

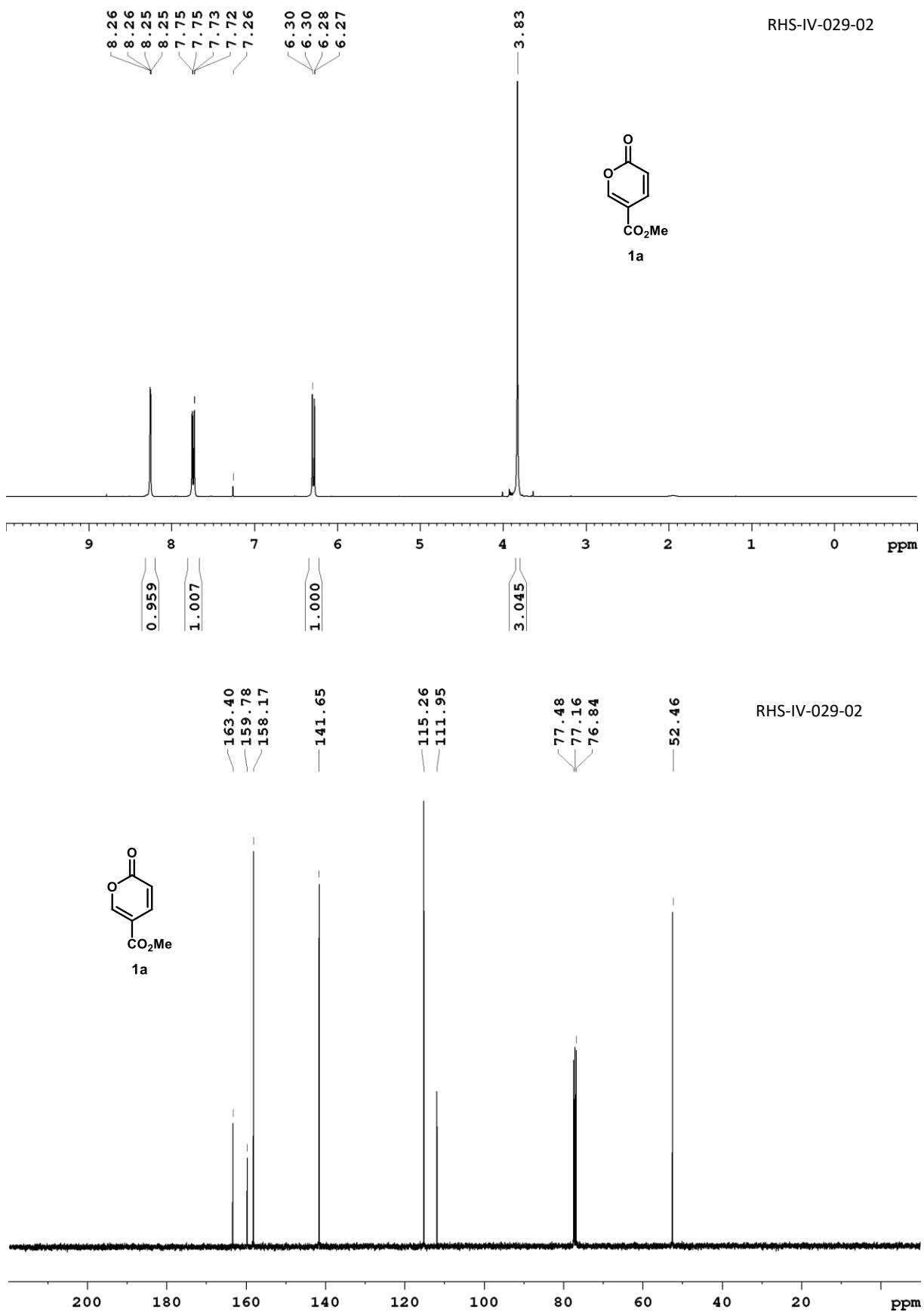
SUPPORTING INFORMATION: PART B

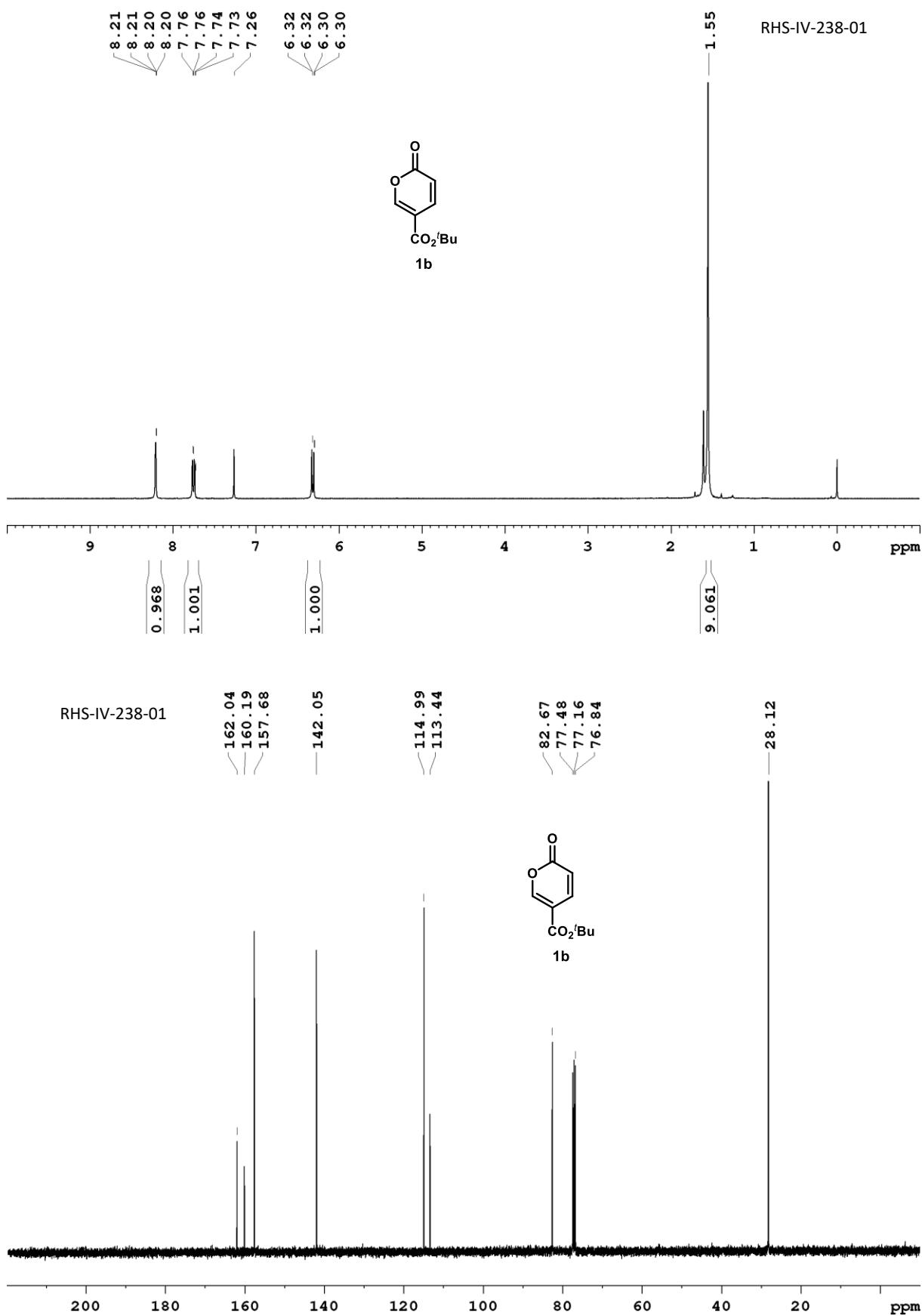
Iridium-catalyzed enantioselective olefinic C(sp²)–H allylic alkylation

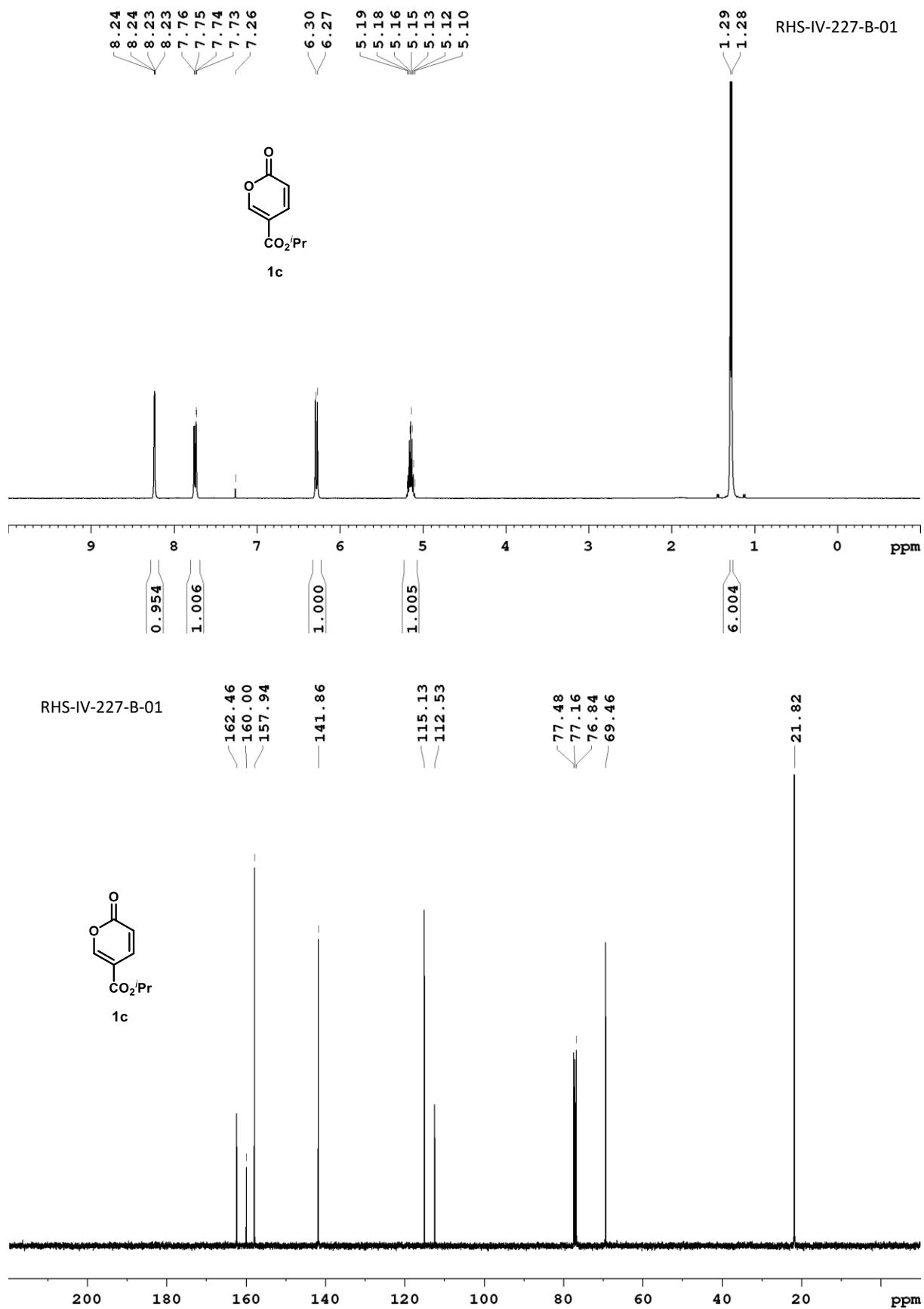
Rahul Sarkar, and Santanu Mukherjee*

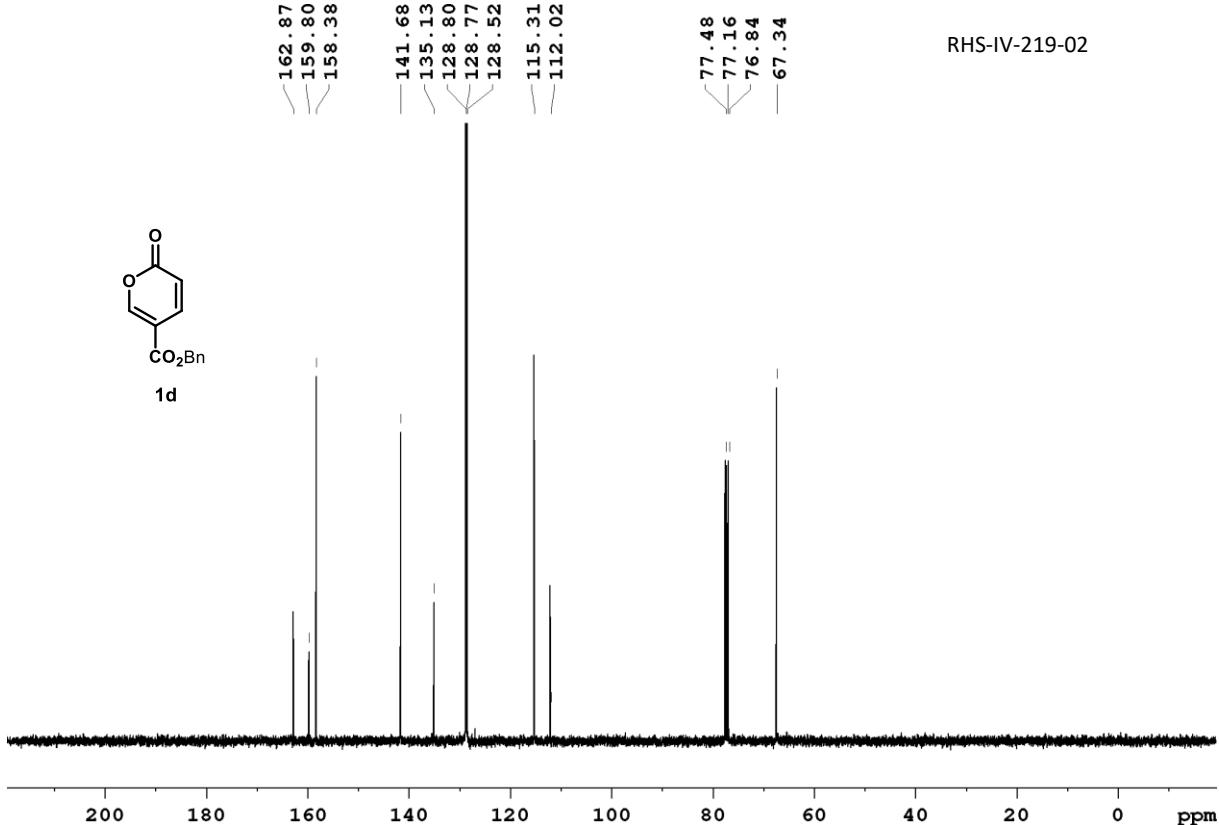
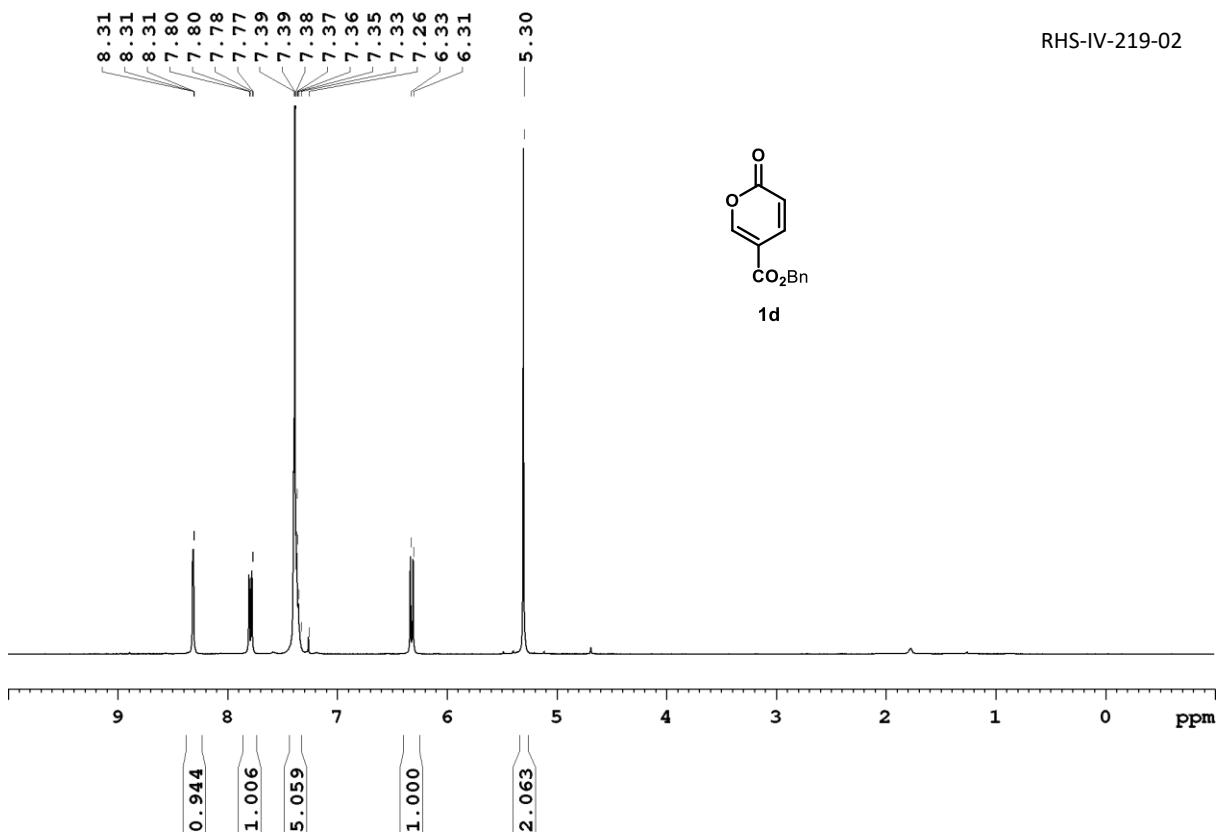
Department of Organic Chemistry, Indian Institute of Science, Bangalore 560 012, INDIA

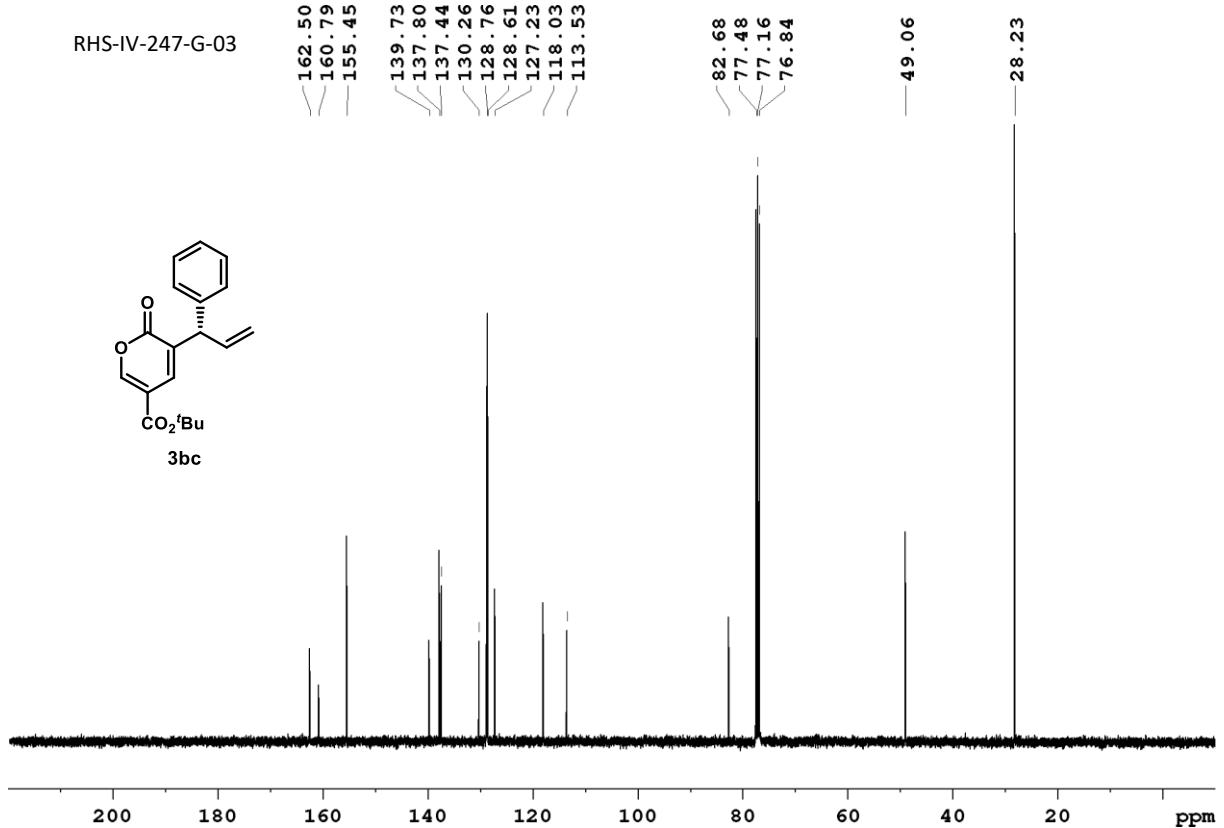
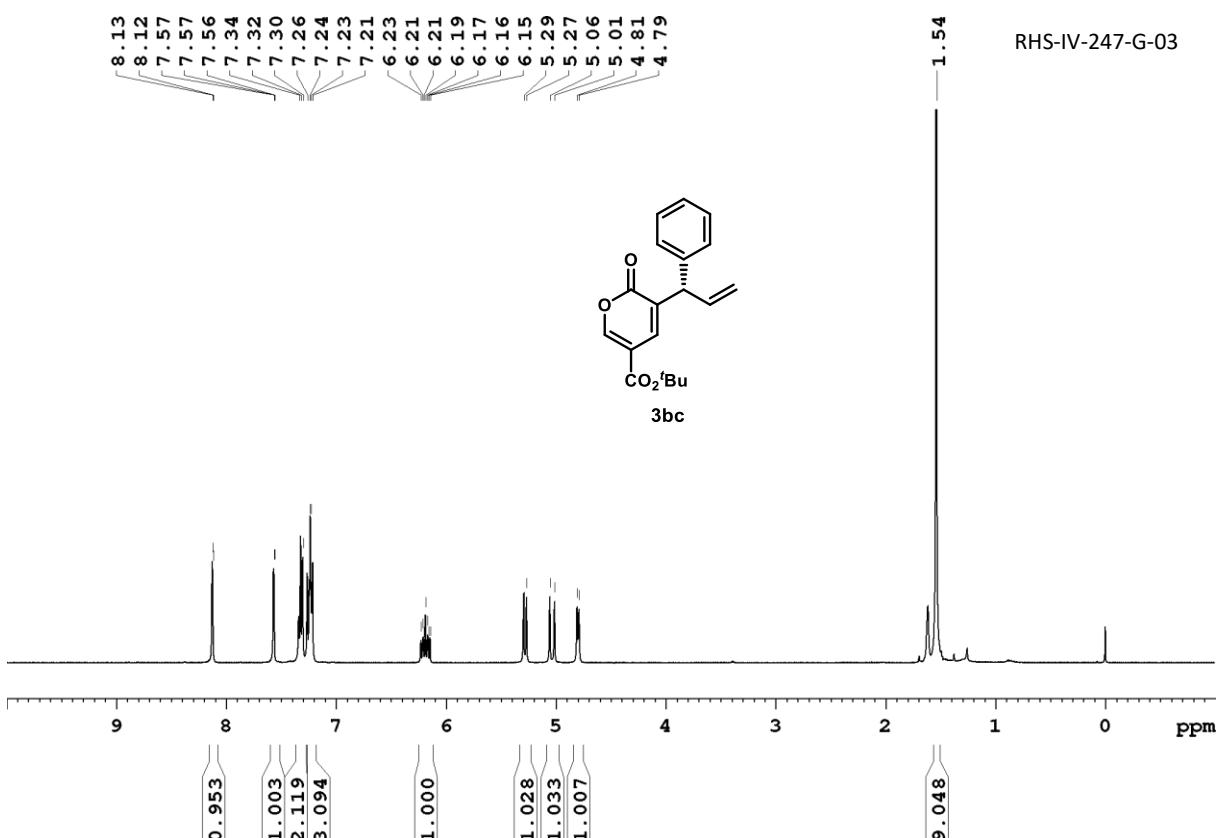
*Corresponding author: E-mail: sm@iisc.ac.in

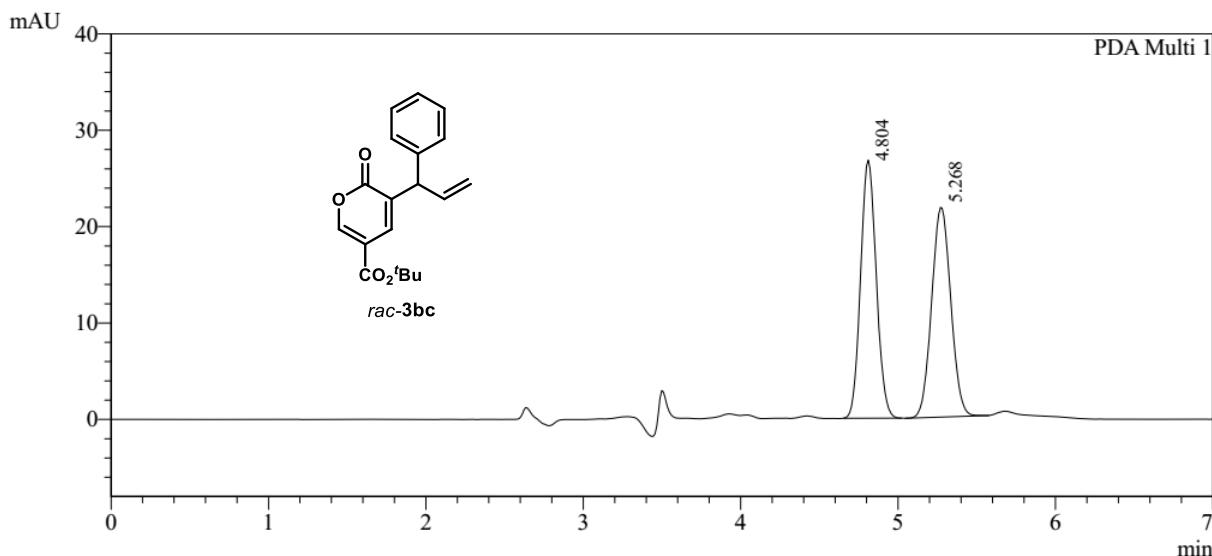










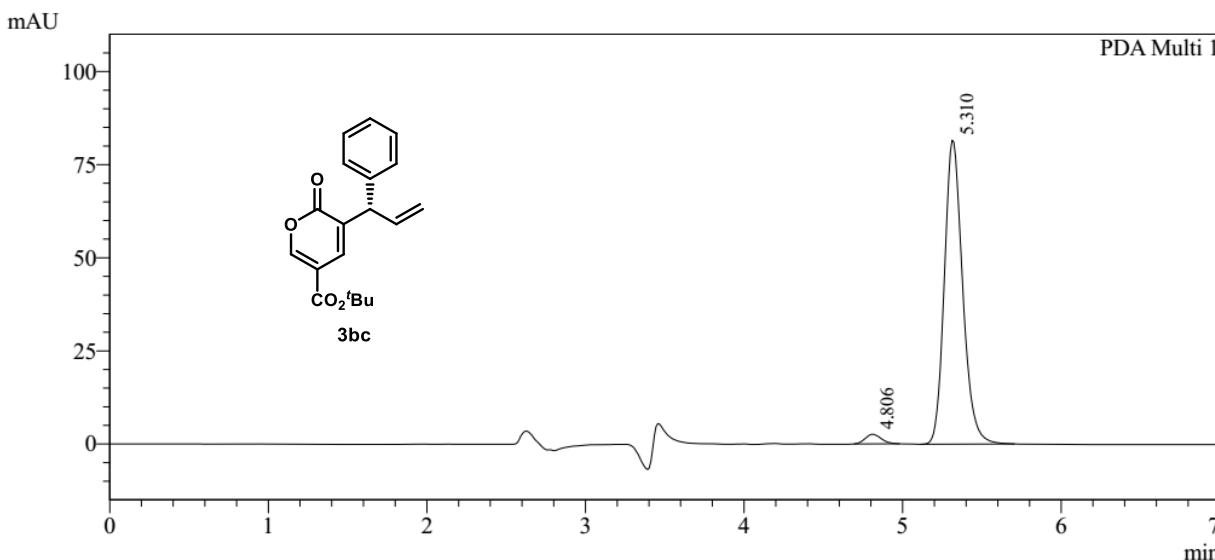


PeakTable

PDA Ch1 290nm 4nm

Peak#	Ret. Time	Area	Area %
1	4.804	185376	50.231
2	5.268	183671	49.769
Total		369047	100.000

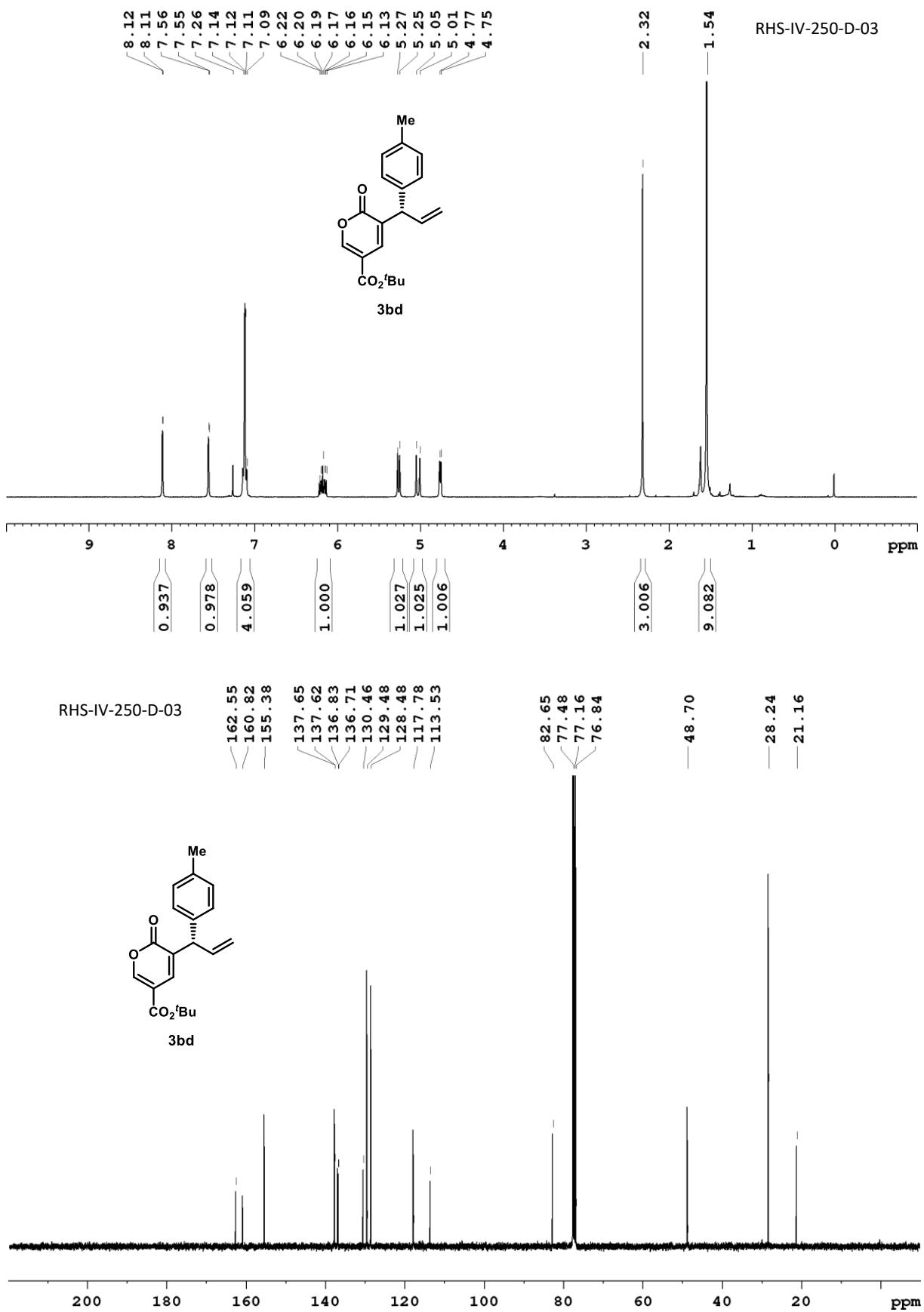
Phenomenex Cellulose-1 column (75:25 *n*-Hexane/EtOH, 1.0 mL/min, 20 °C)

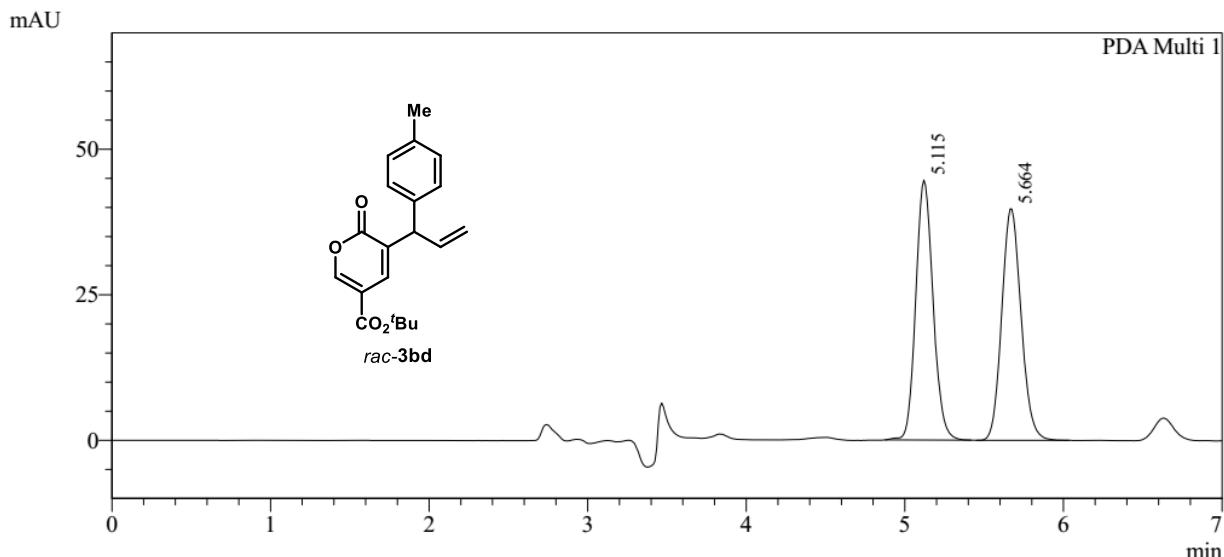


PeakTable

PDA Ch1 290nm 4nm

Peak#	Ret. Time	Area	Area %
1	4.806	18096	2.693
2	5.310	653800	97.307
Total		671896	100.000



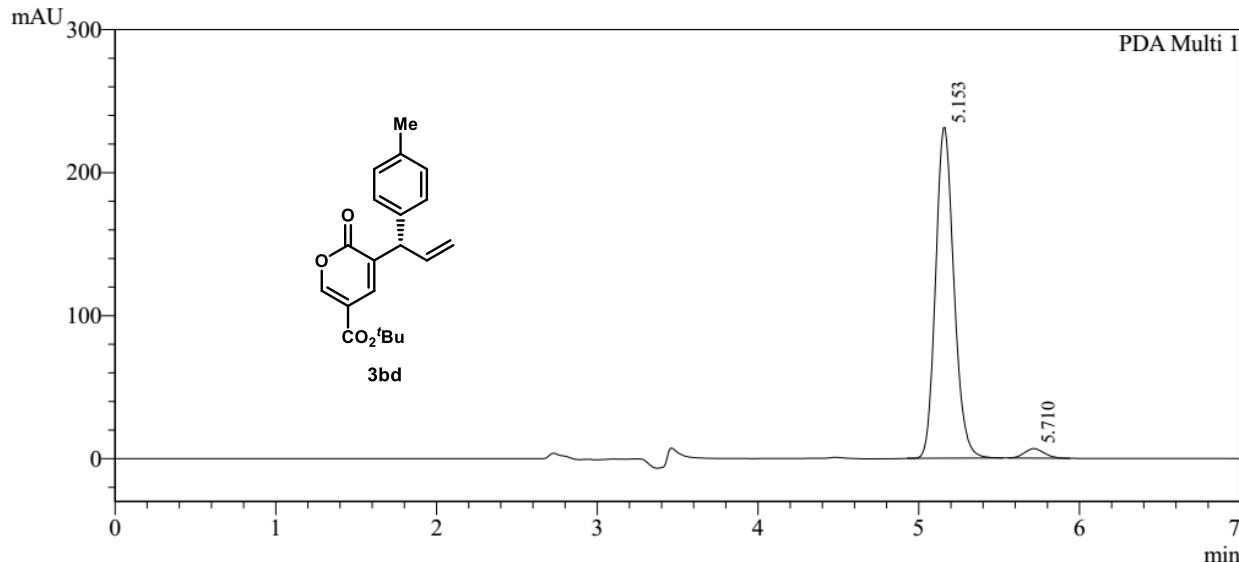


PeakTable

PDA Ch1 252nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.115	338222	50.076
2	5.664	337192	49.924
Total		675414	100.000

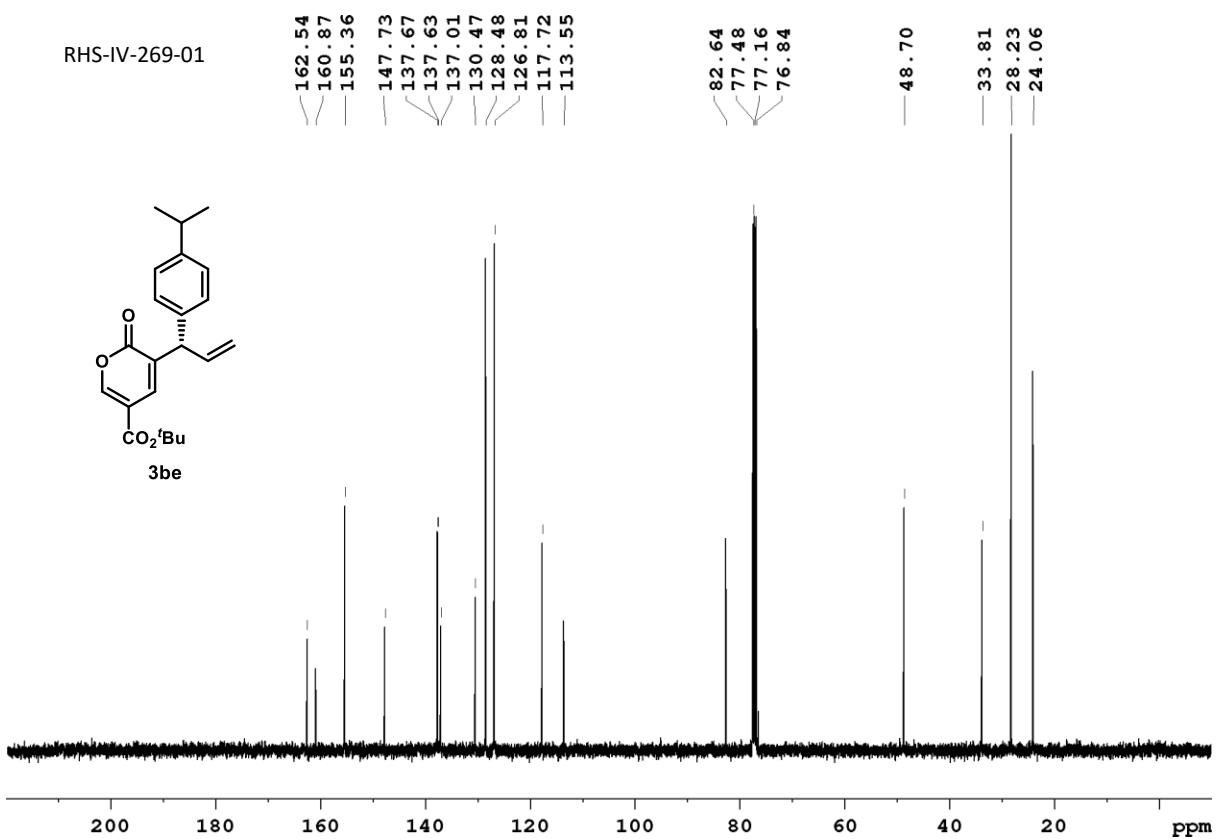
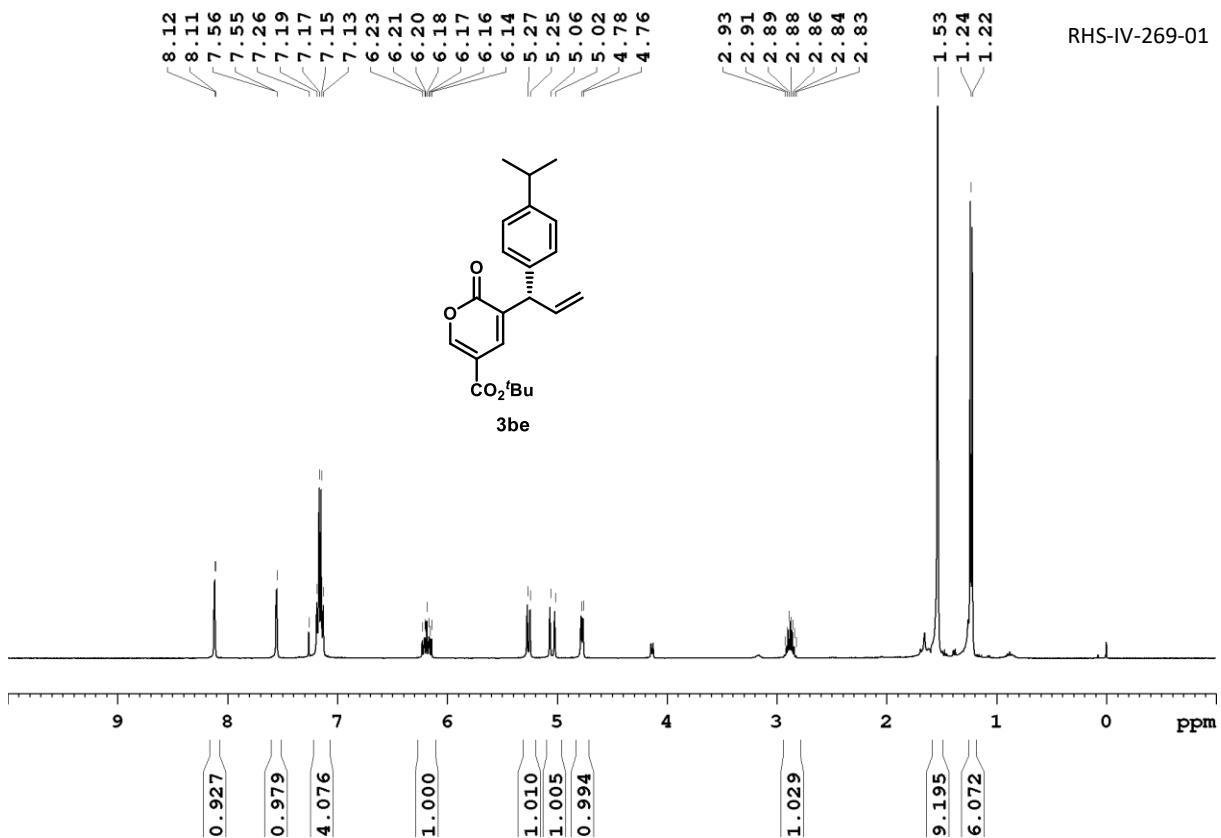
Phenomenex Cellulose-2 column (75:25 *n*-Hexane/EtOH, 1.0 mL/min, 20 °C)

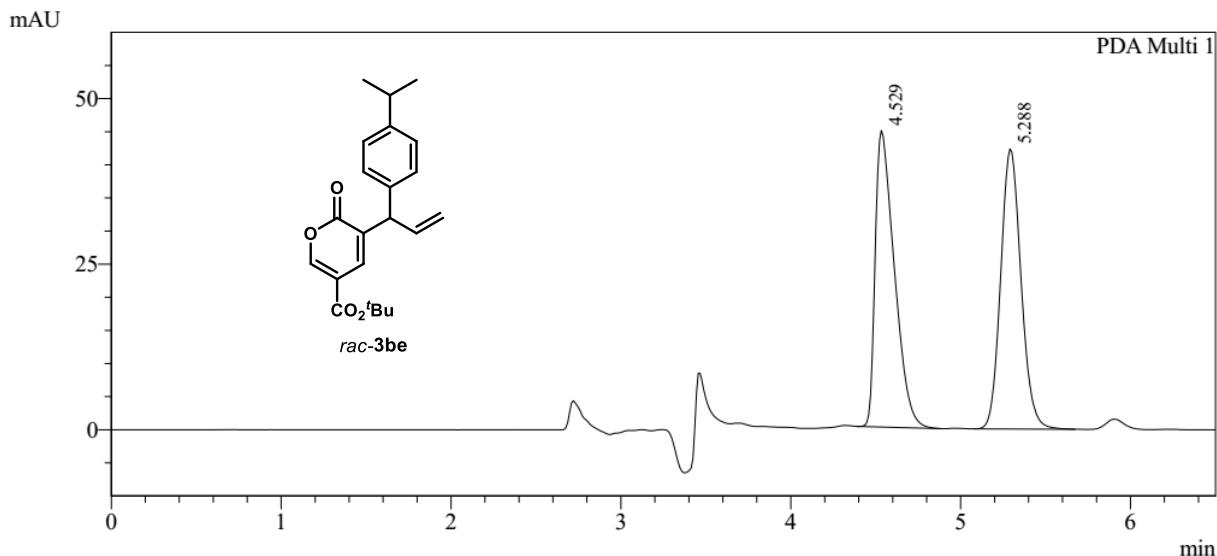


PeakTable

PDA Ch1 252nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.153	1834359	97.015
2	5.710	56438	2.985
Total		1890797	100.000





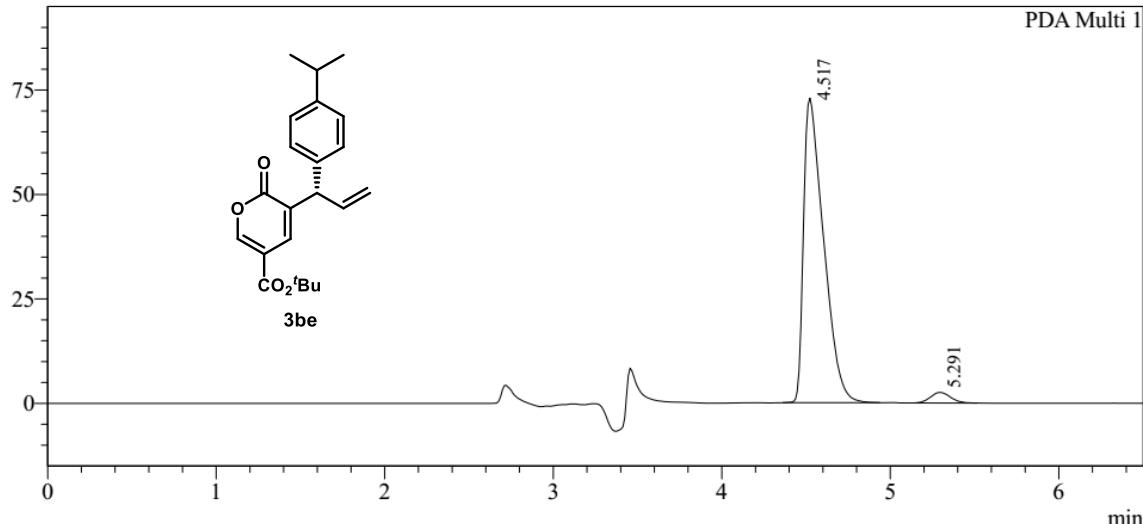
PeakTable

PDA Ch1 252nm 4nm

Peak#	Ret. Time	Area	Area %
1	4.529	350483	49.914
2	5.288	351686	50.086
Total		702169	100.000

Phenomenex Cellulose-2 column (75:25 n-Hexane/EtOH, 1.0 mL/min, 20 °C)

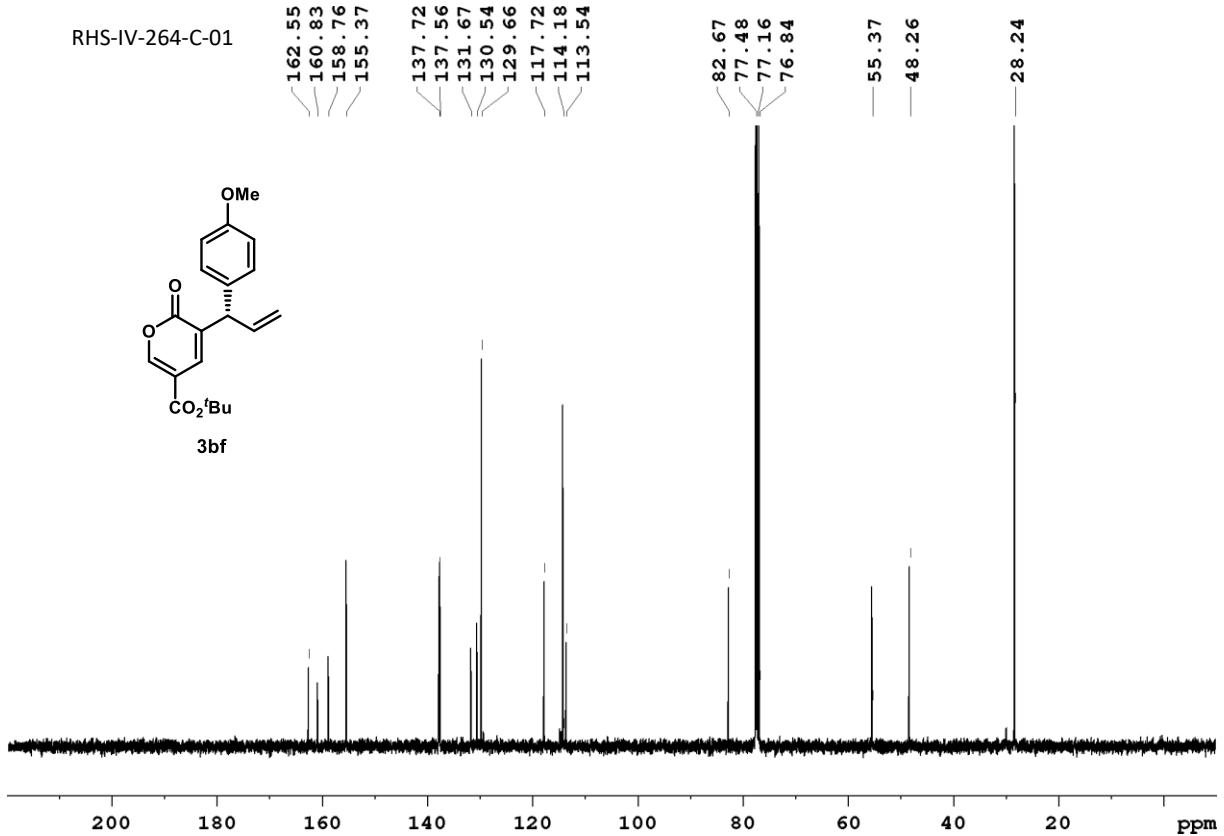
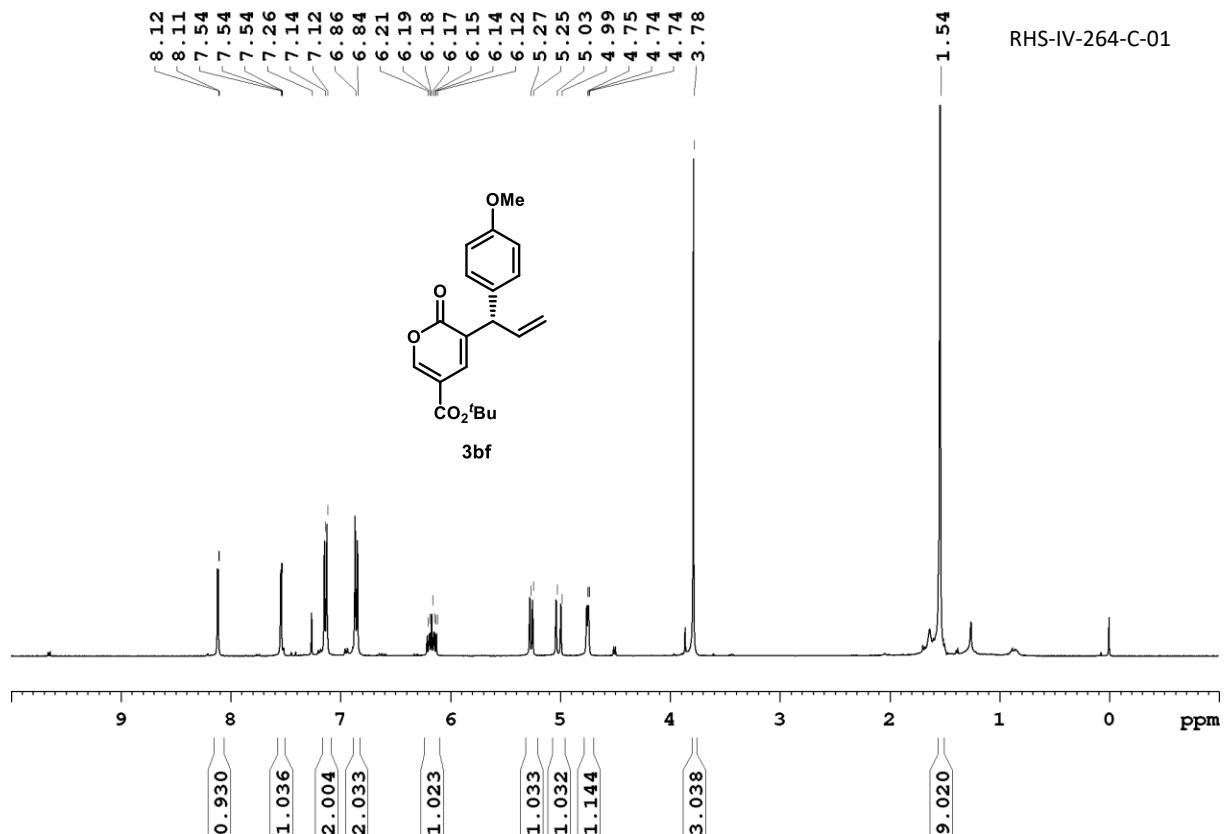
mAU

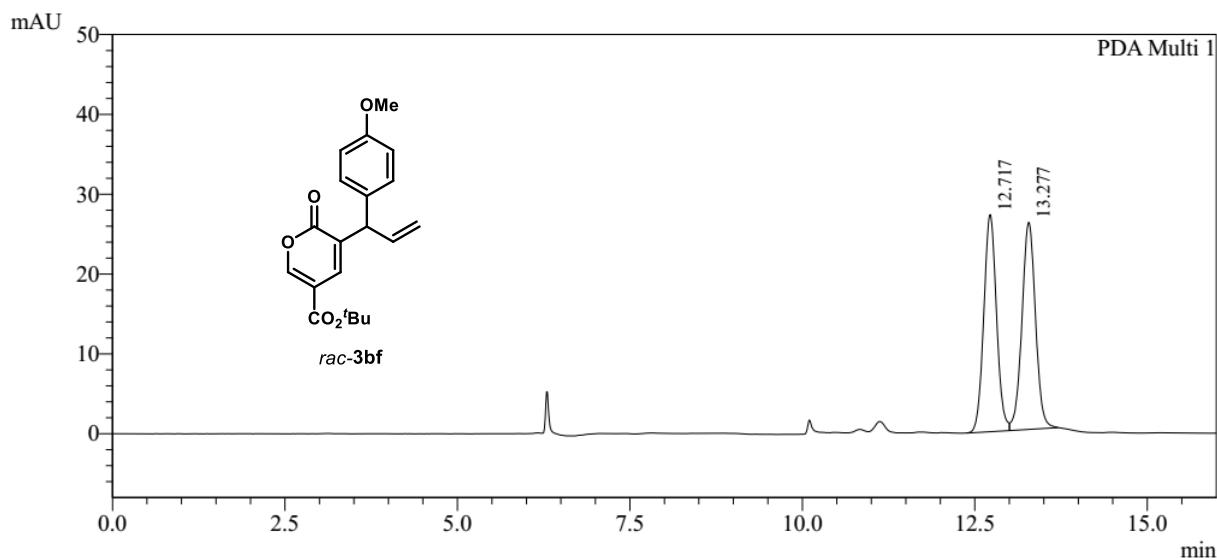


PeakTable

PDA Ch1 252nm 4nm

Peak#	Ret. Time	Area	Area %
1	4.517	602412	96.606
2	5.291	21164	3.394
Total		623576	100.000



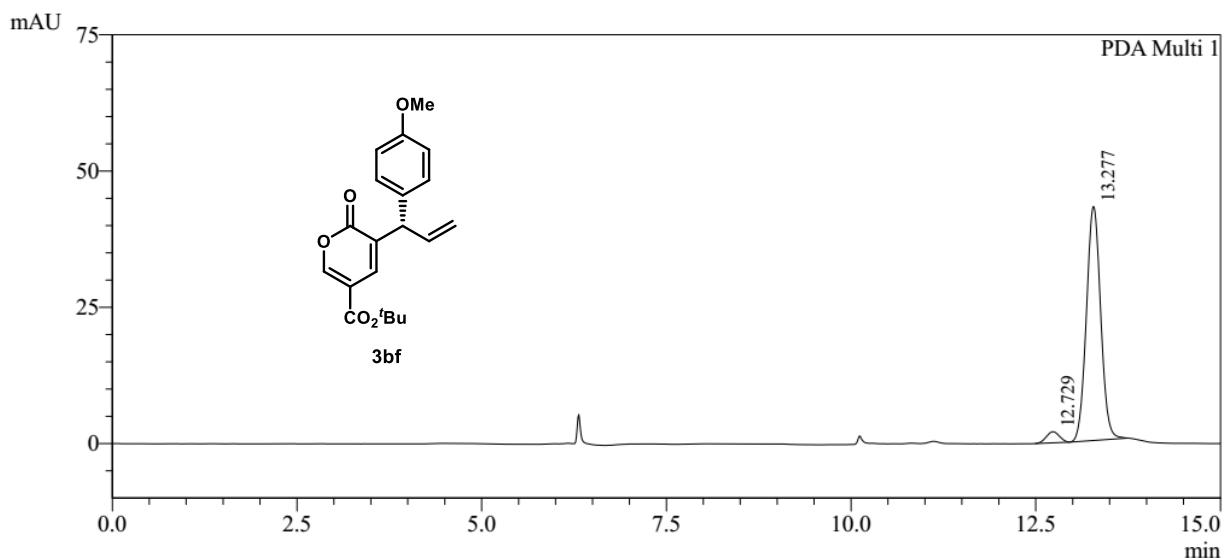


PeakTable

PDA Ch1 295nm 4nm

Peak#	Ret. Time	Area	Area %
1	12.717	349177	49.648
2	13.277	354135	50.352
Total		703313	100.000

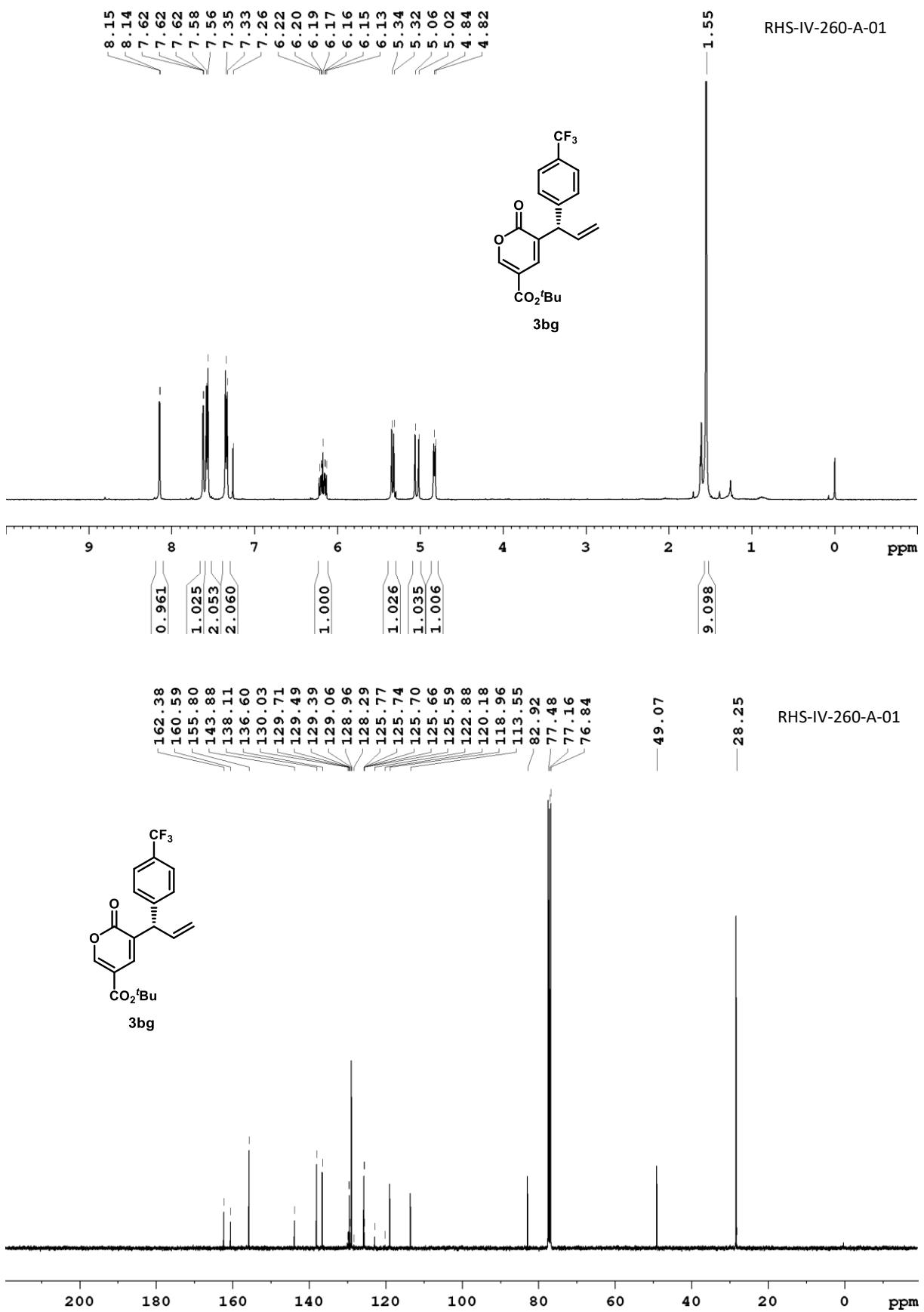
Daicel Chiraldpak IB column (95:5 *n*-Hexane/EtOH, 0.5 mL/min, 20 °C)

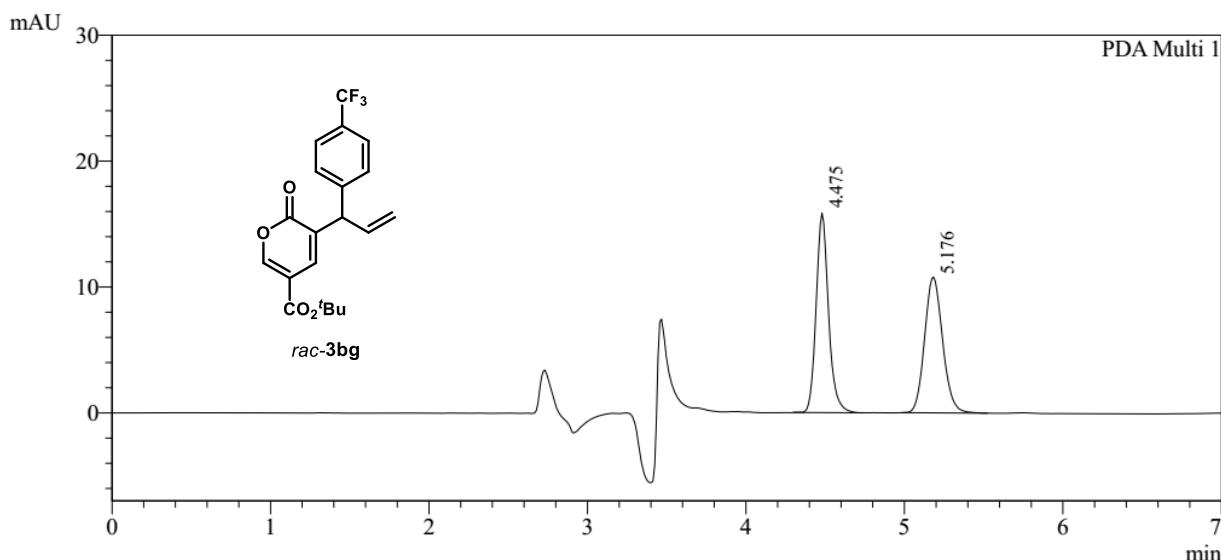


PeakTable

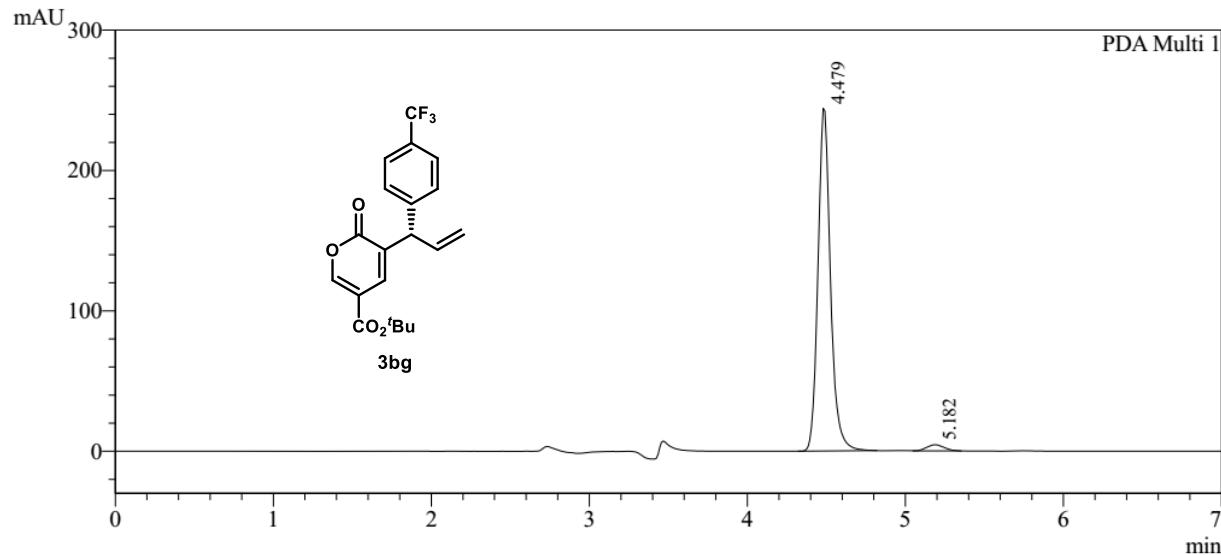
PDA Ch1 295nm 4nm

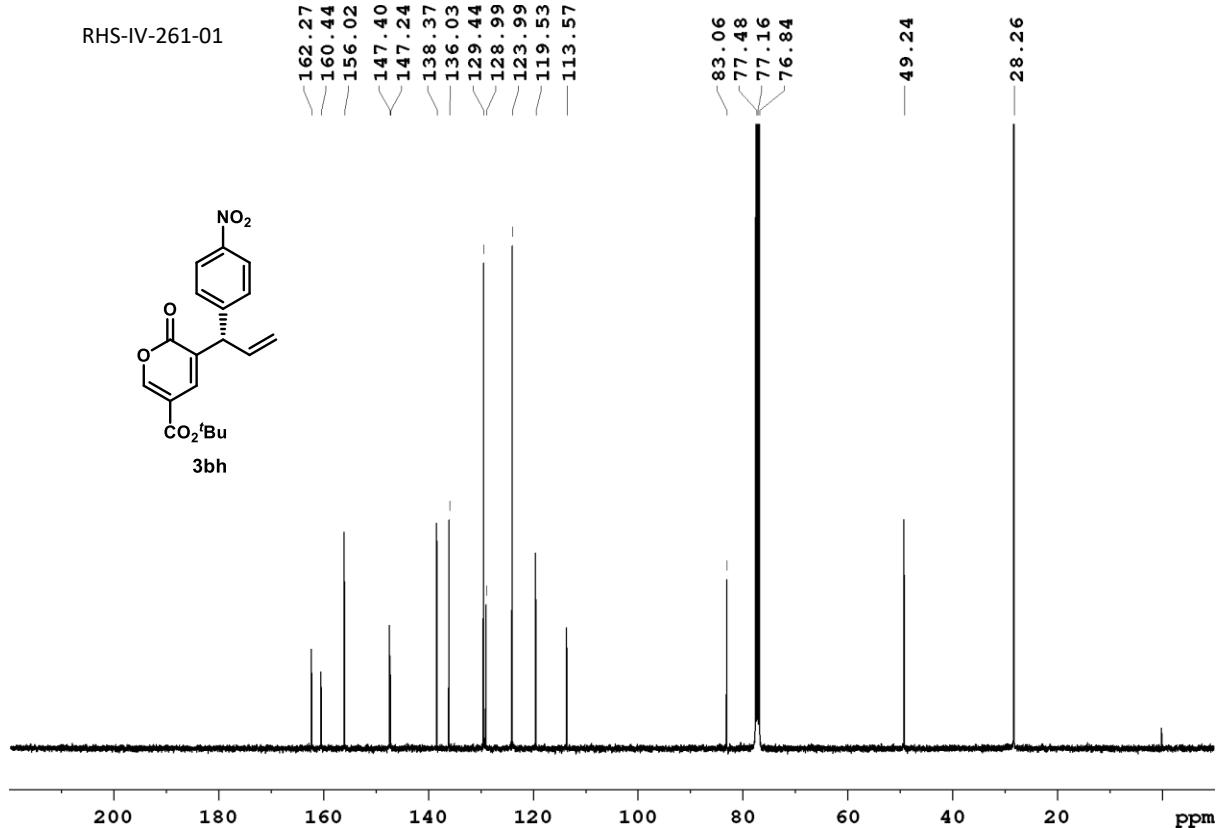
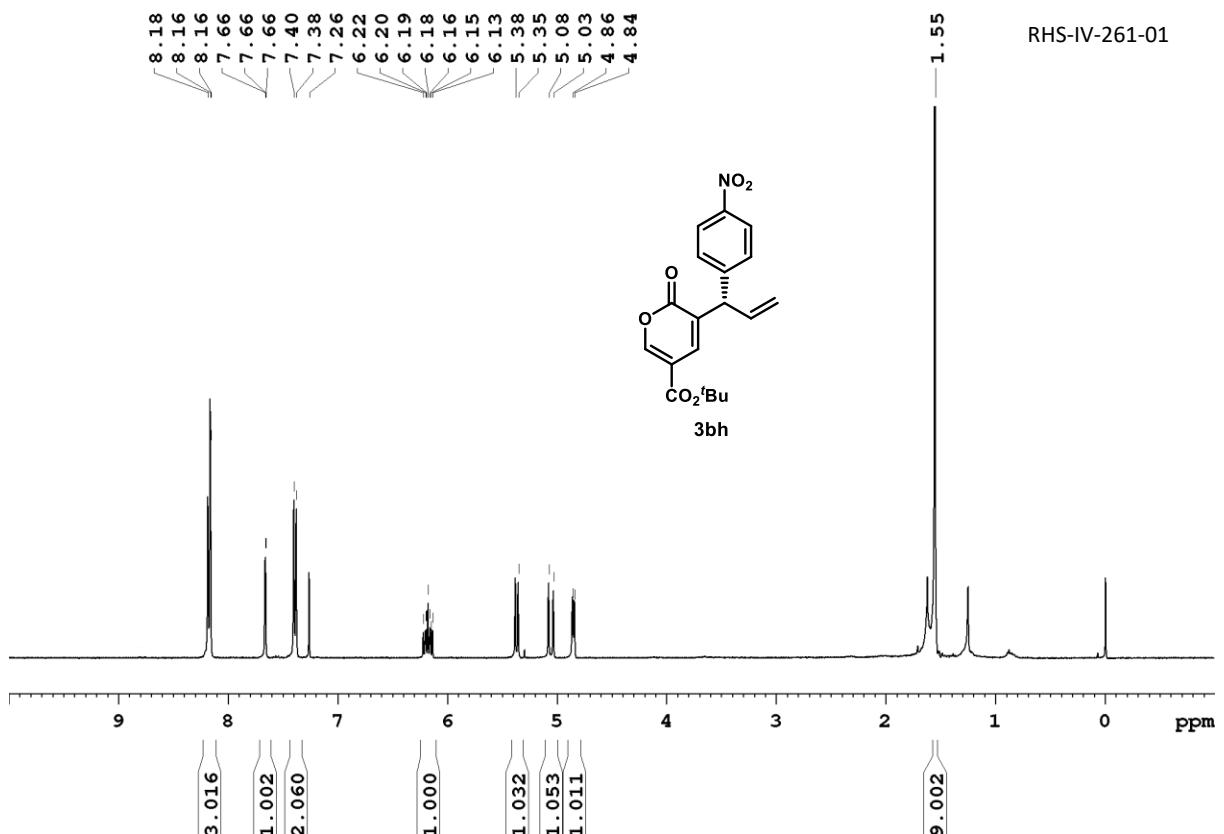
Peak#	Ret. Time	Area	Area %
1	12.729	25060	4.180
2	13.277	574465	95.820
Total		599526	100.000

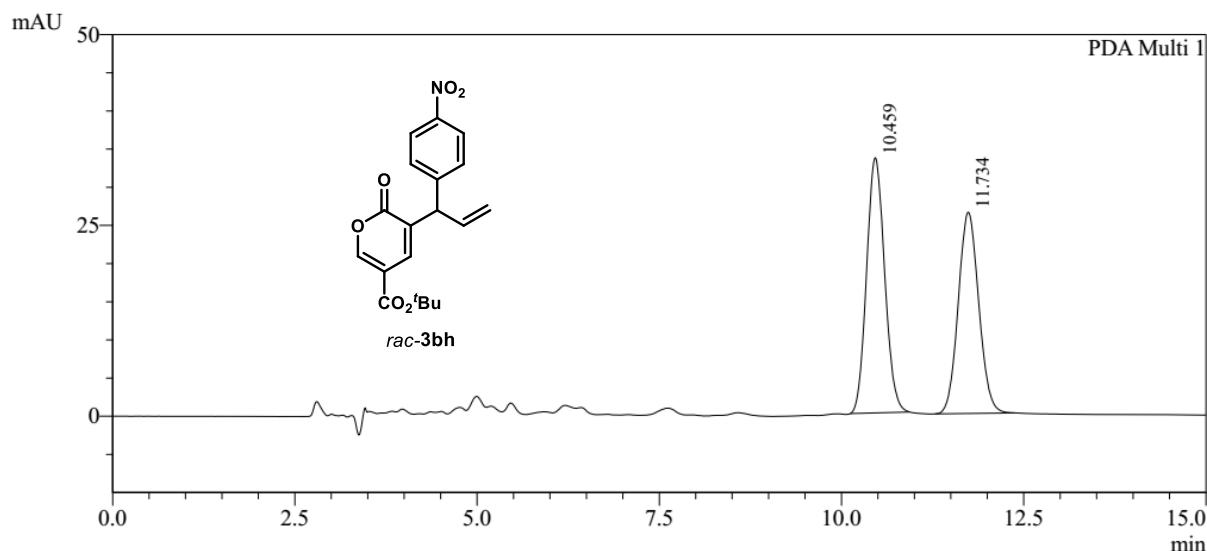




Phenomenex Cellulose-2 column (75:25 *n*-Hexane/EtOH, 1.0 mL/min, 20 °C)





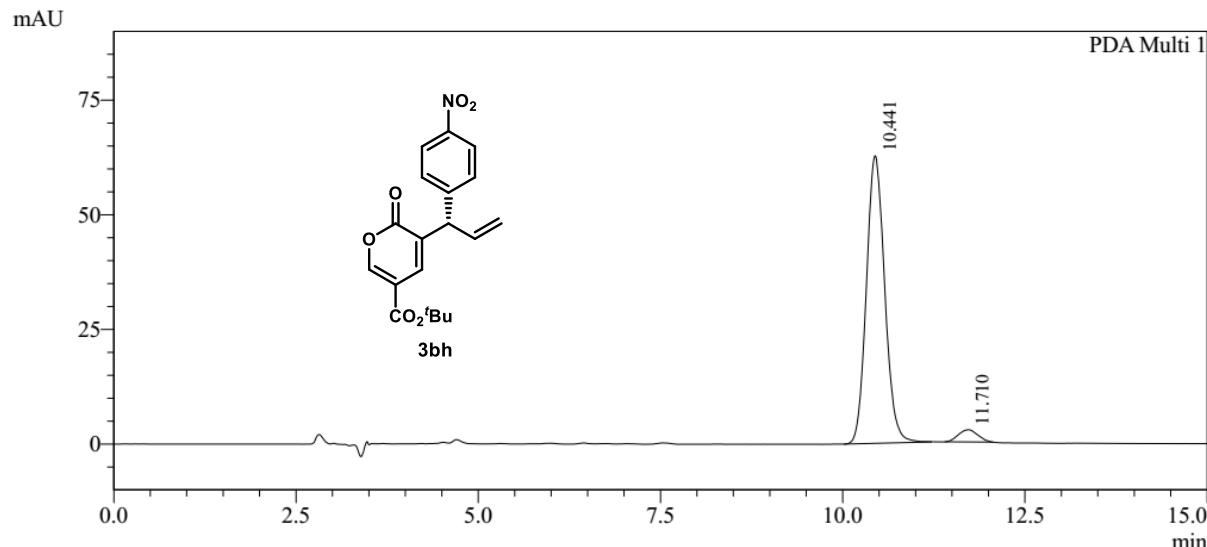


PeakTable

PDA Ch1 252nm 4nm

Peak#	Ret. Time	Area	Area %
1	10.459	575144	52.646
2	11.734	517326	47.354
Total		1092470	100.000

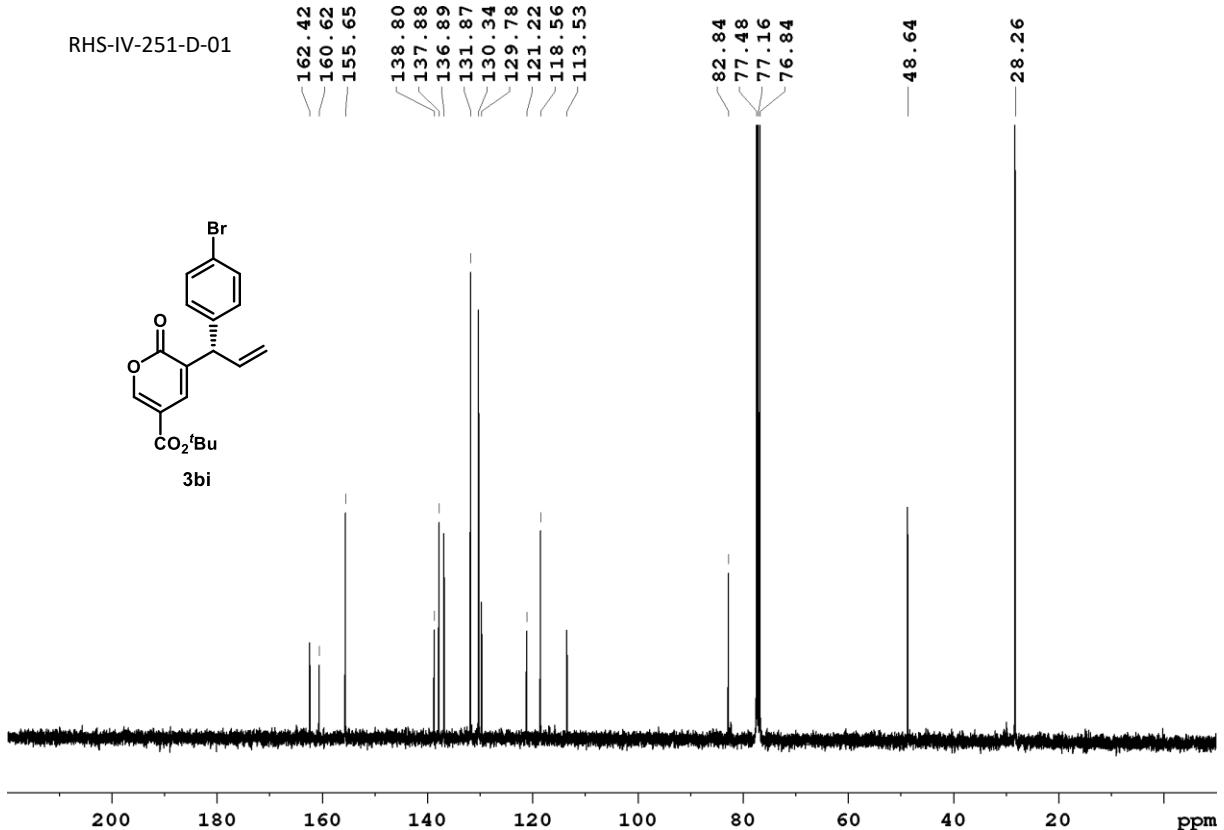
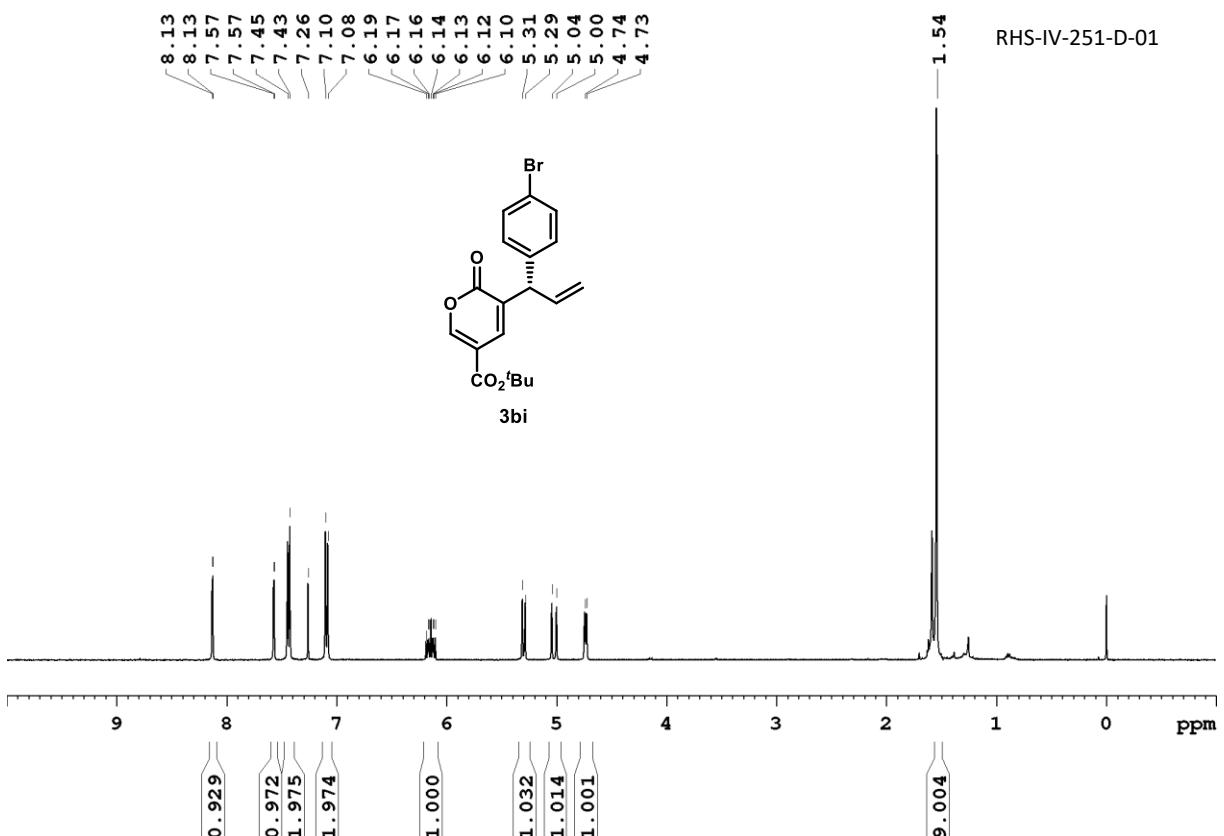
Phenomenex Cellulose-2 column (75:25 *n*-Hexane/EtOH, 1.0 mL/min, 20 °C)

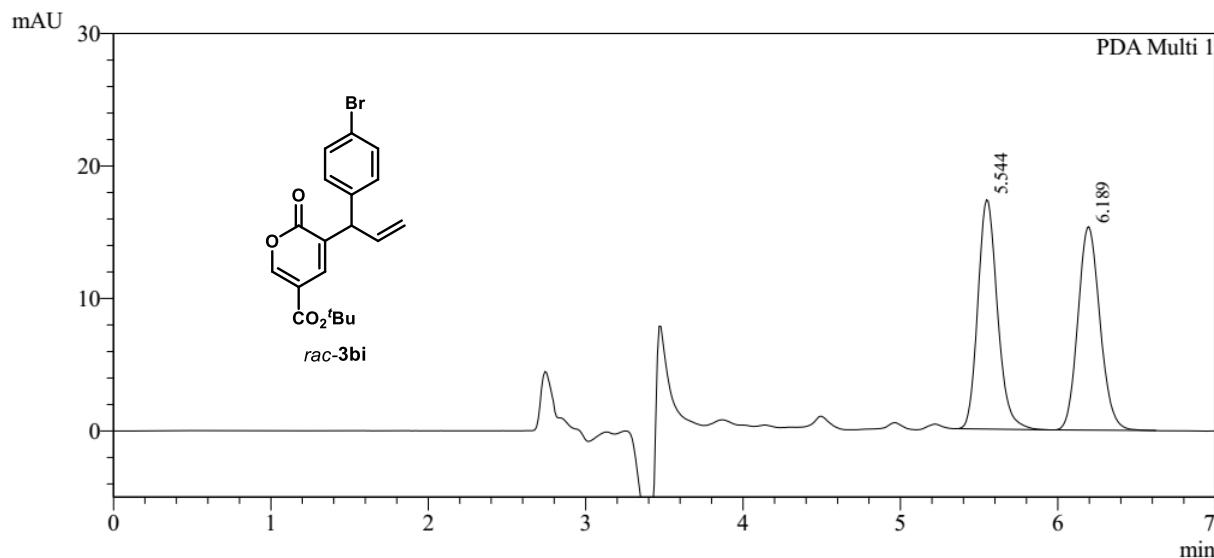


PeakTable

PDA Ch1 252nm 4nm

Peak#	Ret. Time	Area	Area %
1	10.441	1097237	95.681
2	11.710	49533	4.319
Total		1146770	100.000



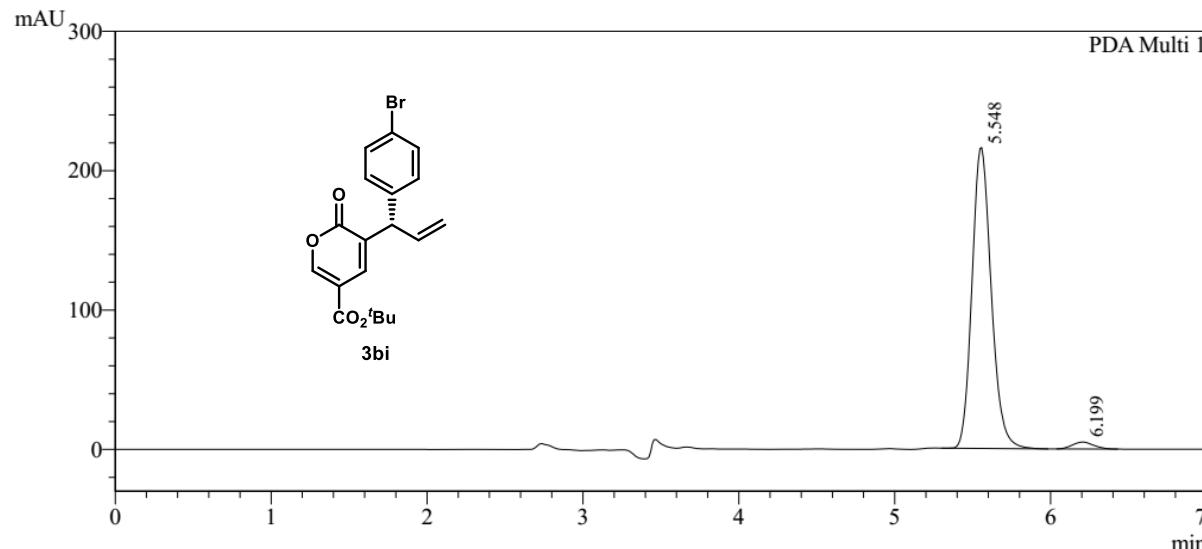


PeakTable

PDA Ch1 247nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.544	150239	50.141
2	6.189	149395	49.859
Total		299633	100.000

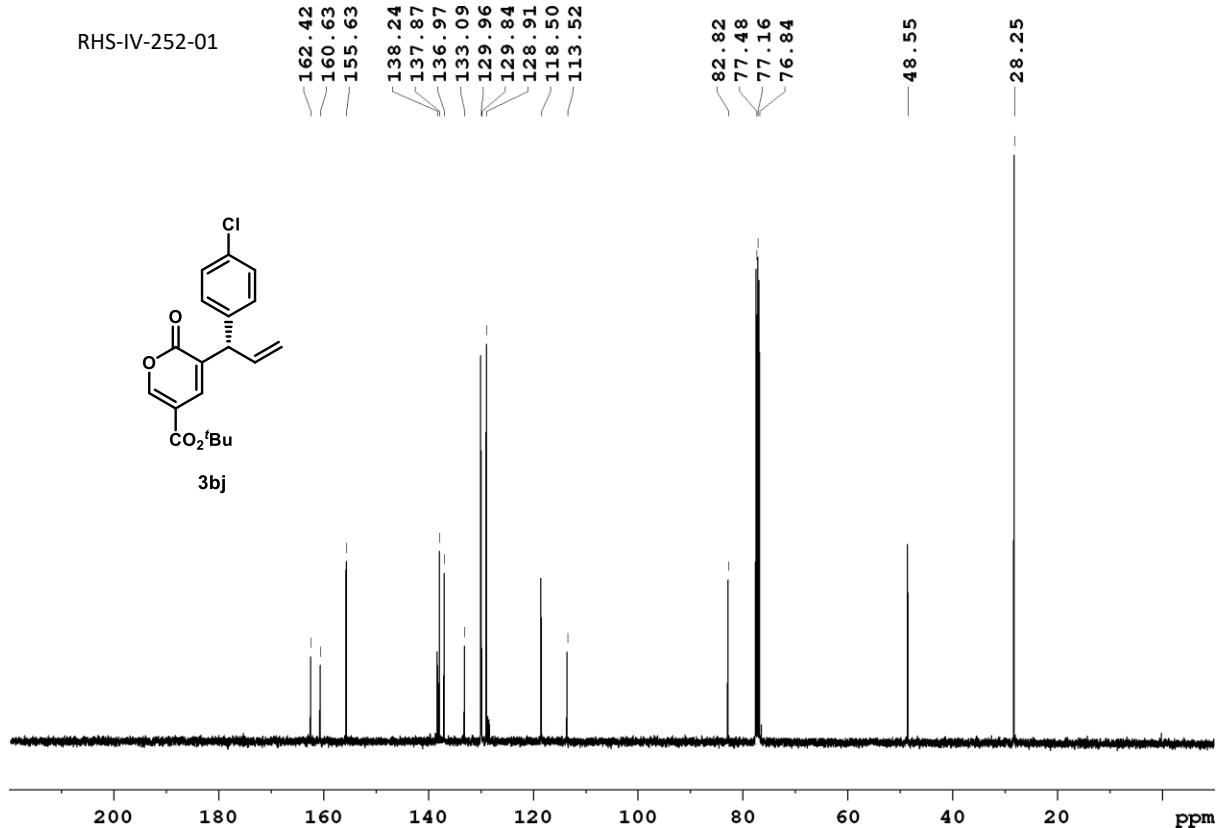
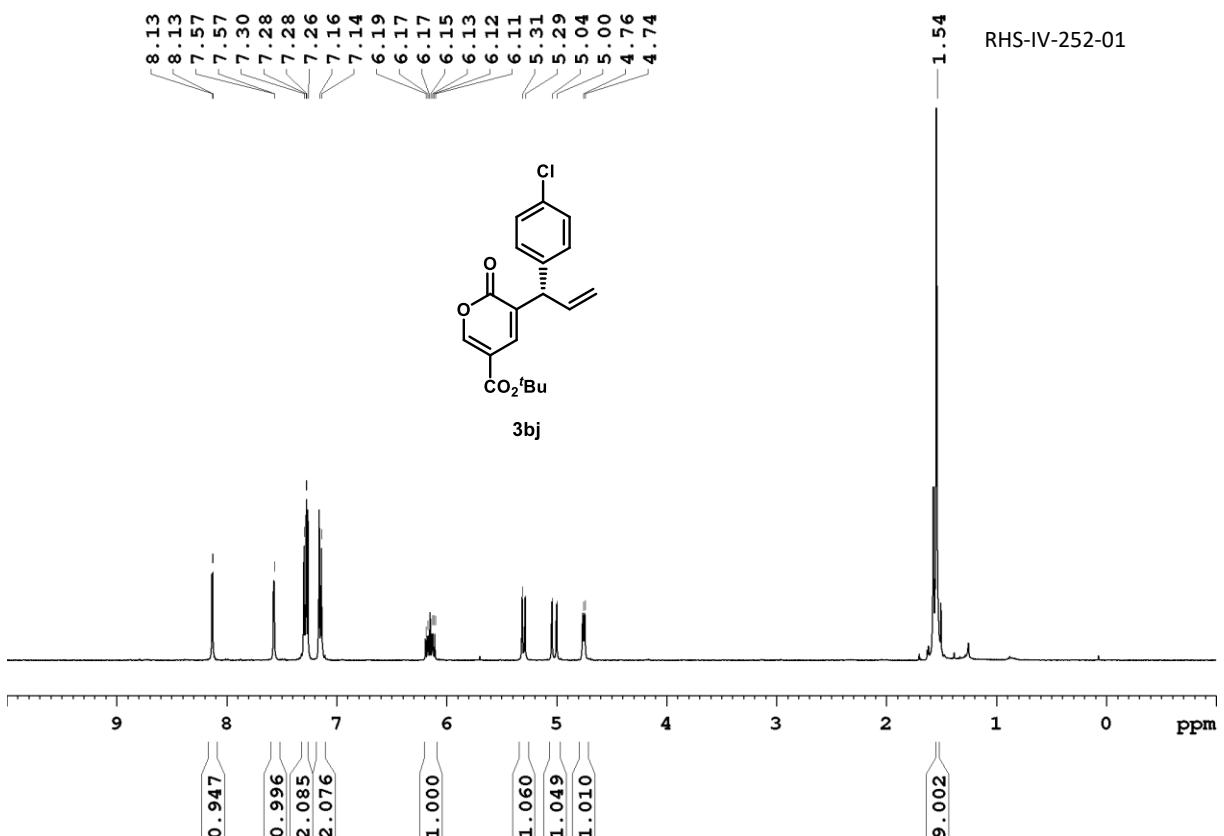
Phenomenex Cellulose-2 column (75:25 *n*-Hexane/EtOH, 1.0 mL/min, 20 °C)

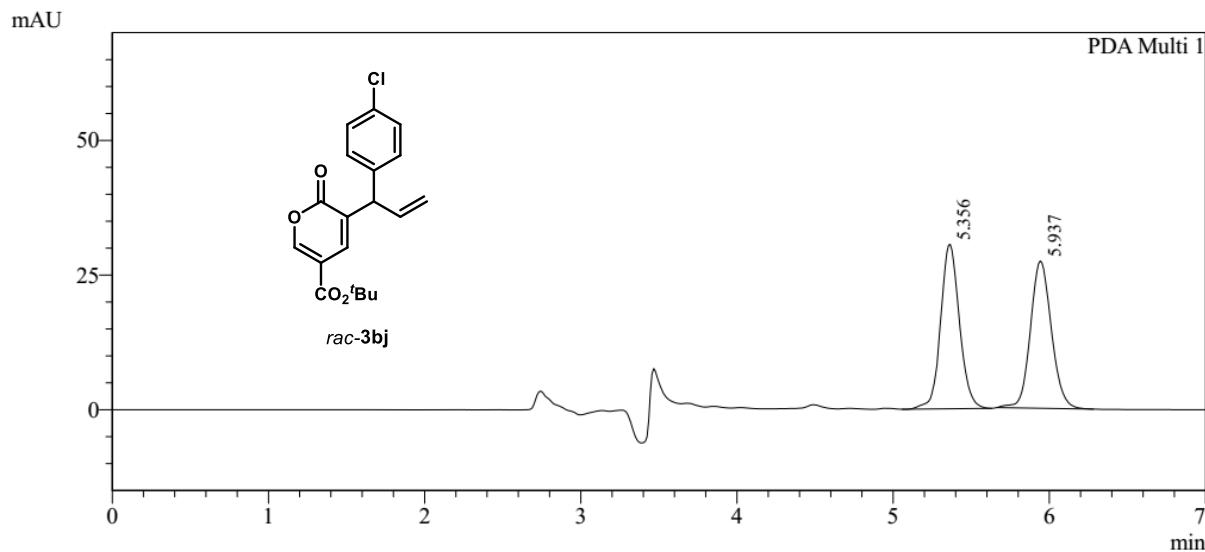


PeakTable

PDA Ch1 247nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.548	1852617	97.547
2	6.199	46584	2.453
Total		1899201	100.000



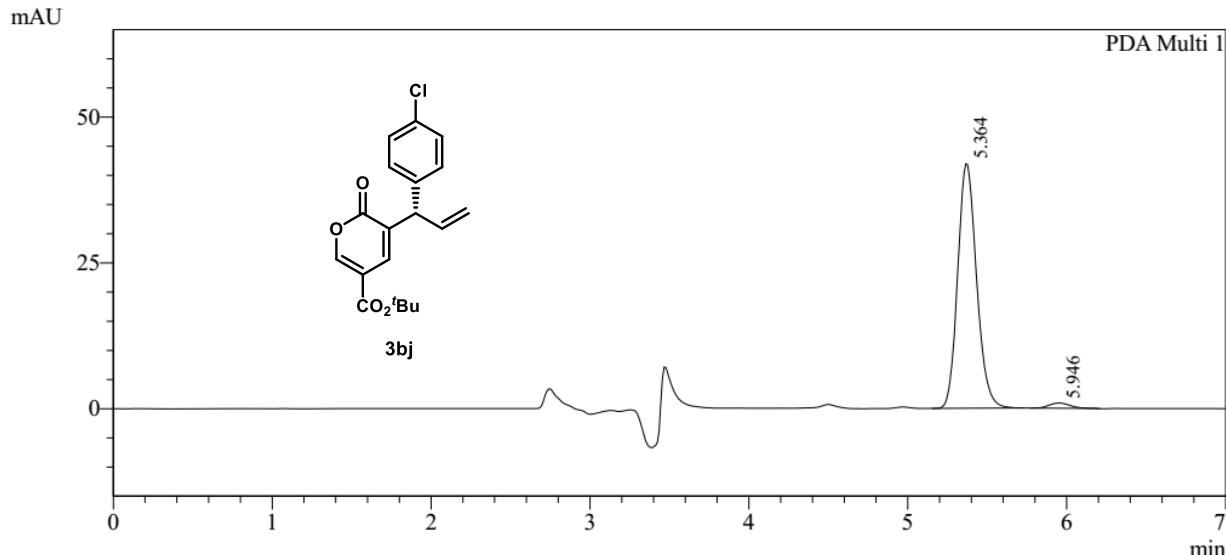


PeakTable

PDA Ch1 252nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.356	256066	50.054
2	5.937	255511	49.946
Total		511577	100.000

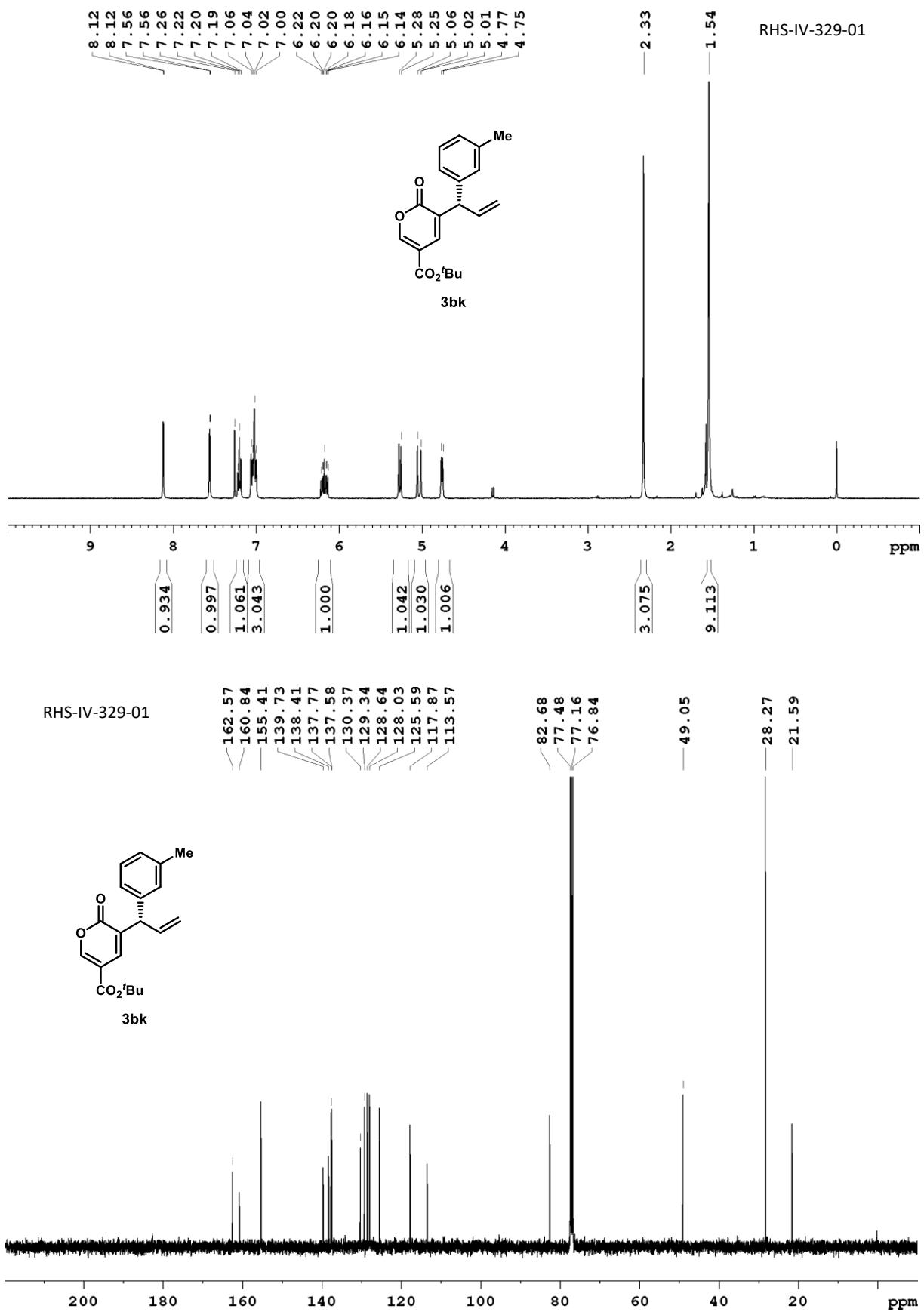
Phenomenex Cellulose-2 column (75:25 *n*-Hexane/EtOH, 1.0 mL/min, 20 °C)

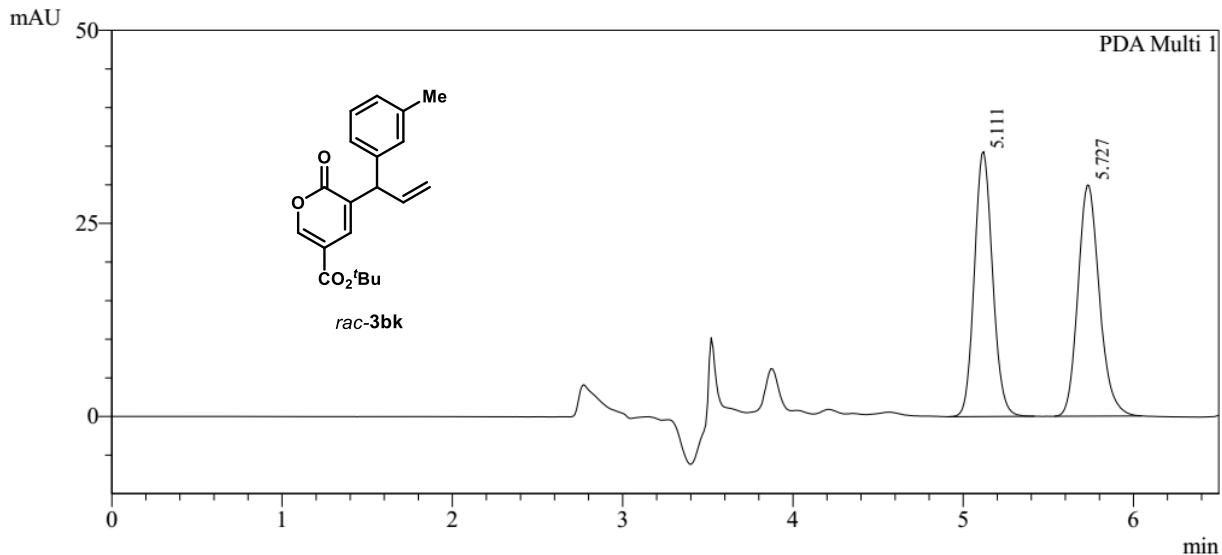


PeakTable

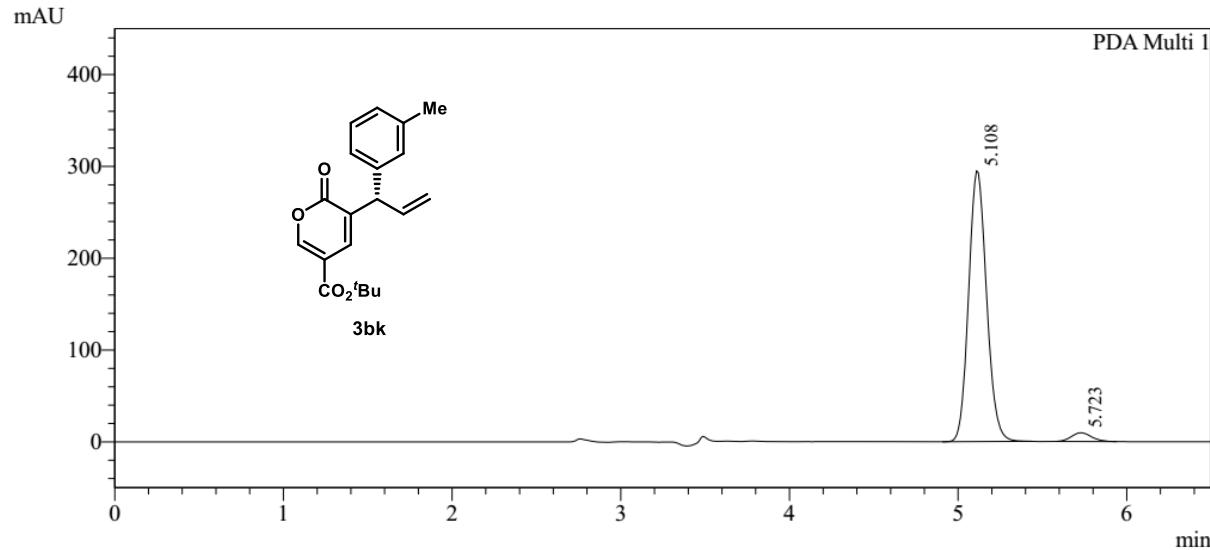
PDA Ch1 252nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.364	346423	97.665
2	5.946	8282	2.335
Total		354704	100.000

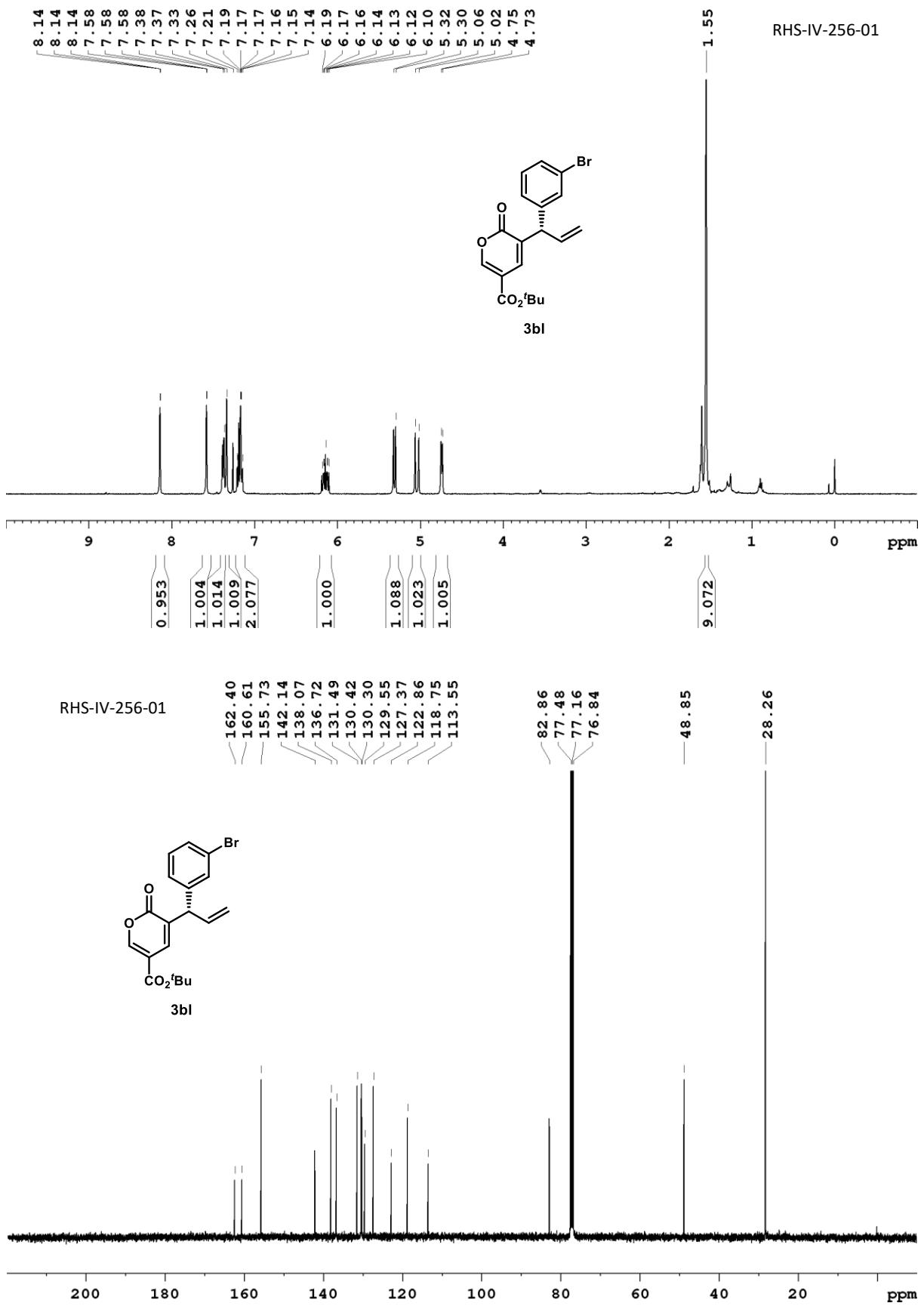


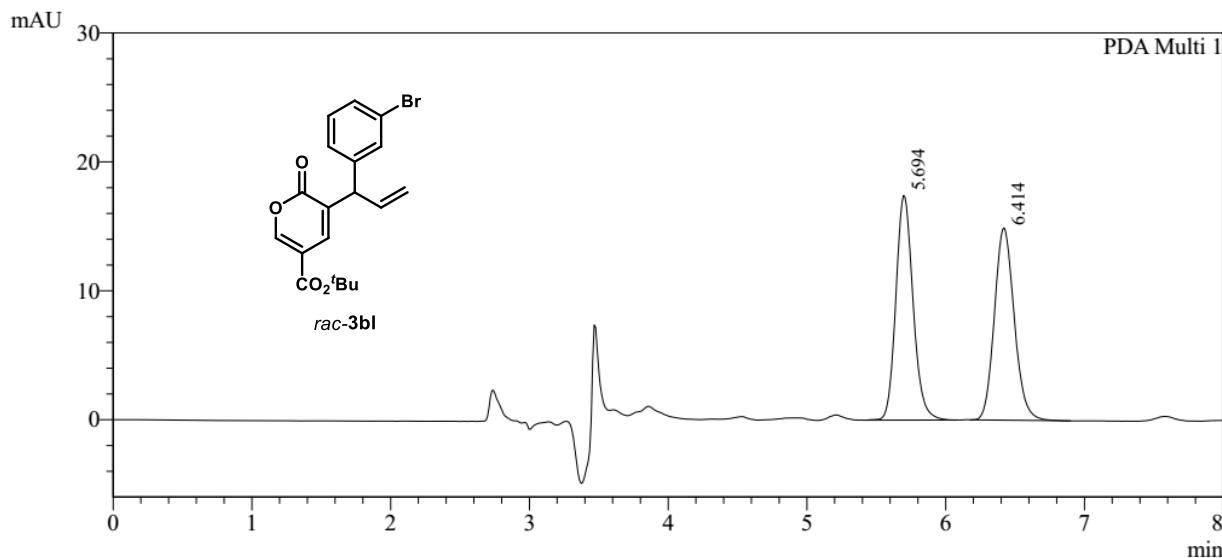


Phenomenex Cellulose-2 column (75:25 *n*-Hexane/EtOH, 1.0 mL/min, 20 °C)

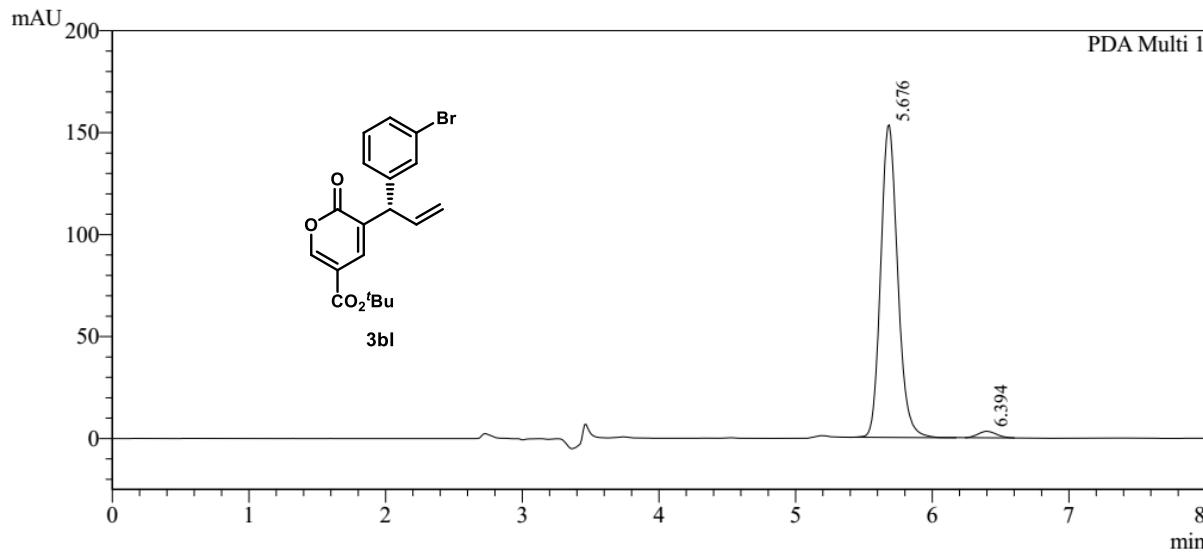


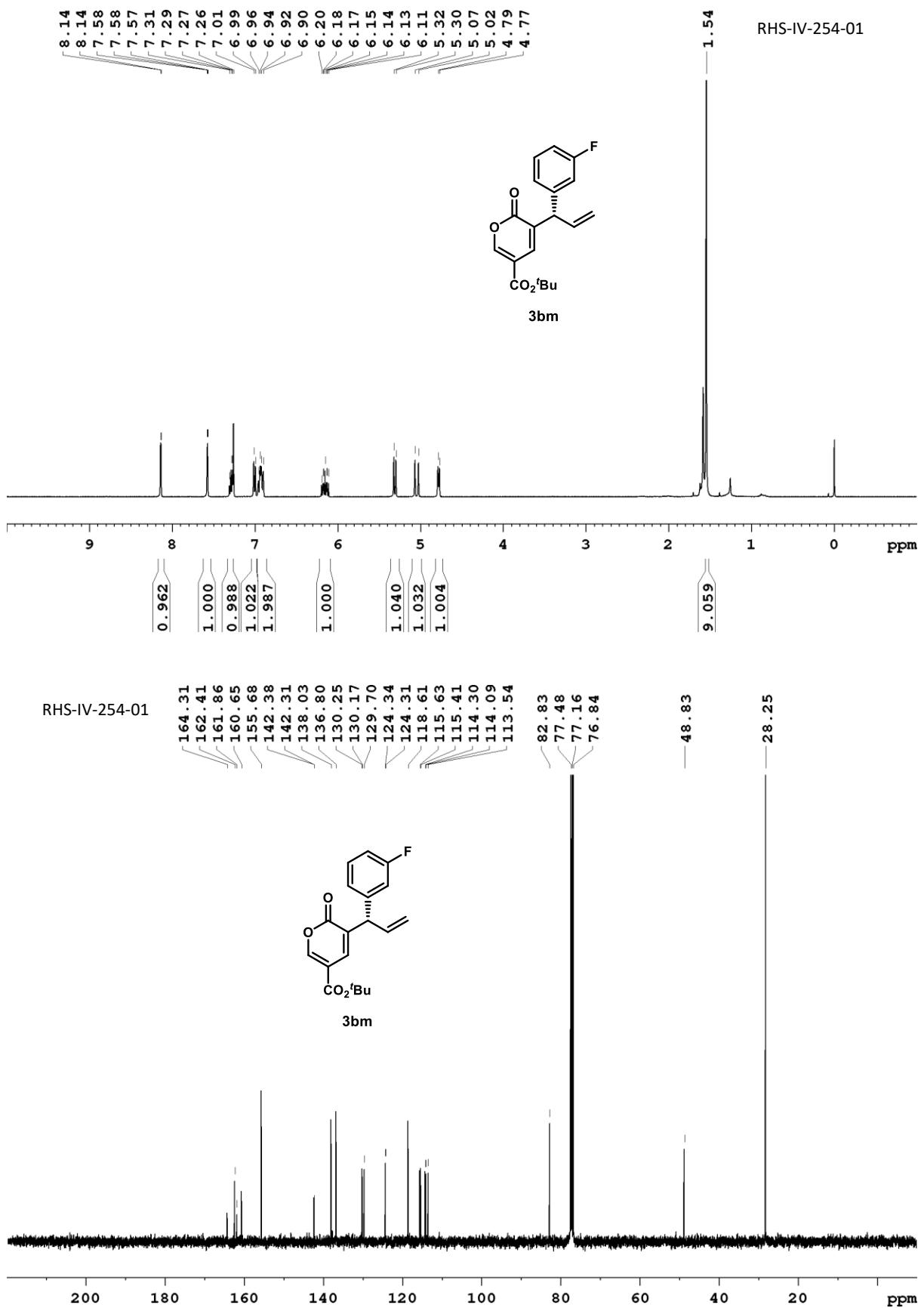
Peak#	Ret. Time	Area	Area %
1	5.108	2182604	96.542
2	5.723	78189	3.458
Total		2260793	100.000

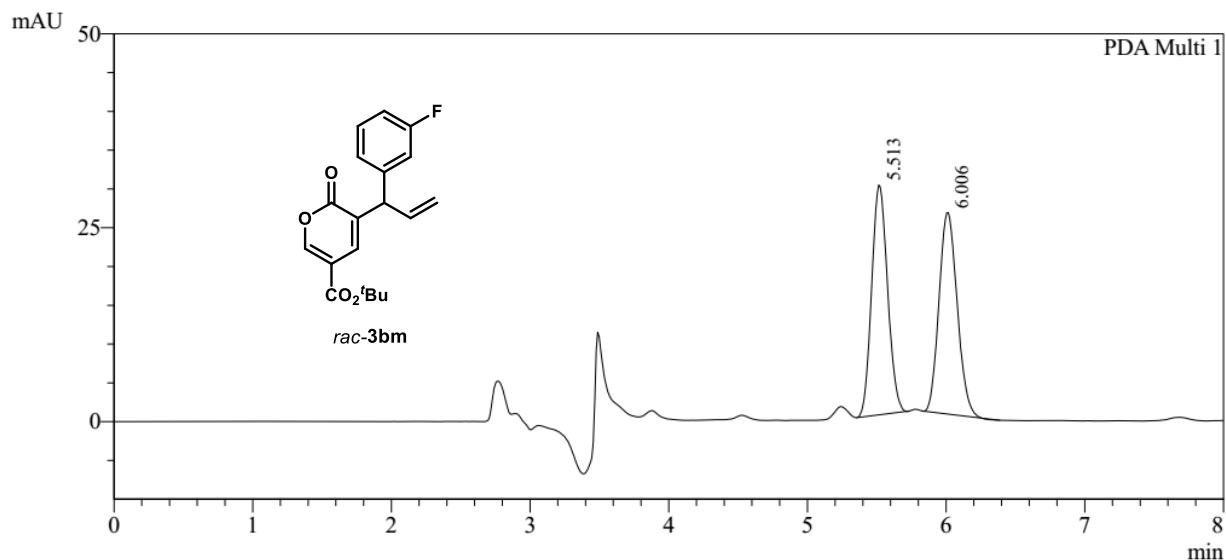




Phenomenex Cellulose-2 column (75:25 *n*-Hexane/EtOH, 1.0 mL/min, 20 °C)





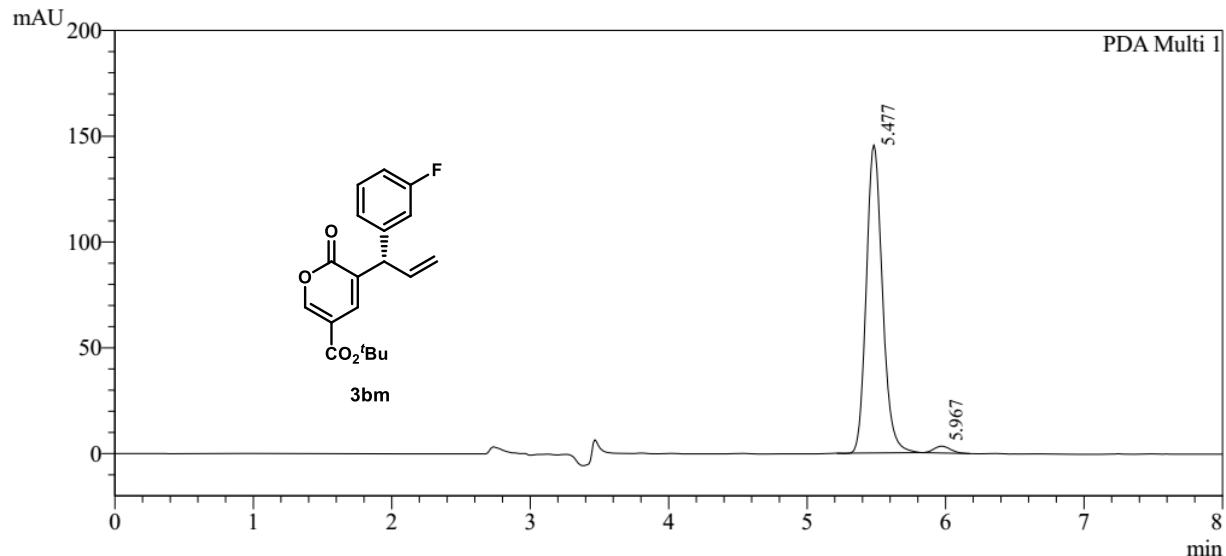


PeakTable

PDA Ch1 250nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.513	235860	50.032
2	6.006	235563	49.968
Total		471423	100.000

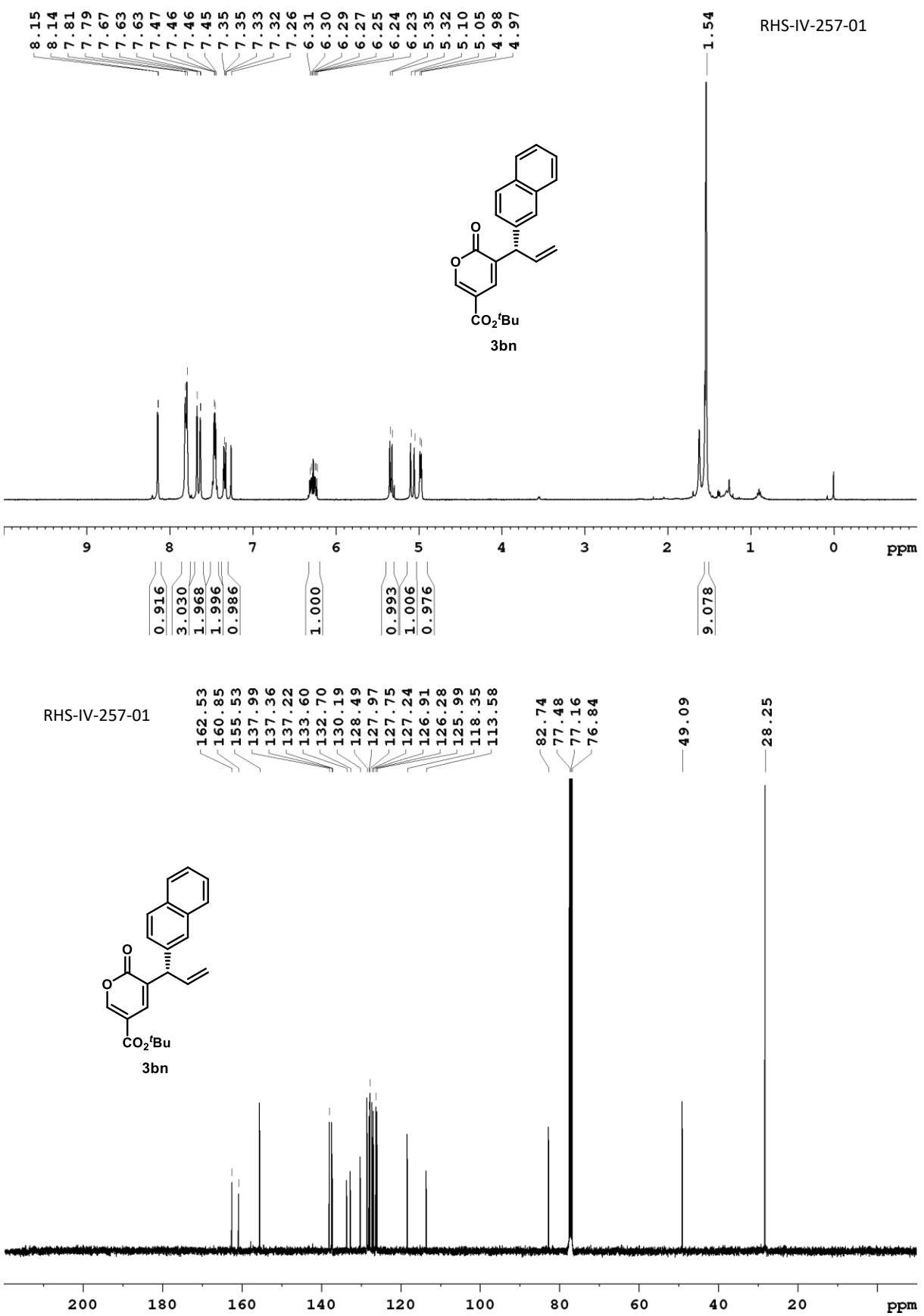
Phenomenex Cellulose-2 column (75:25 *n*-Hexane/EtOH, 1.0 mL/min, 20 °C)

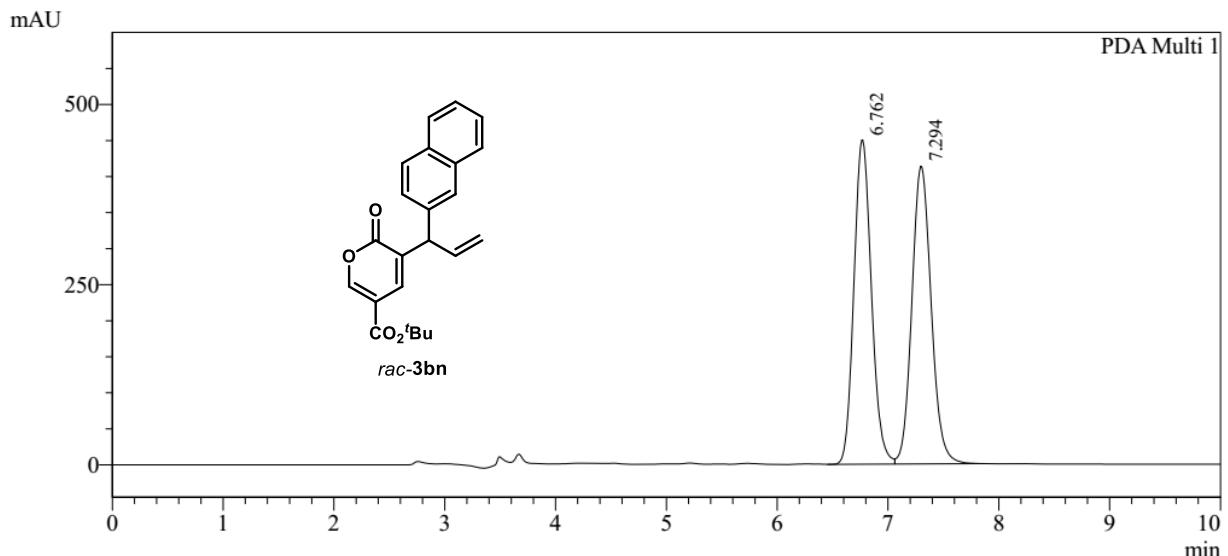


PeakTable

PDA Ch1 250nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.477	1179255	97.785
2	5.967	26713	2.215
Total		1205968	100.000





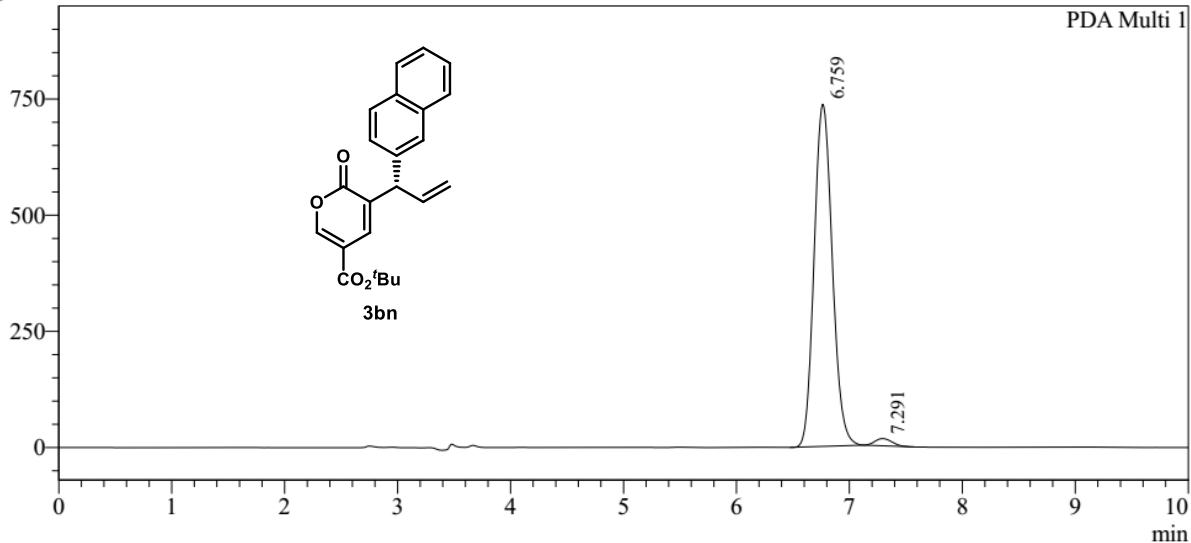
PeakTable

PDA Ch1 230nm 4nm

Peak#	Ret. Time	Area	Area %
1	6.762	4941669	49.662
2	7.294	5008911	50.338
Total		9950580	100.000

Phenomenex Cellulose-2 column (75:25 *n*-Hexane/EtOH, 1.0 mL/min, 20 °C)

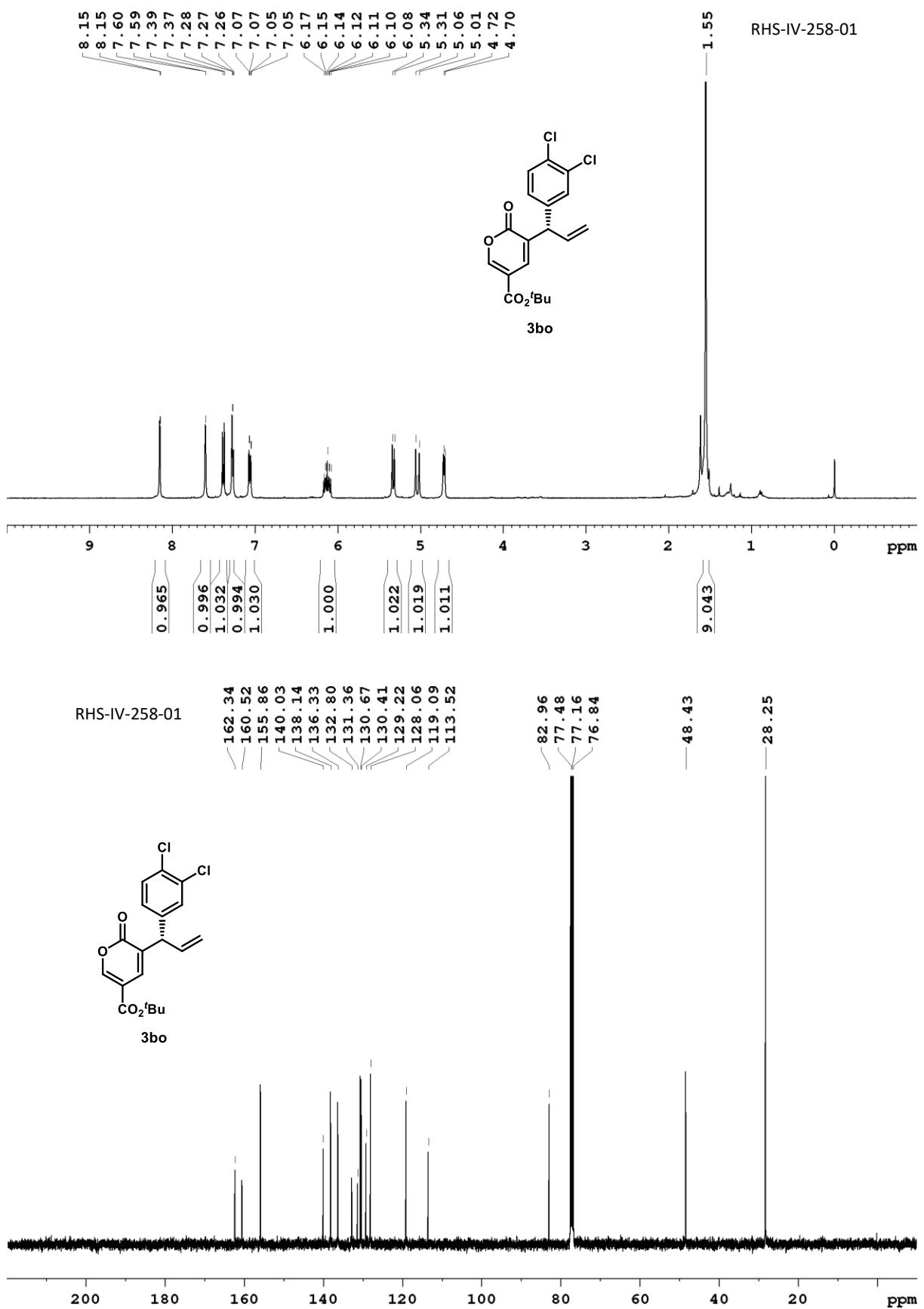
mAU

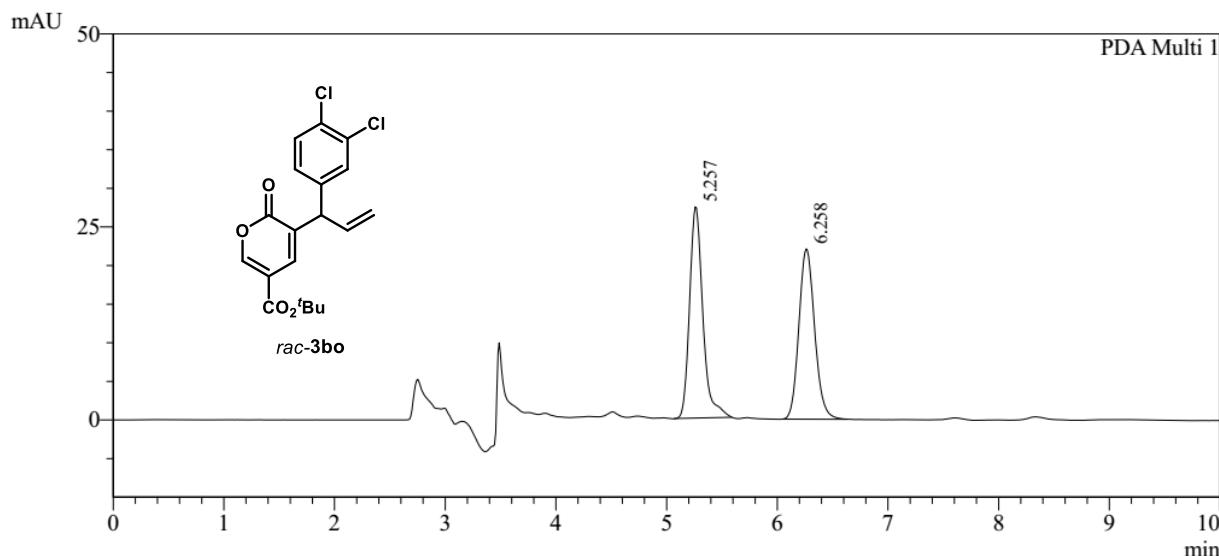


PeakTable

PDA Ch1 230nm 4nm

Peak#	Ret. Time	Area	Area %
1	6.759	8230090	98.040
2	7.291	164571	1.960
Total		8394661	100.000



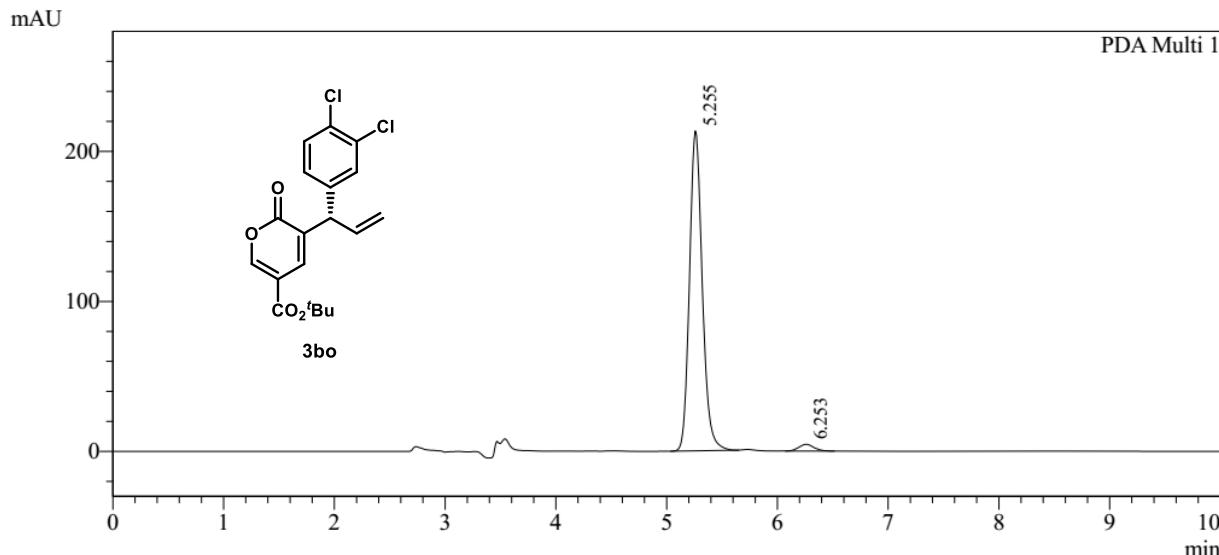


PeakTable

PDA Ch1 247nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.257	228296	51.144
2	6.258	218081	48.856
Total		446377	100.000

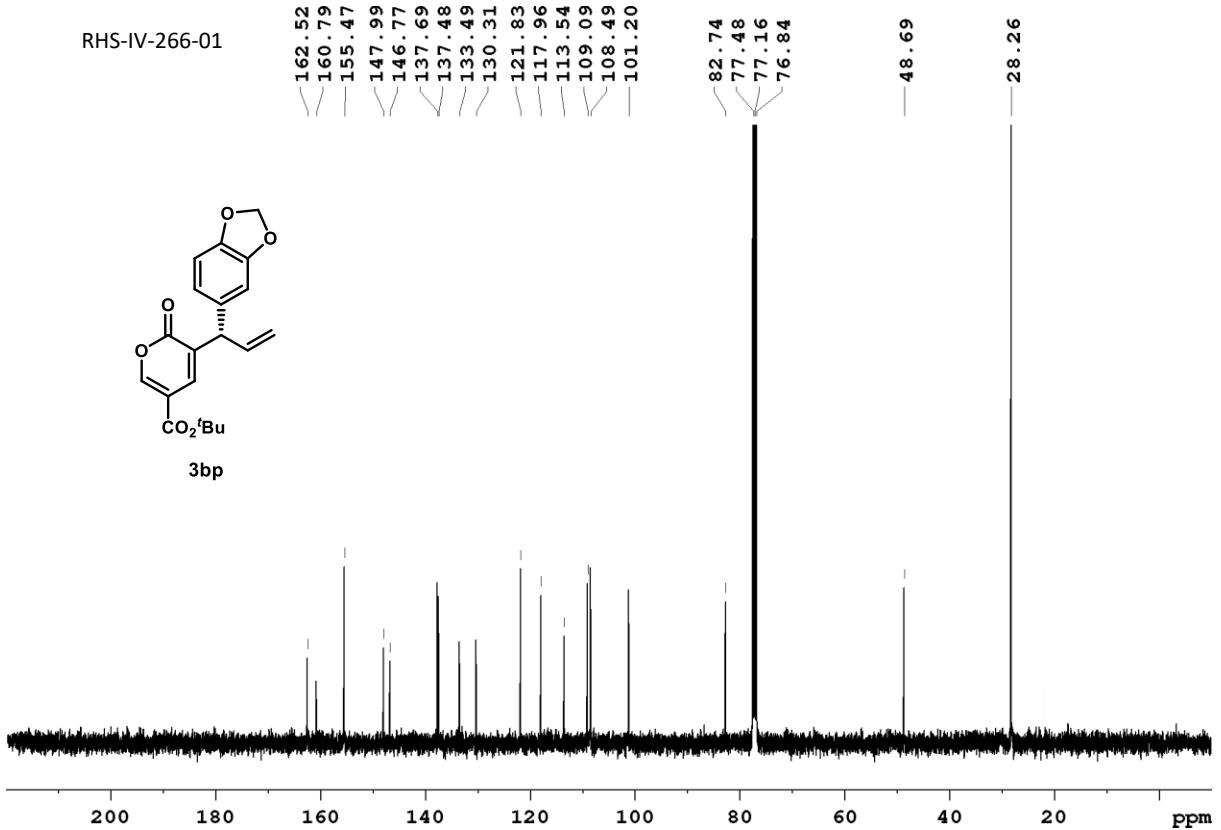
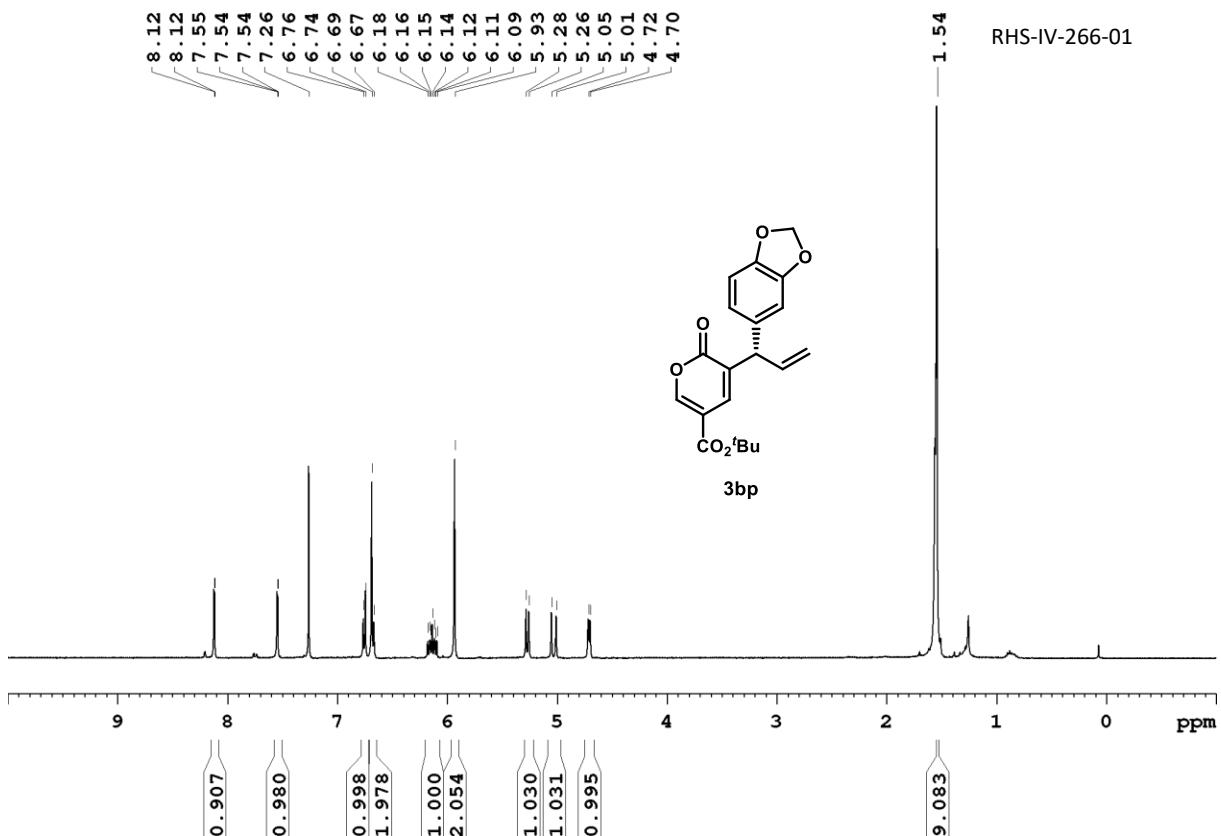
Phenomenex Cellulose-2 column (75:25 *n*-Hexane/EtOH, 1.0 mL/min, 20 °C)

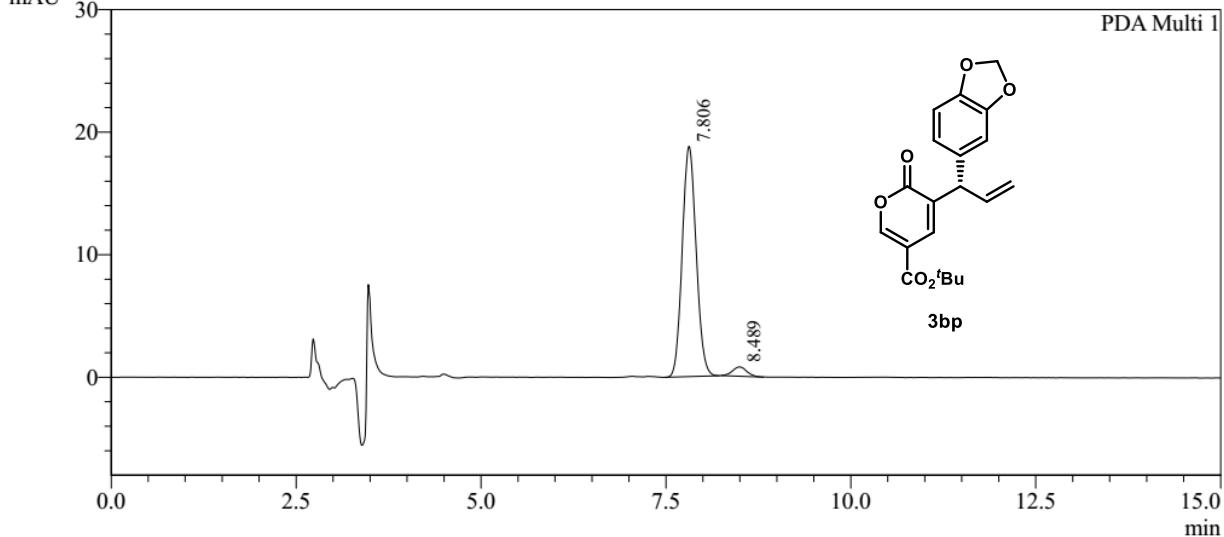
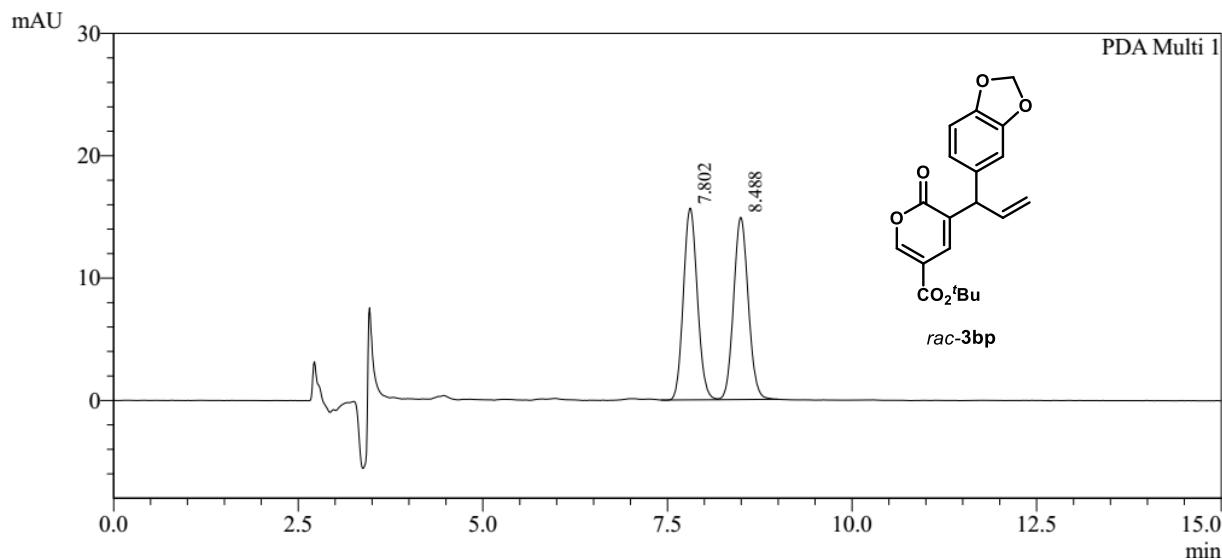


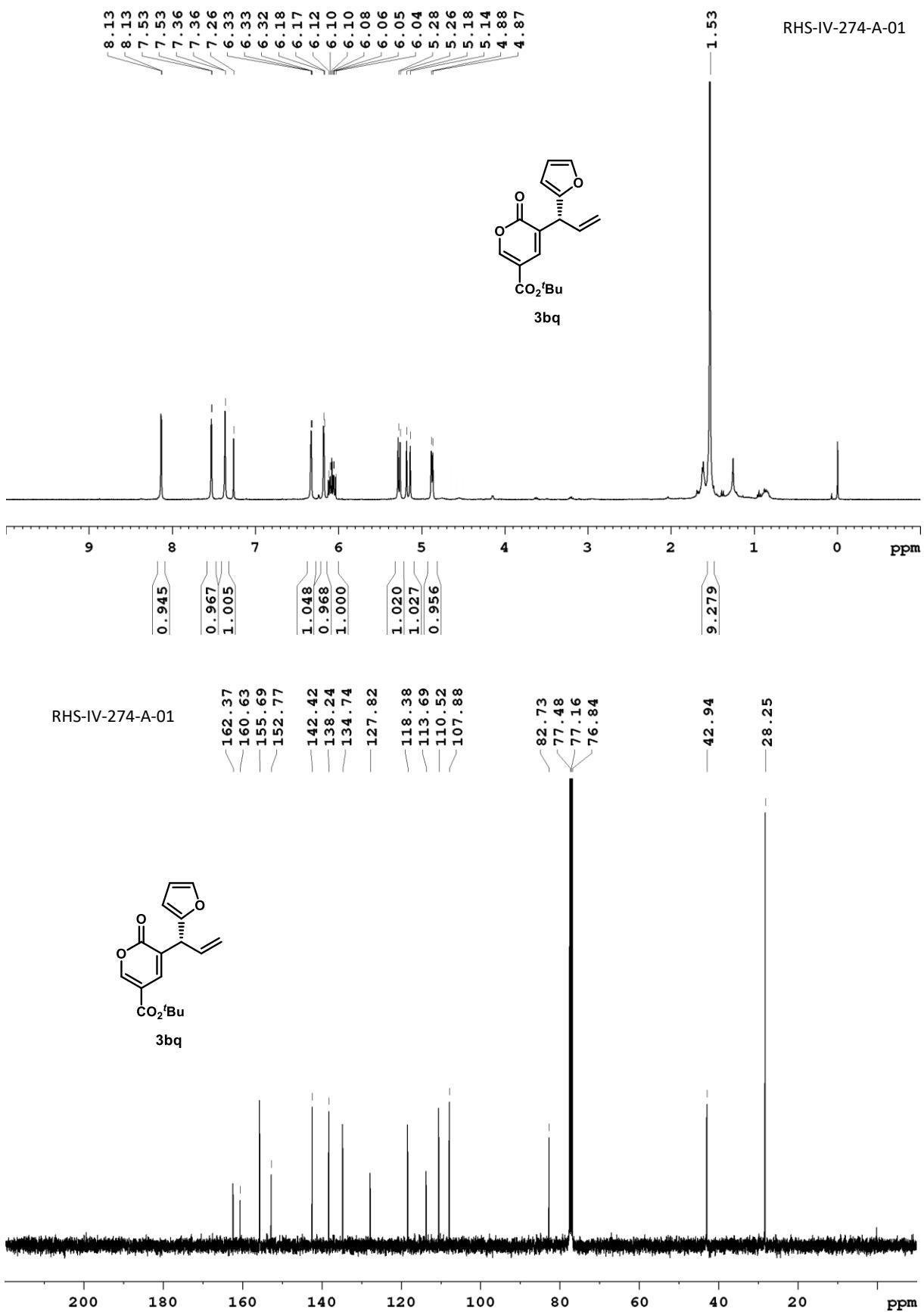
PeakTable

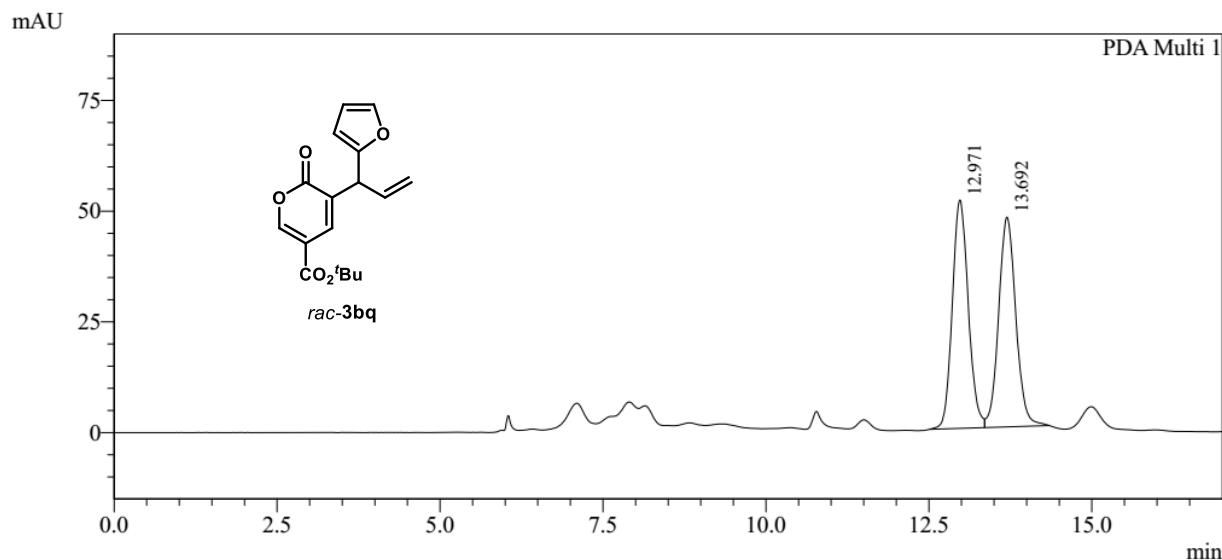
PDA Ch1 247nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.255	1714566	97.563
2	6.253	42835	2.437
Total		1757401	100.000







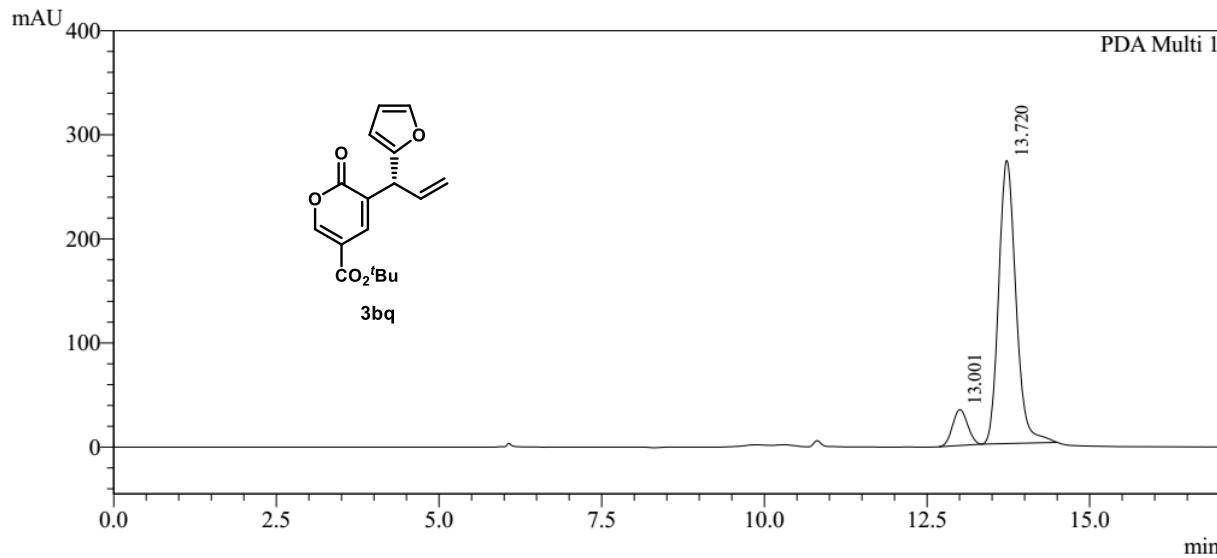


PeakTable

PDA Ch1 252nm 4nm

Peak#	Ret. Time	Area	Area %
1	12.971	878598	50.271
2	13.692	869124	49.729
Total		1747722	100.000

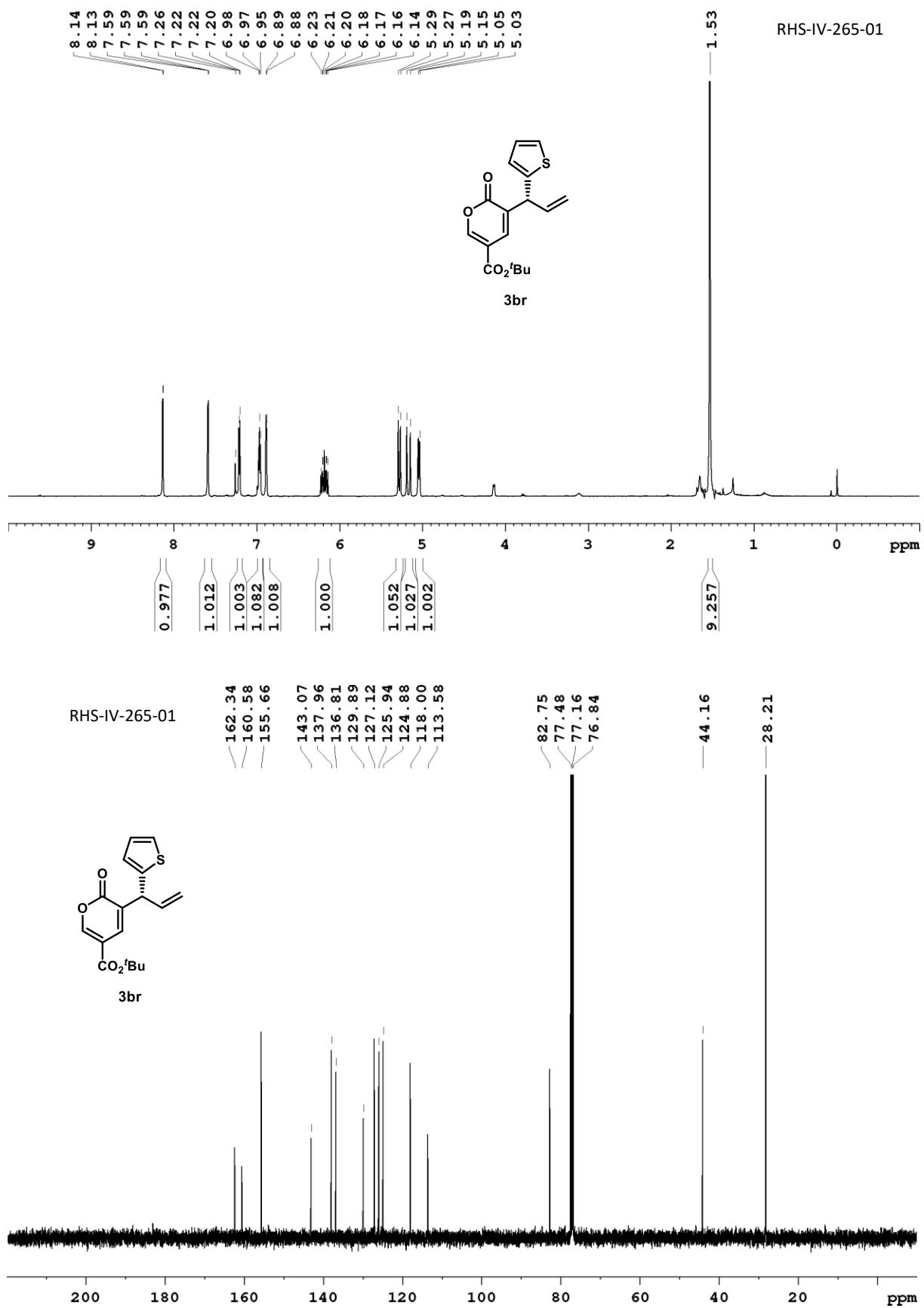
Phenomenex Cellulose-1 column (75:25 *n*-Hexane/EtOH, 0.5 mL/min, 20 °C)

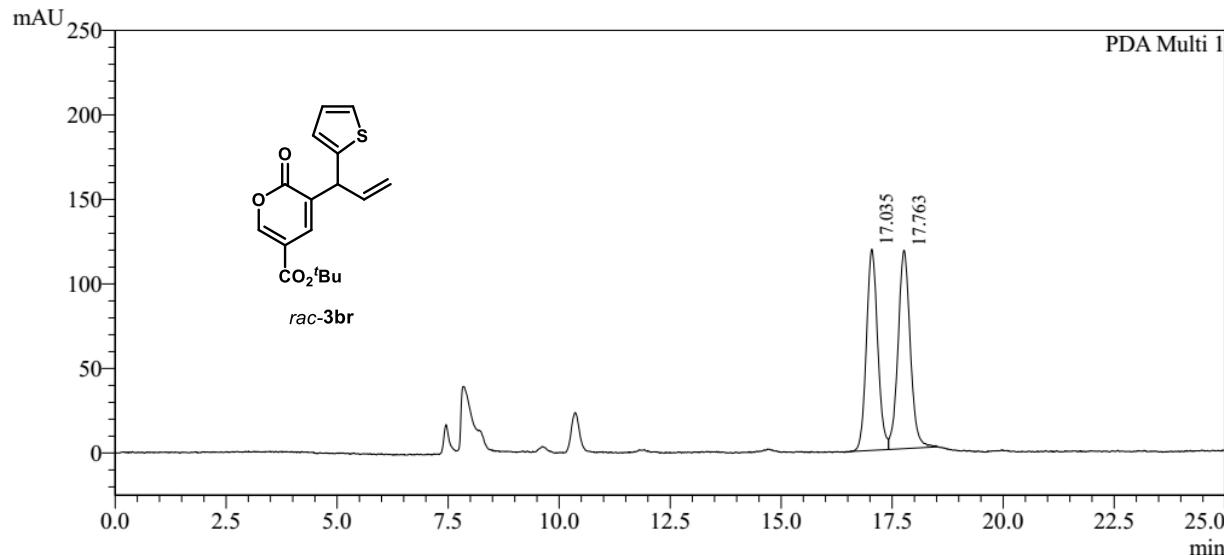


PeakTable

PDA Ch1 252nm 4nm

Peak#	Ret. Time	Area	Area %
1	13.001	555878	9.976
2	13.720	5016320	90.024
Total		5572199	100.000



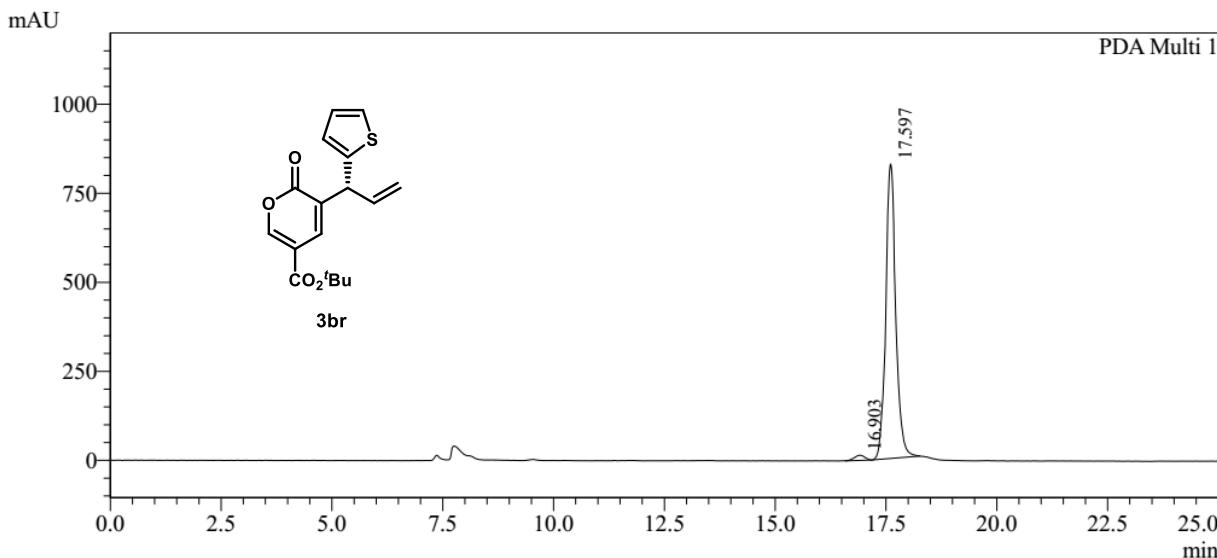


PeakTable

PDA Ch1 195nm 4nm

Peak#	Ret. Time	Area	Area %
1	17.035	2111970	48.442
2	17.763	2247789	51.558
Total		4359759	100.000

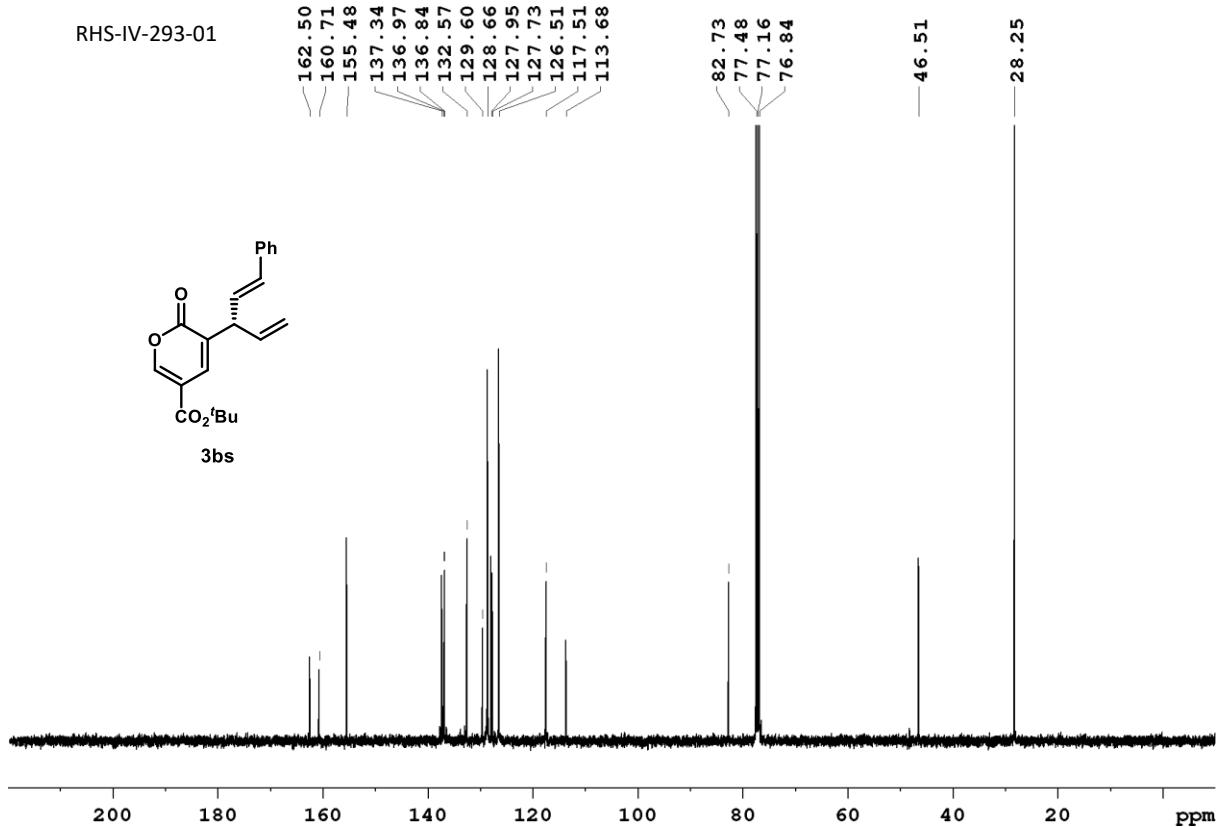
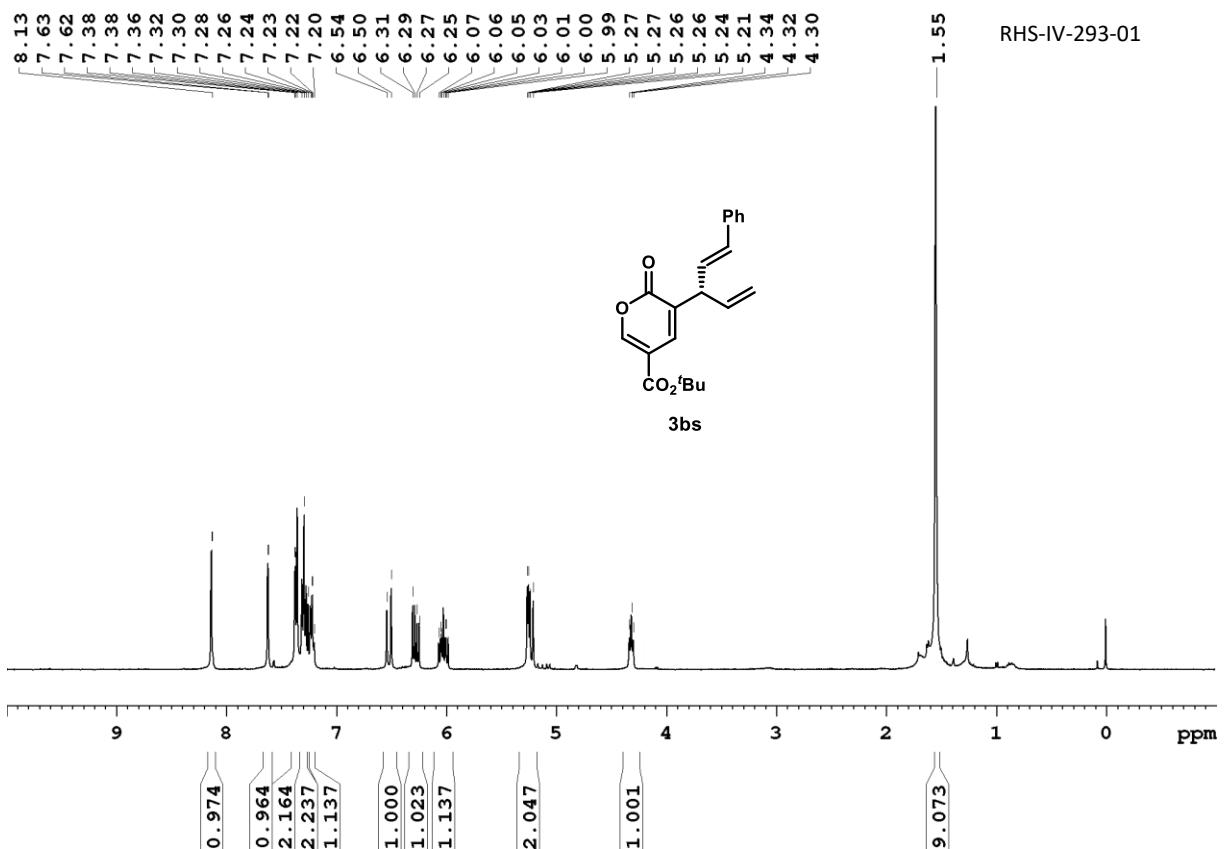
Daicel Chiraldex IB column (95:5 *n*-Hexane/*i*-PrOH, 0.4 mL/min, 20 °C)

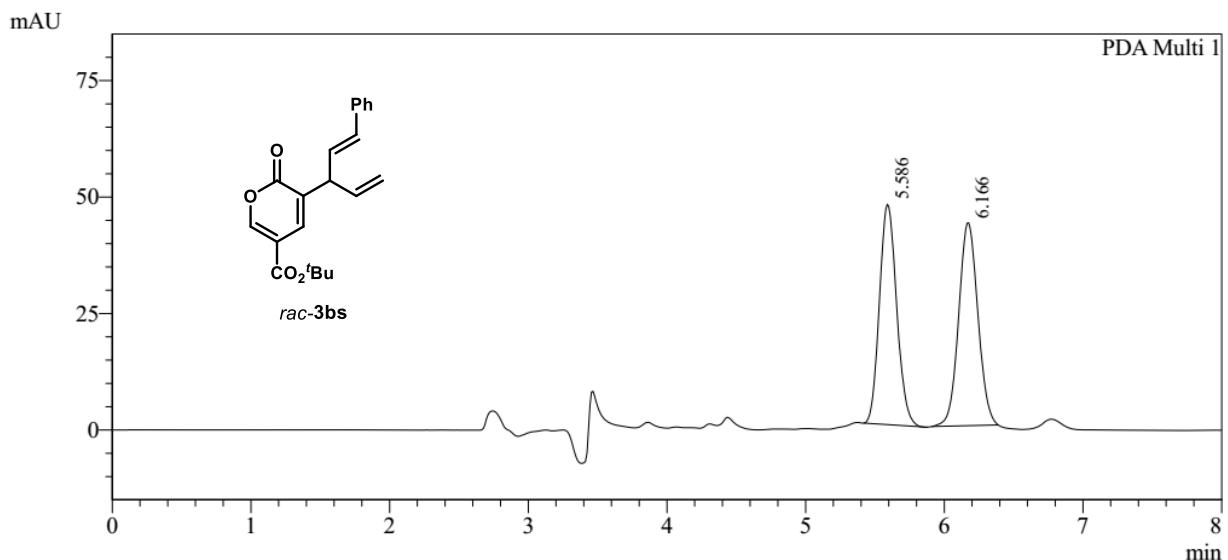


PeakTable

PDA Ch1 195nm 4nm

Peak#	Ret. Time	Area	Area %
1	16.903	234749	1.798
2	17.597	12824734	98.202
Total		13059483	100.000



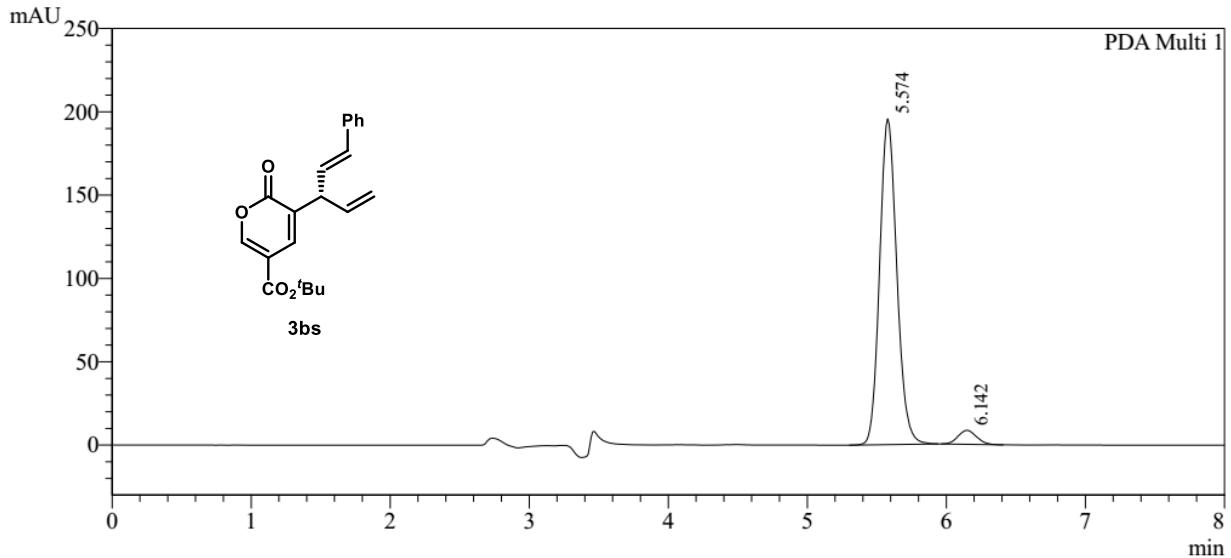


PeakTable

PDA Ch1 252nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.586	407797	49.298
2	6.166	419411	50.702
Total		827209	100.000

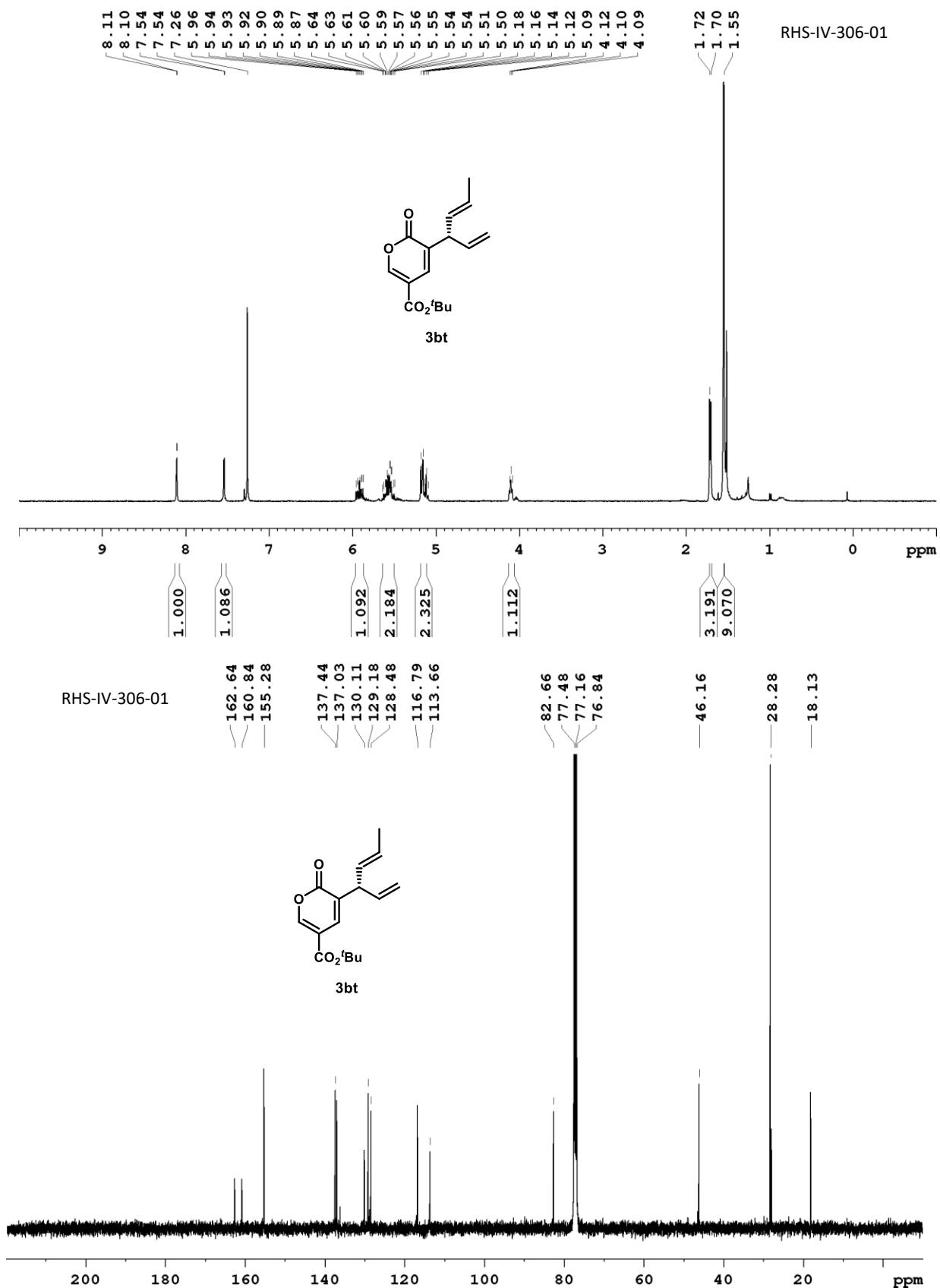
Phenomenex Cellulose-2 column (75:25 n-Hexane/EtOH, 1.0 mL/min, 20 °C)

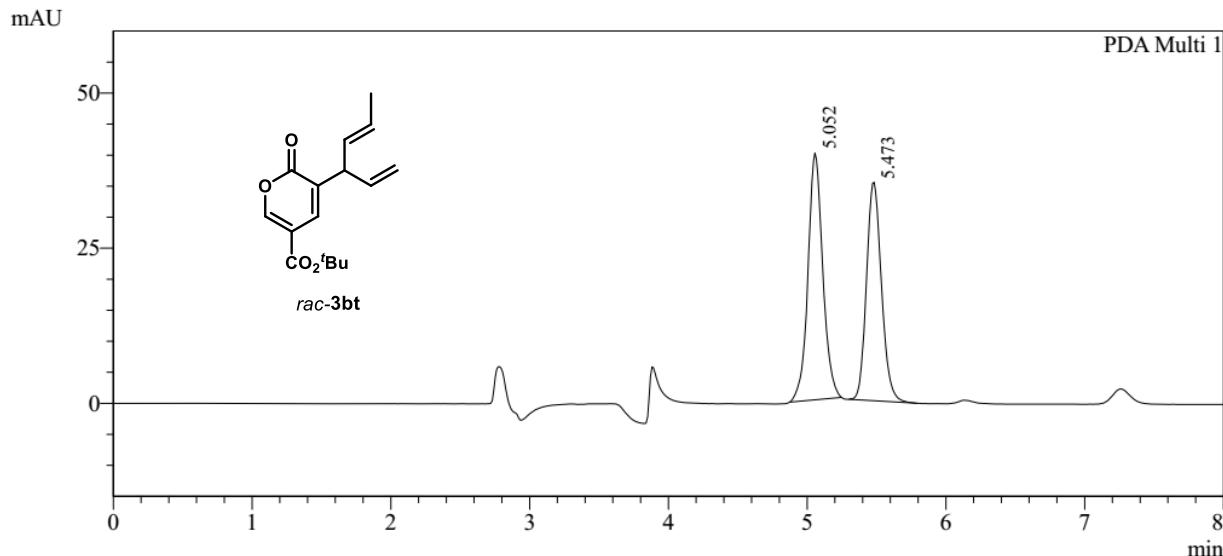


PeakTable

PDA Ch1 252nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.574	1681799	95.591
2	6.142	77563	4.409
Total		1759361	100.000



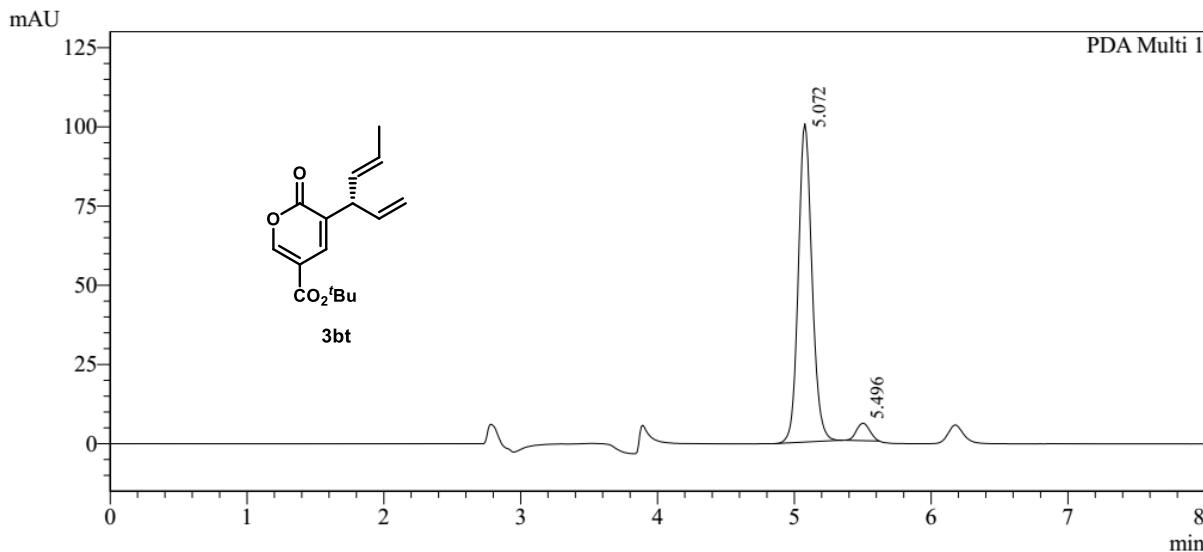


PeakTable

PDA Ch1 295nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.052	294073	52.723
2	5.473	263693	47.277
Total		557766	100.000

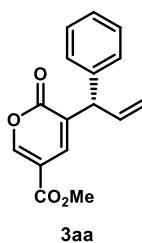
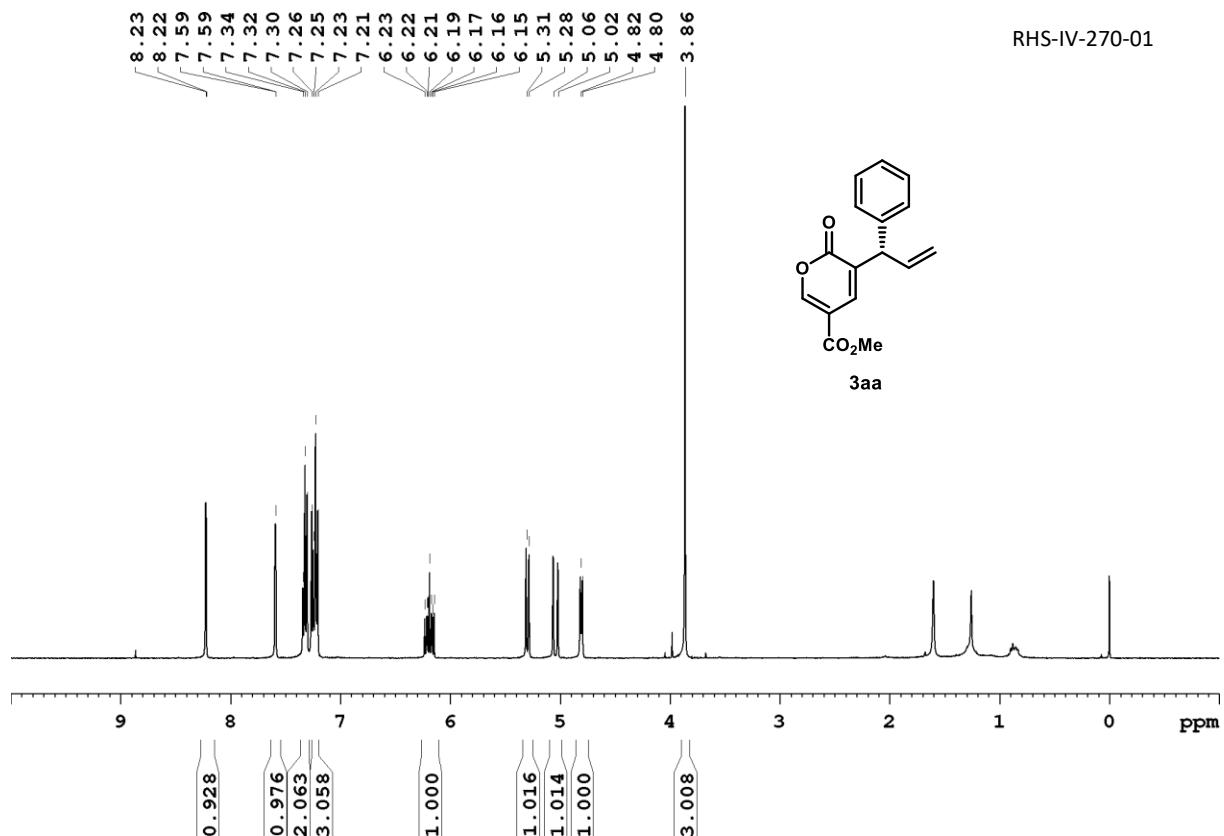
Phenomenex Cellulose-2 column (85:15 *n*-Hexane/EtOH, 1.0 mL/min, 20 °C)



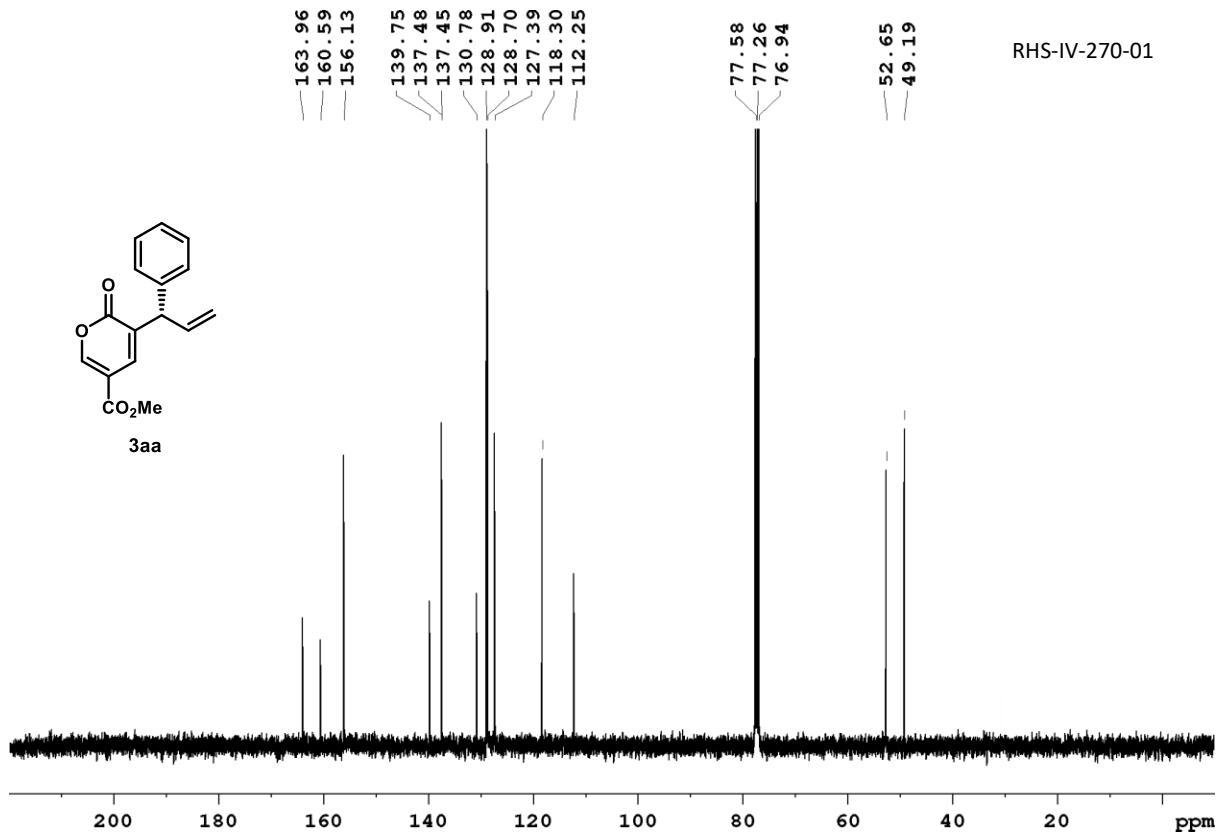
PeakTable

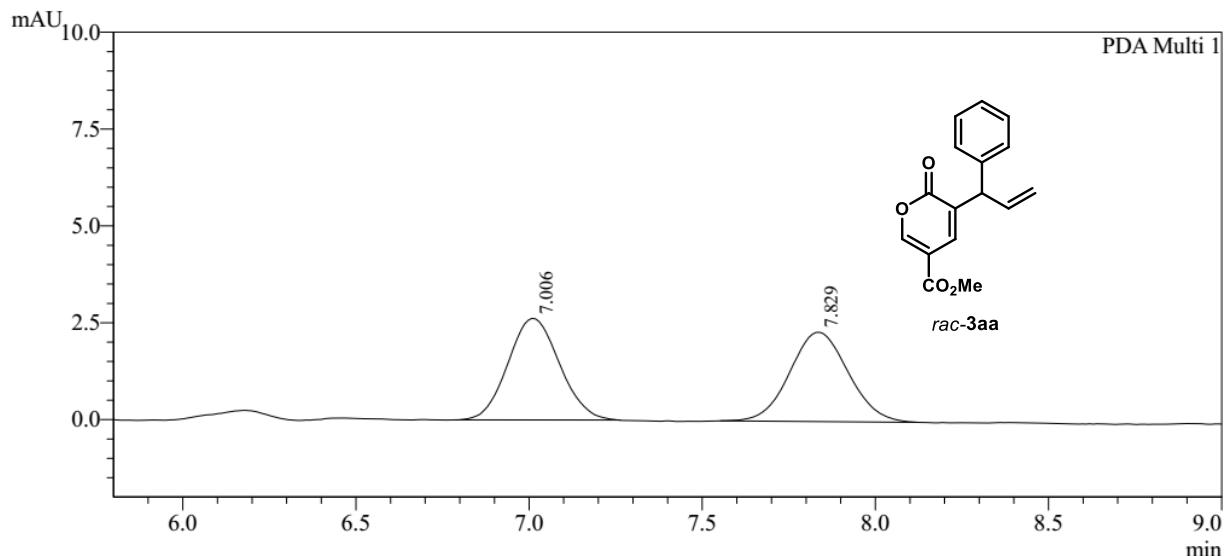
PDA Ch1 295nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.072	700079	94.949
2	5.496	37242	5.051
Total		737321	100.000

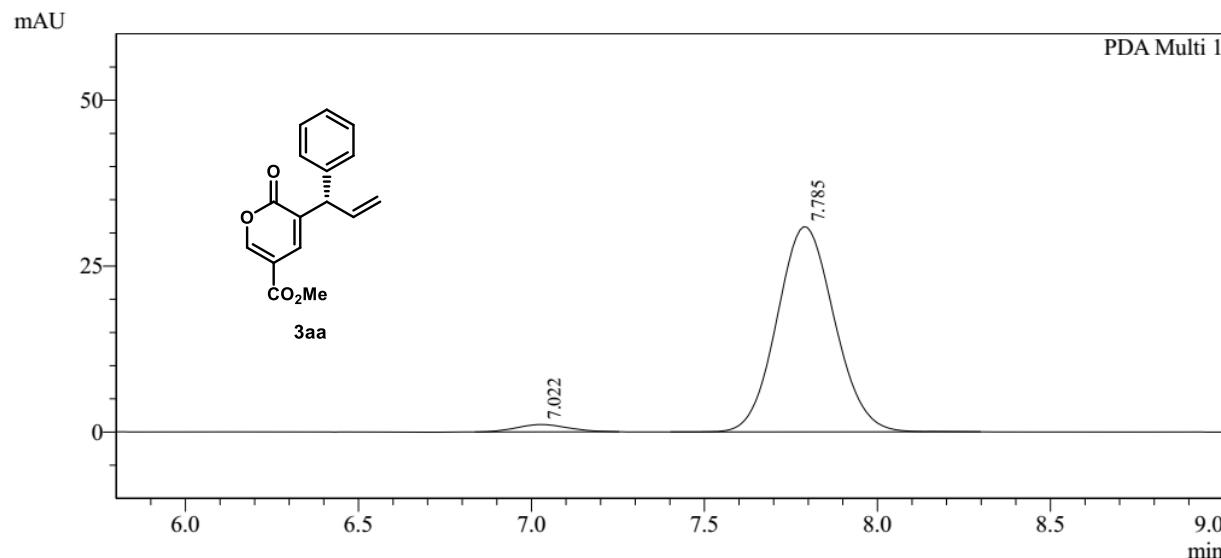


3aa





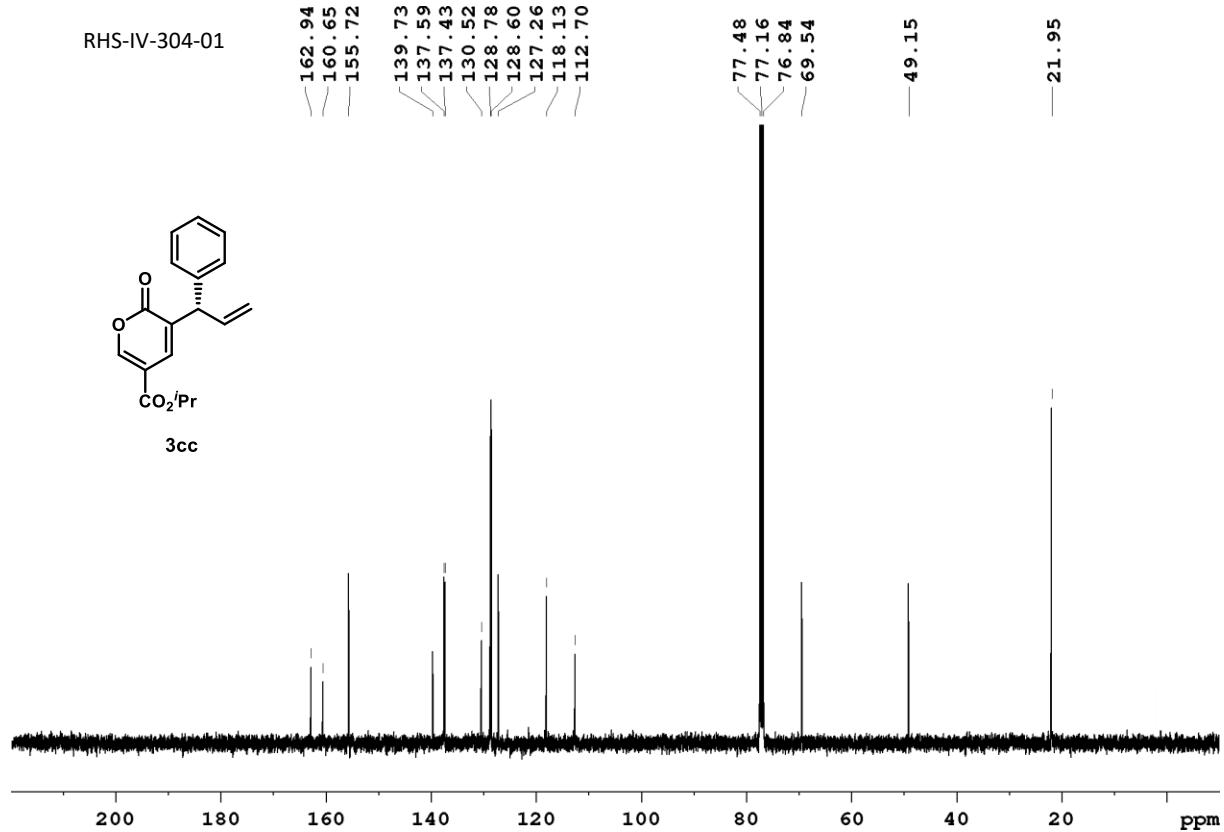
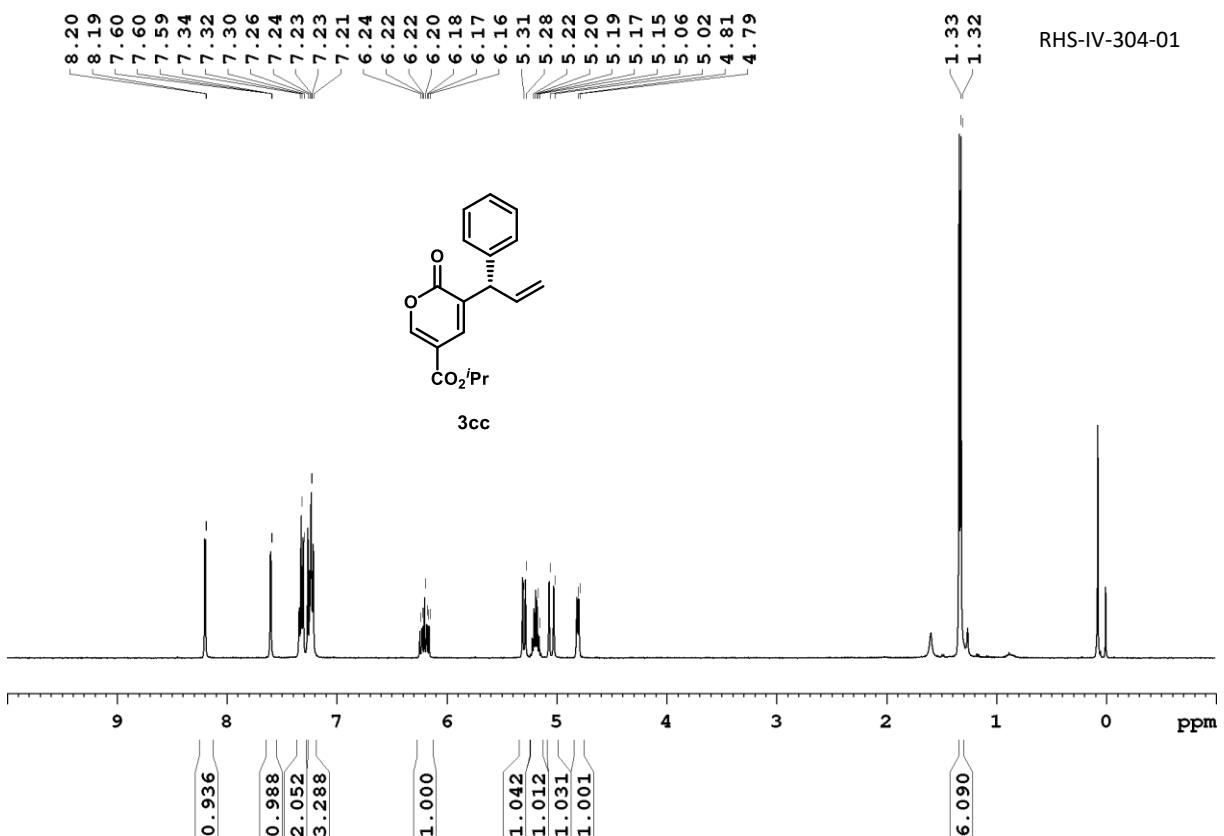
Phenomenex Cellulose-1 column (75:25 *n*-Hexane/EtOH, 1.0 mL/min, 20 °C)

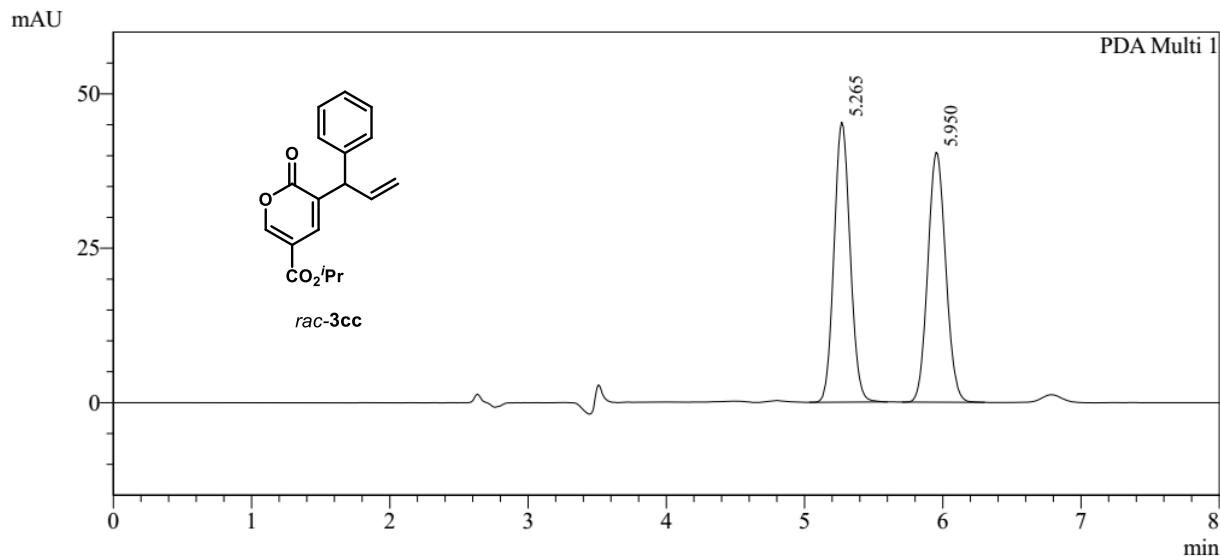


PeakTable

PDA Ch1 282nm 4nm

Peak#	Ret. Time	Area	Area %
1	7.022	11407	3.095
2	7.785	357118	96.905
Total		368524	100.000



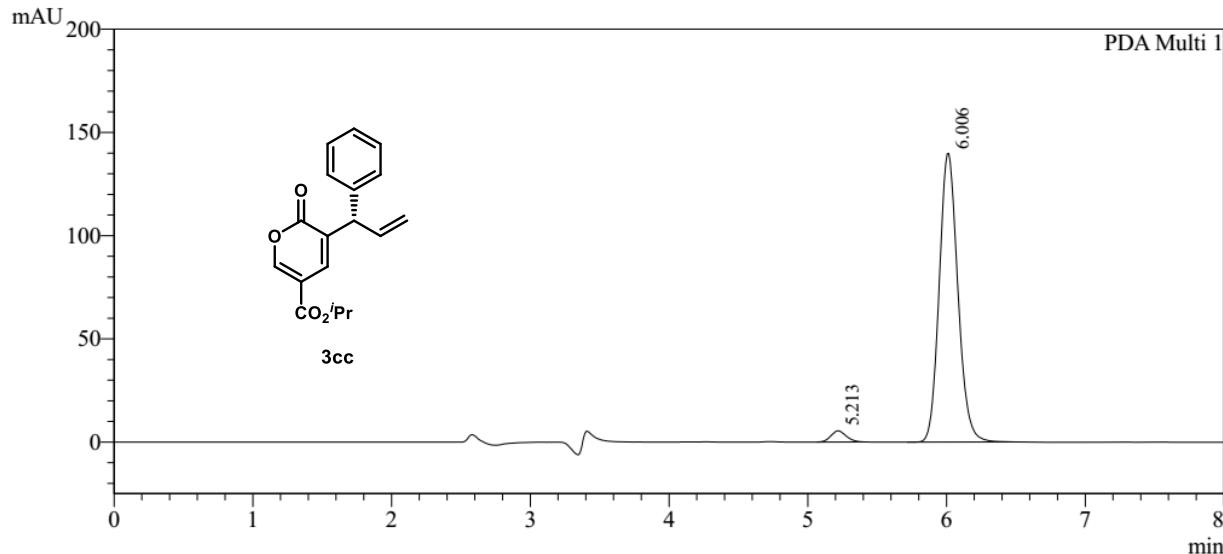


PeakTable

PDA Ch1 300nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.265	367205	50.182
2	5.950	364539	49.818
Total		731744	100.000

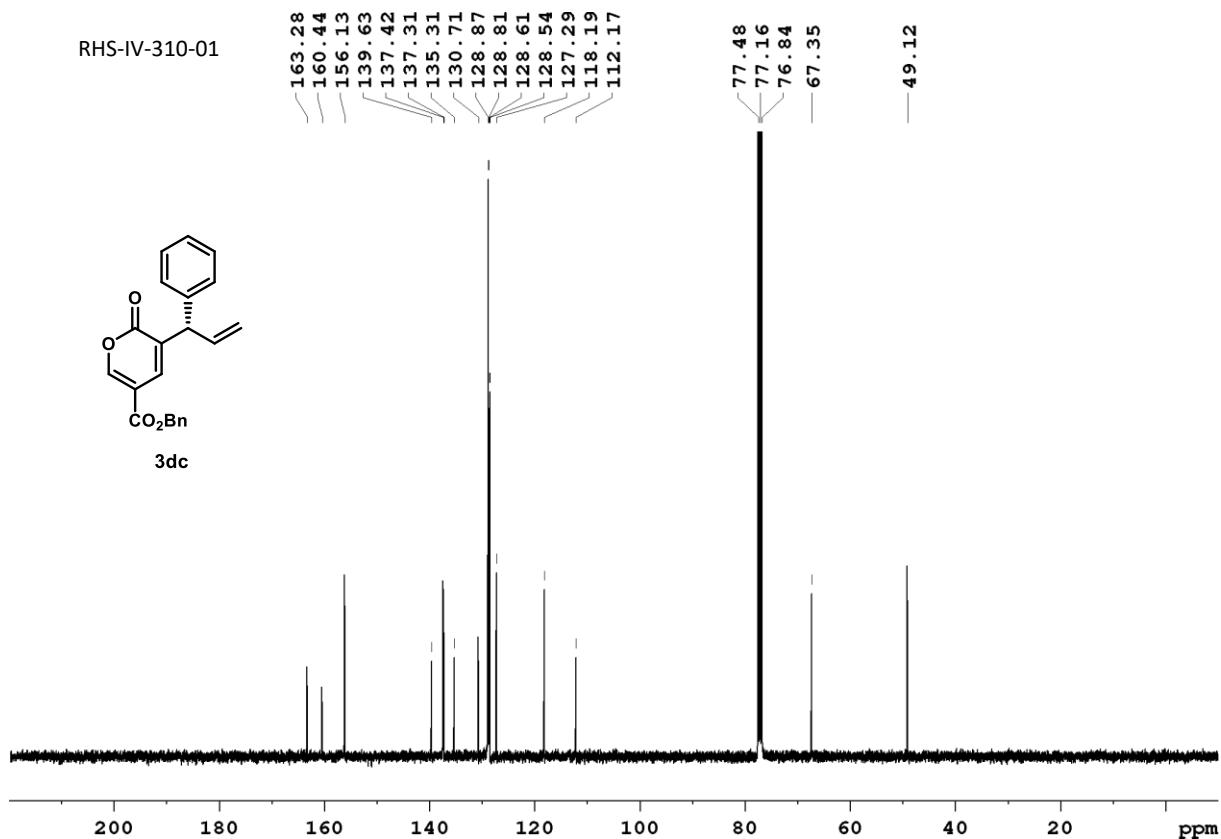
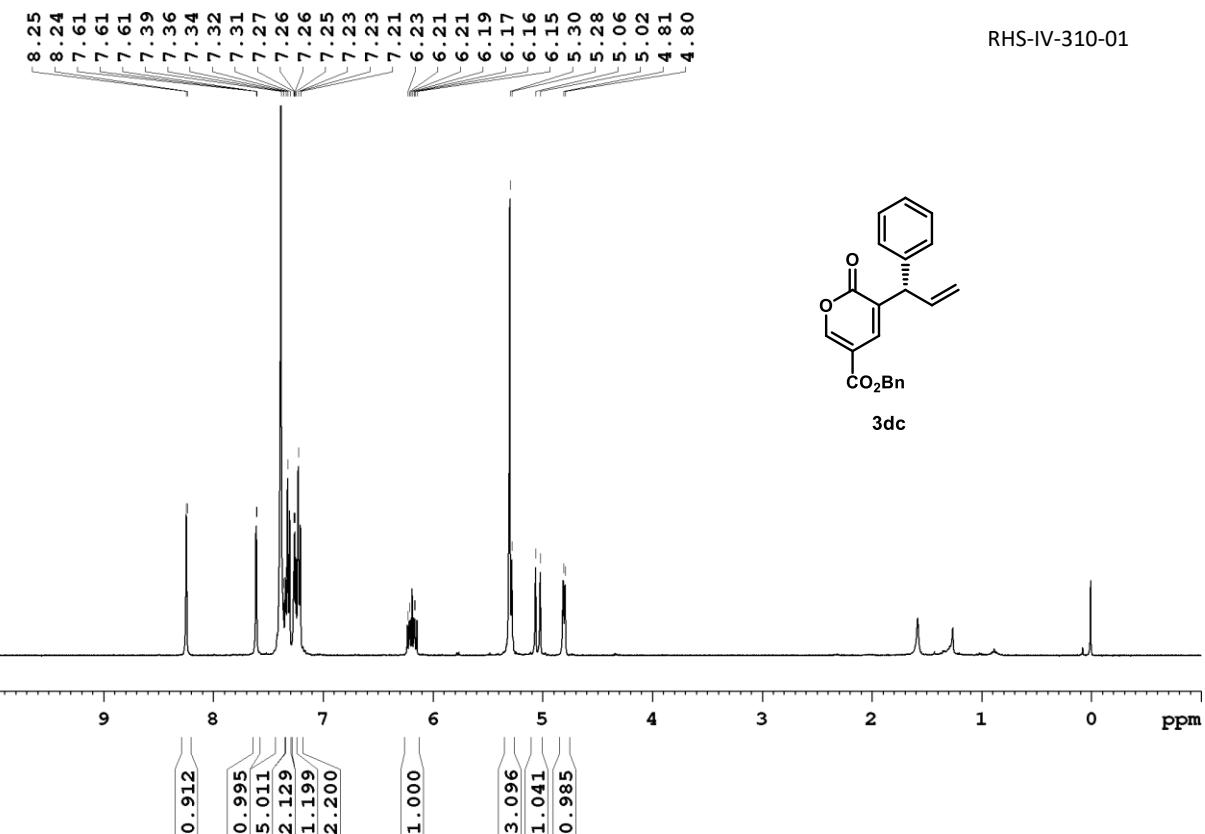
Phenomenex Cellulose-1 column (75:25 *n*-Hexane/EtOH, 1.0 mL/min, 20 °C)

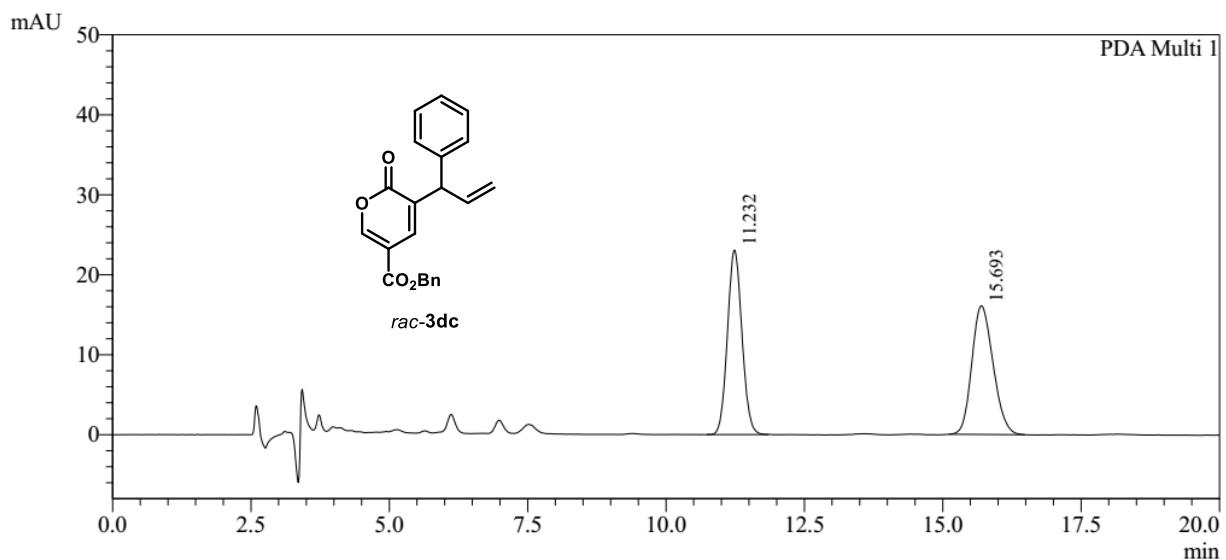


PeakTable

PDA Ch1 300nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.213	41646	3.088
2	6.006	1306936	96.912
Total		1348582	100.000



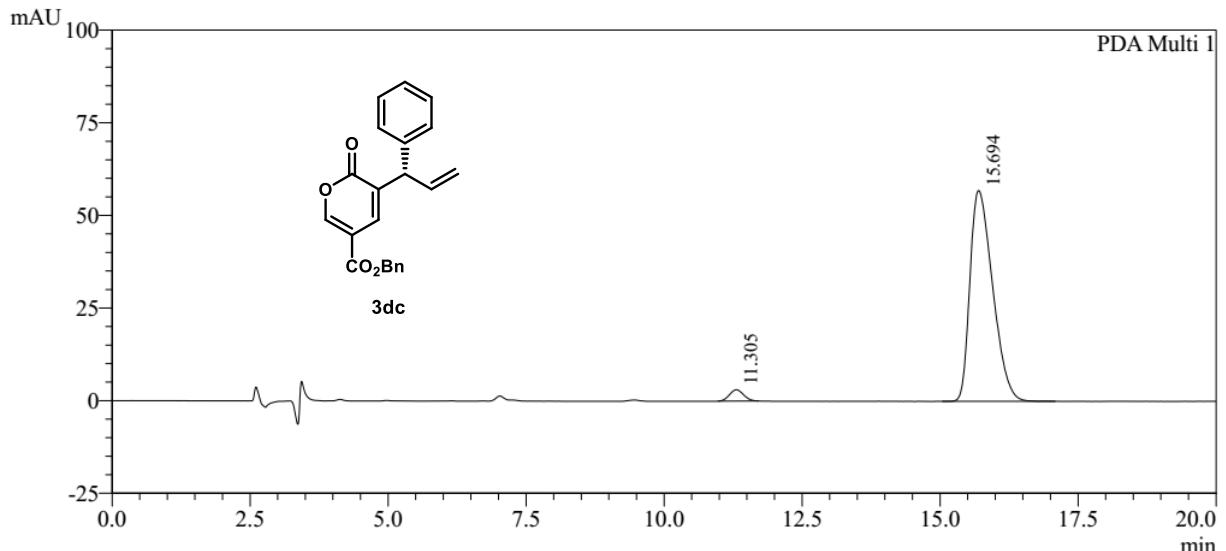


PeakTable

PDA Ch1 300nm 4nm

Peak#	Ret. Time	Area	Area %
1	11.232	420984	49.477
2	15.693	429890	50.523
Total		850875	100.000

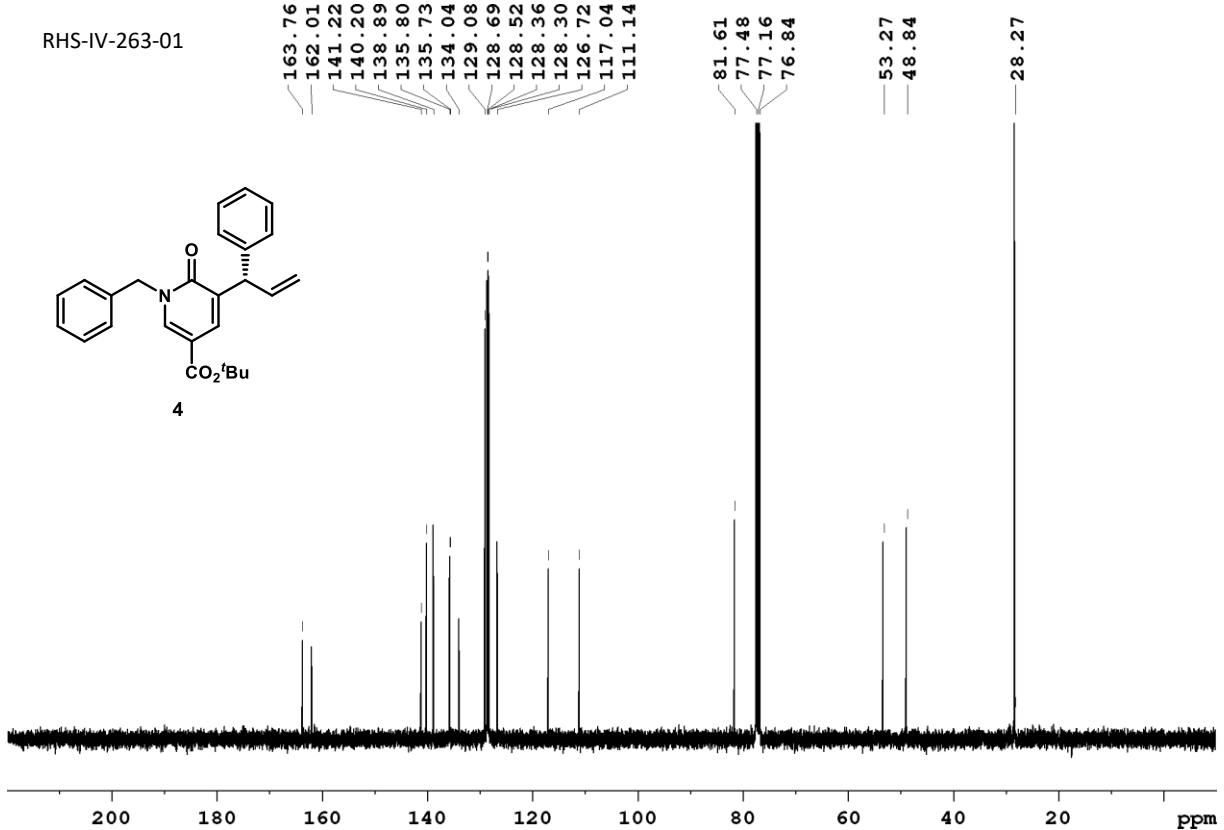
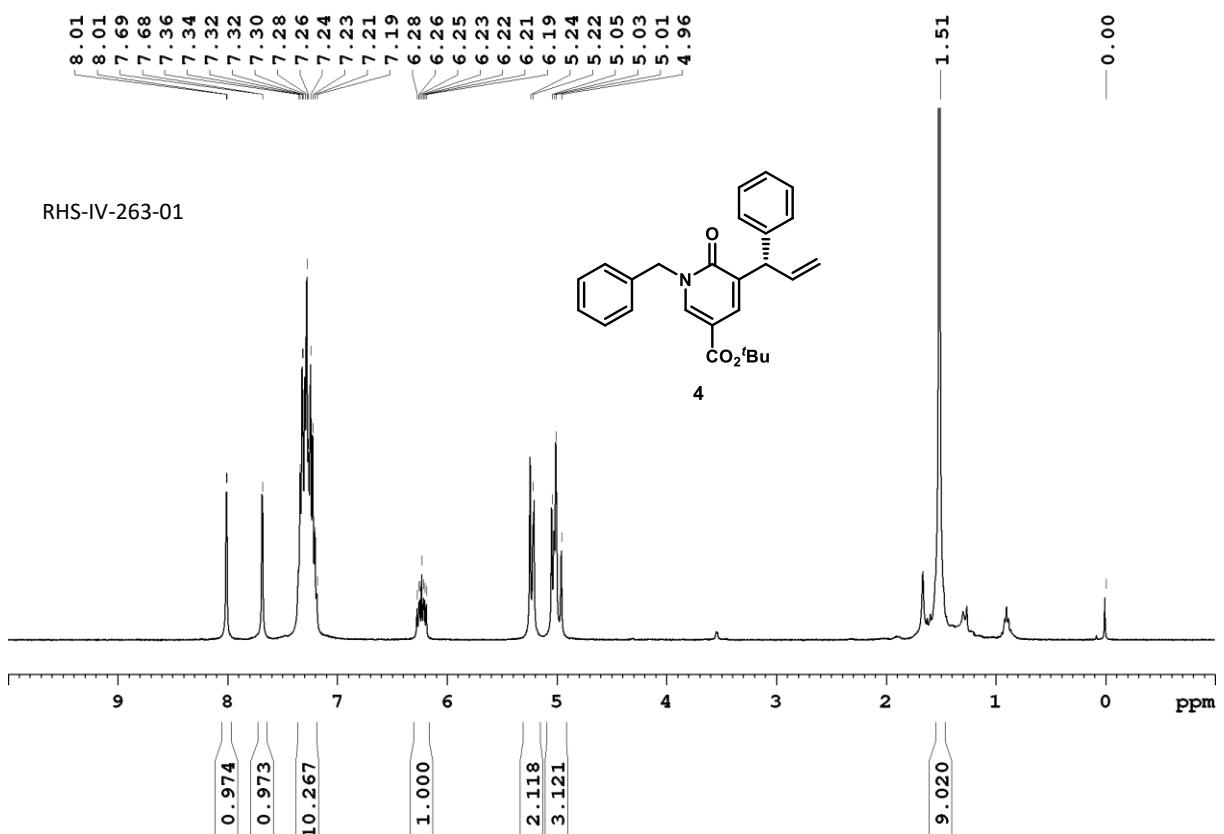
Phenomenex Cellulose-1 column (75:25 n-Hexane/EtOH, 1.0 mL/min, 20 °C)

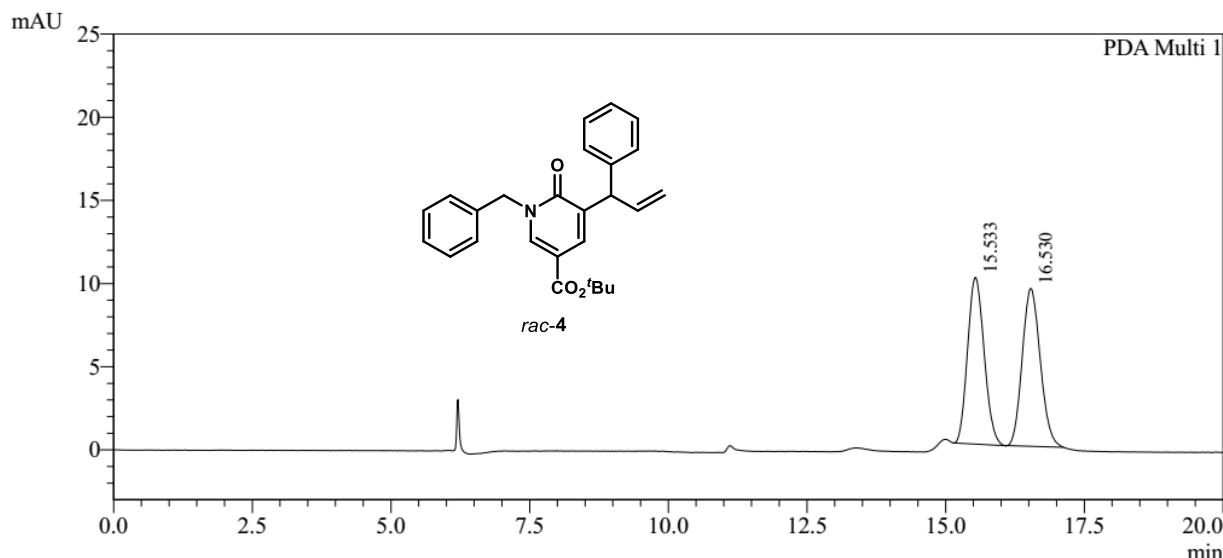


PeakTable

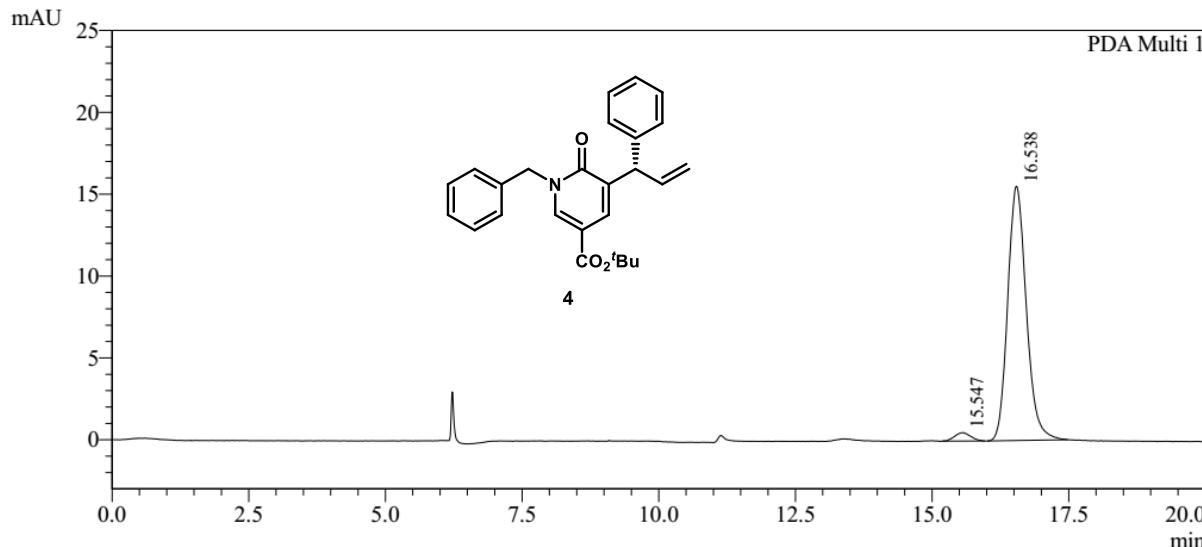
PDA Ch1 300nm 4nm

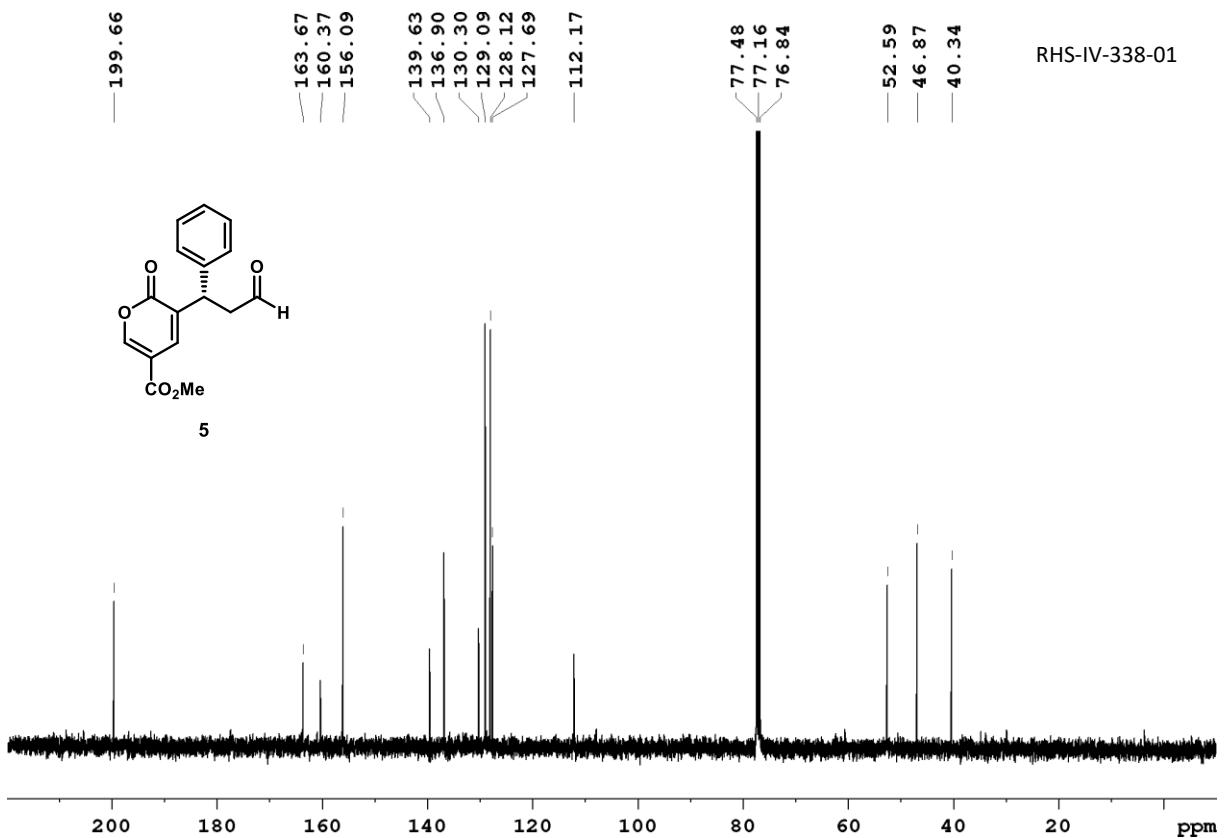
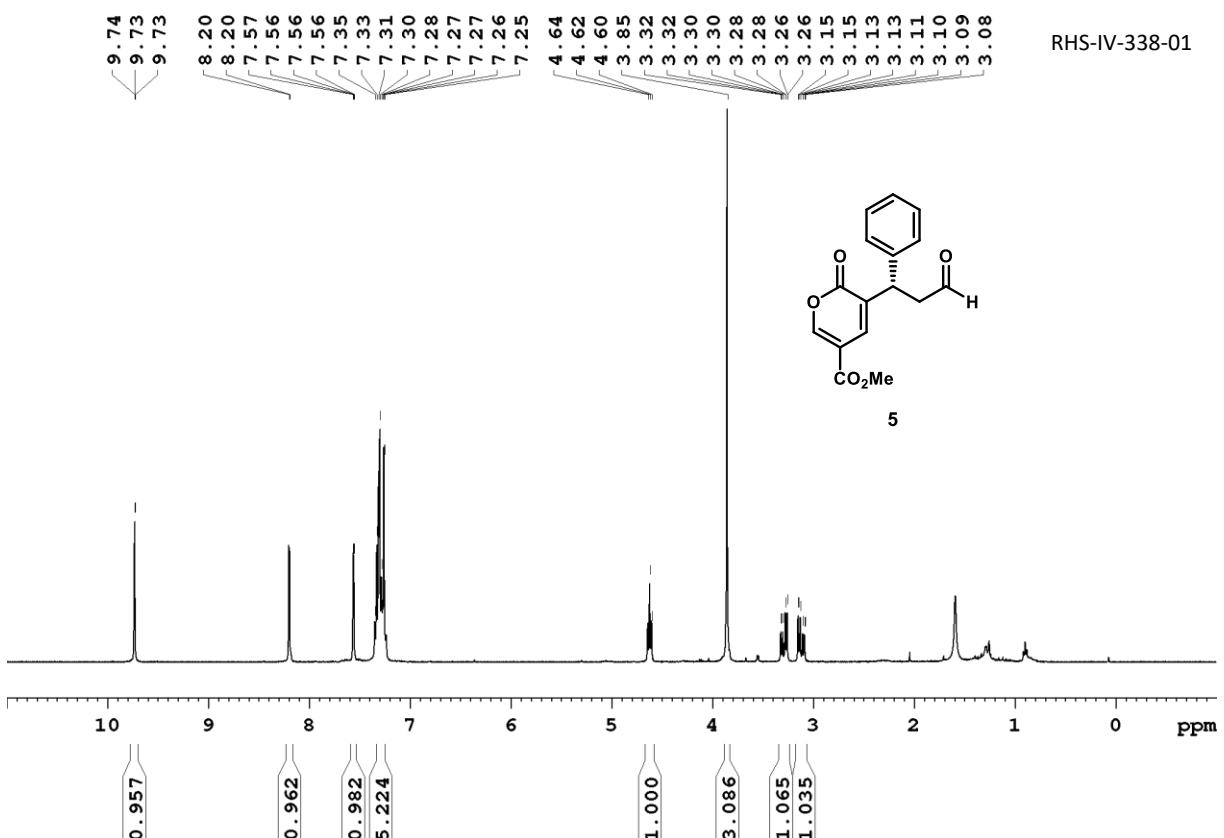
Peak#	Ret. Time	Area	Area %
1	11.305	54009	3.210
2	15.694	1628304	96.790
Total		1682312	100.000

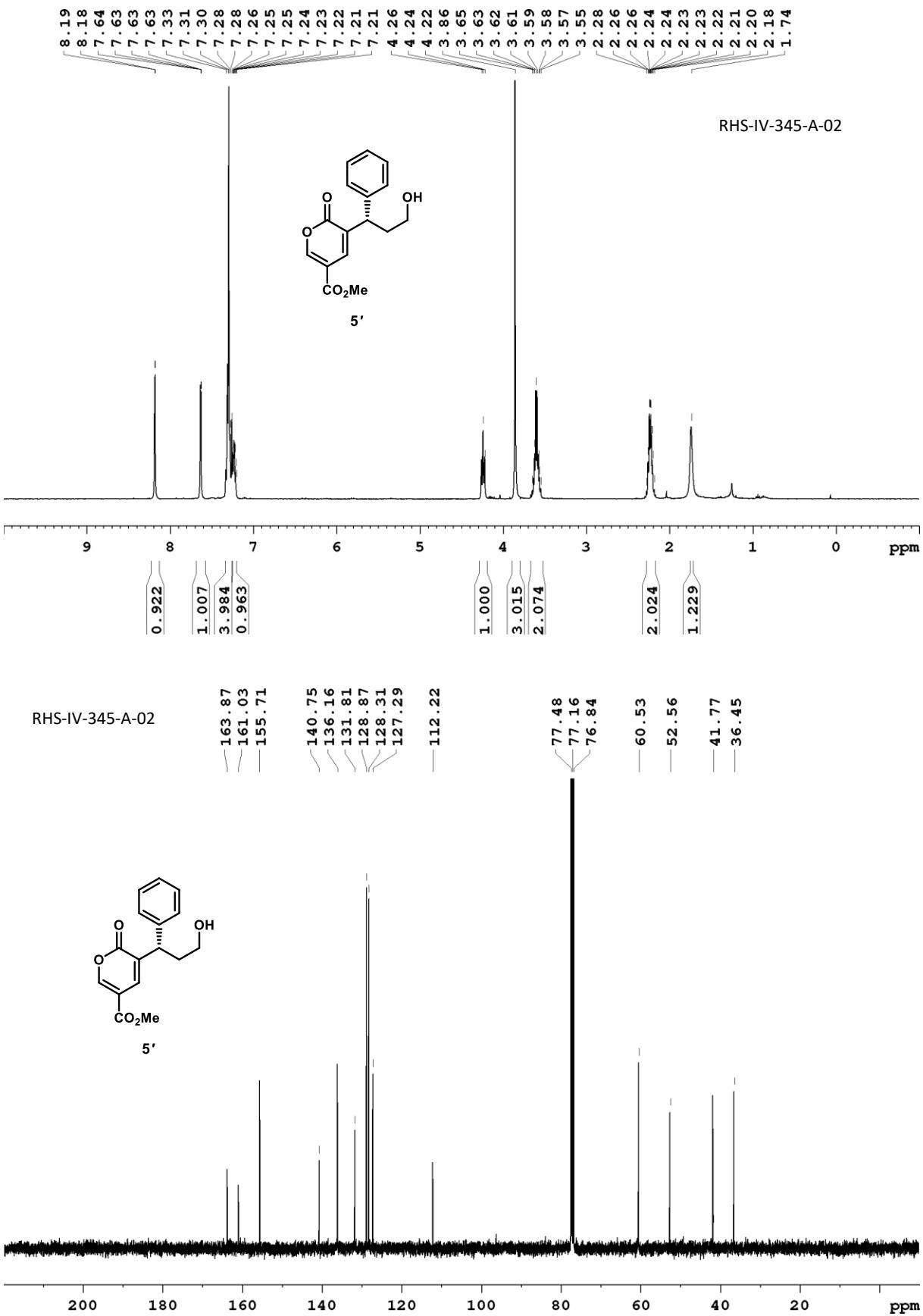


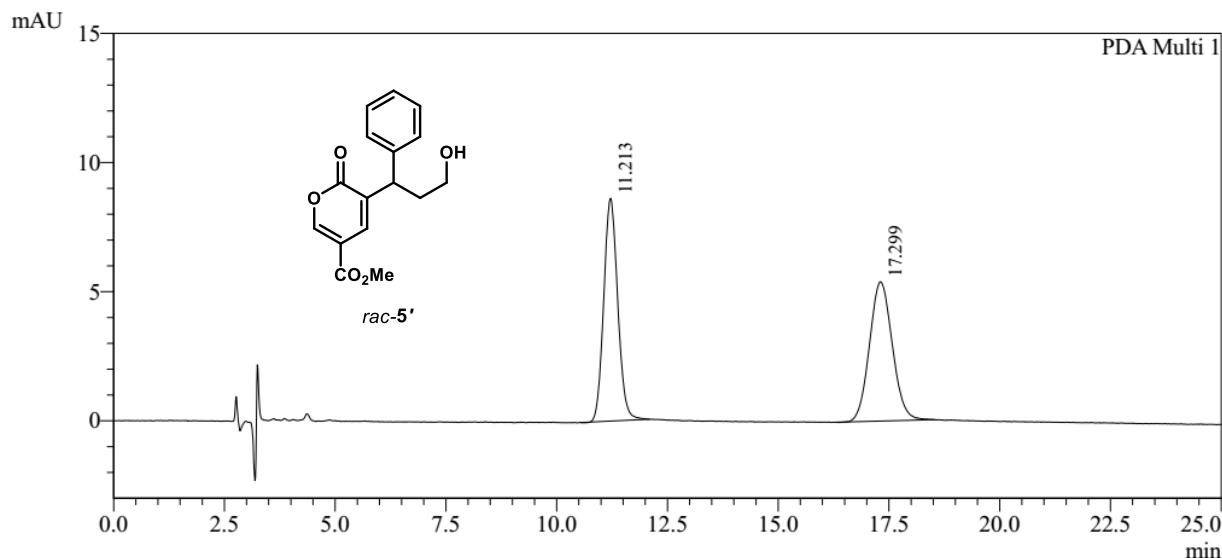


Phenomenex Cellulose-1 column (95:5 *n*-Hexane/EtOH, 0.5 mL/min, 20 °C)







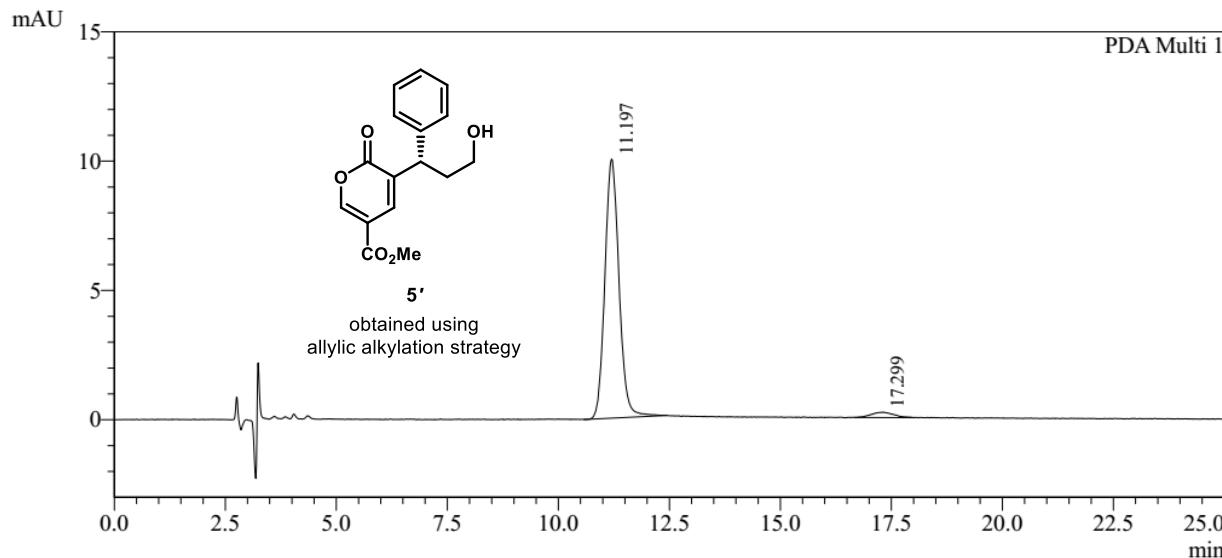


PeakTable

PDA Ch1 300nm 4nm

Peak#	Ret. Time	Area	Area %
1	11.213	189592	49.506
2	17.299	193379	50.494
Total		382971	100.000

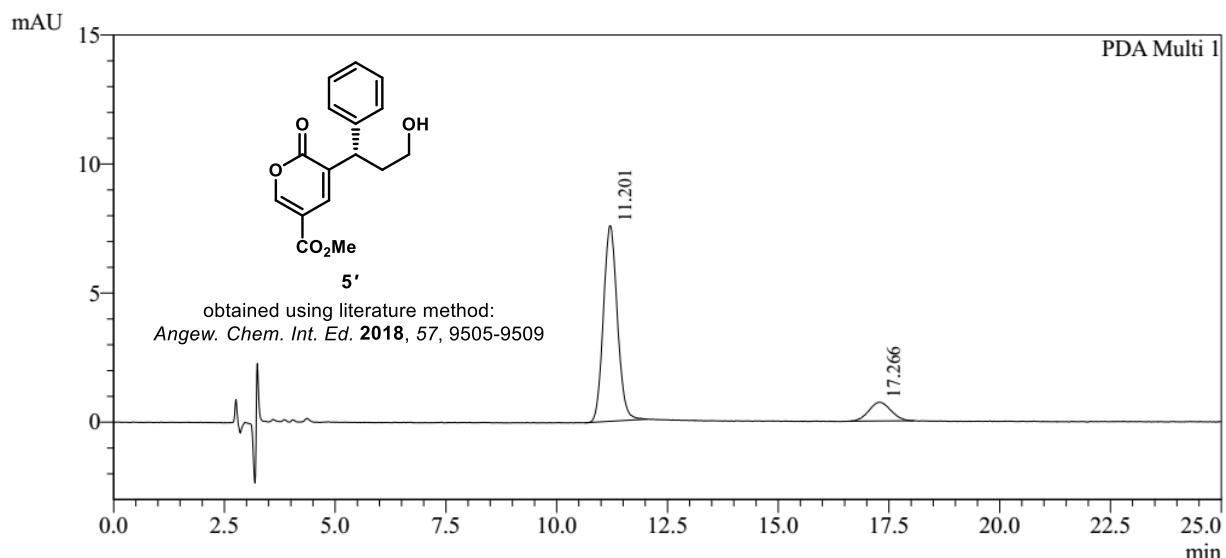
Phenomenex Cellulose-2 column (60:40 *n*-Hexane/EtOH, 1.0 mL/min, 20 °C)



PeakTable

PDA Ch1 300nm 4nm

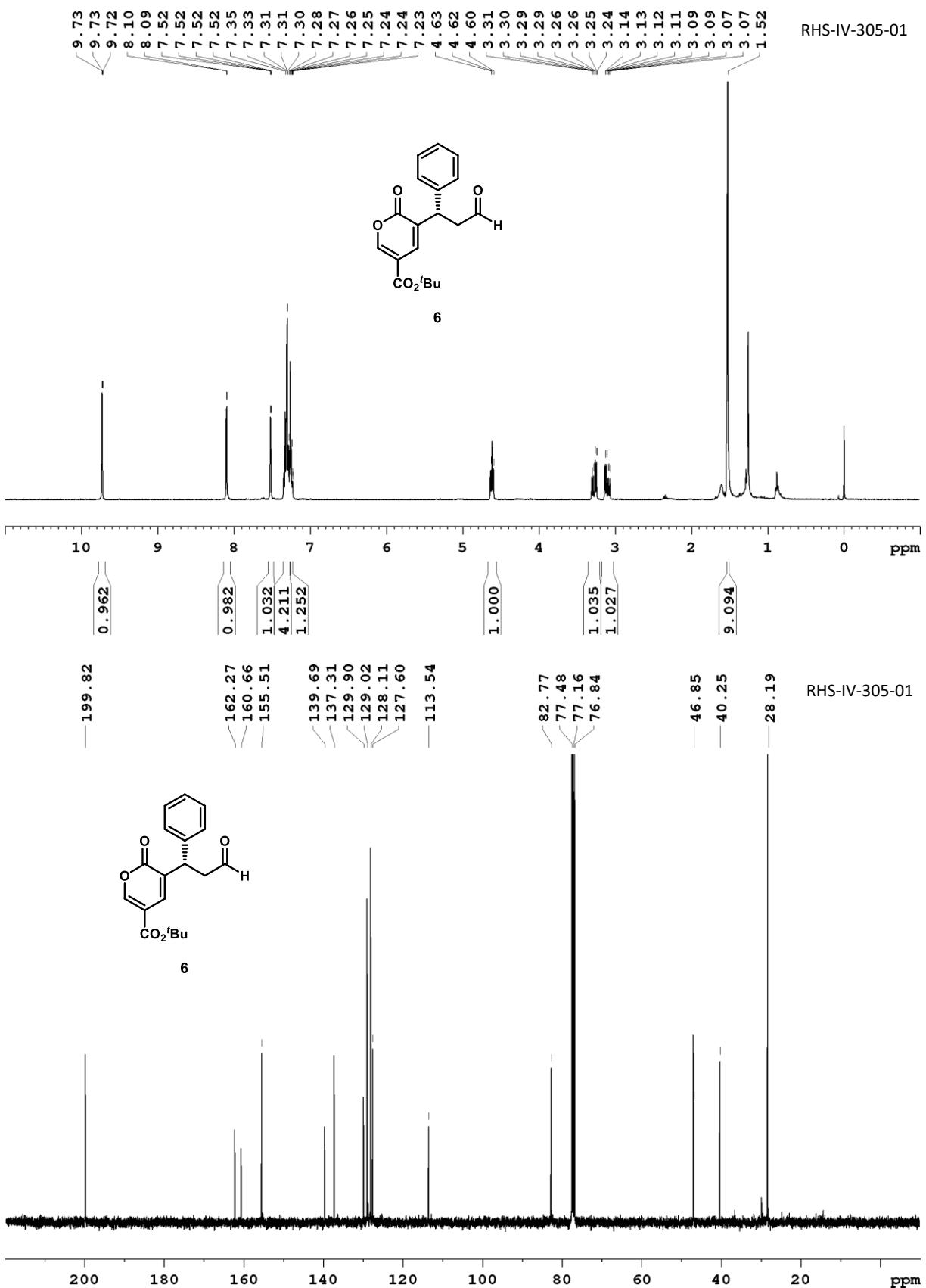
Peak#	Ret. Time	Area	Area %
1	11.197	222965	96.904
2	17.299	7124	3.096
Total		230089	100.000

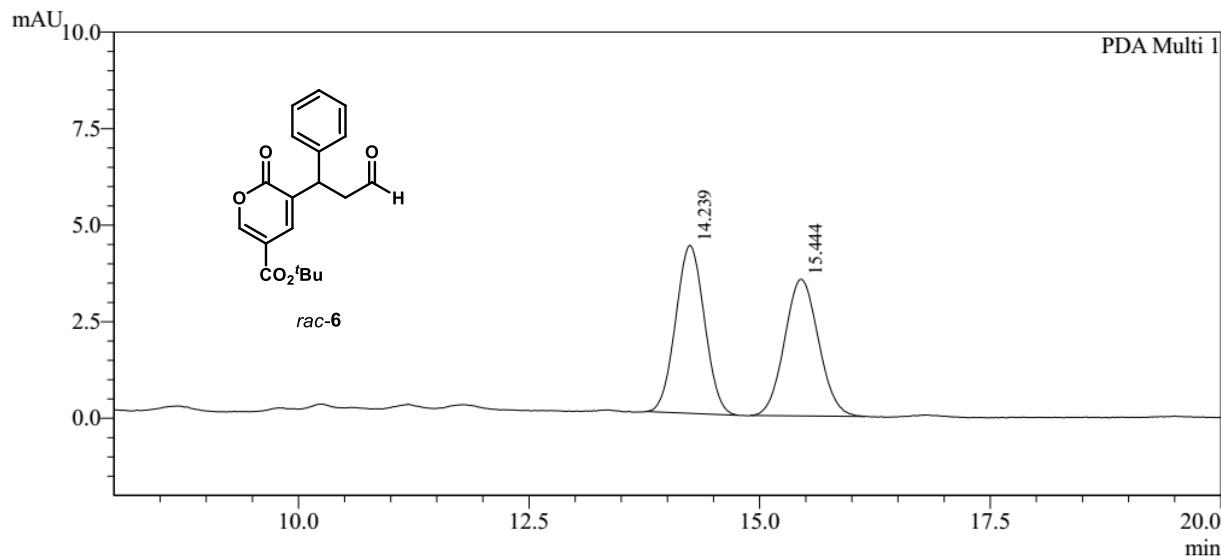


PeakTable

PDA Ch1 300nm 4nm

Peak#	Ret. Time	Area	Area %
1	11.201	166774	86.940
2	17.266	25052	13.060
Total		191825	100.000



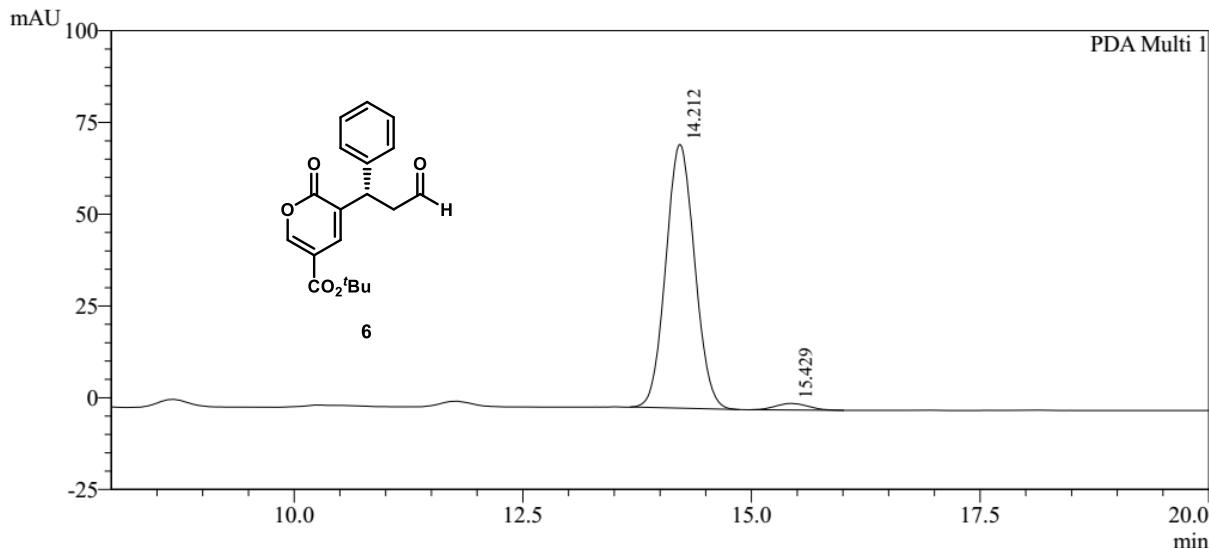


PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	14.239	94647	51.026
2	15.444	90839	48.974
Total		185485	100.000

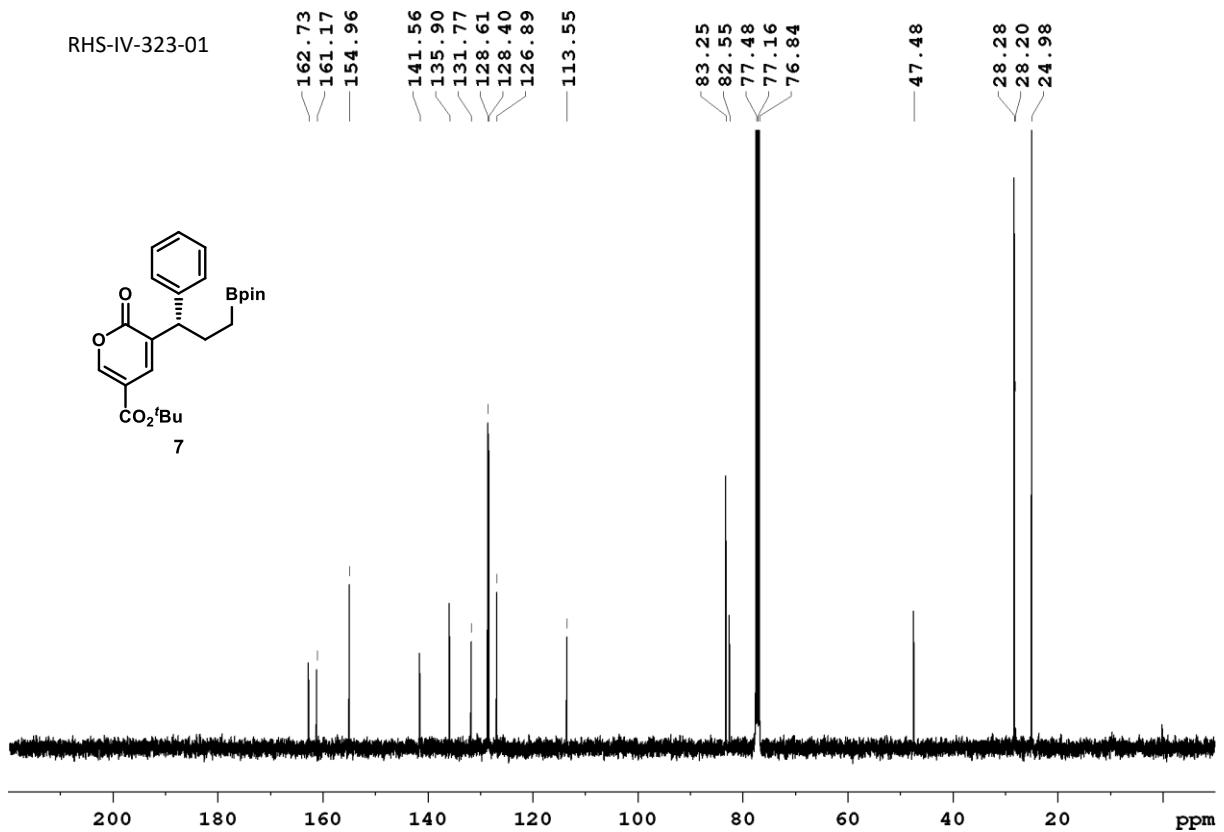
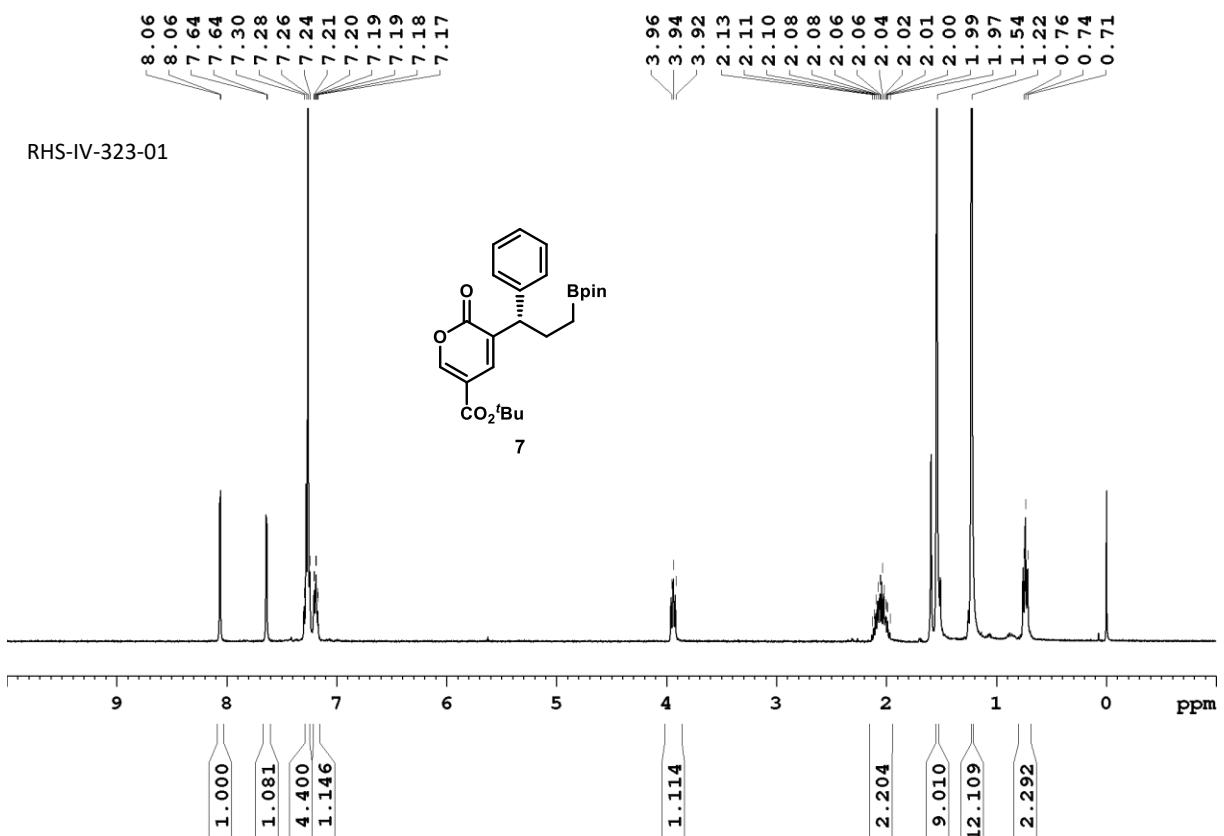
Daicel Chiraldex IG column (75:25 n-Hexane/EtOH, 1.0 mL/min, 20 °C)

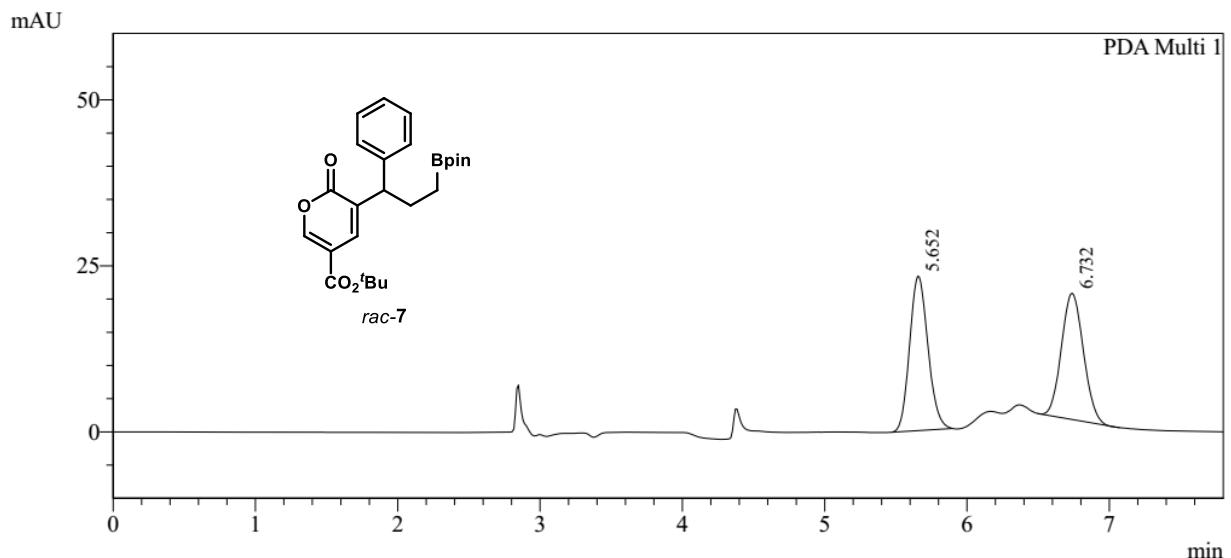


PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Area %
1	14.212	1582134	97.285
2	15.429	44154	2.715
Total		1626288	100.000



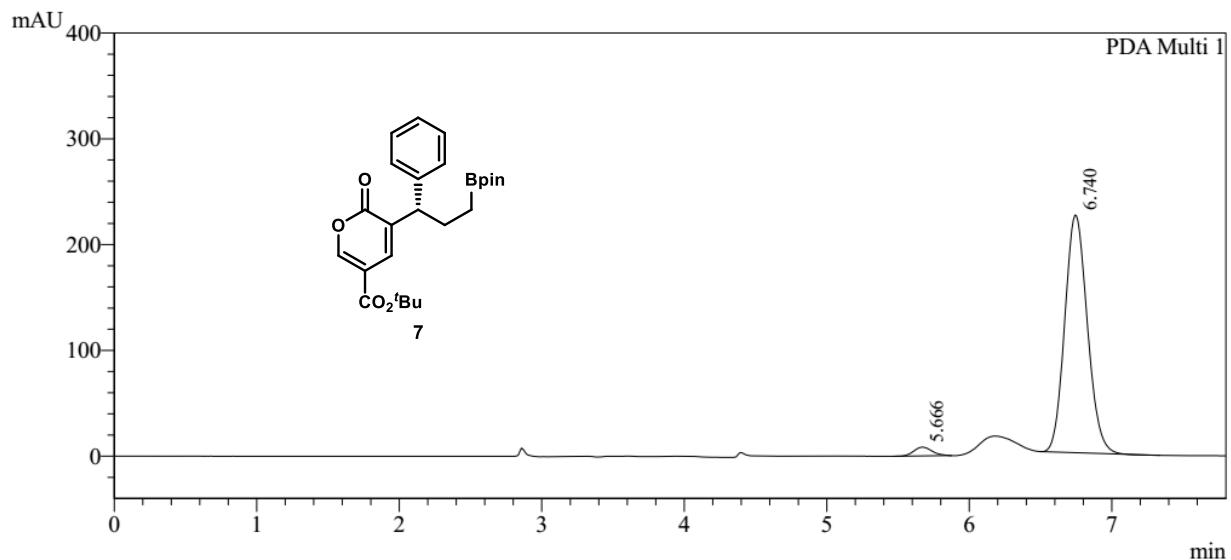


PeakTable

PDA Ch1 258nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.652	208250	50.605
2	6.732	203267	49.395
Total		411517	100.000

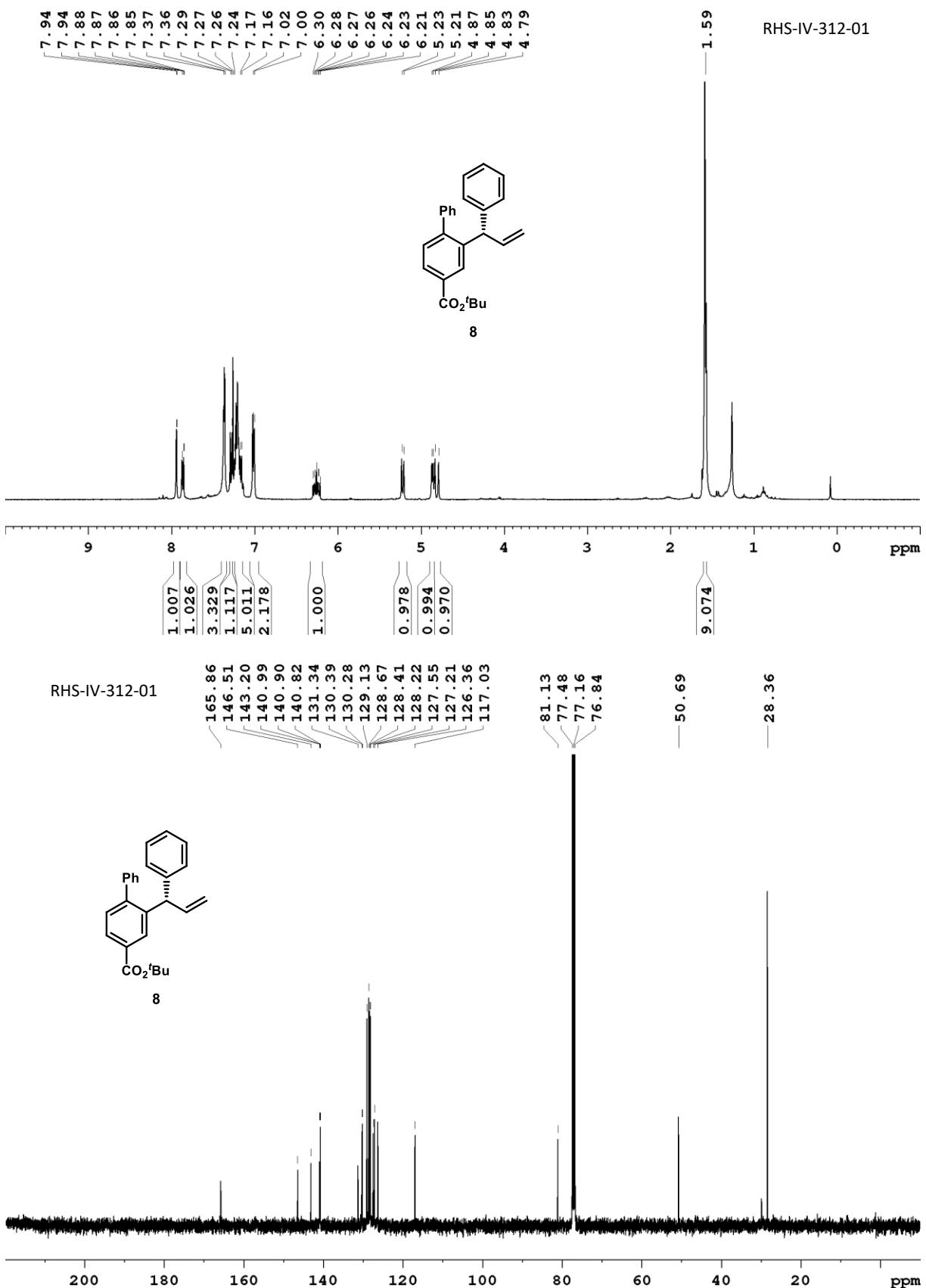
Phenomenex Cellulose-1 column (90:10 *n*-Hexane/EtOH, 1.0 mL/min, 20 °C)

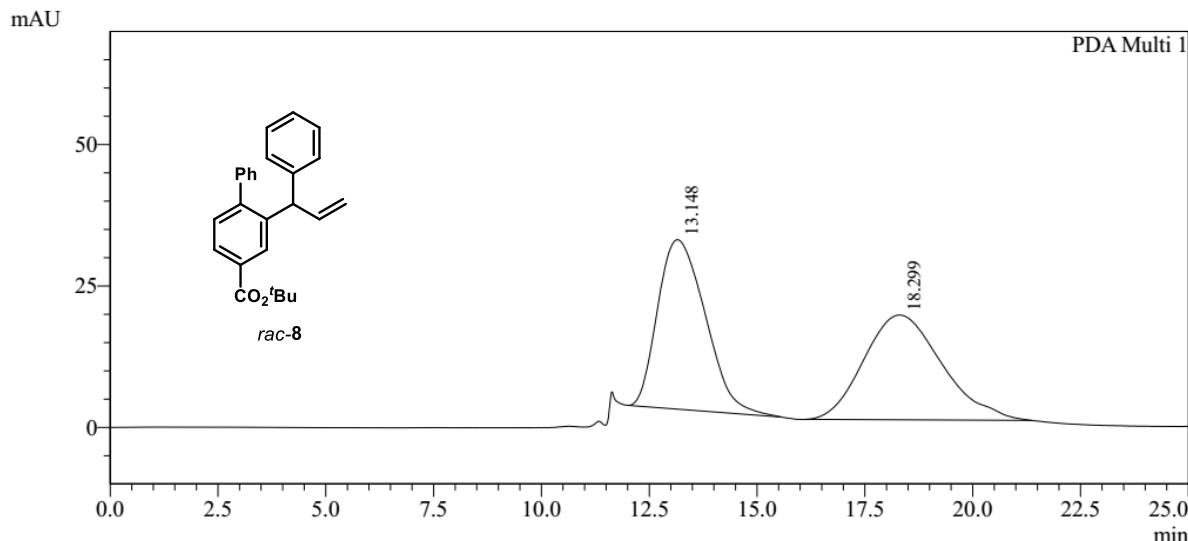


PeakTable

PDA Ch1 258nm 4nm

Peak#	Ret. Time	Area	Area %
1	5.666	73015	2.871
2	6.740	2470410	97.129
Total		2543426	100.000



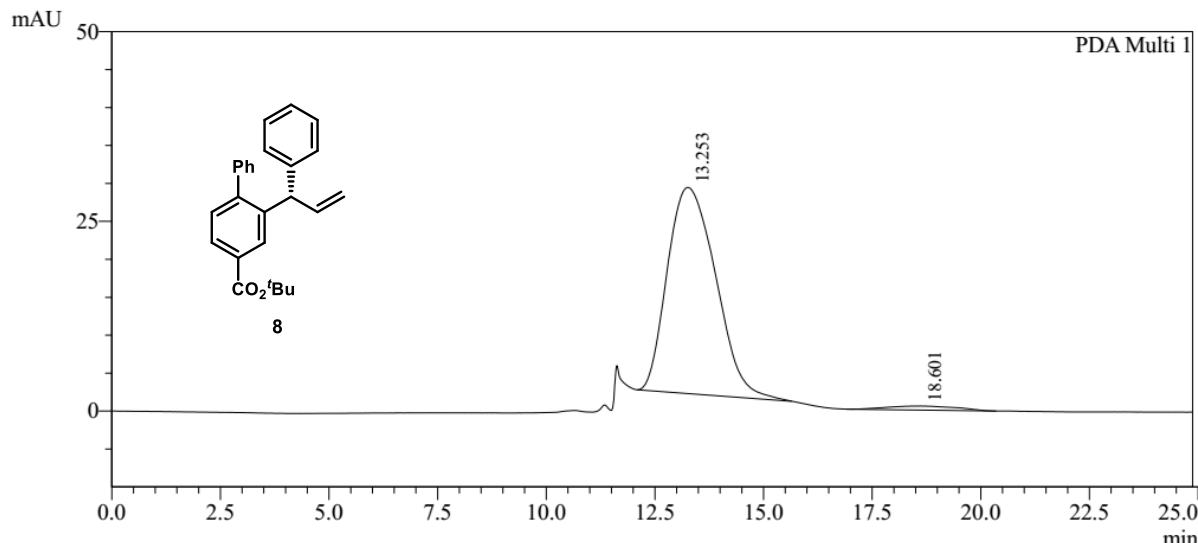


PeakTable

PDA Ch1 248nm 4nm

Peak#	Ret. Time	Area	Area %
1	13.148	2301732	49.667
2	18.299	2332590	50.333
Total		4634322	100.000

Phenomenex Cellulose-3 column (99:1 *n*-Hexane/*i*-PrOH, 0.3 mL/min, 20 °C)



PeakTable

PDA Ch1 248nm 4nm

Peak#	Ret. Time	Area	Area %
1	13.253	2109072	97.266
2	18.601	59284	2.734
Total		2168356	100.000