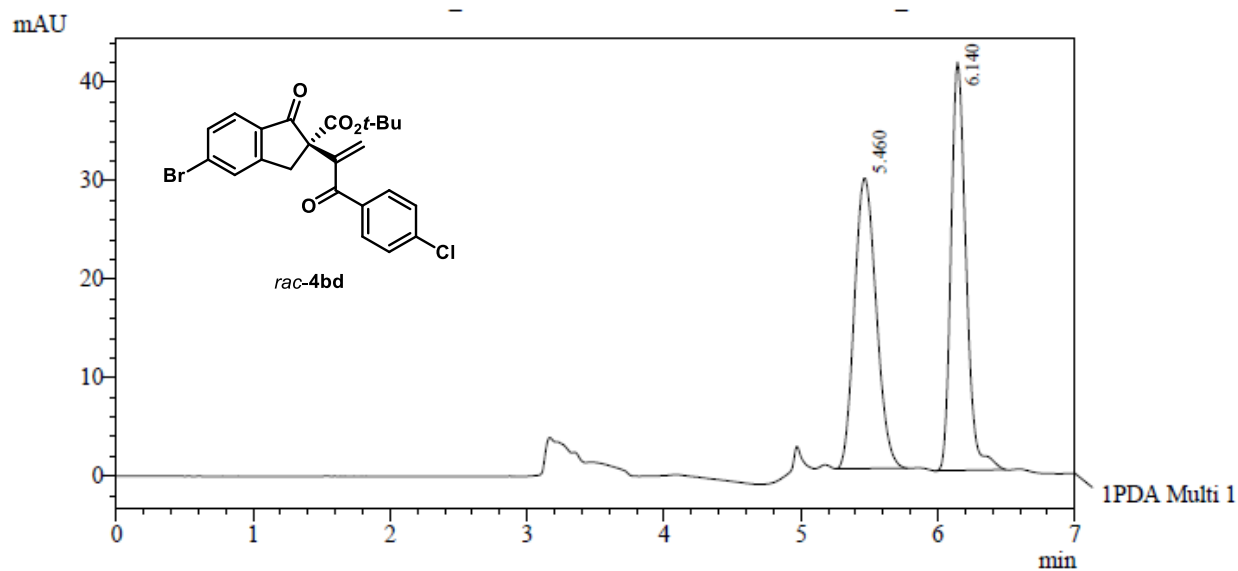
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.987	1086190	3.414
2	8.989	30731302	96.586
Total		31817492	100.000





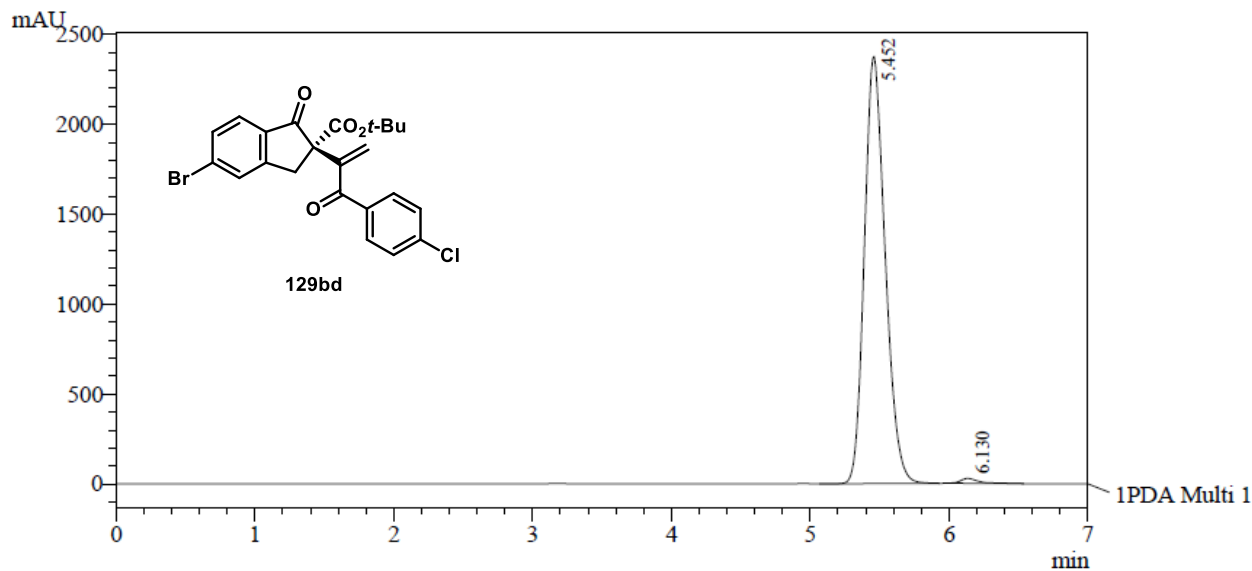
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.460	326919	50.773
2	6.140	316967	49.227
Total		643886	100.000

Daicel Chiralpak AS-H column (*n*-Hexane/EtOH = 95:5, 1.0 mL min⁻¹, 20 °C, 254 nm)

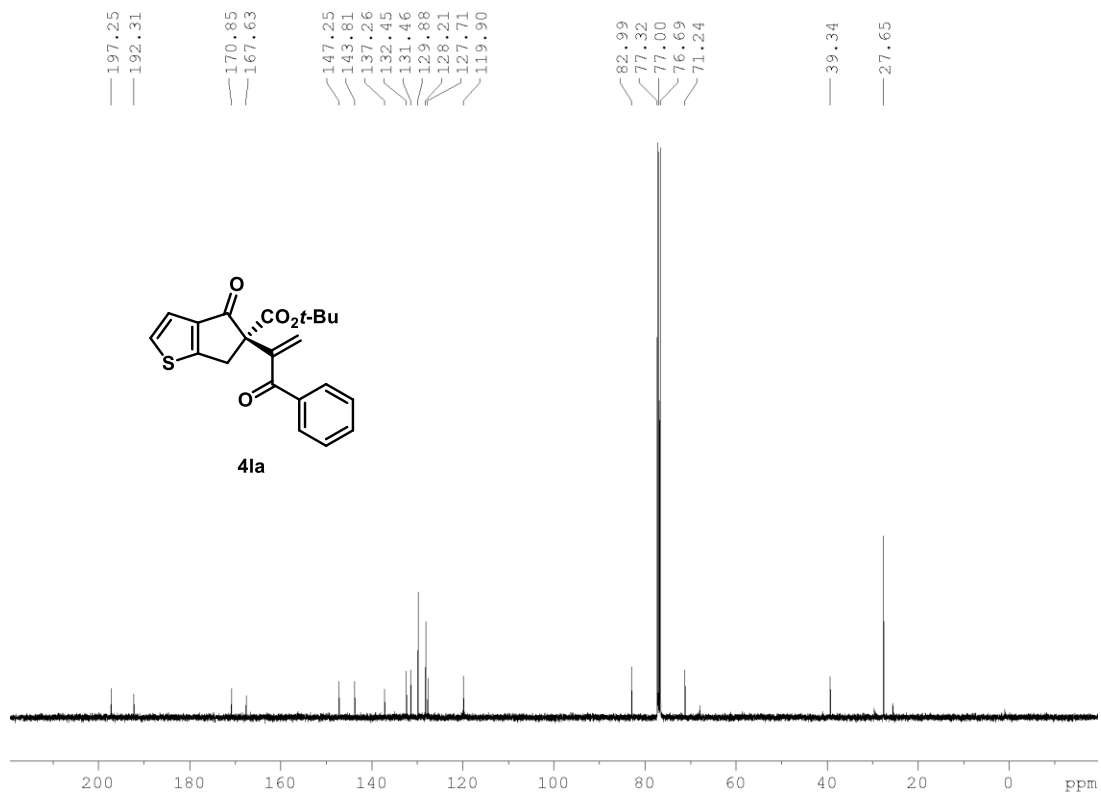
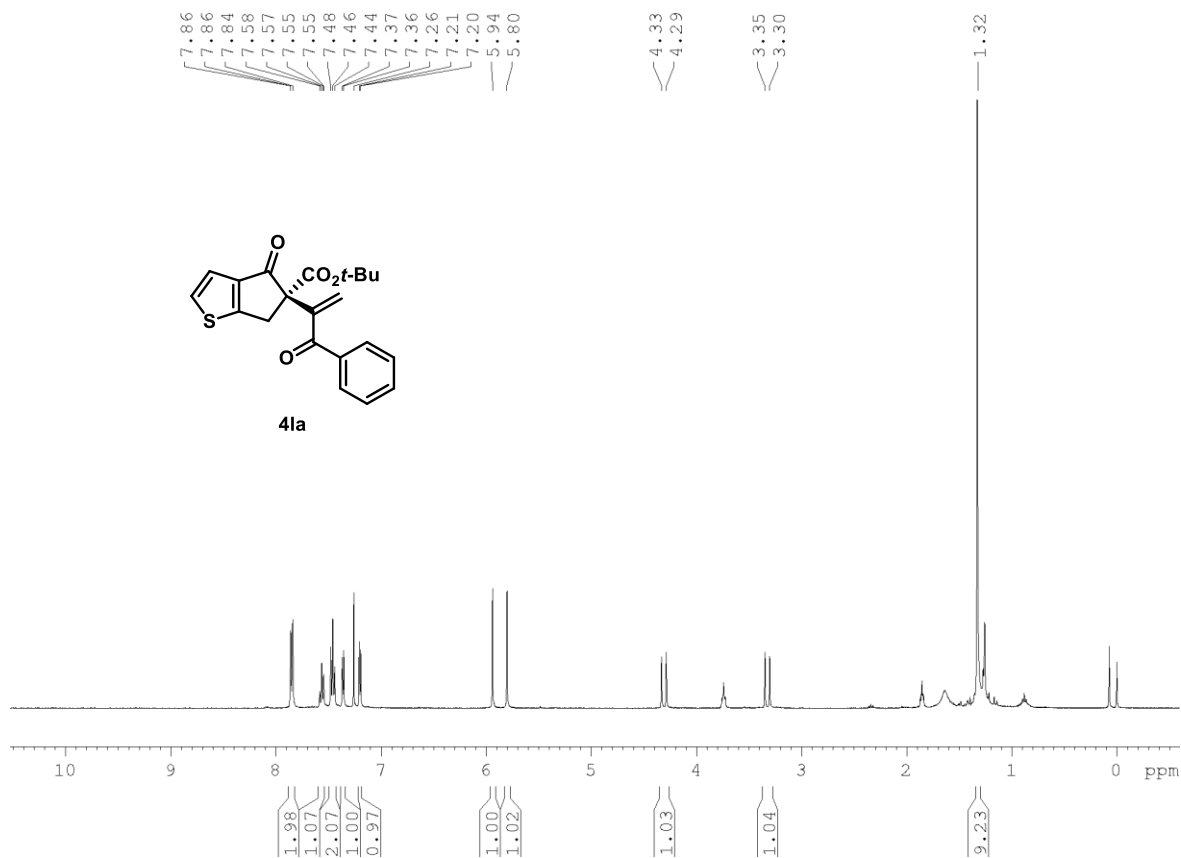


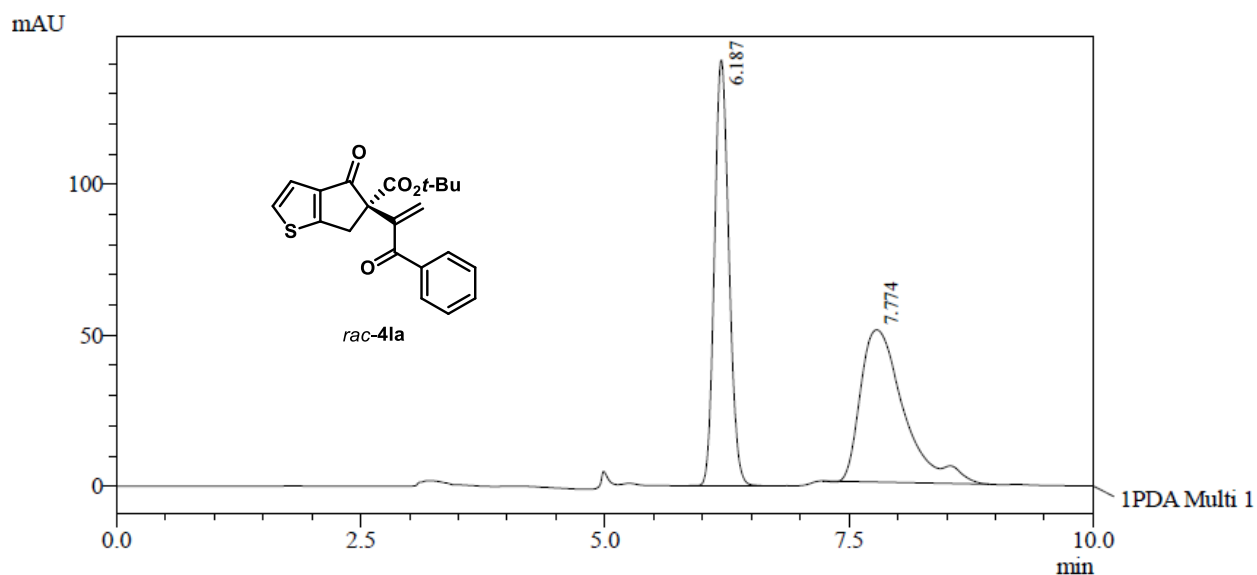
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.452	24769208	99.030
2	6.130	242613	0.970
Total		25011821	100.000





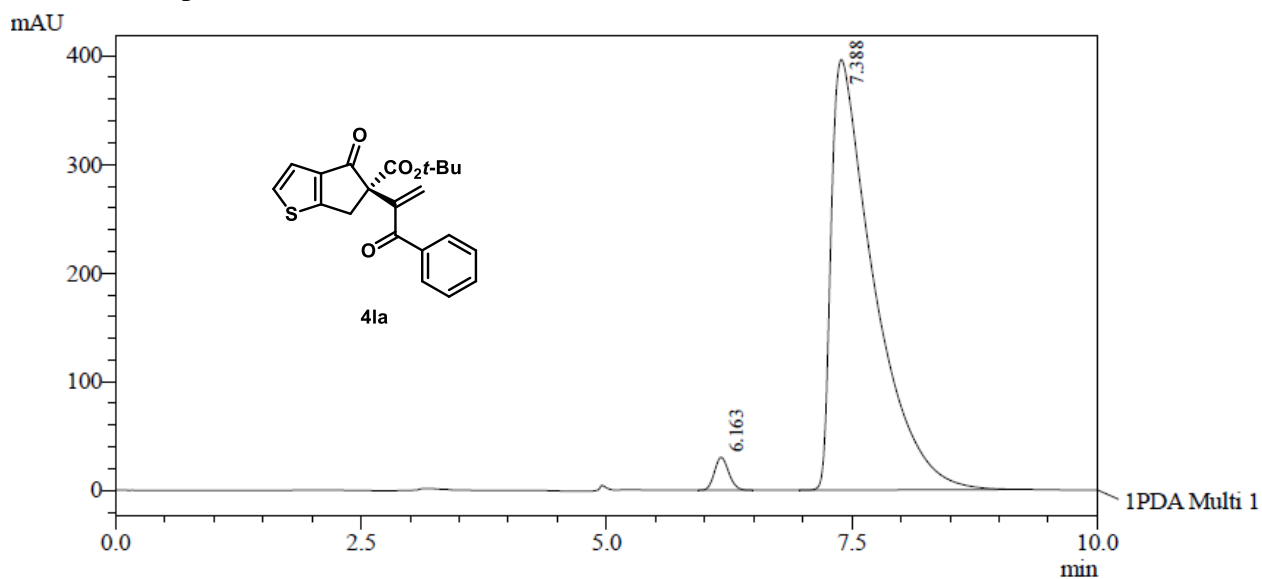
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	6.187	1458242	48.255
2	7.774	1563683	51.745
Total		3021925	100.000

Daicel Chiralpak AS-H column (*n*-Hexane/EtOH = 95:5, 1.0 mL min⁻¹, 20 °C, 254 nm)

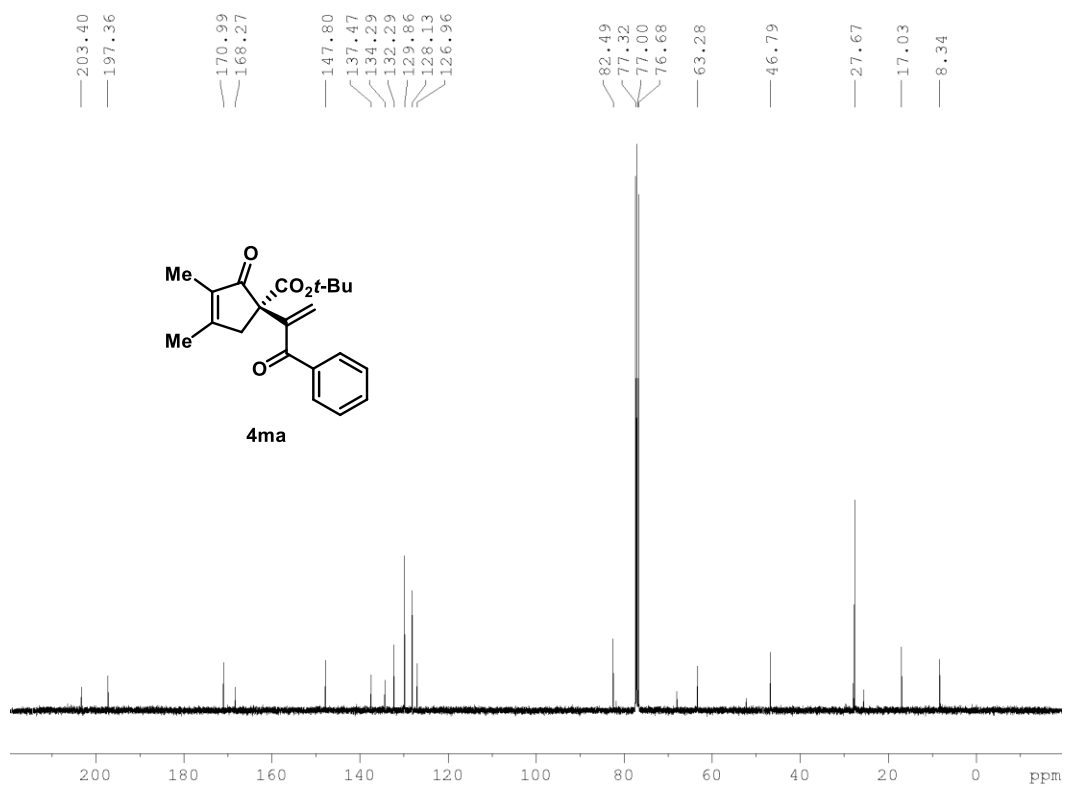
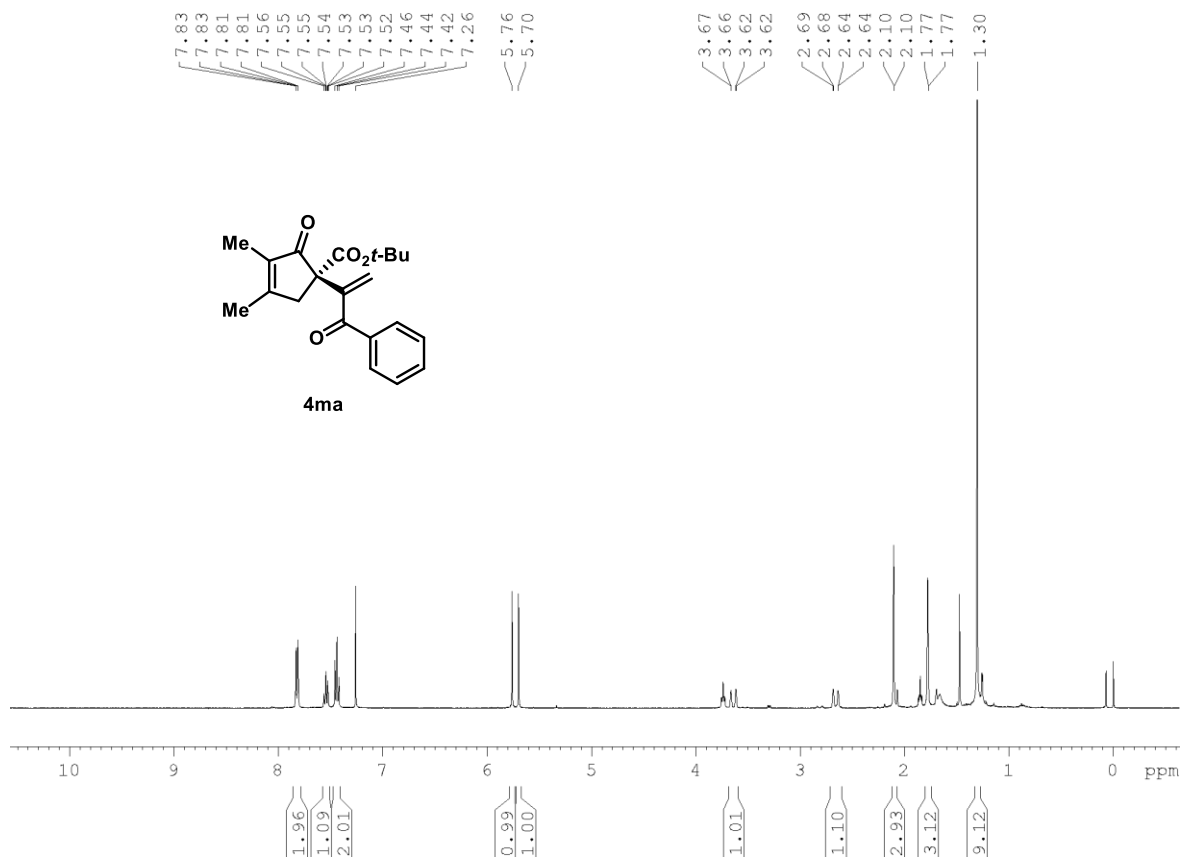


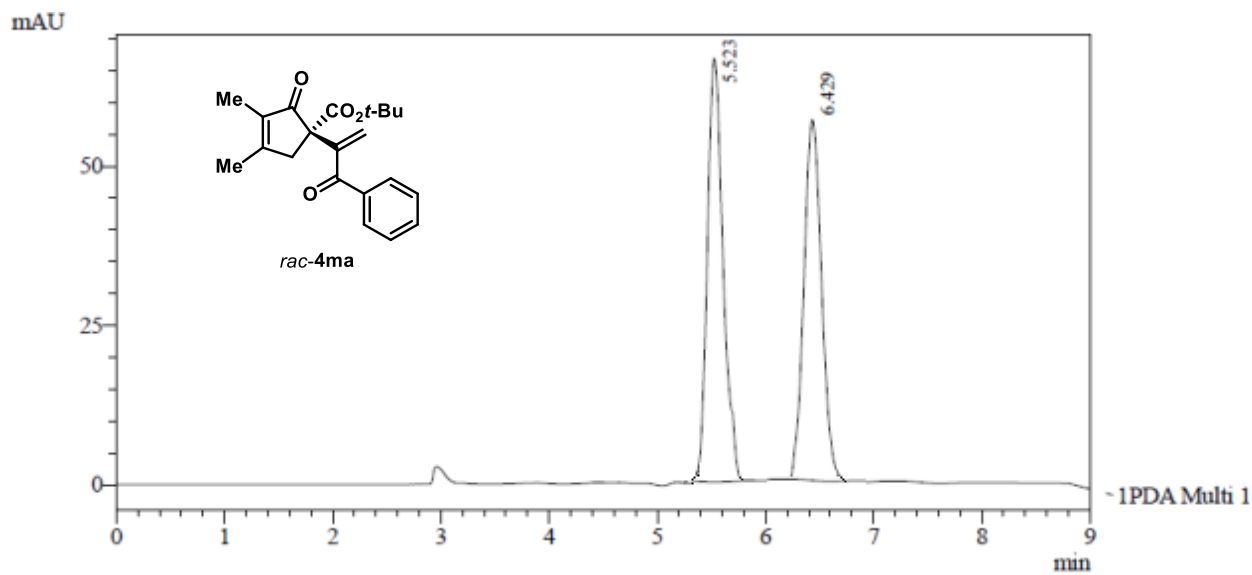
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	6.163	305797	2.491
2	7.388	11969175	97.509
Total		12274972	100.000





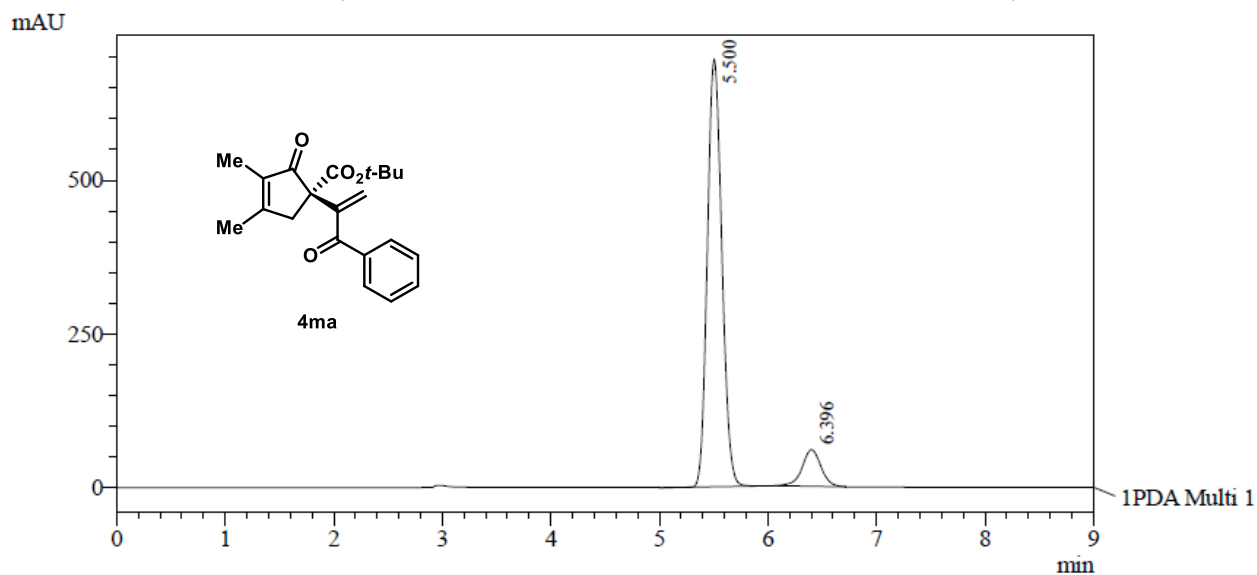
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.523	588263	49.363
2	6.429	603439	50.637
Total		1191702	100.000

Phenomenex C1 column (*n*-Hexane/IPA = 95:5, 1.0 mL min⁻¹, 20 °C, 254 nm)

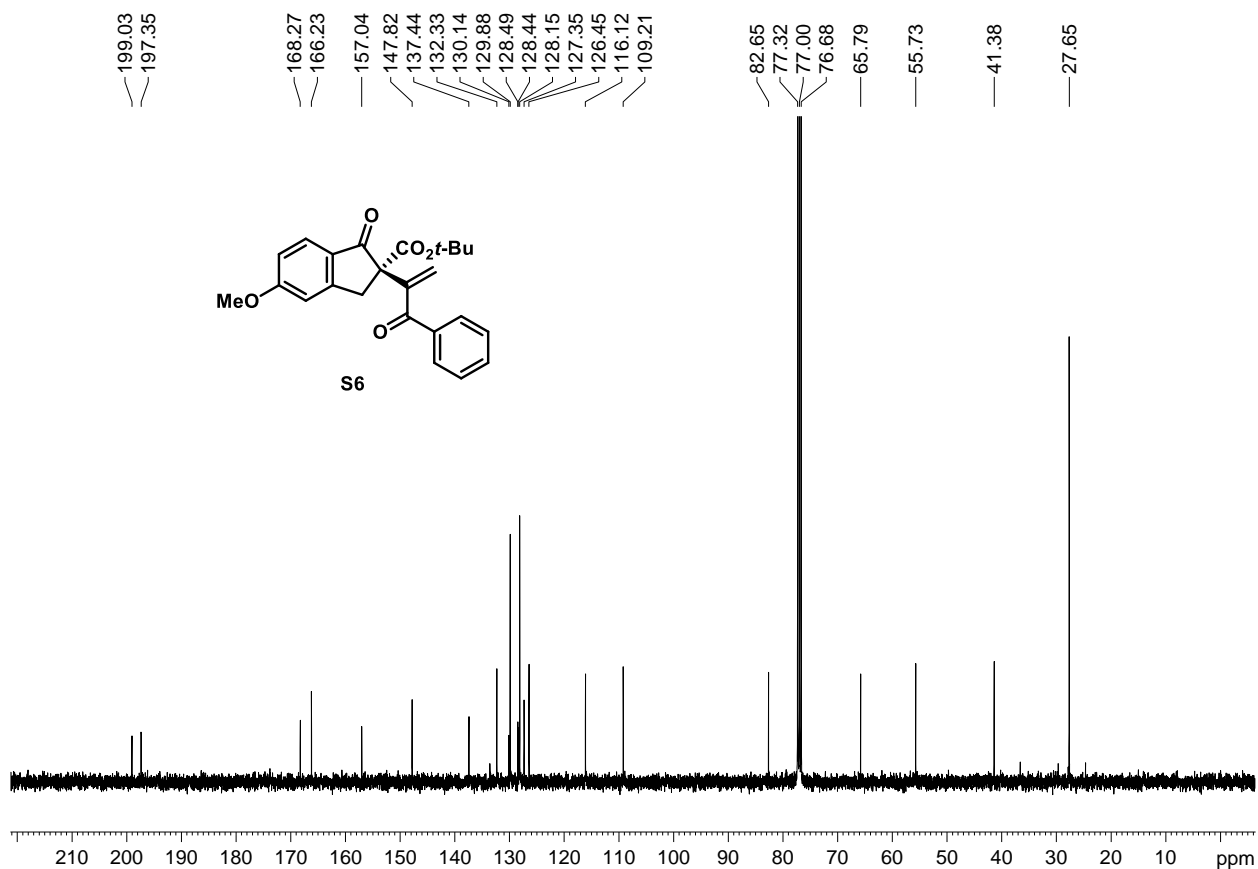
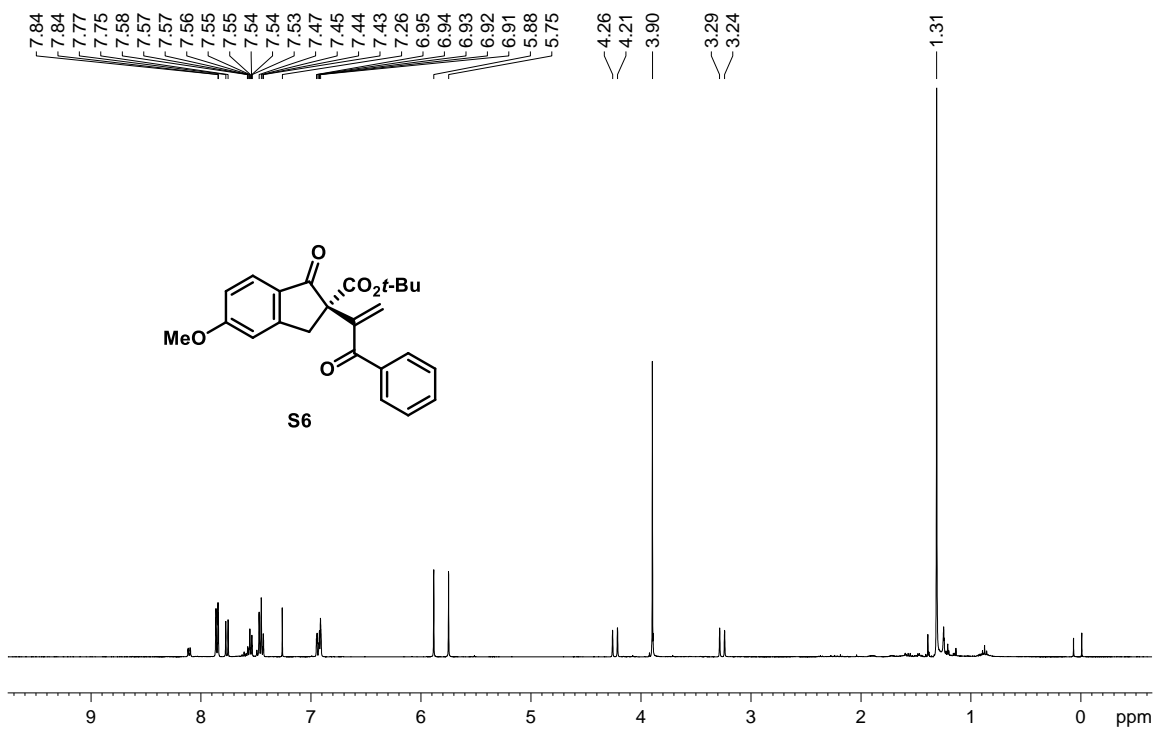


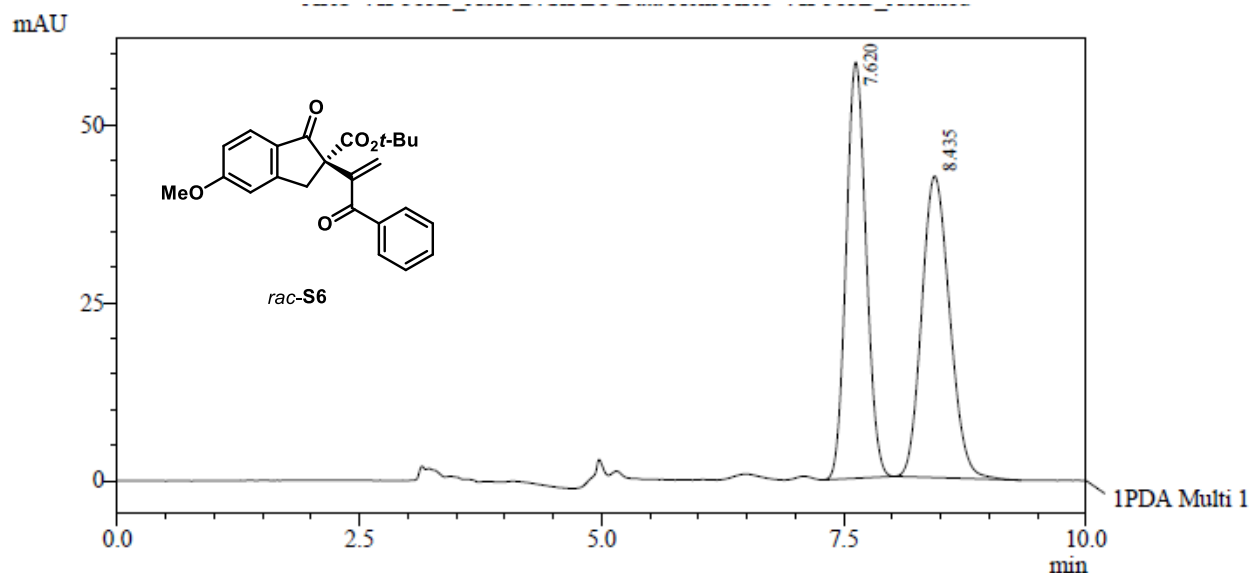
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.500	6452425	89.952
2	6.396	720761	10.048
Total		7173186	100.000





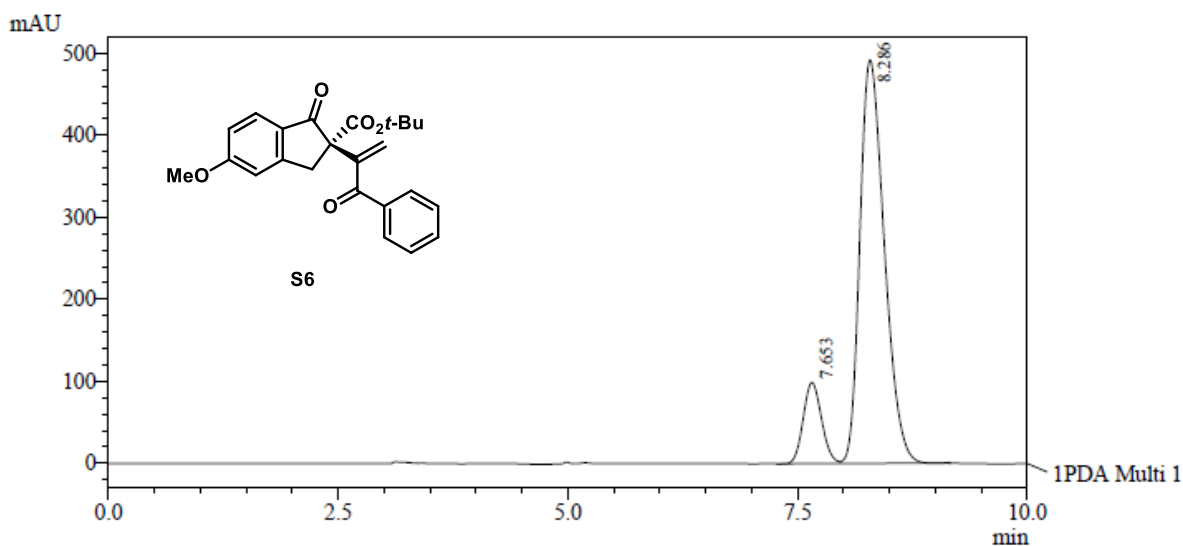
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	7.620	836145	49.586
2	8.435	850102	50.414
Total		1686248	100.000

Daicel Chiralpak AS-H column (*n*-Hexane/EtOH = 95:5, 1.0 mL min⁻¹, 20 °C, 254 nm)

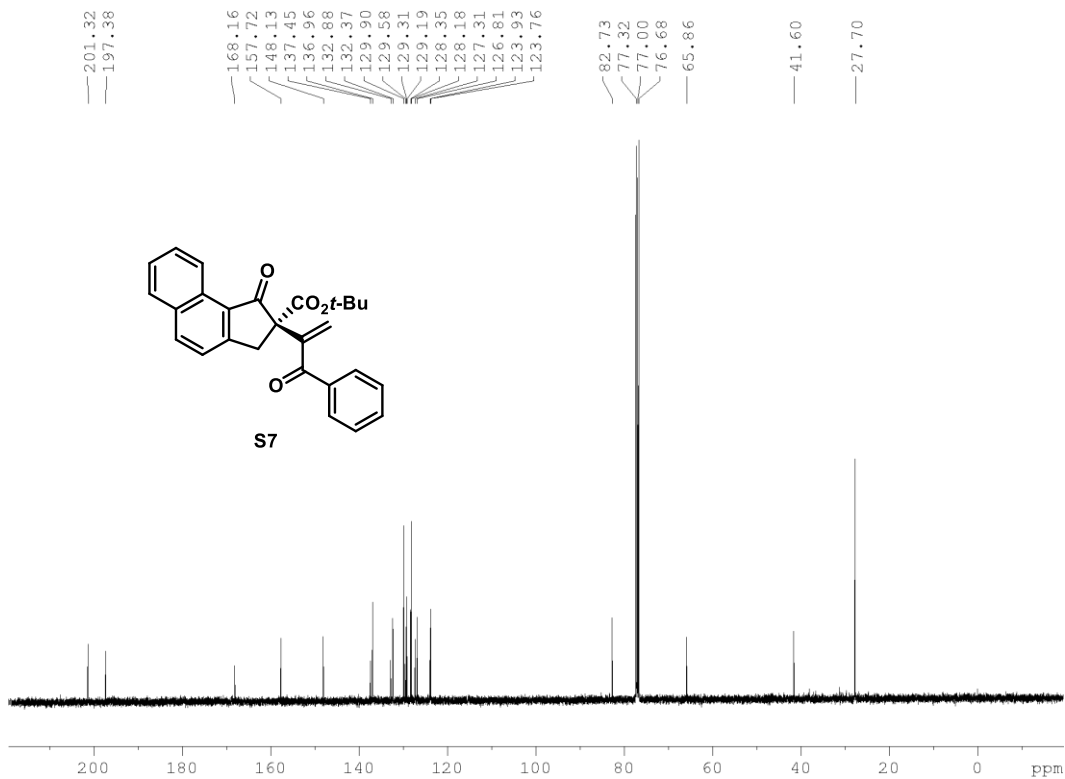
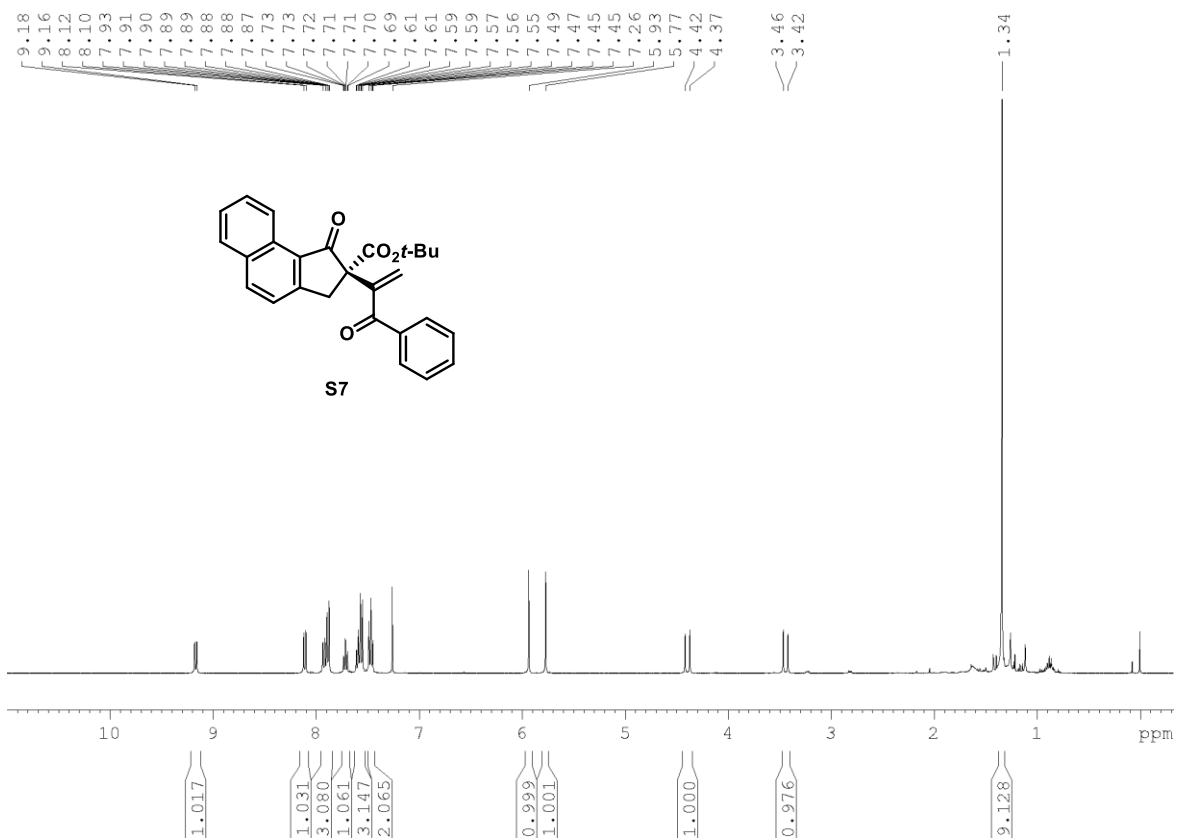


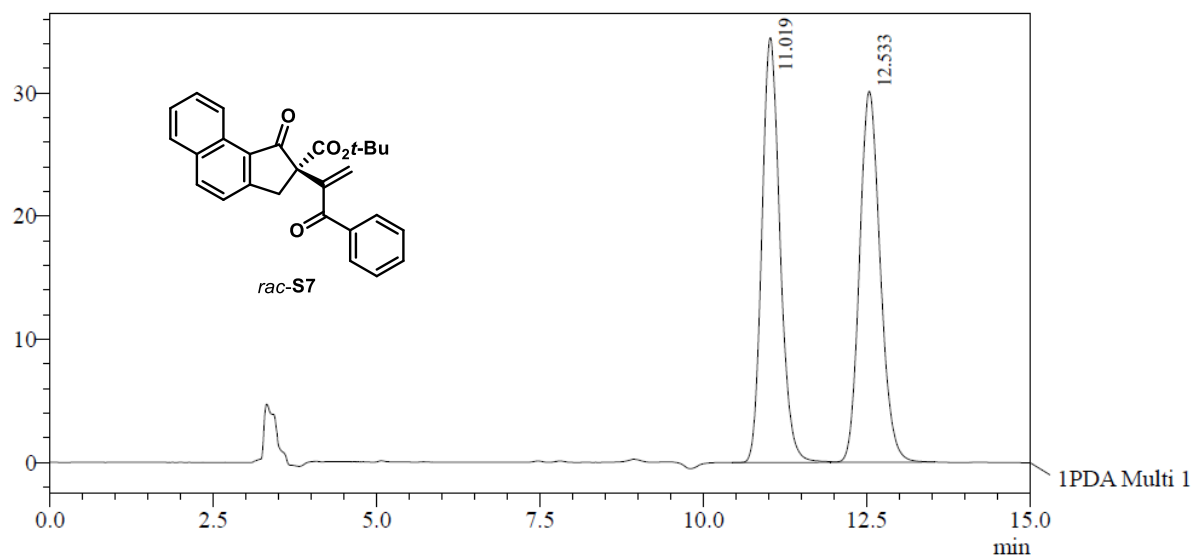
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	7.653	1373932	13.110
2	8.286	9106220	86.890
Total		10480151	100.000





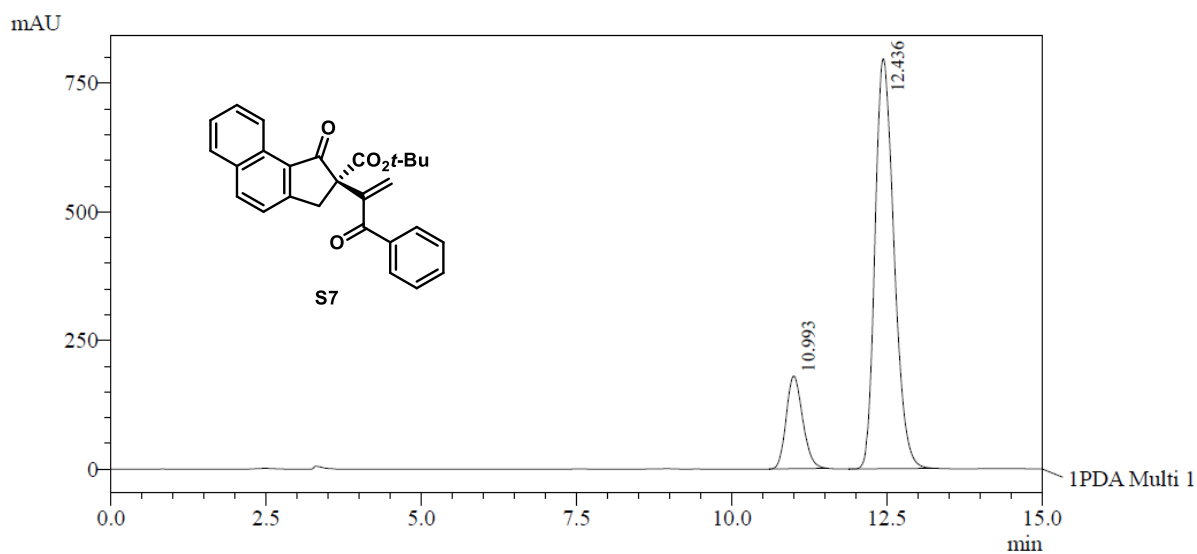
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	11.019	665186	50.010
2	12.533	664911	49.990
Total		1330097	100.000

Daicel Chiralpak IC column (*n*-Hexane/IPA = 95:5, 1.0 mL min⁻¹, 20 °C, 254 nm)

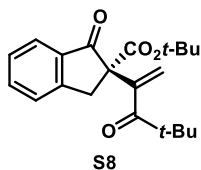
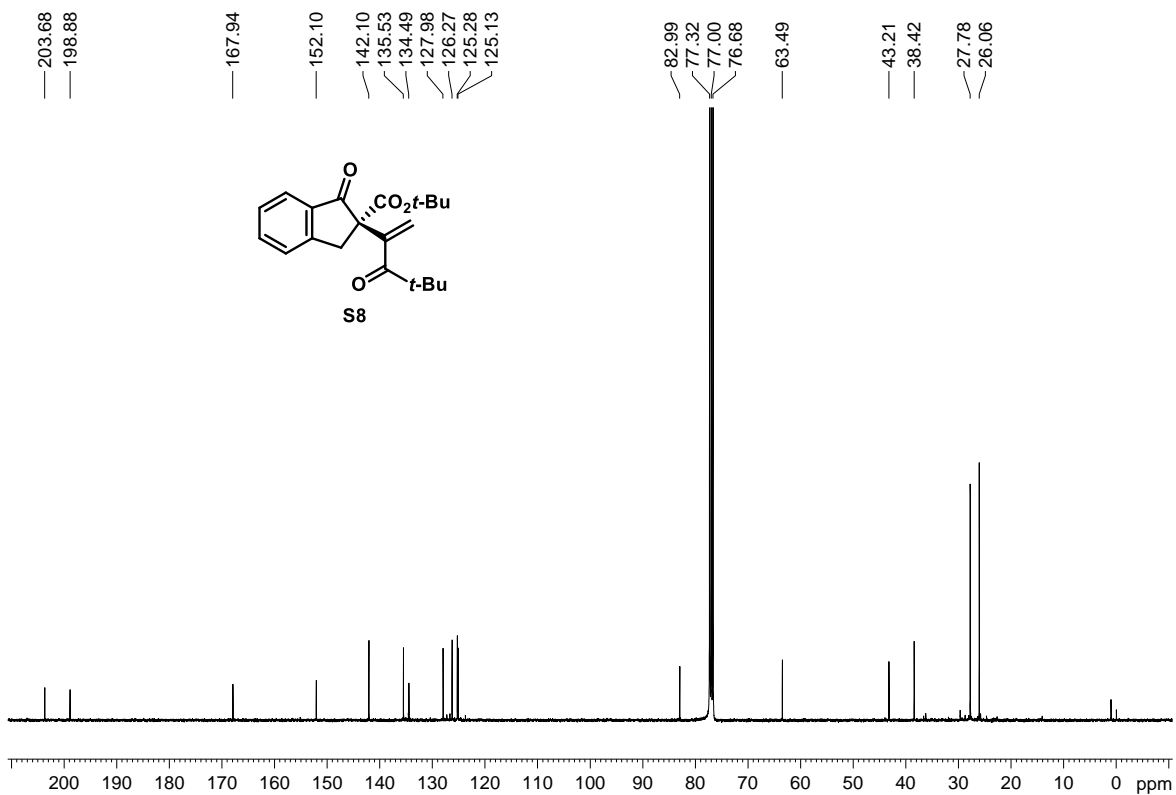
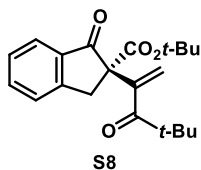
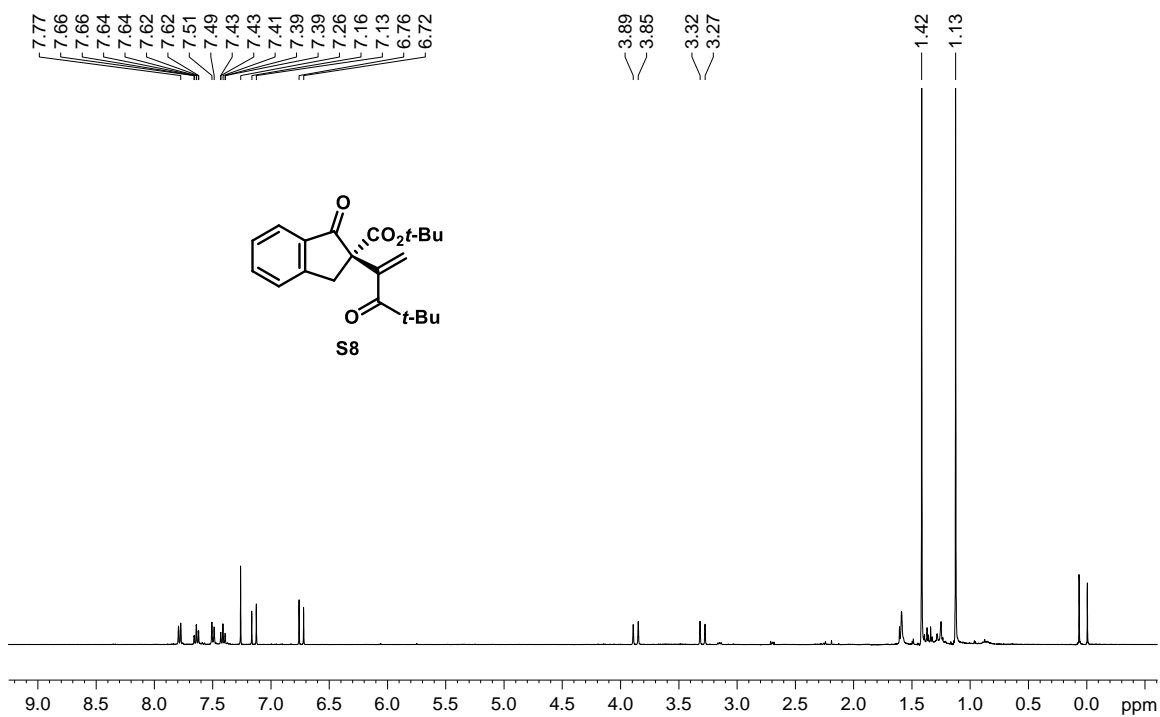


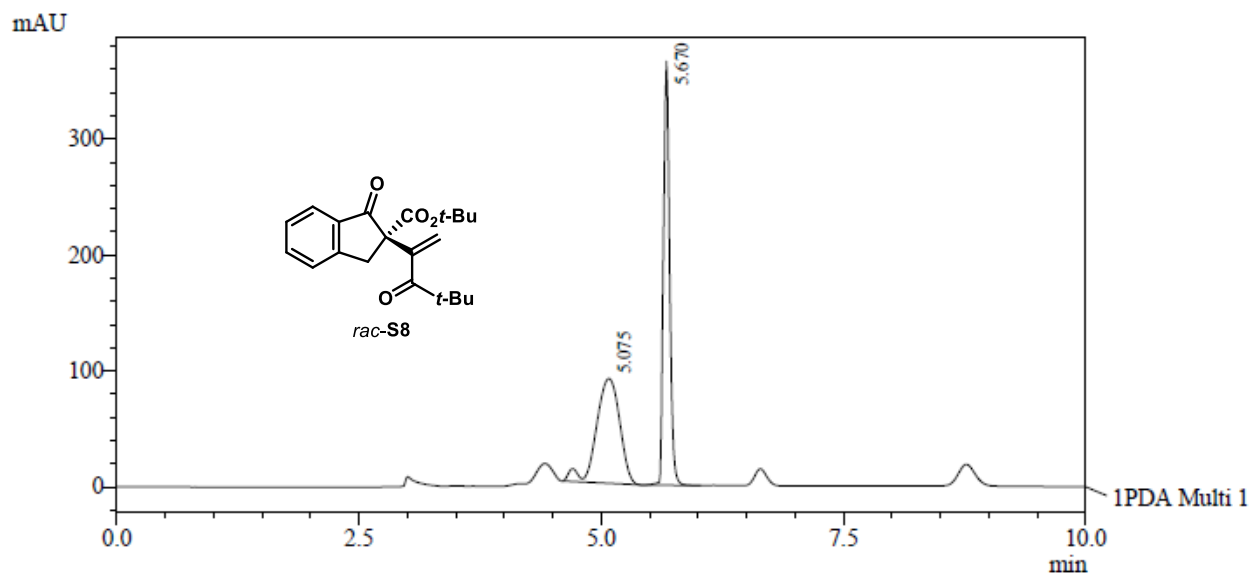
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	10.993	3329740	16.386
2	12.436	16990640	83.614
Total		20320380	100.000





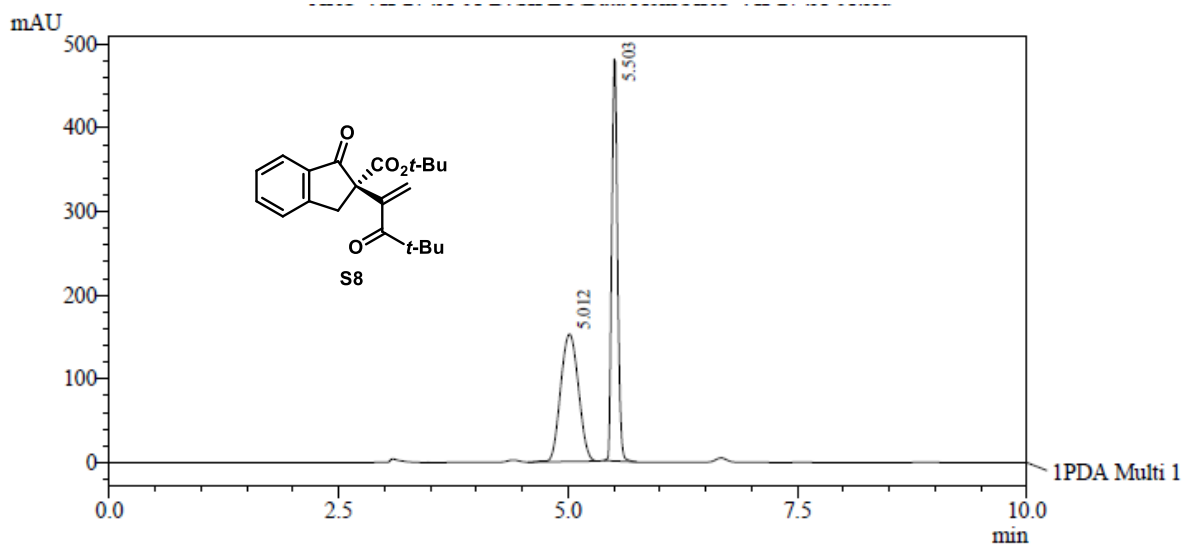
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.075	1525132	48.332
2	5.670	1630390	51.668
Total		3155522	100.000

Phenomenex C-1 column (*n*-Hexane/EtOH = 95:5, 1.0 mL min⁻¹, 20 °C, 254 nm)

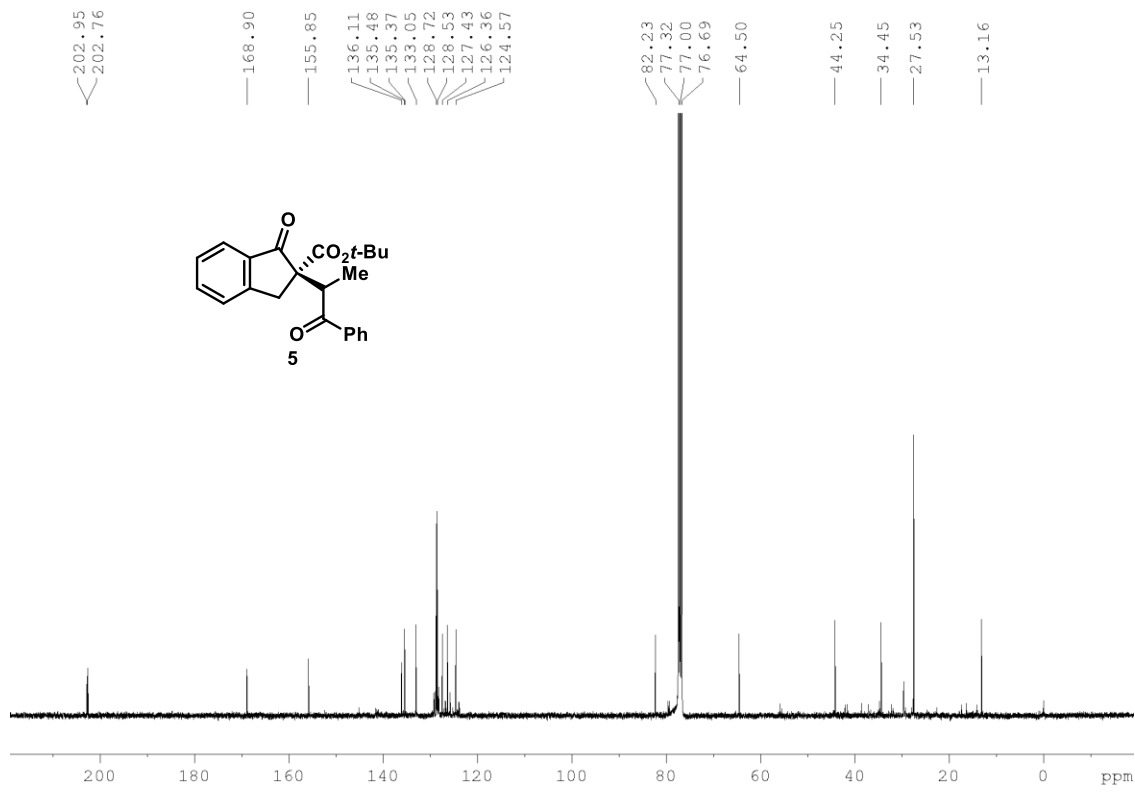
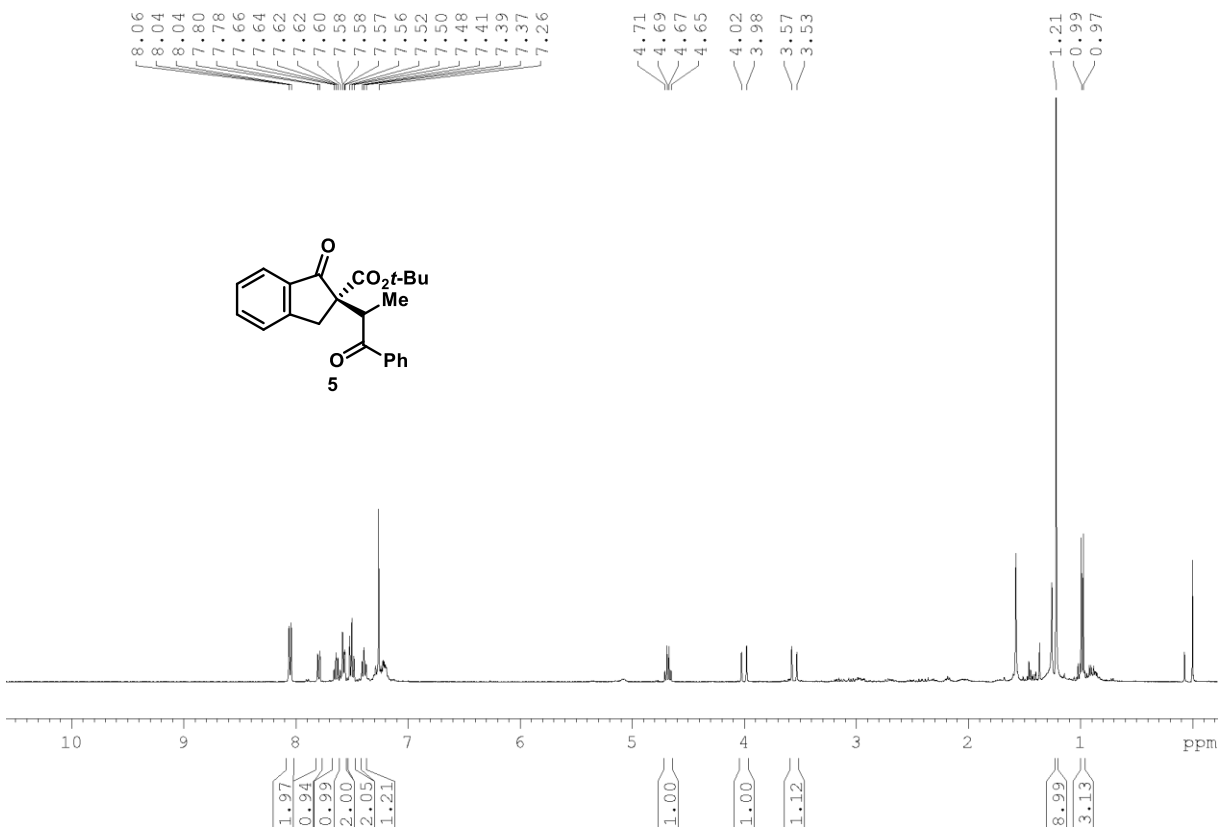


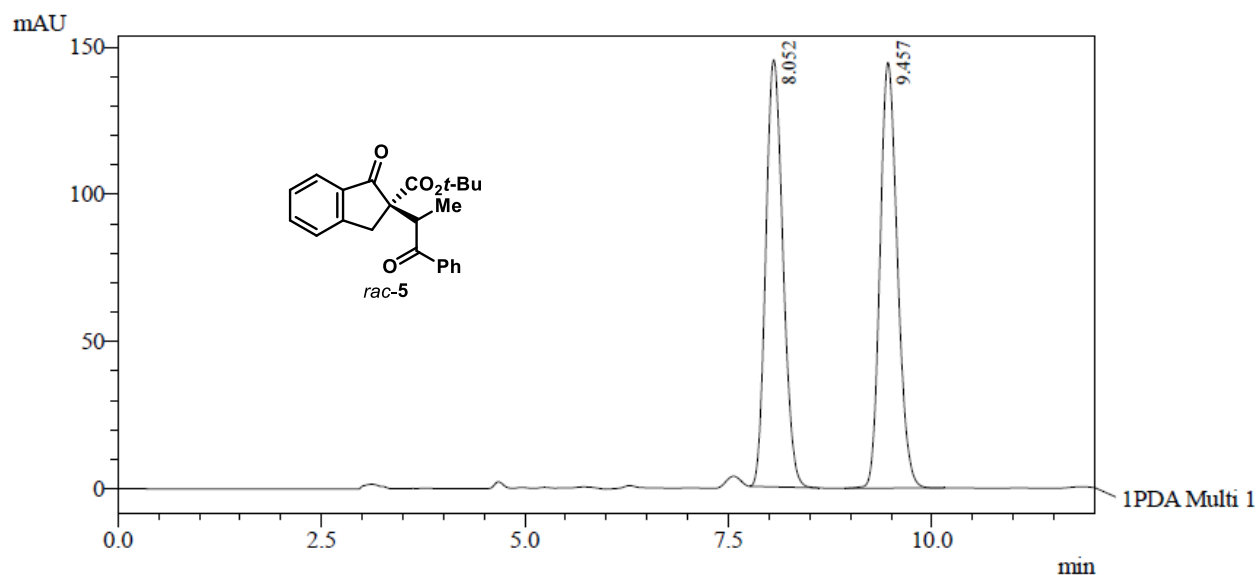
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.012	2057338	49.543
2	5.503	2095281	50.457
Total		4152619	100.000





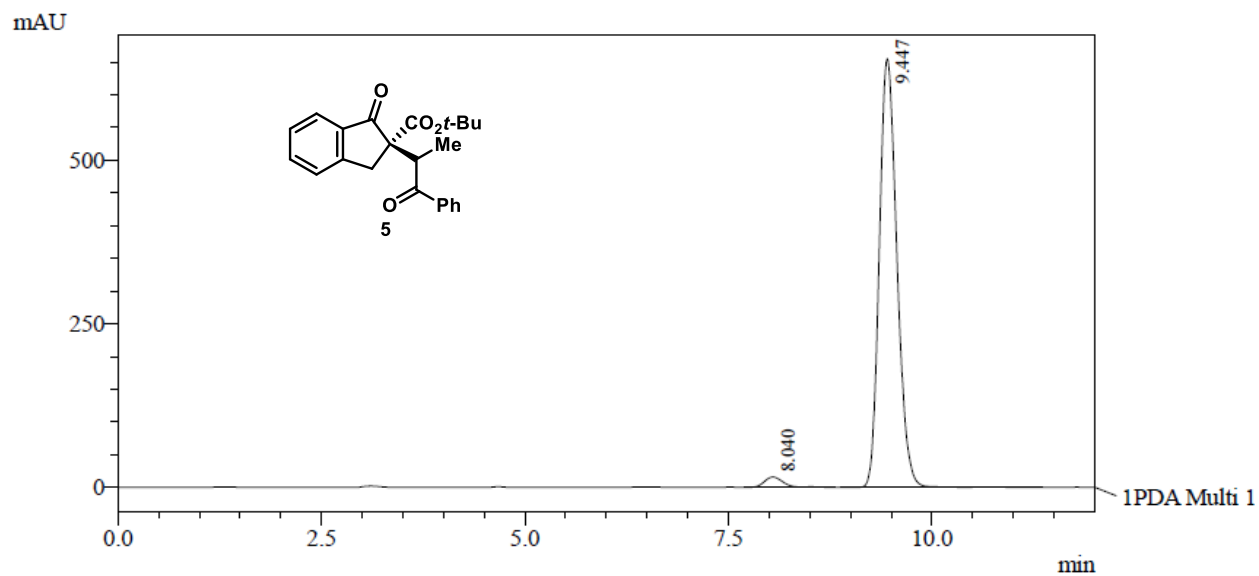
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	8.052	2128640	49.718
2	9.457	2152816	50.282
Total		4281456	100.000

Daicel Chiralpak AD-H column (*n*-Hexane/IPA = 90:10, 1.0 mL min⁻¹, 20 °C, 254 nm)

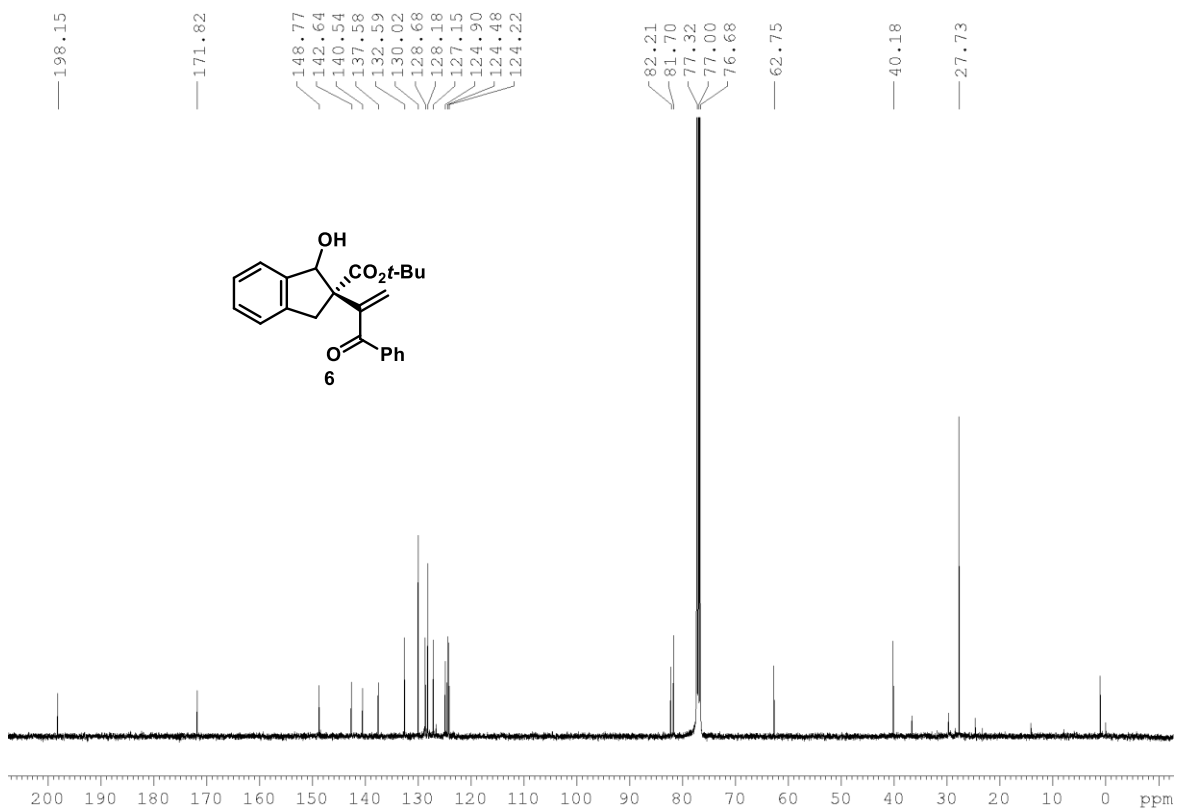
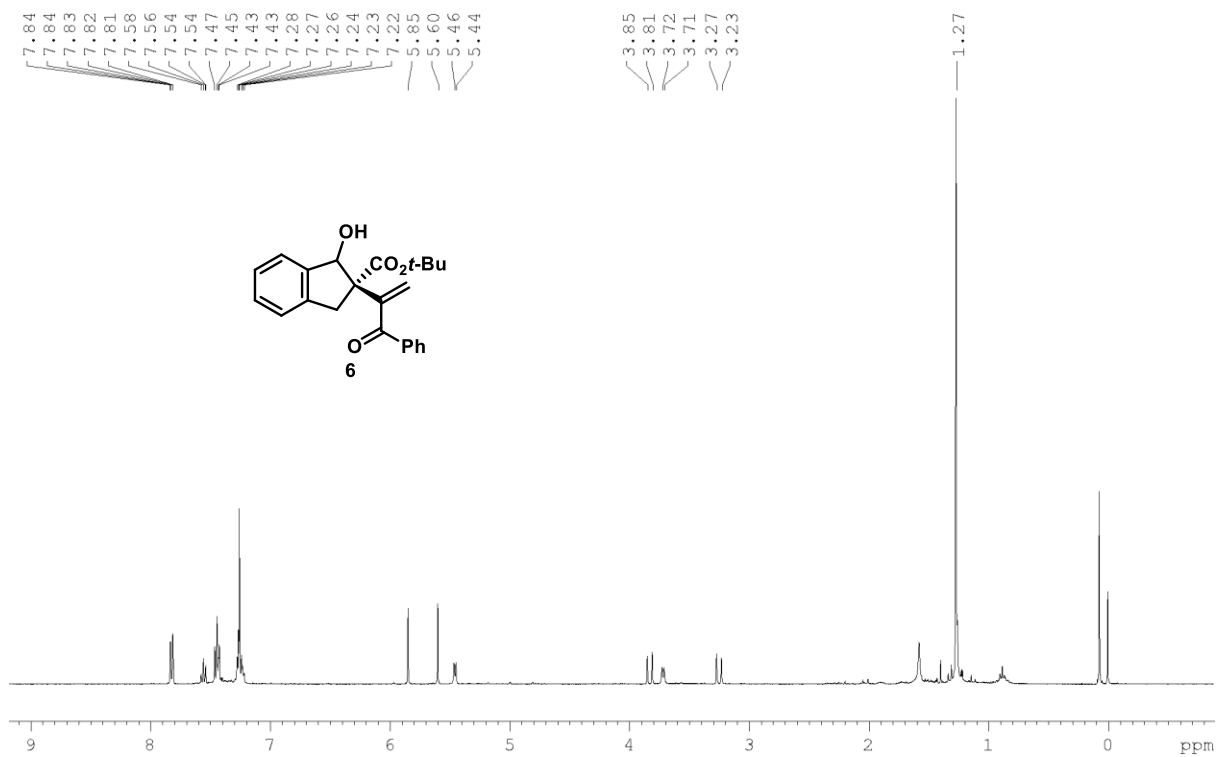


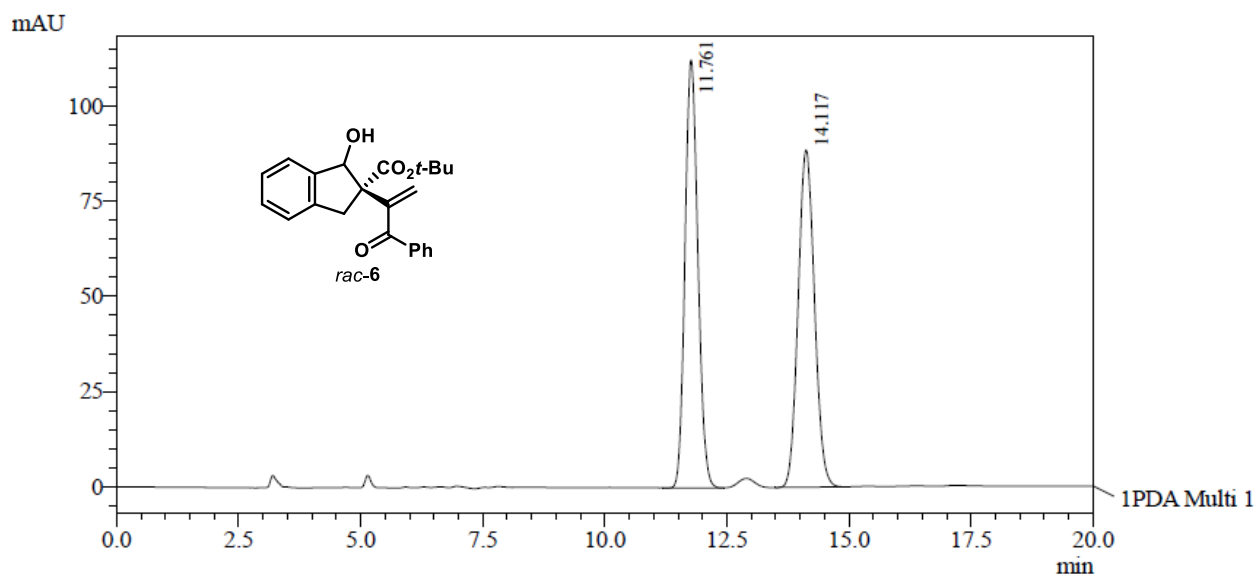
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	8.040	251657	2.491
2	9.447	9852156	97.509
Total		10103813	100.000





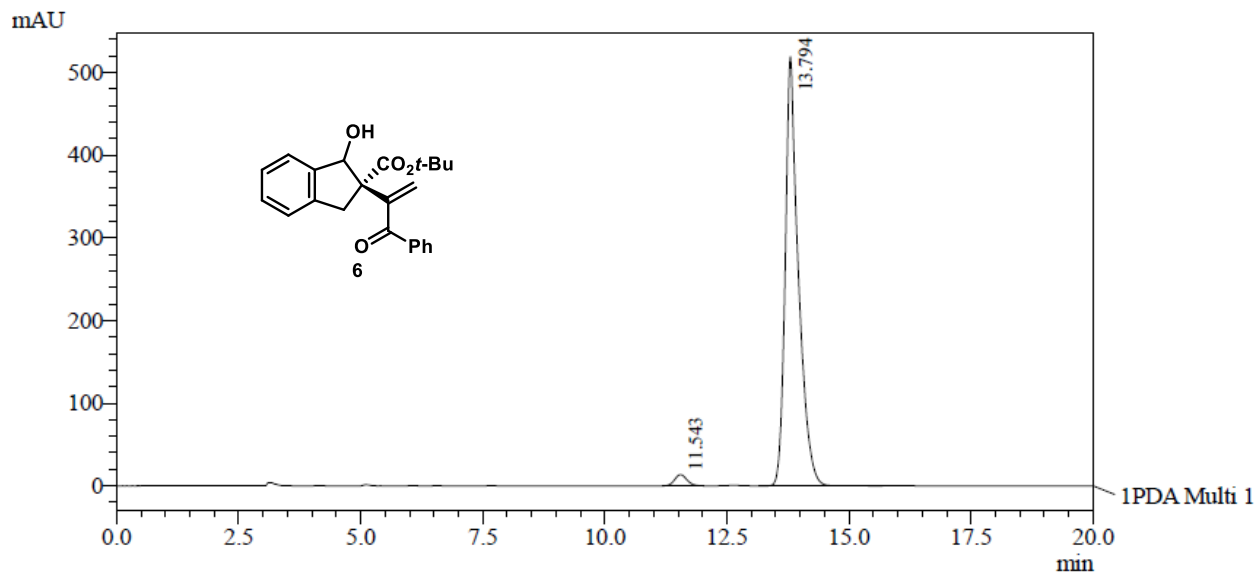
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	11.761	2062410	49.963
2	14.117	2065502	50.037
Total		4127912	100.000

Daicel Chiralpak AD-H column (*n*-Hexane/EtOH = 95:5, 1.0 mL min⁻¹, 20 °C, 254 nm)

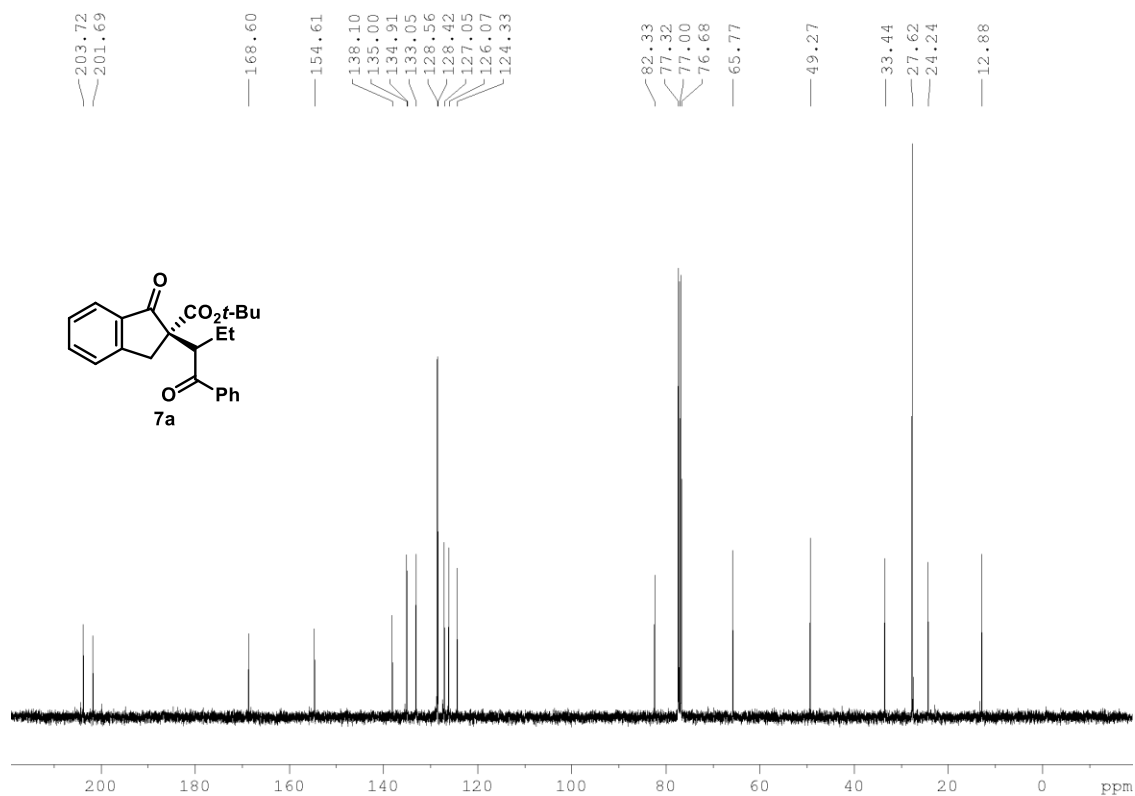
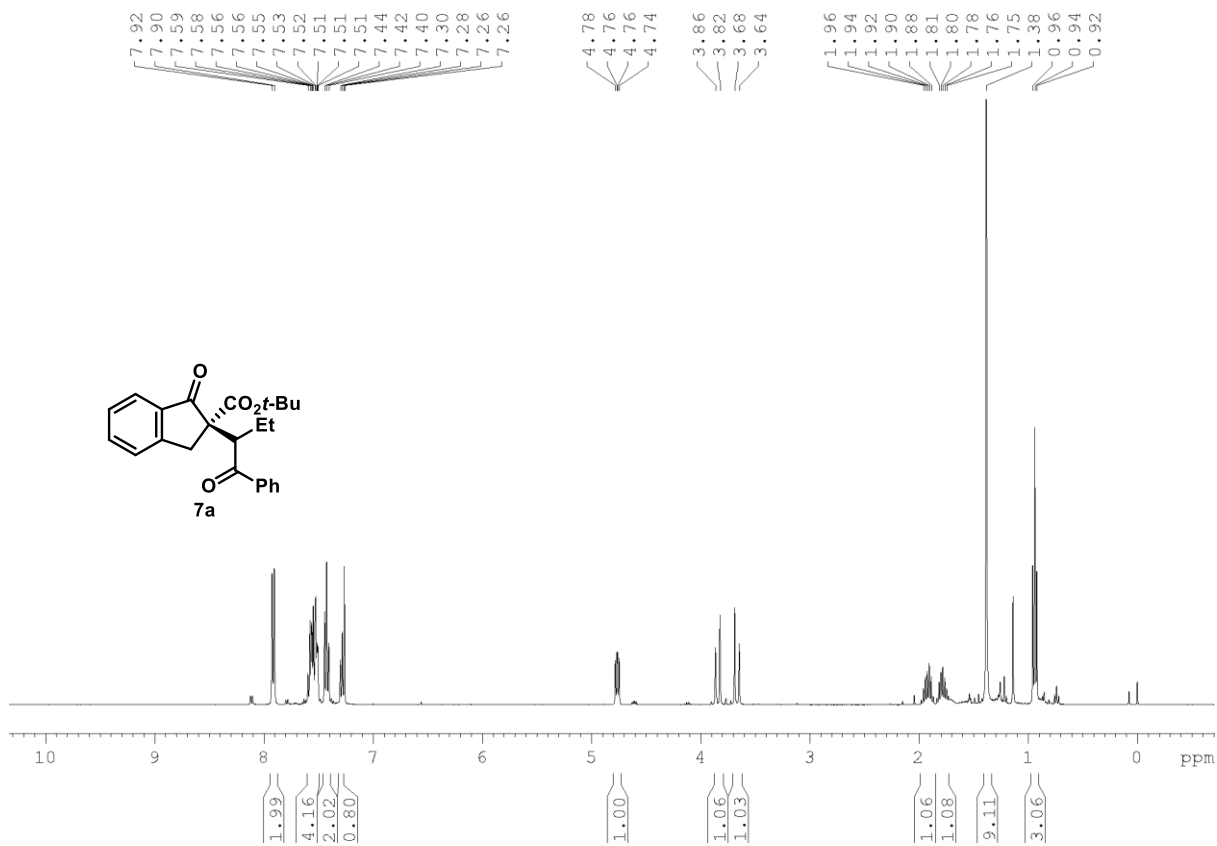


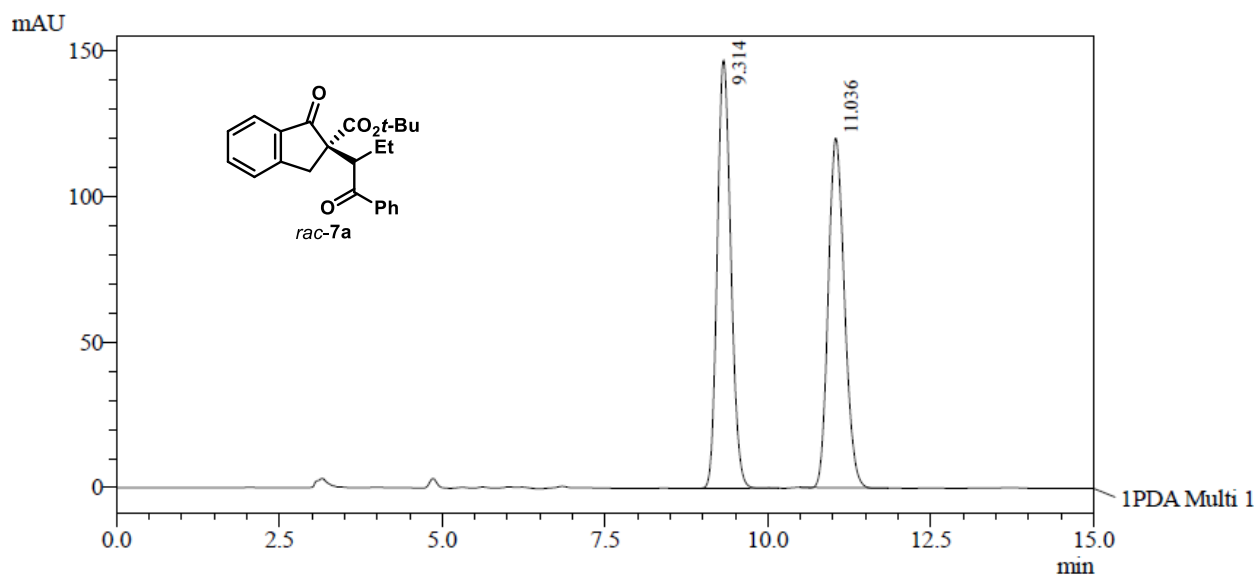
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	11.543	235909	2.365
2	13.794	9739268	97.635
Total		9975177	100.000





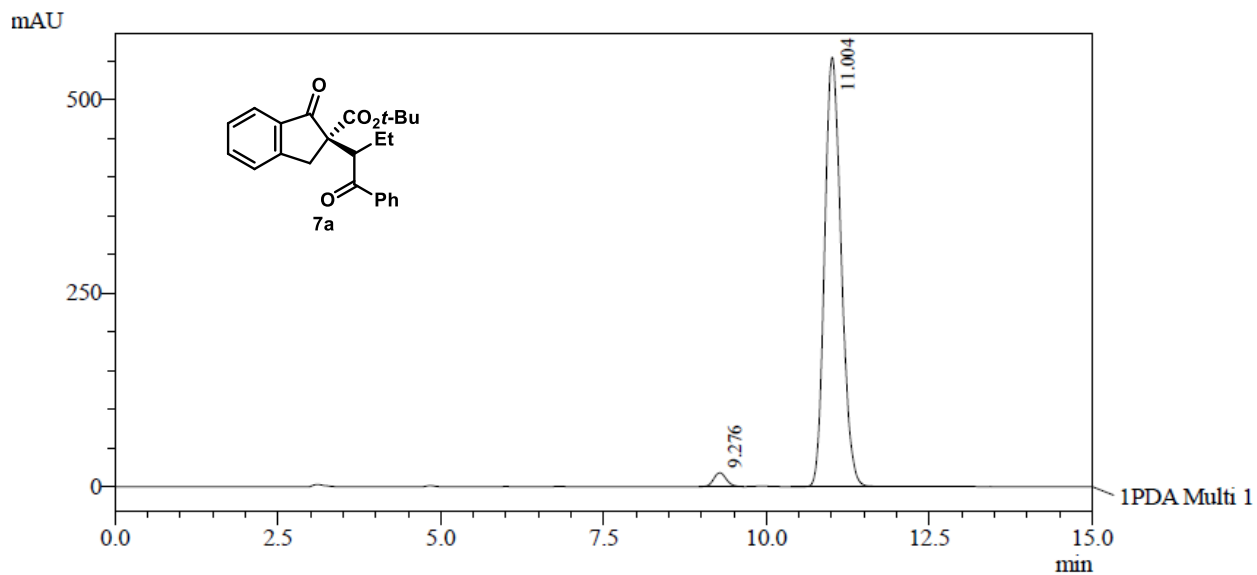
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	9.314	2141246	50.749
2	11.036	2078019	49.251
Total		4219264	100.000

Daicel Chiralpak AD-H column (*n*-Hexane/EtOH = 95:5, 1.0 mL min⁻¹, 20 °C, 254 nm)

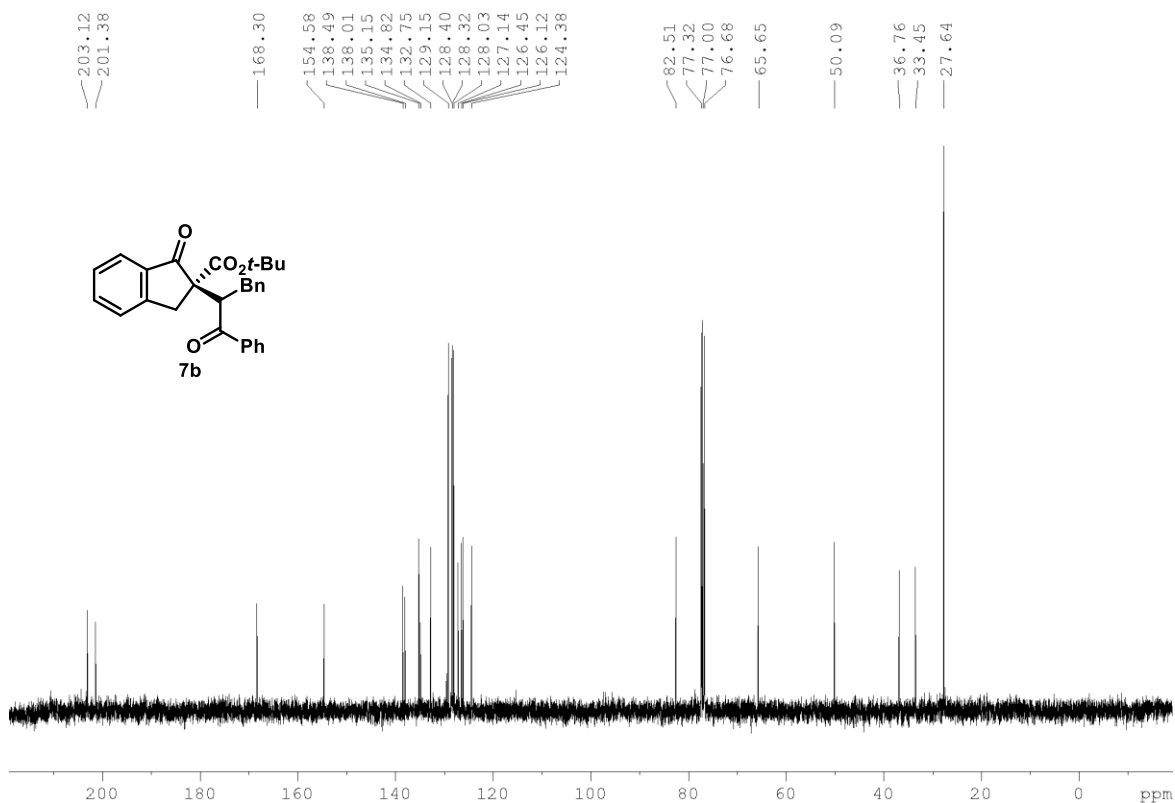
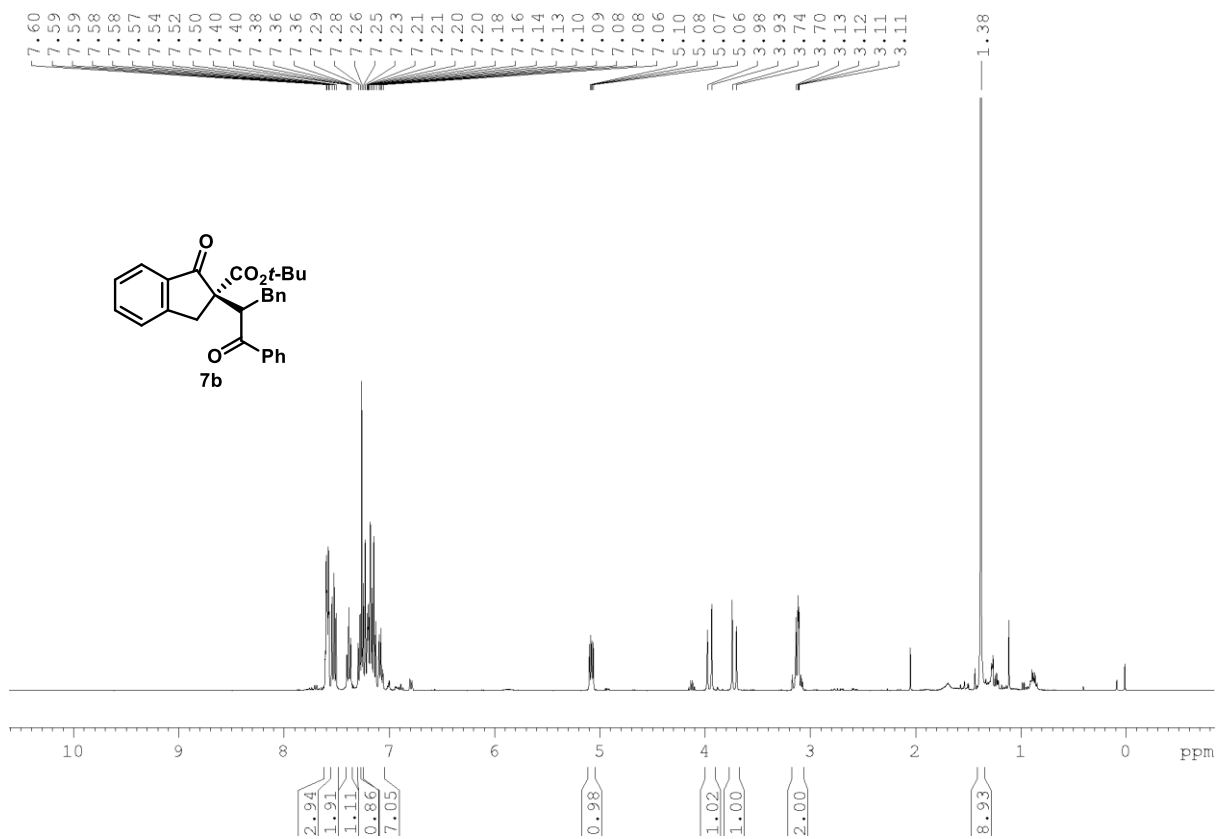


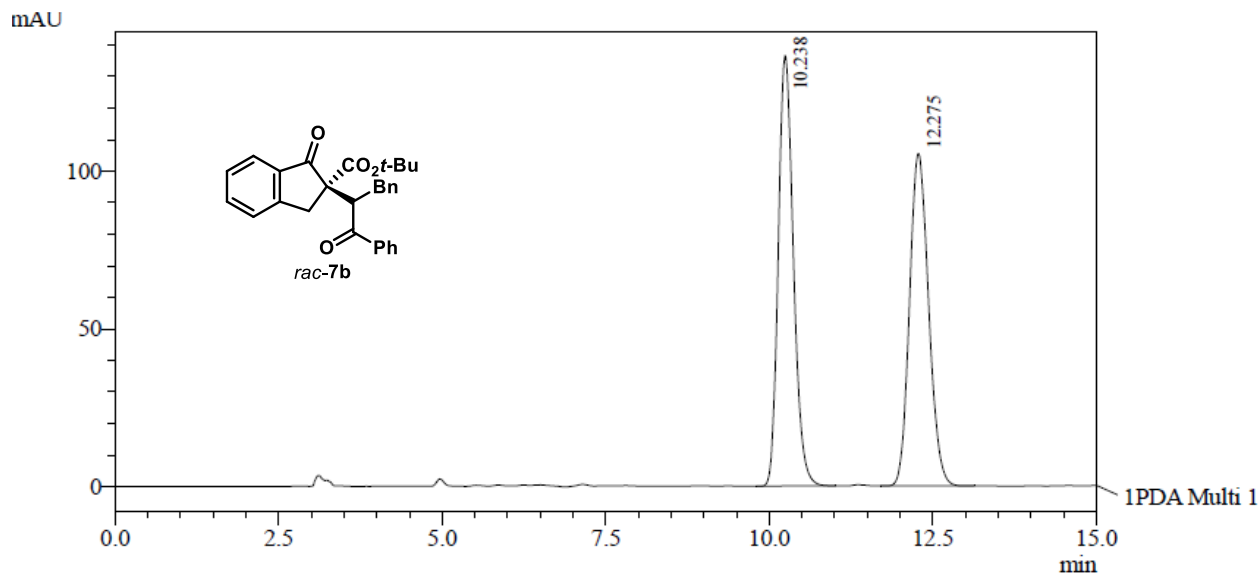
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	9.276	240631	2.389
2	11.004	9833890	97.611
Total		10074520	100.000





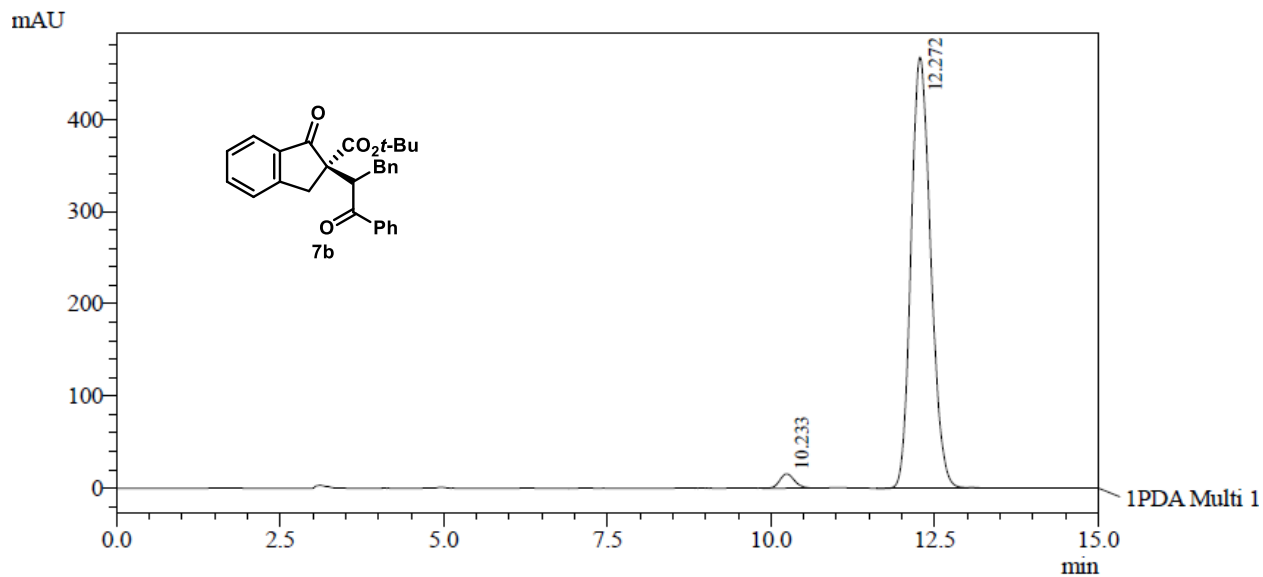
1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	10.238	2193416	50.612
2	12.275	2140394	49.388
Total		4333810	100.000

Daicel Chiralpak AD-H column (*n*-Hexane/IPA = 90:10, 1.0 mL min⁻¹, 20 °C, 254 nm)



1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	10.233	238508	2.379
2	12.272	9788262	97.621
Total		10026770	100.000