

Supporting Information

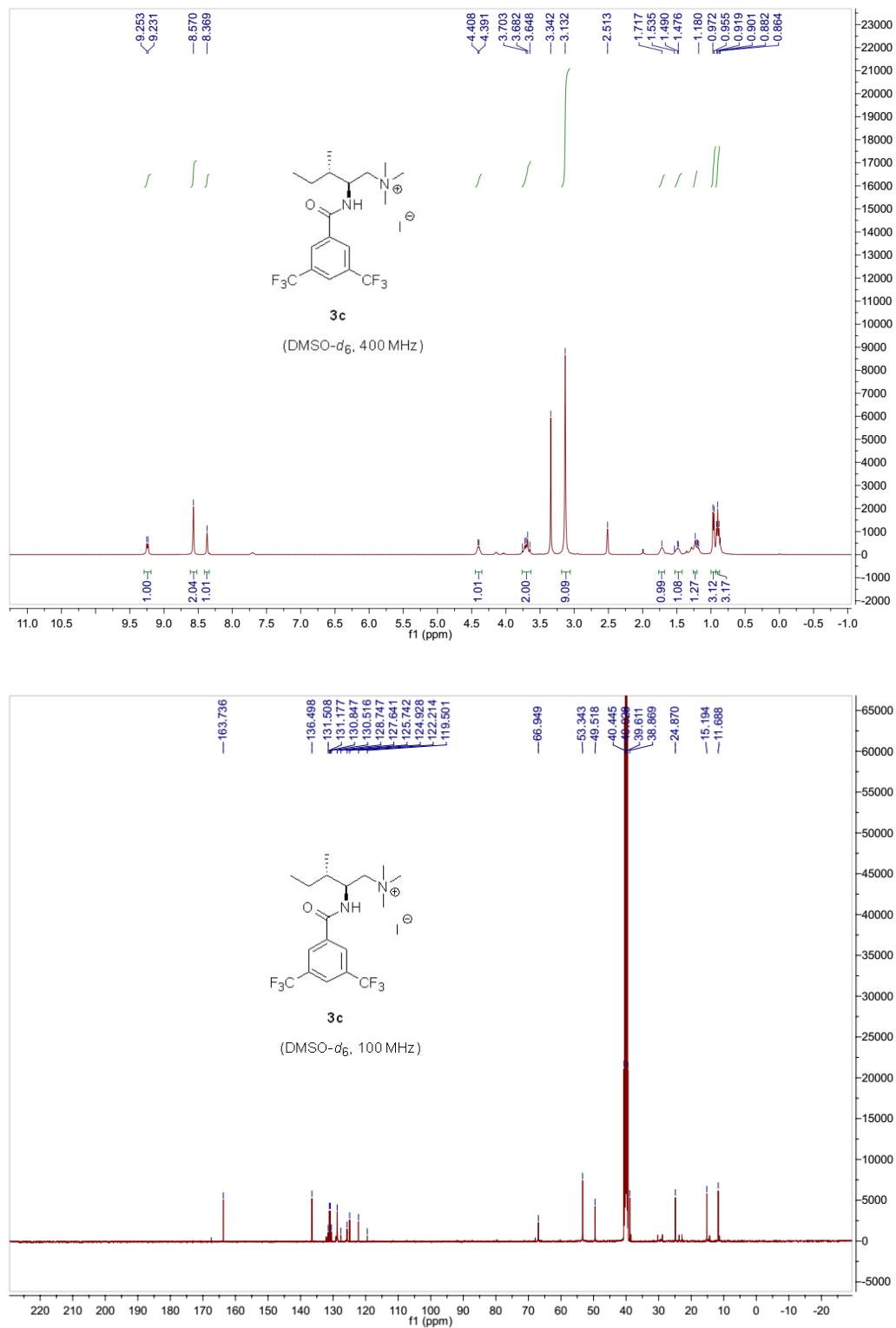
Bifunctional Quaternary Ammonium Salts Catalyzed Stereoselective Conjugate Addition of Oxindoles to Electron-Deficient β -Haloalkenes

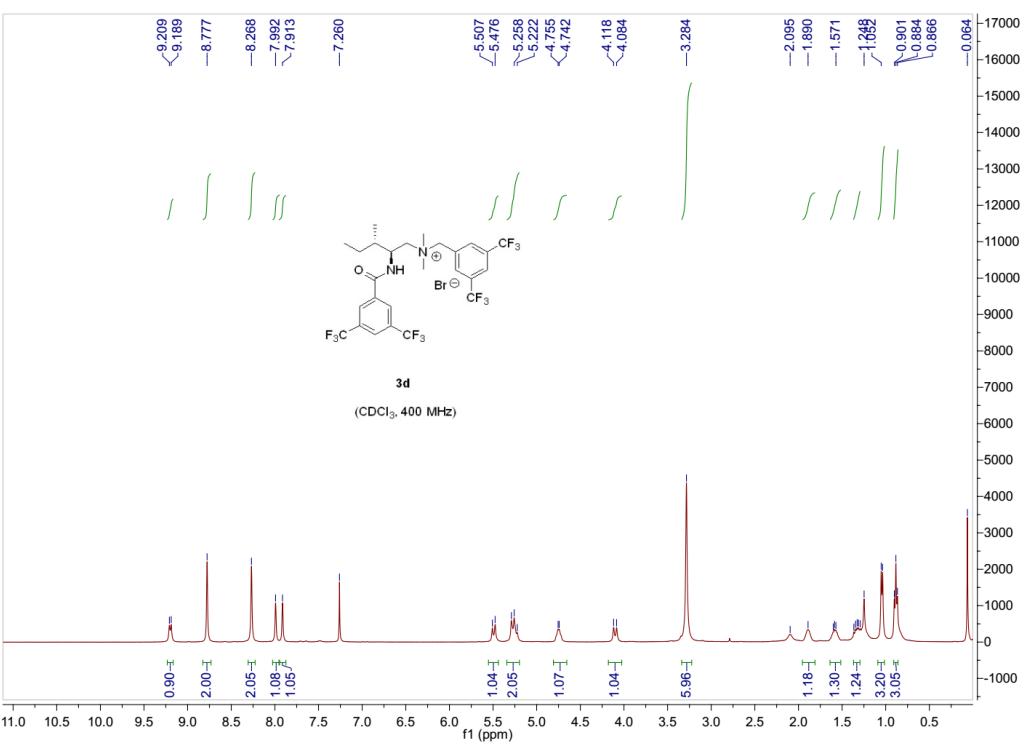
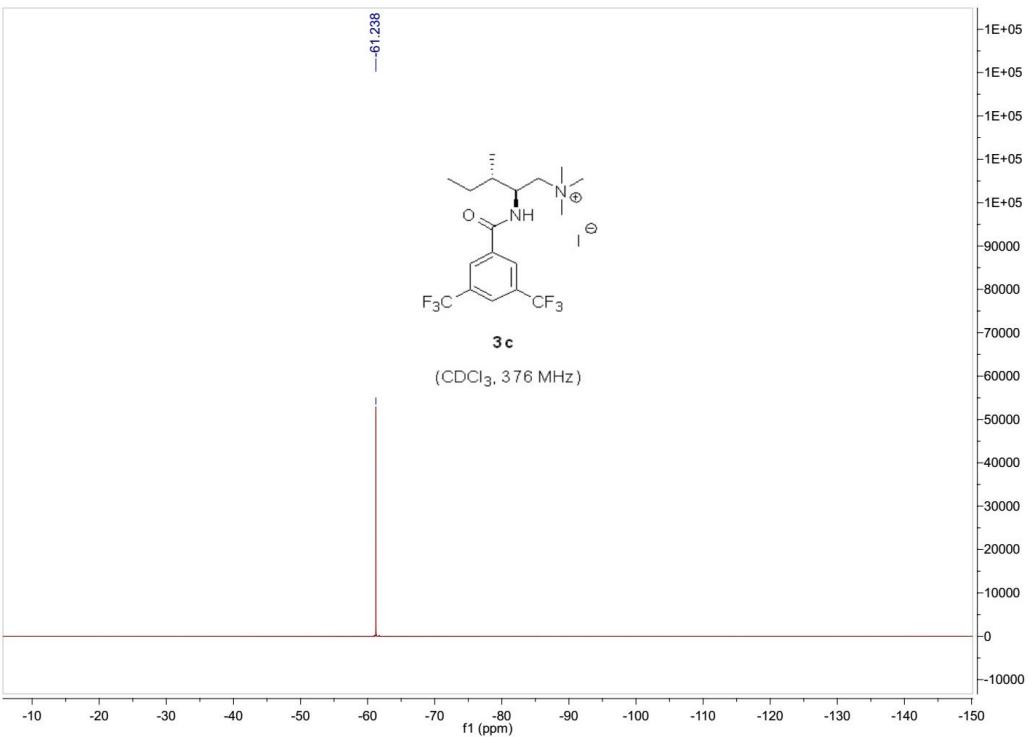
Qiaowen Jin,[†] Changwu Zheng,[‡] Gang Zhao,^{*,‡} and Gang Zou^{*,†}

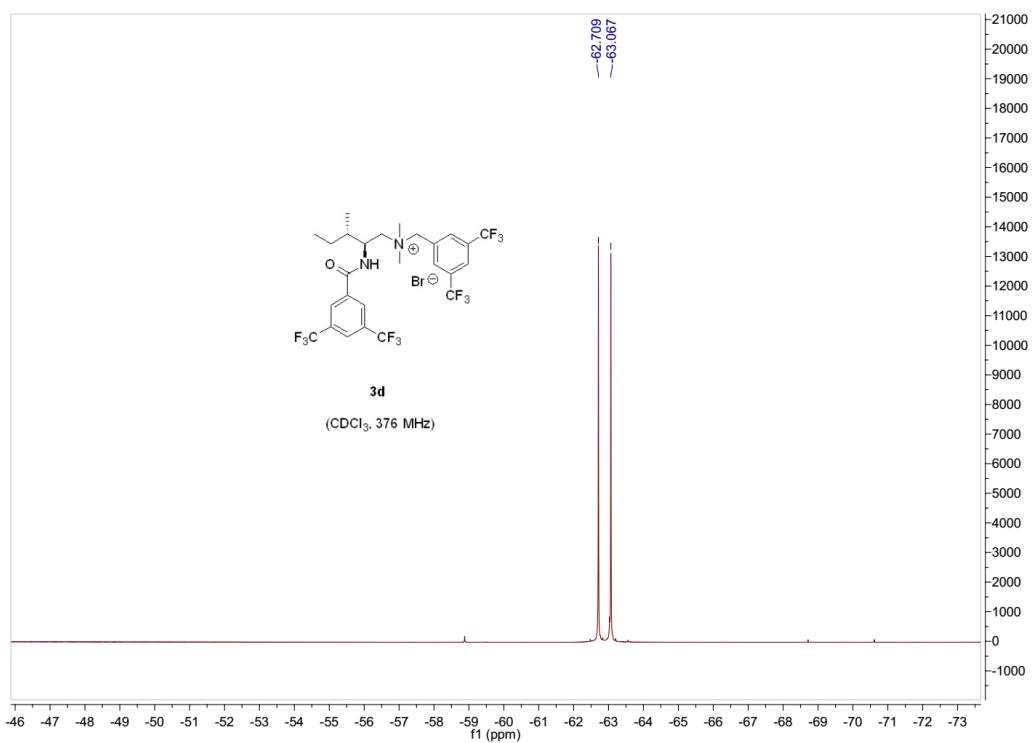
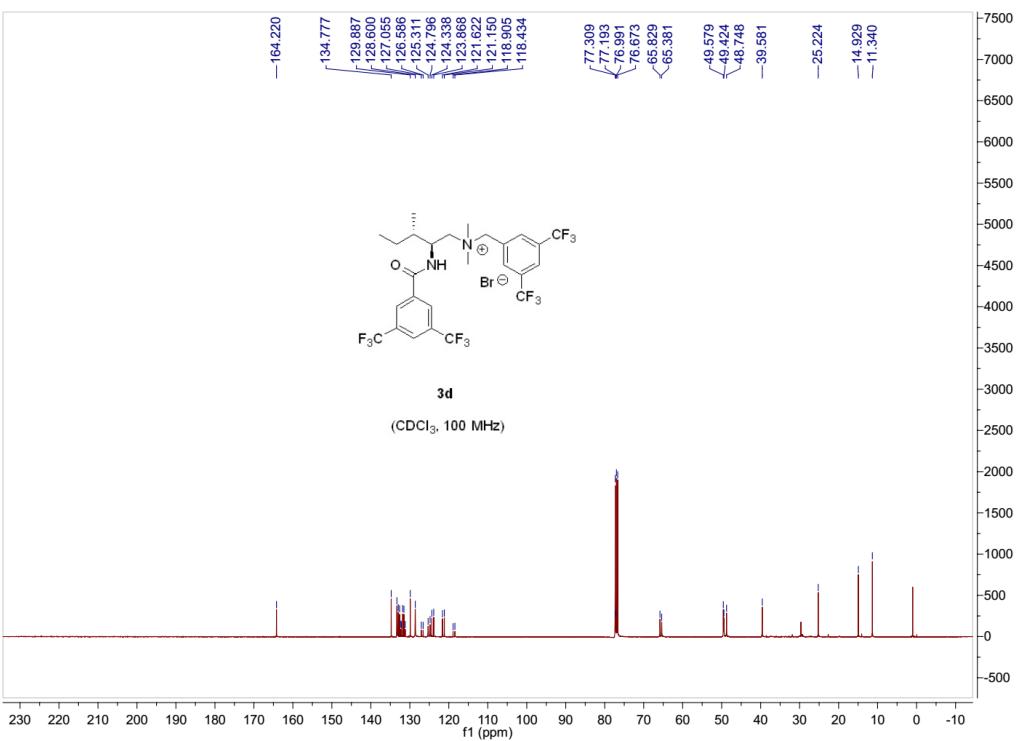
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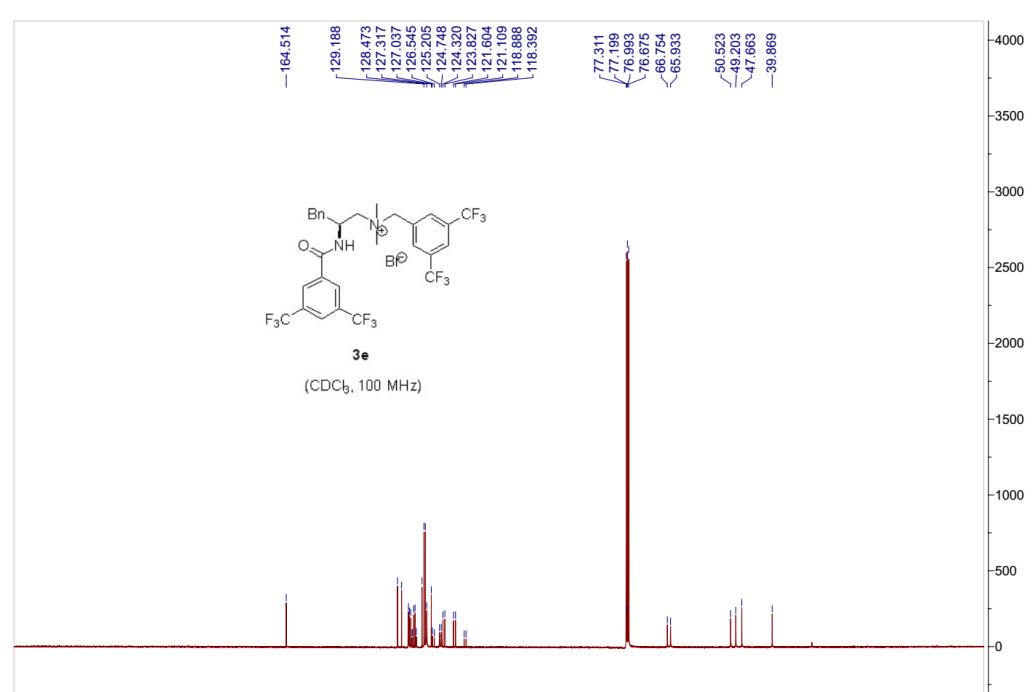
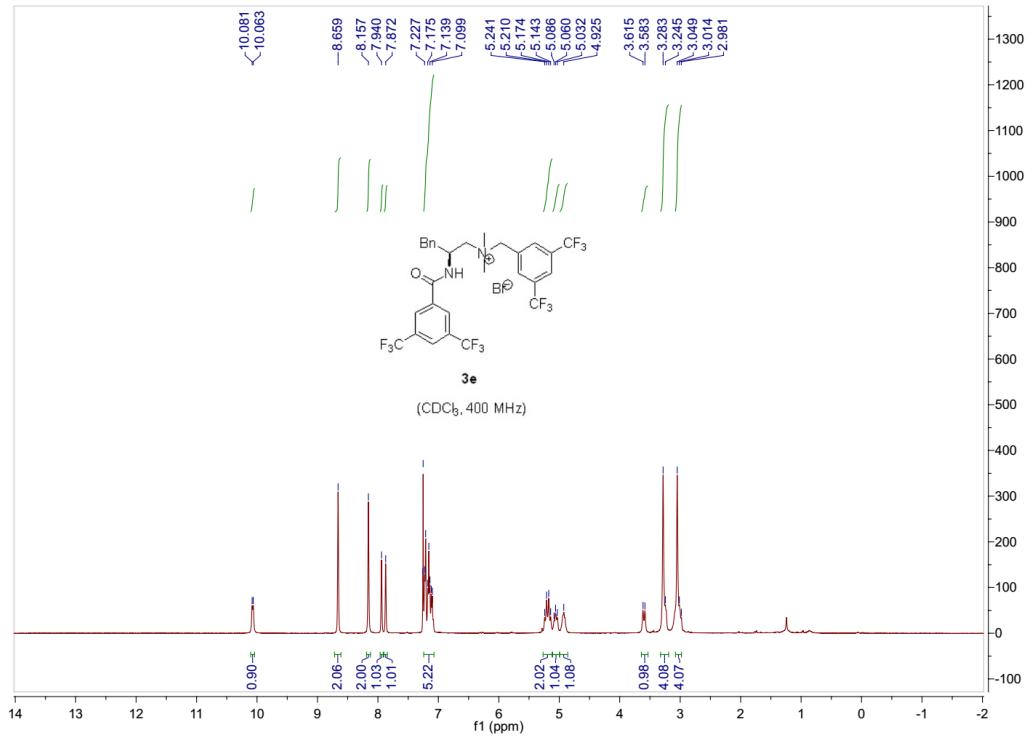
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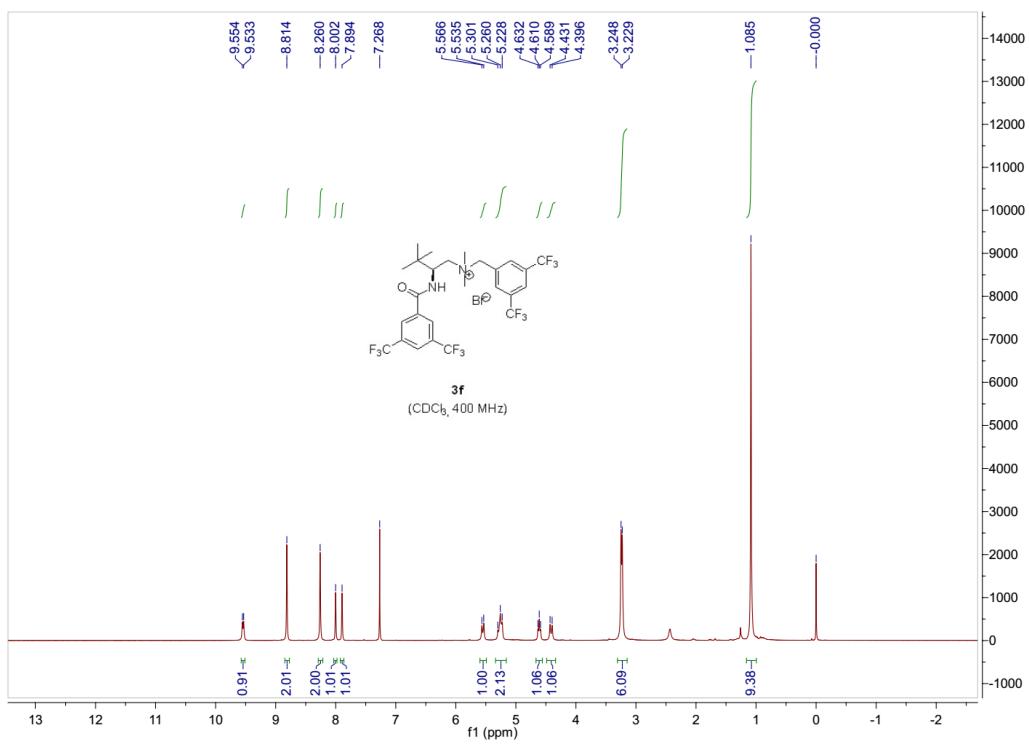
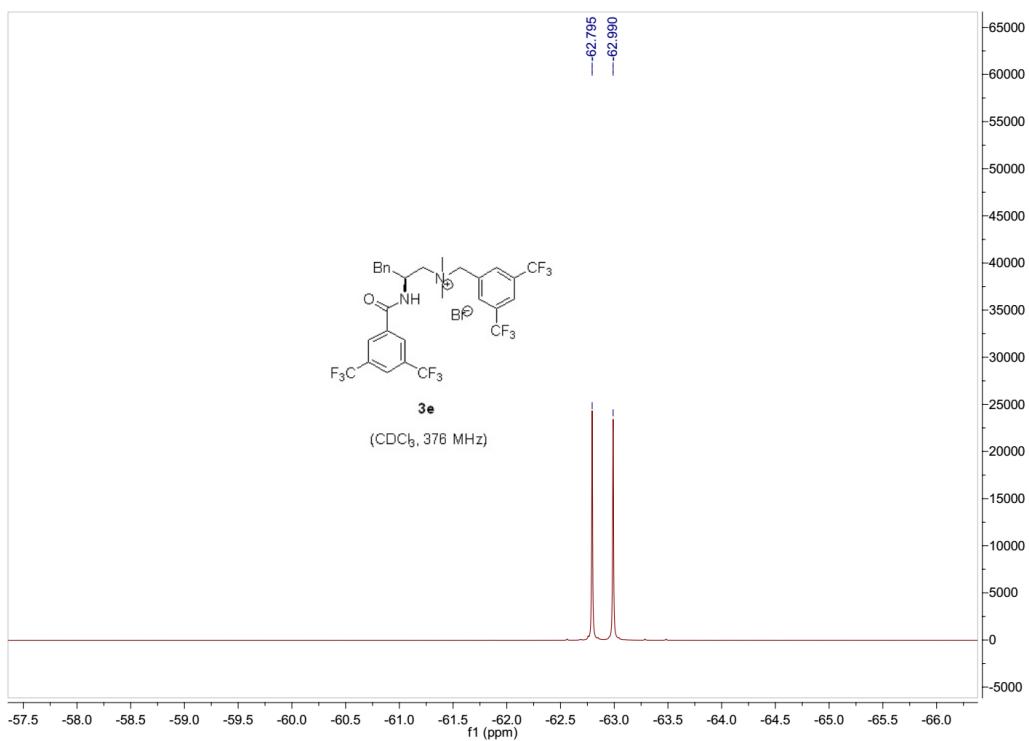
Part I. NMR Spectra for catalysts 3

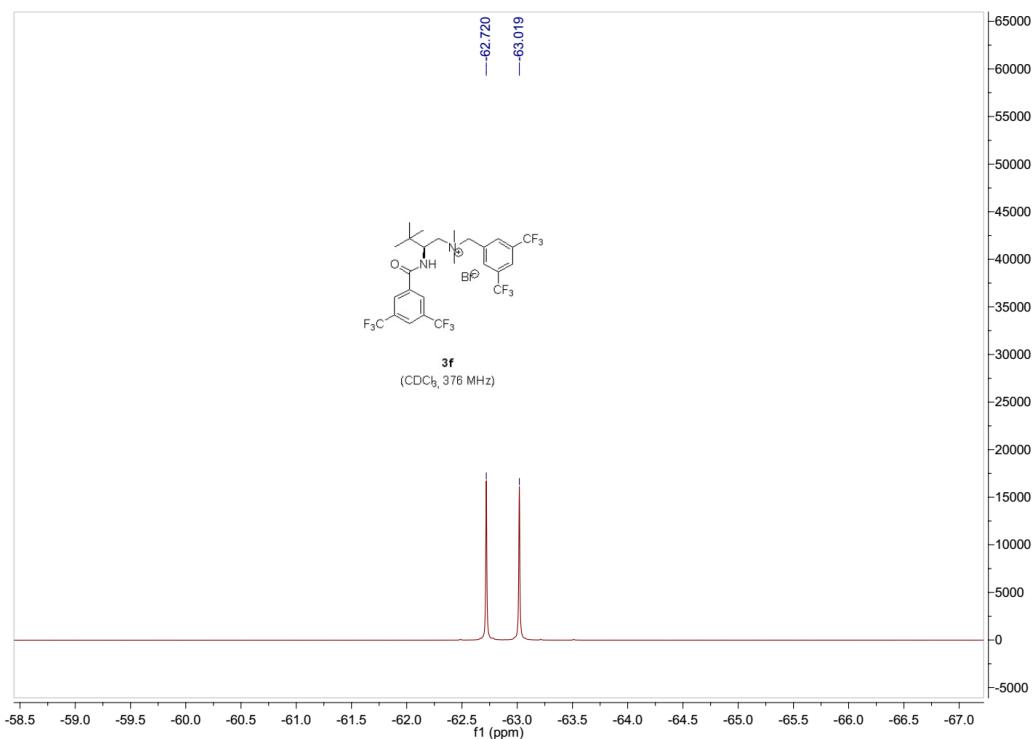
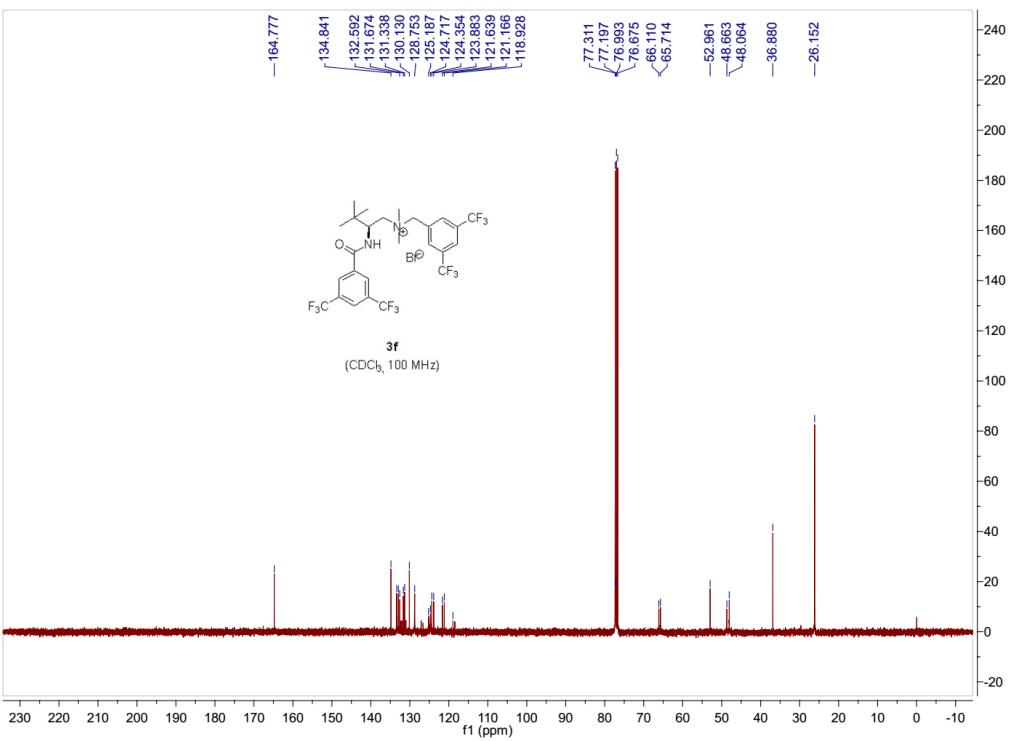


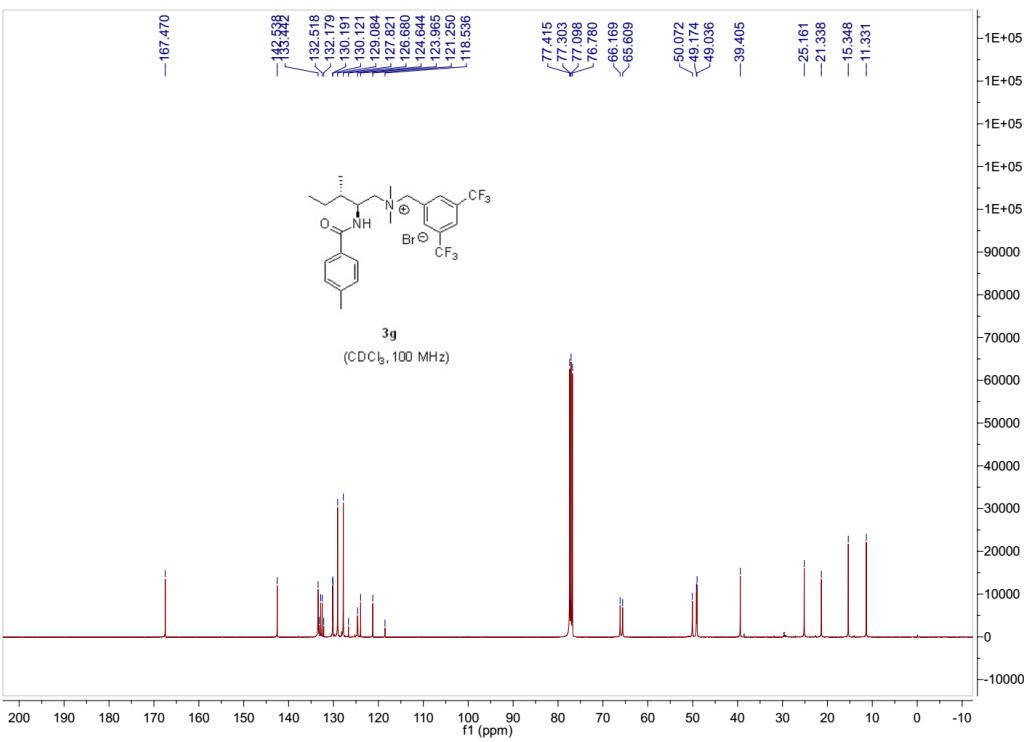
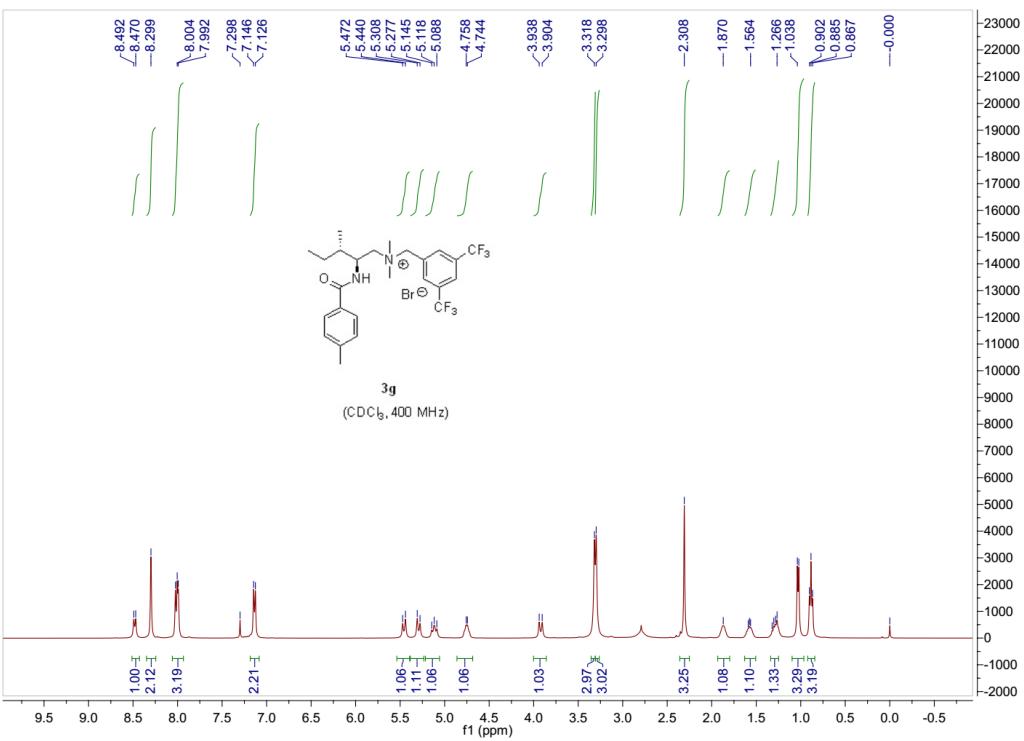


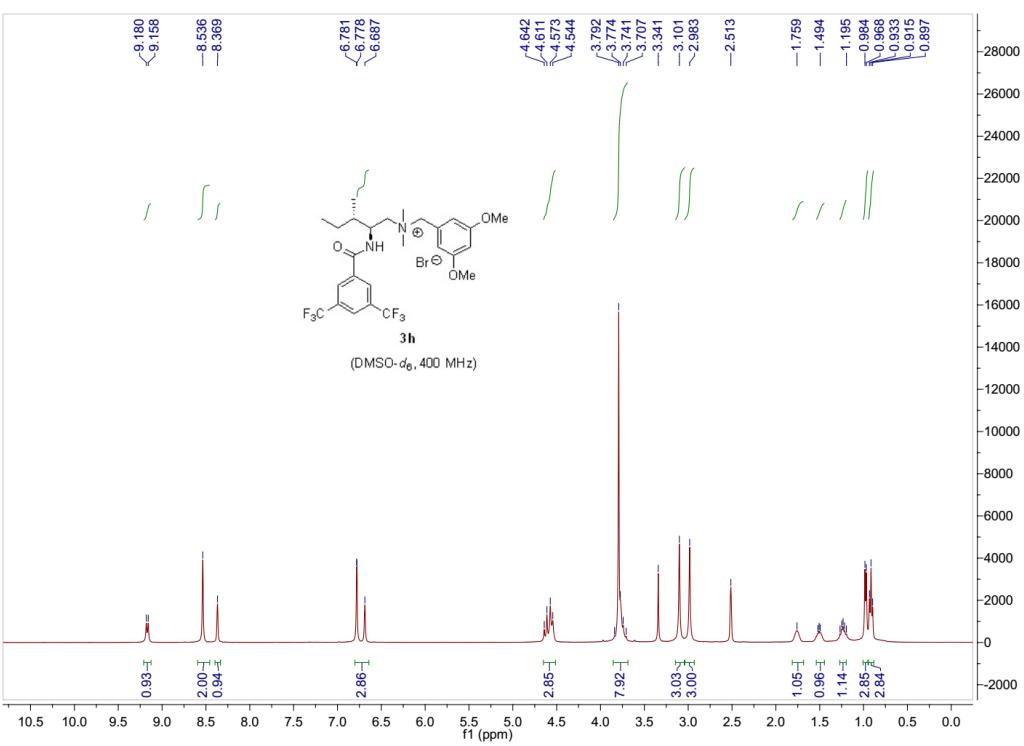
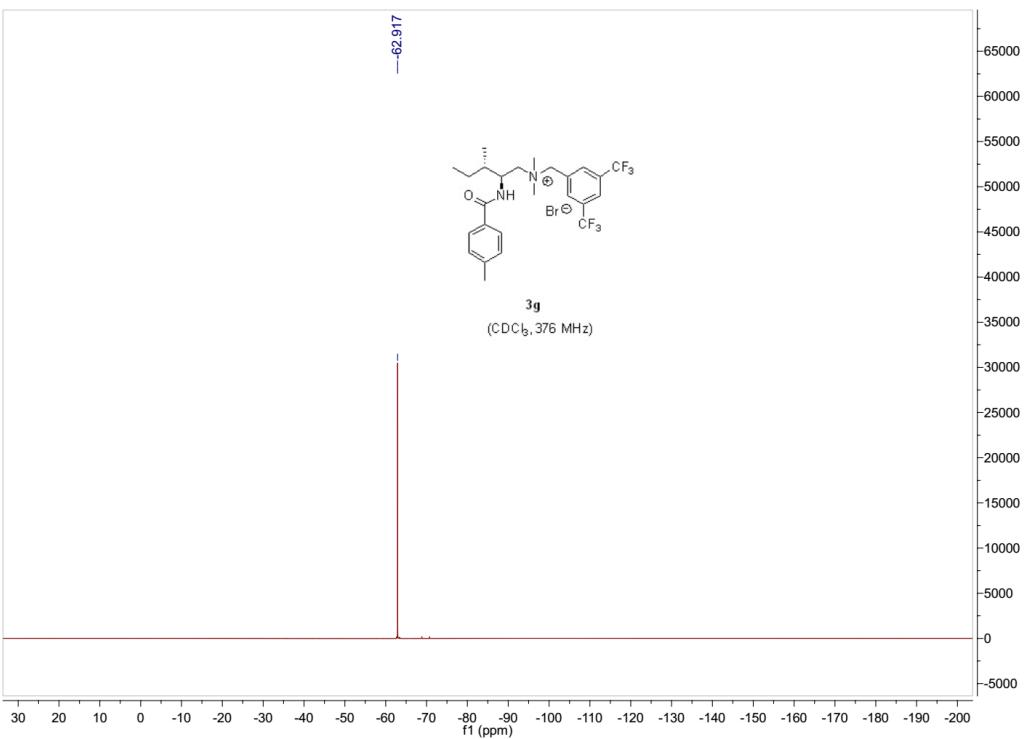


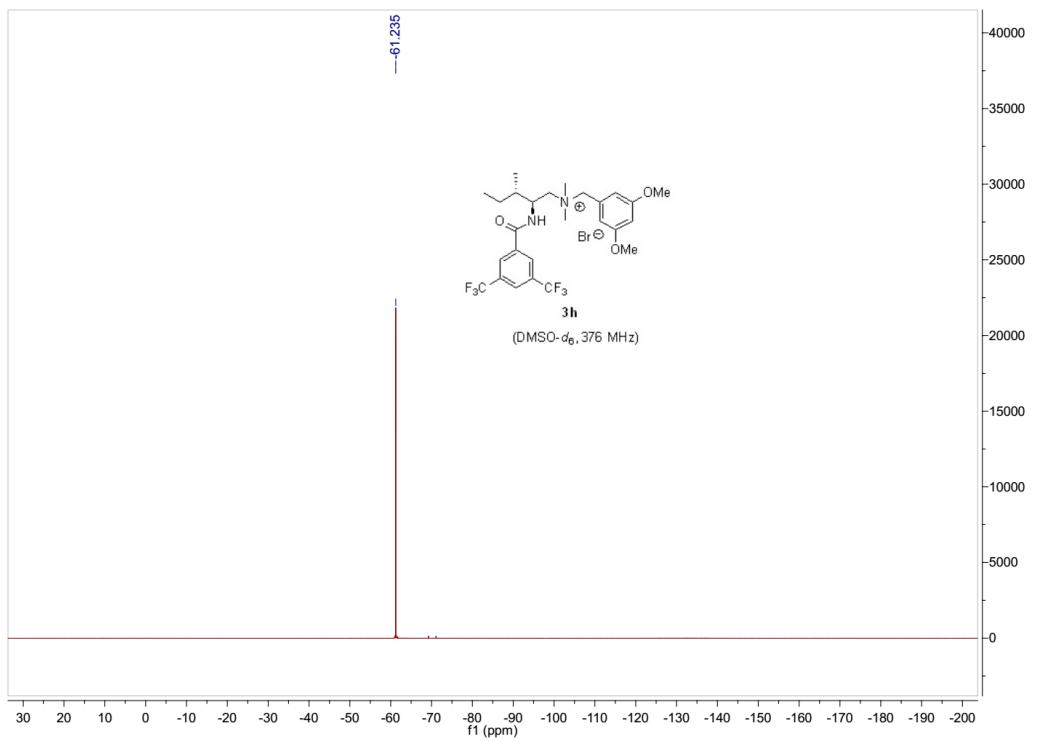
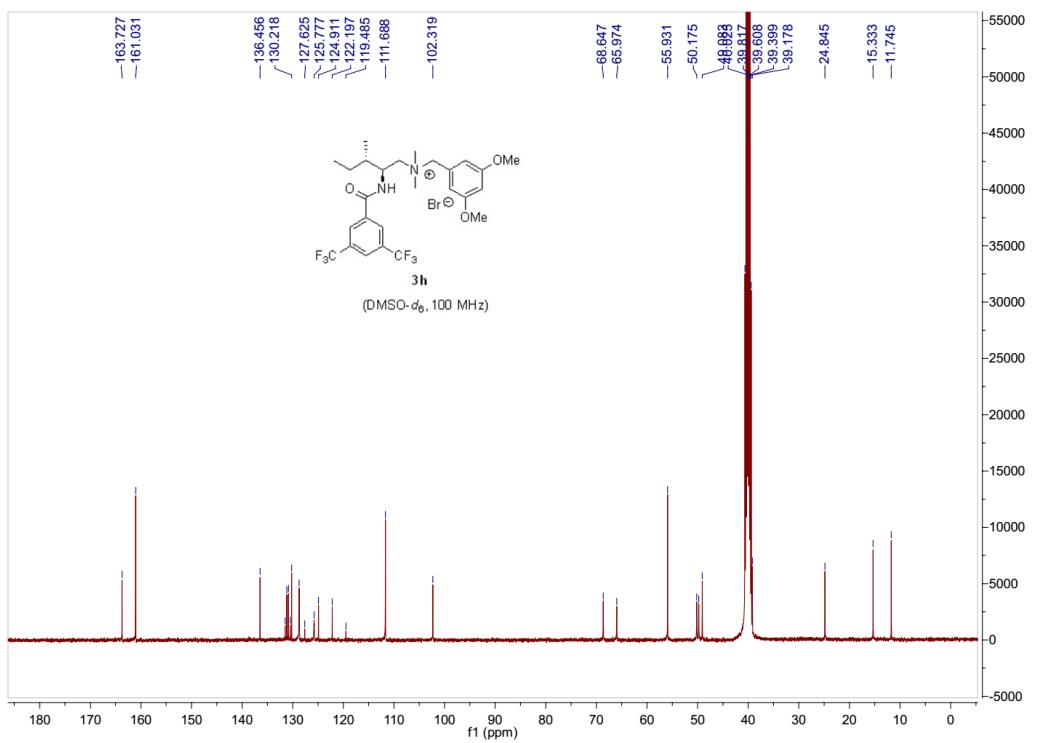


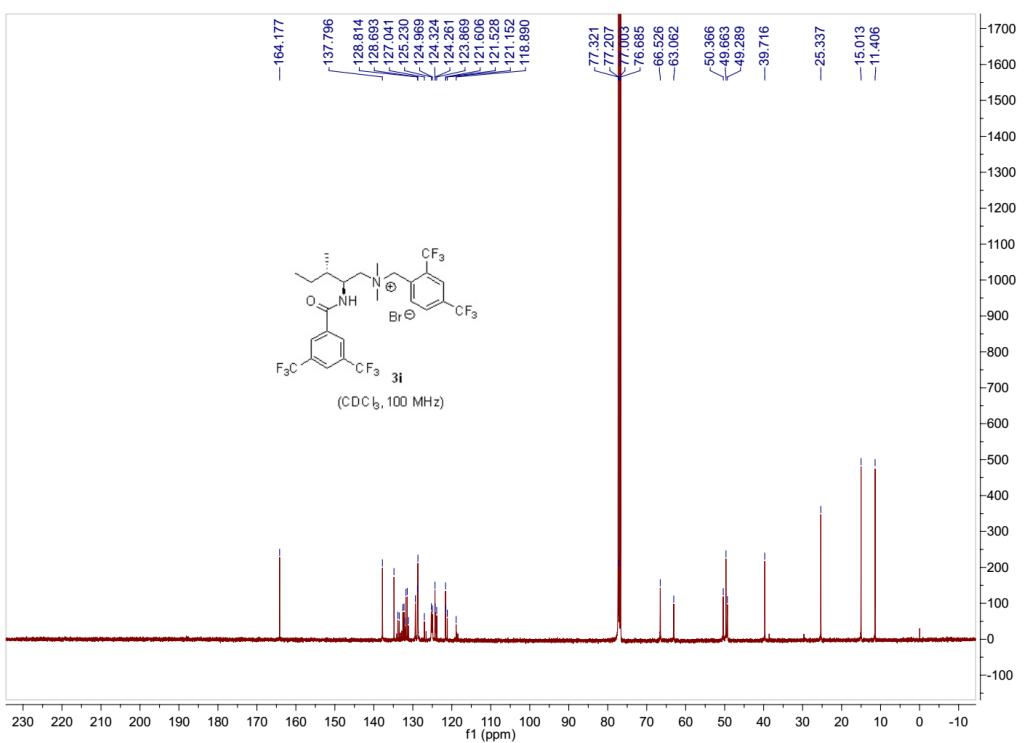
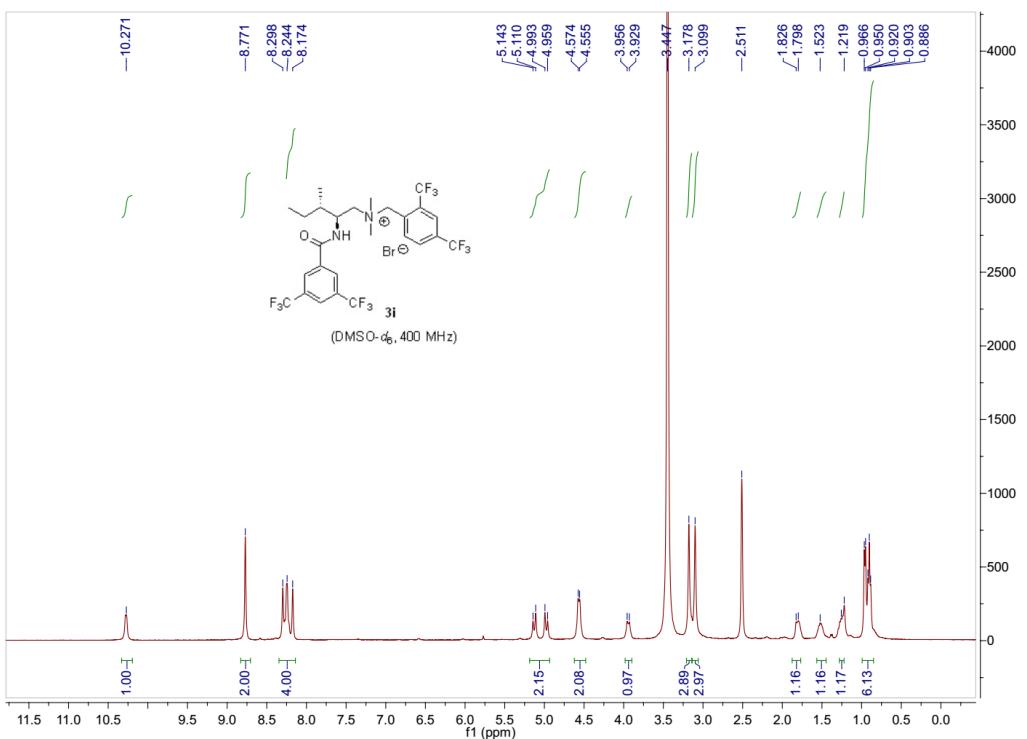


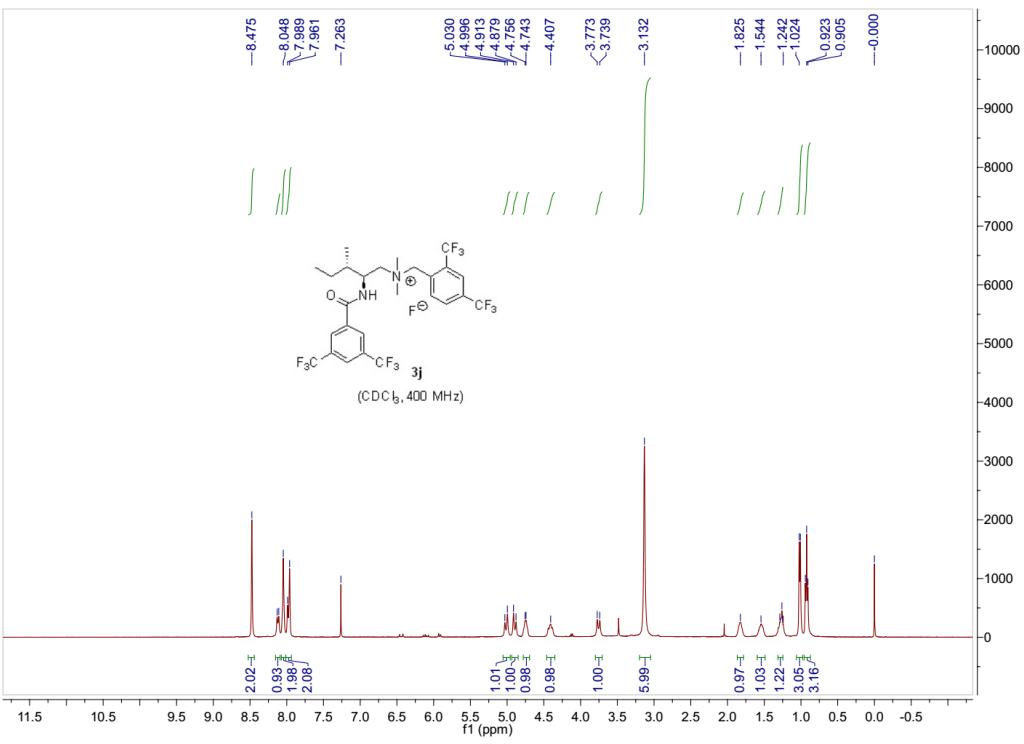
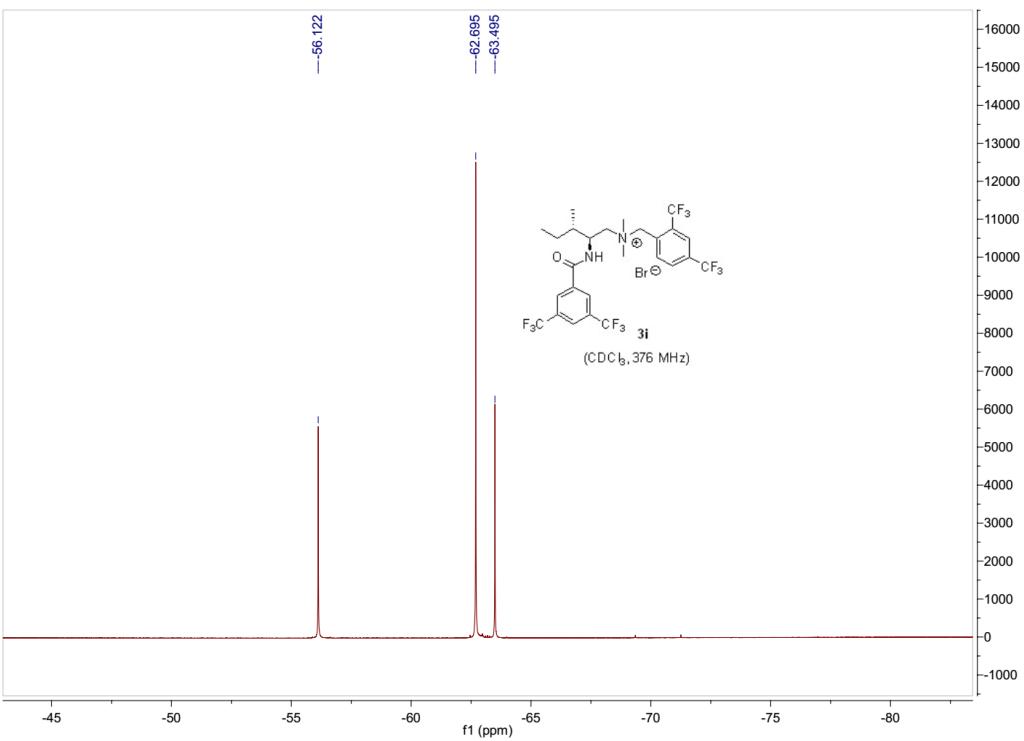


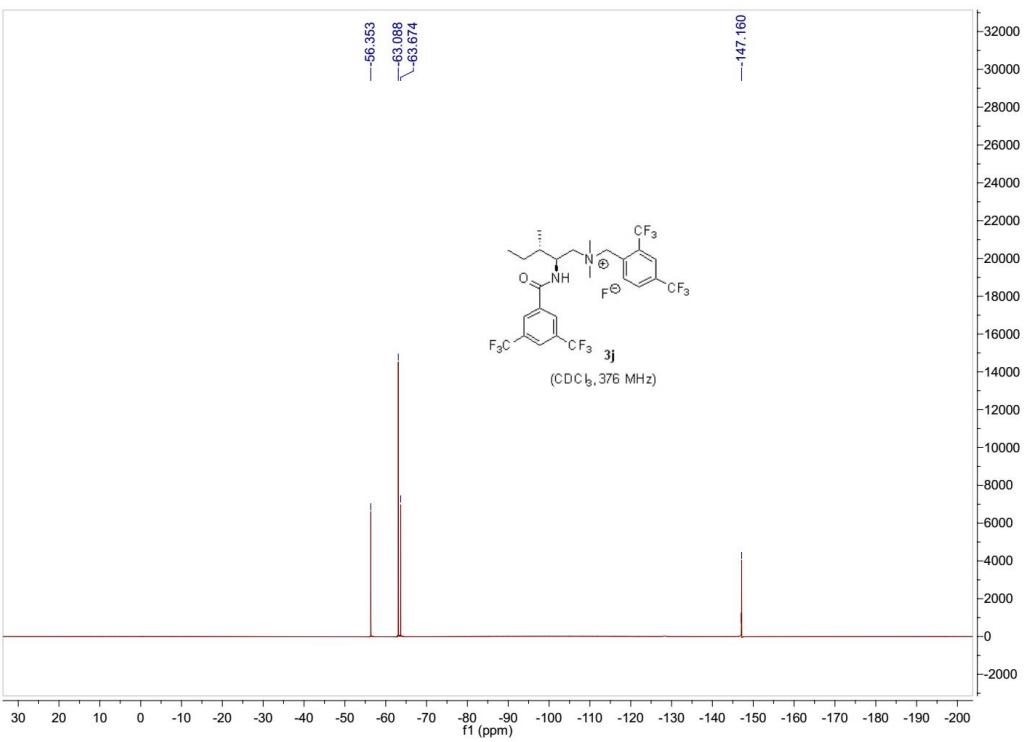
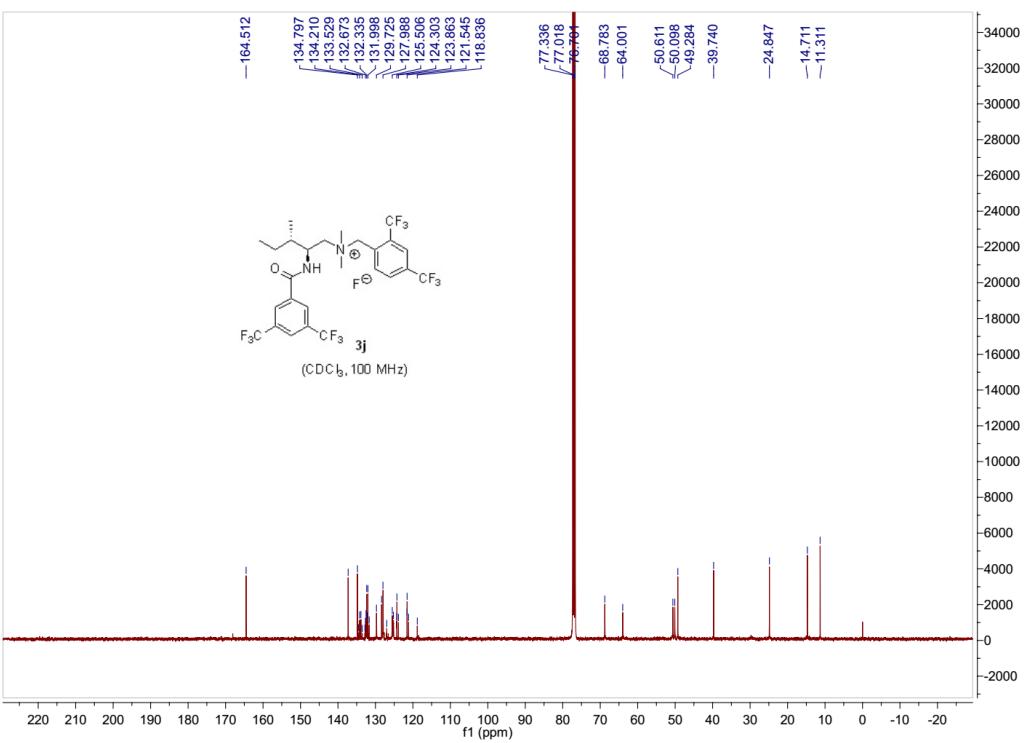


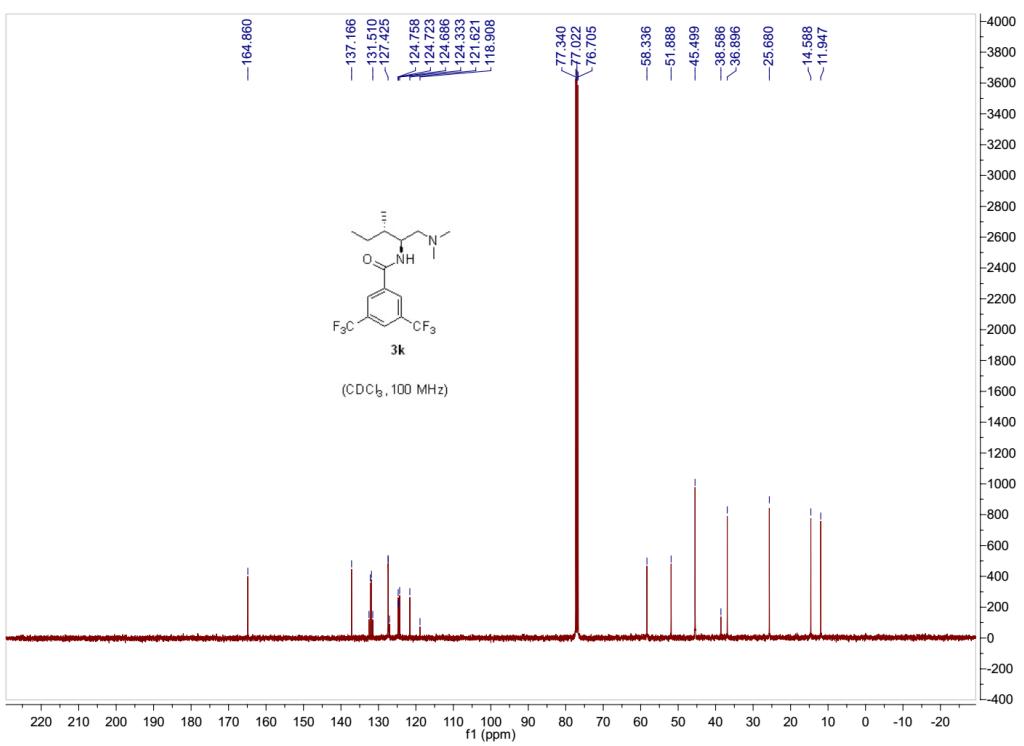
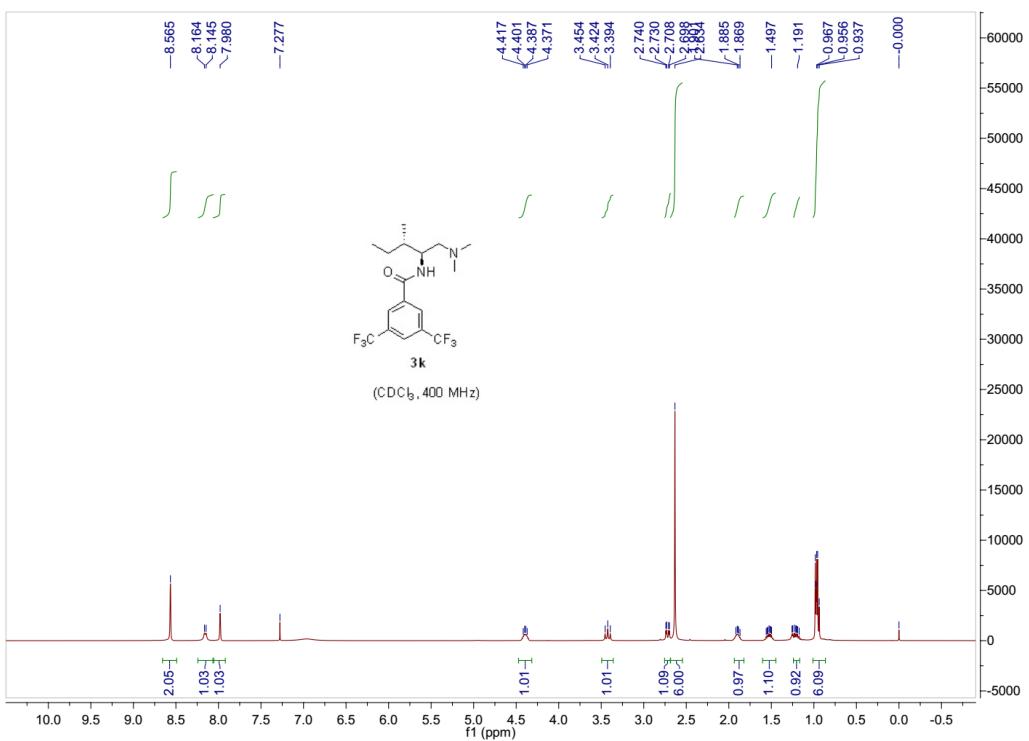


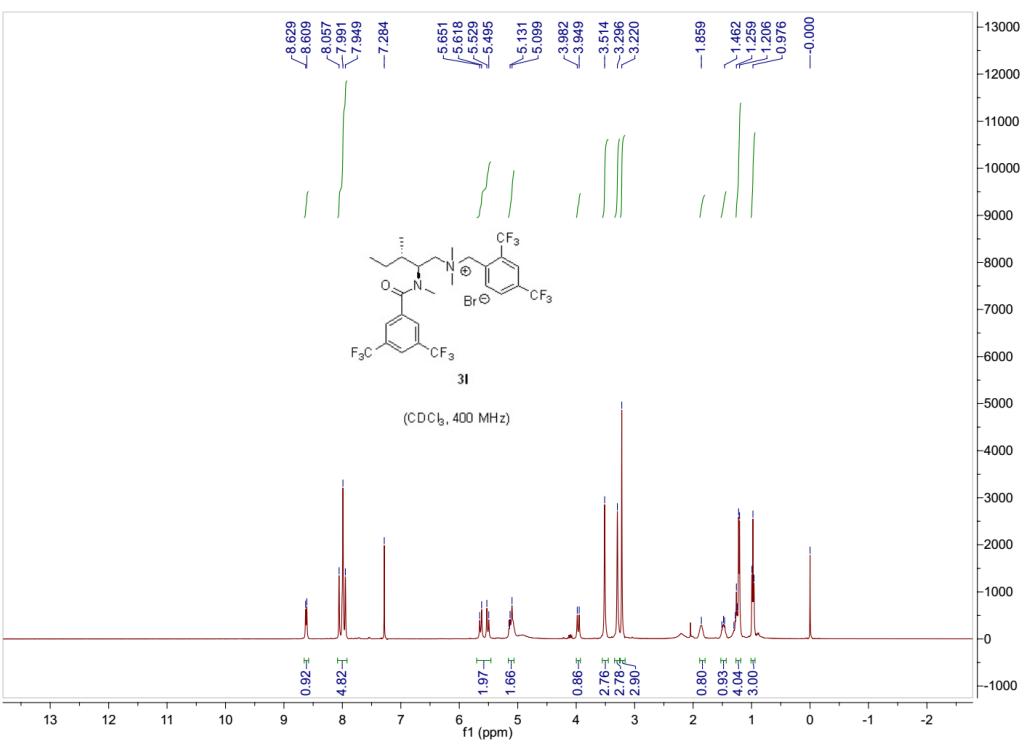
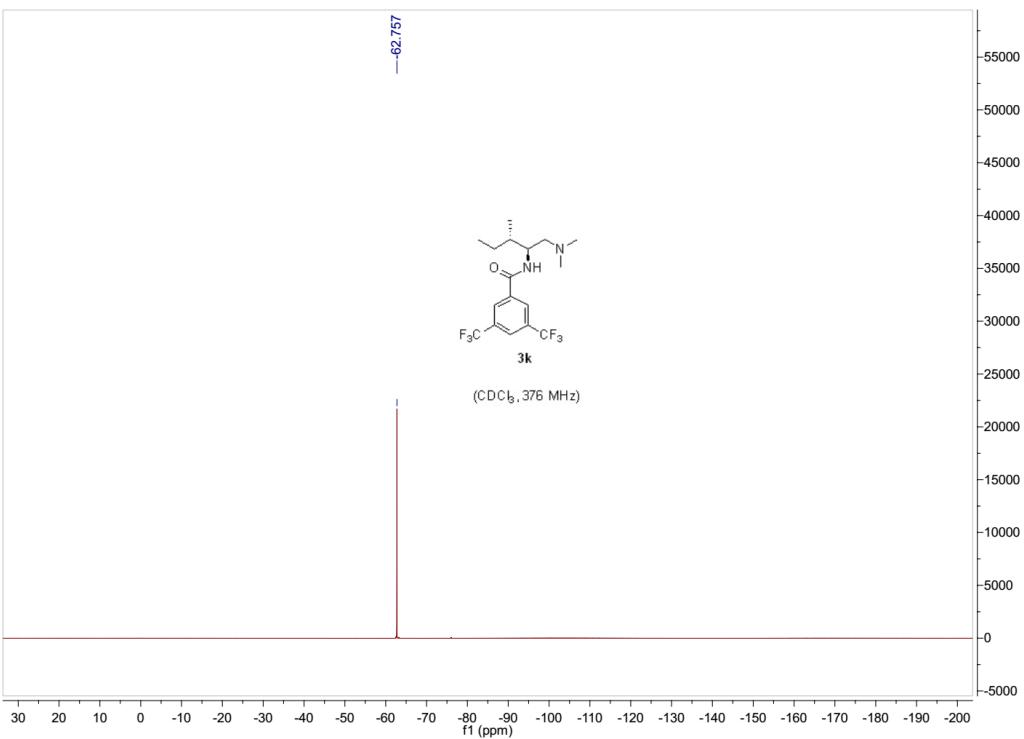


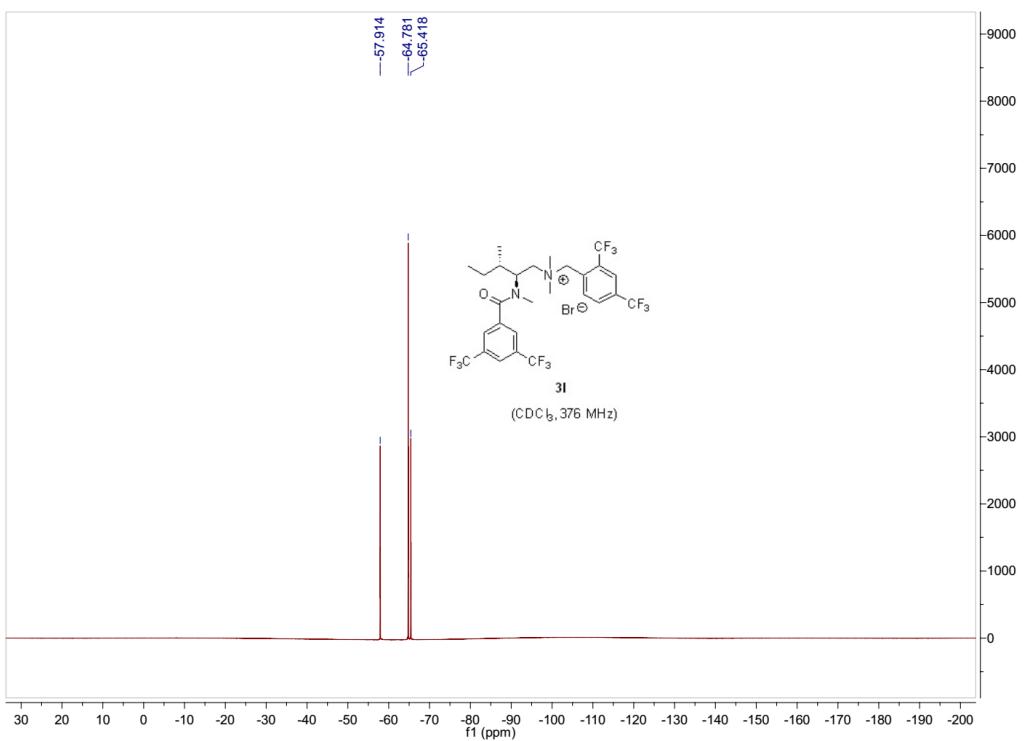
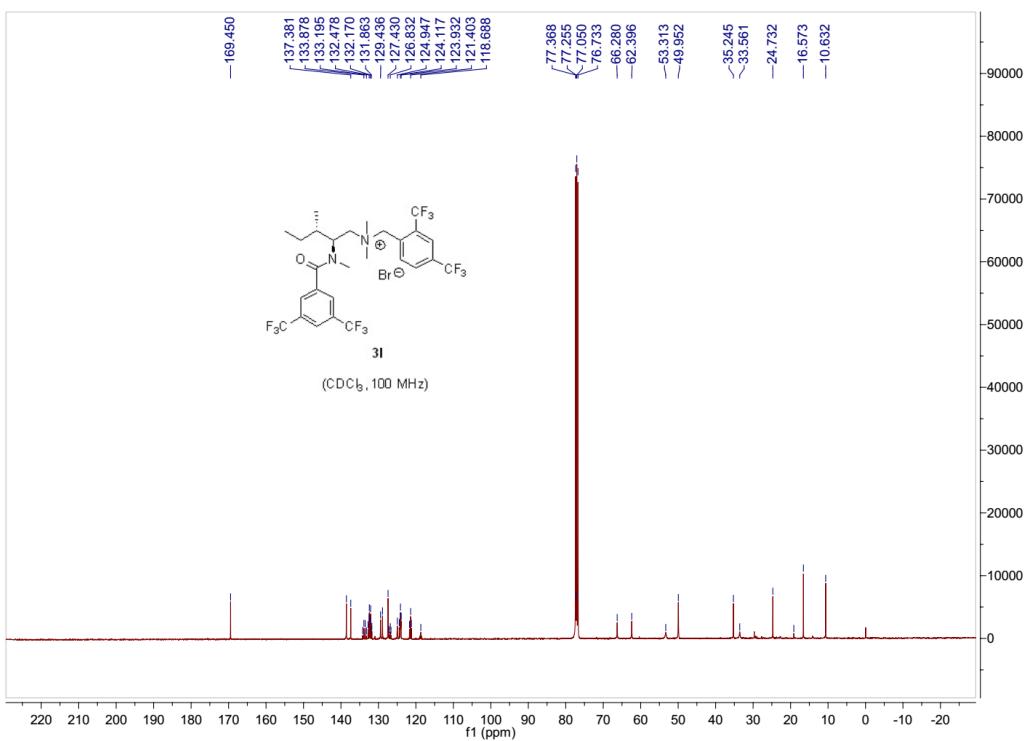




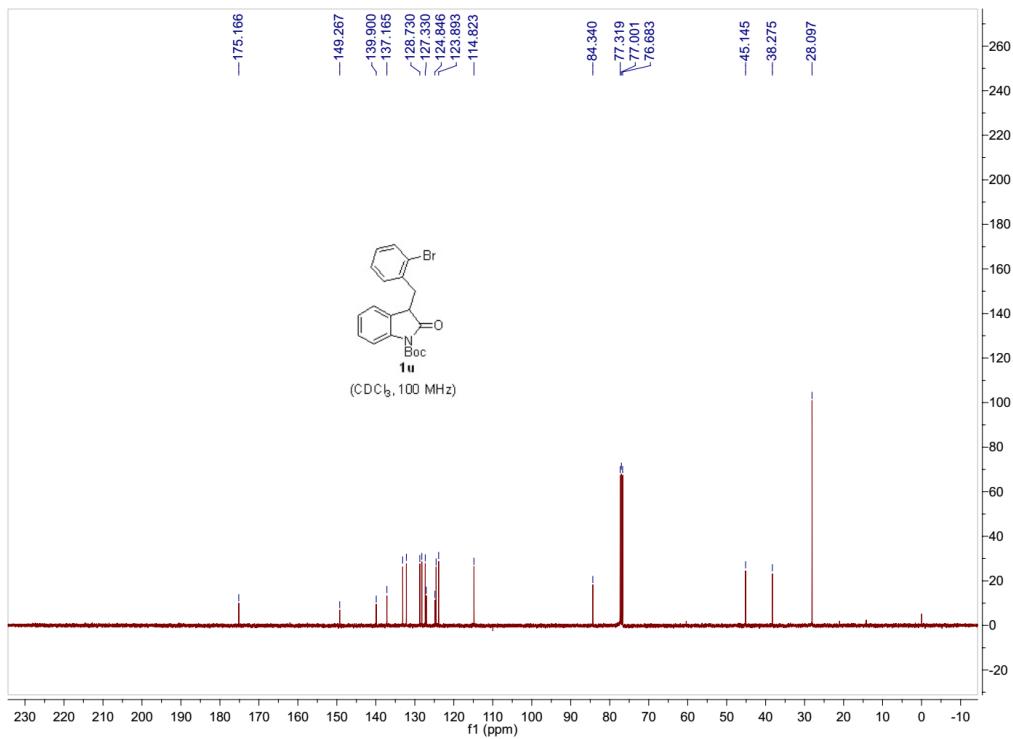
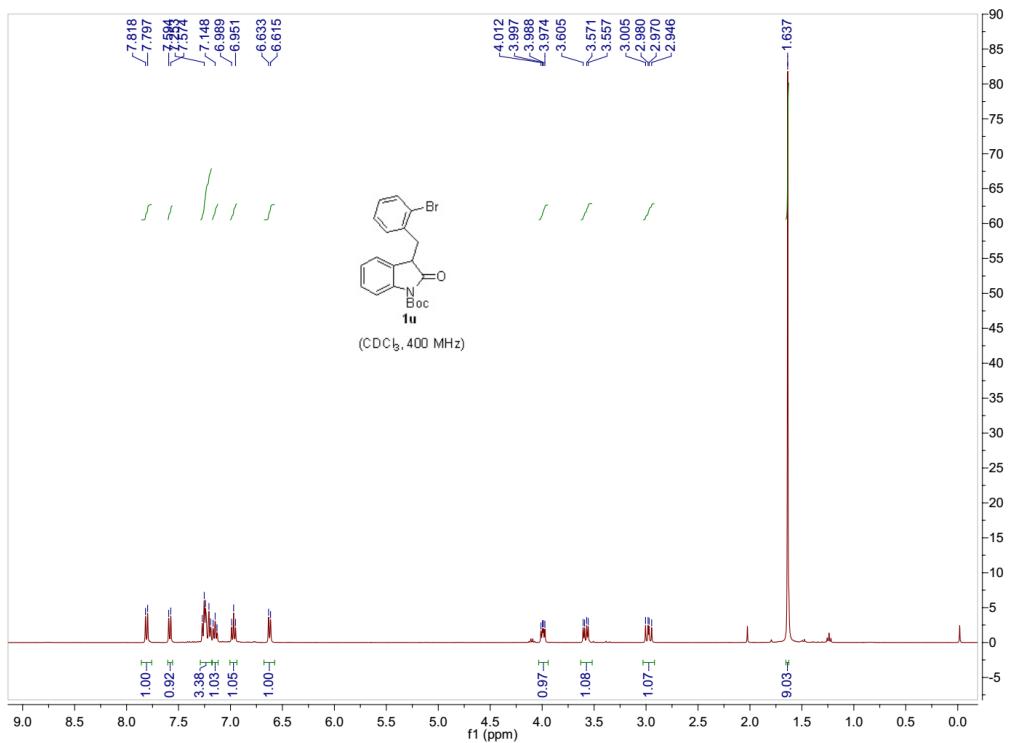


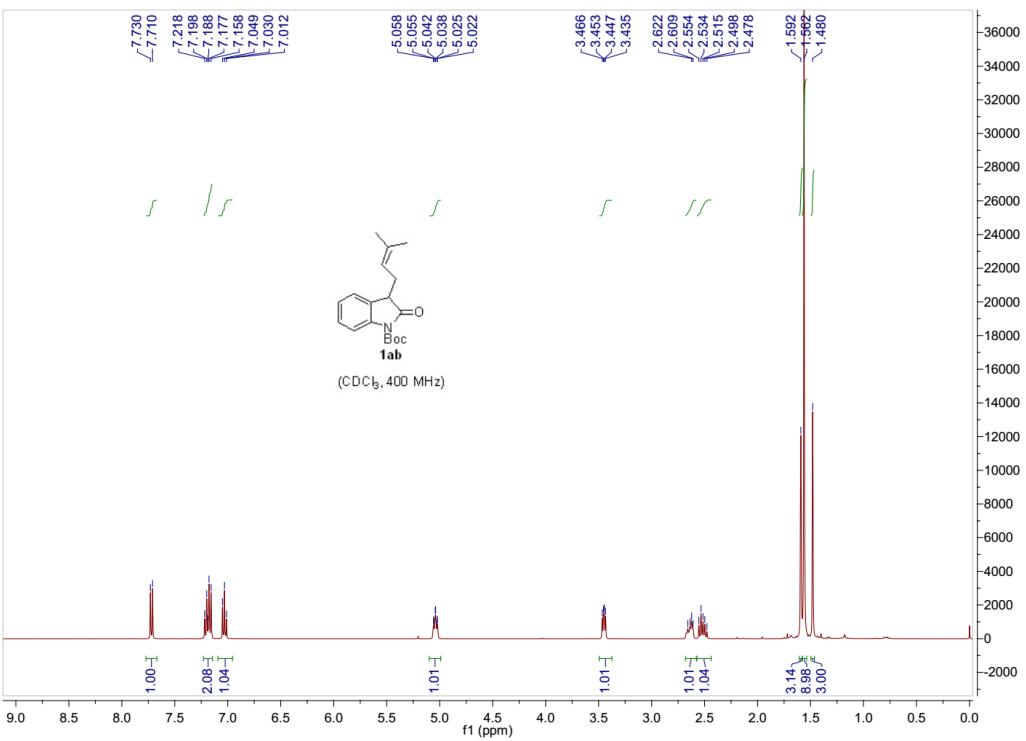


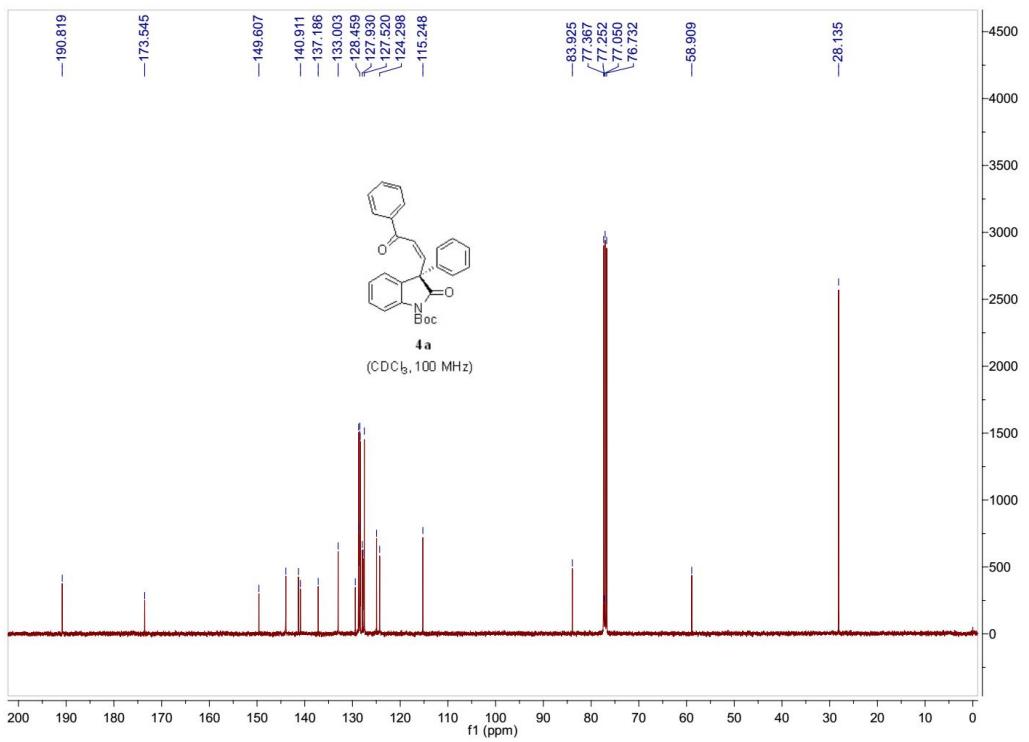
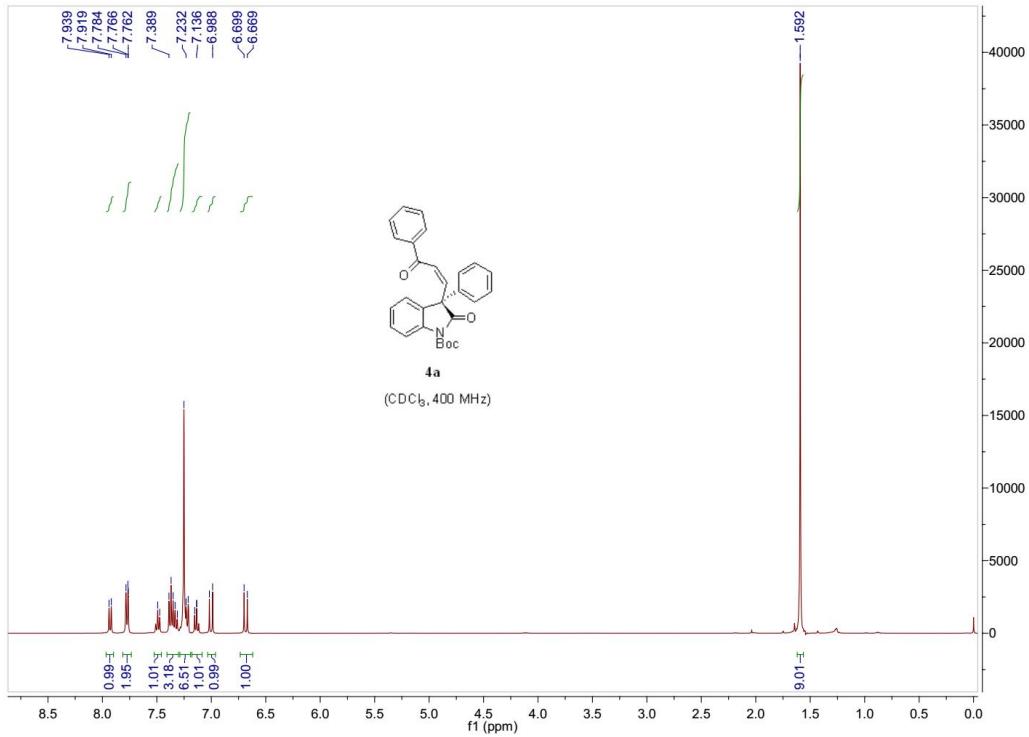


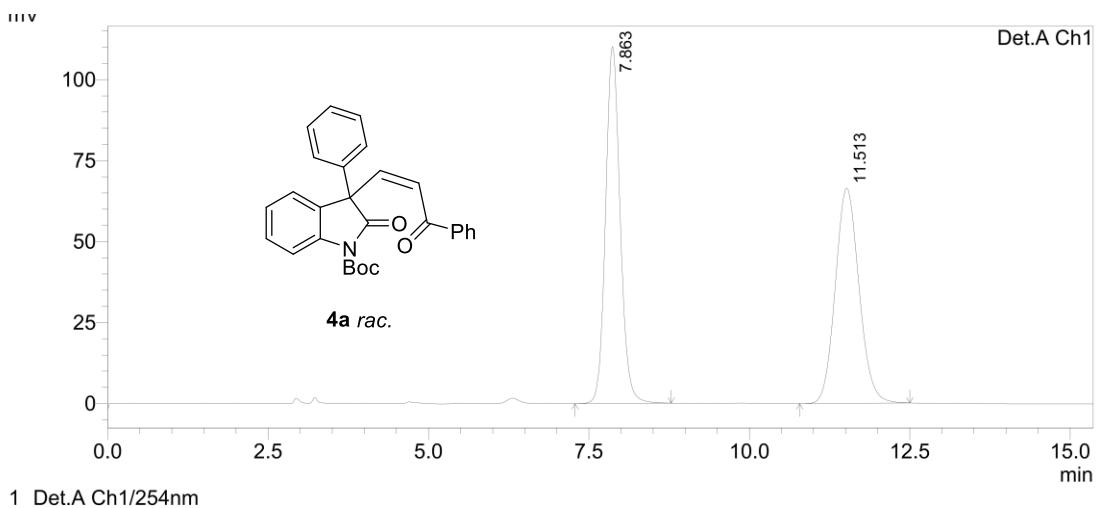


Part II. NMR Spectra and HPLC Chromatography for products 1, 4, 5, 6 and 7







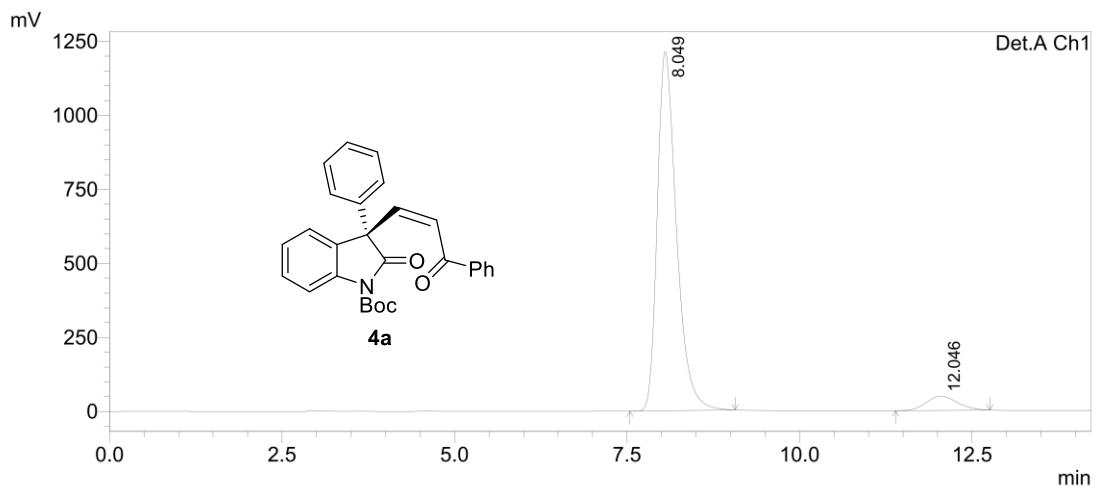


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.863	1743429	110239	50.477	62.395
2	11.513	1710511	66440	49.523	37.605
Total		3453940	176679	100.000	100.000

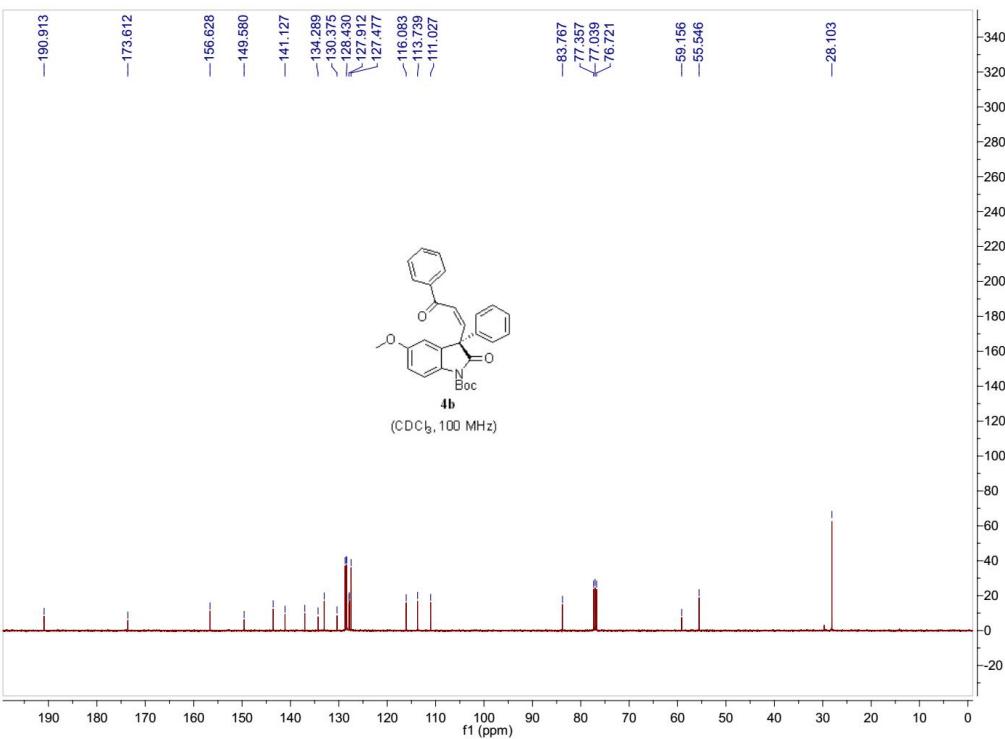
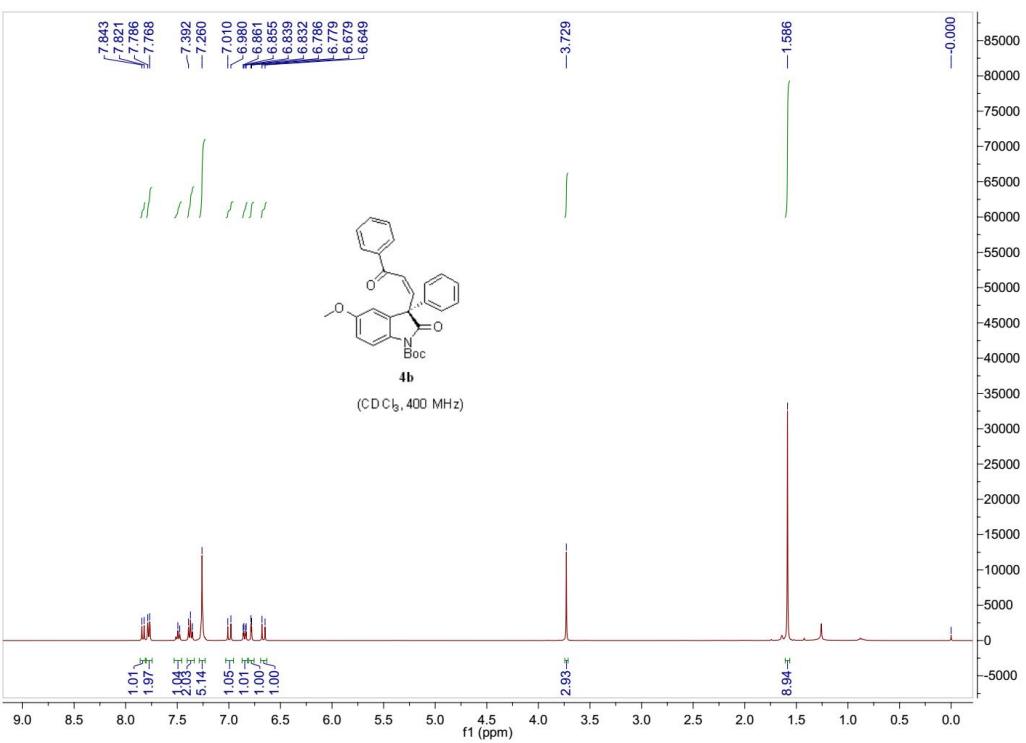


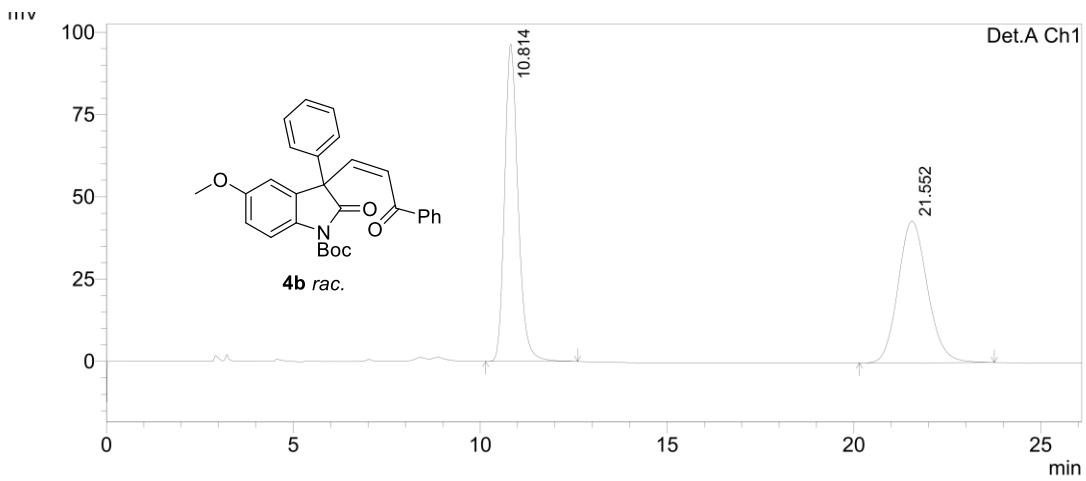
1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.049	23481041	1213387	93.947	96.188
2	12.046	1512755	48083	6.053	3.812
Total		24993796	1261470	100.000	100.000



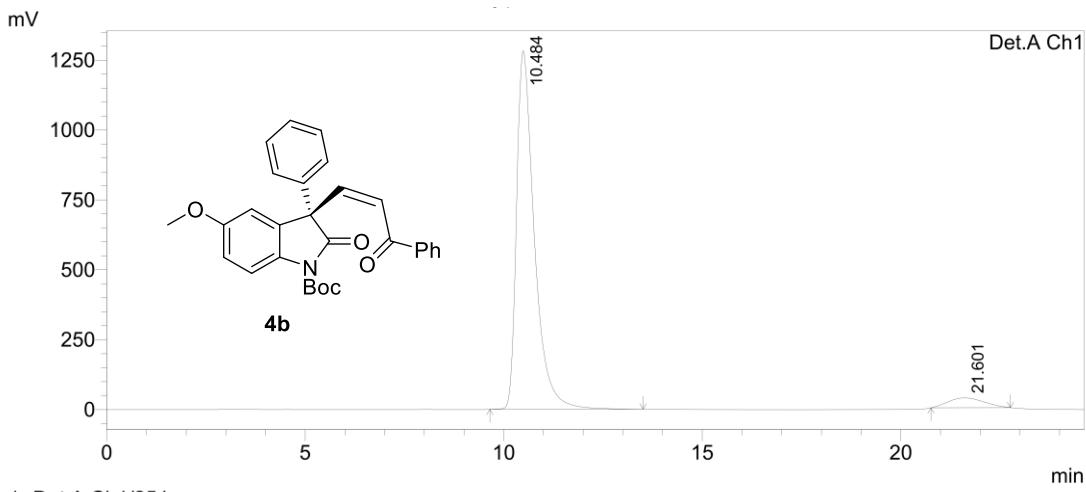


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.814	2408755	96407	50.634	69.117
2	21.552	2348455	43076	49.366	30.883
Total		4757211	139483	100.000	100.000

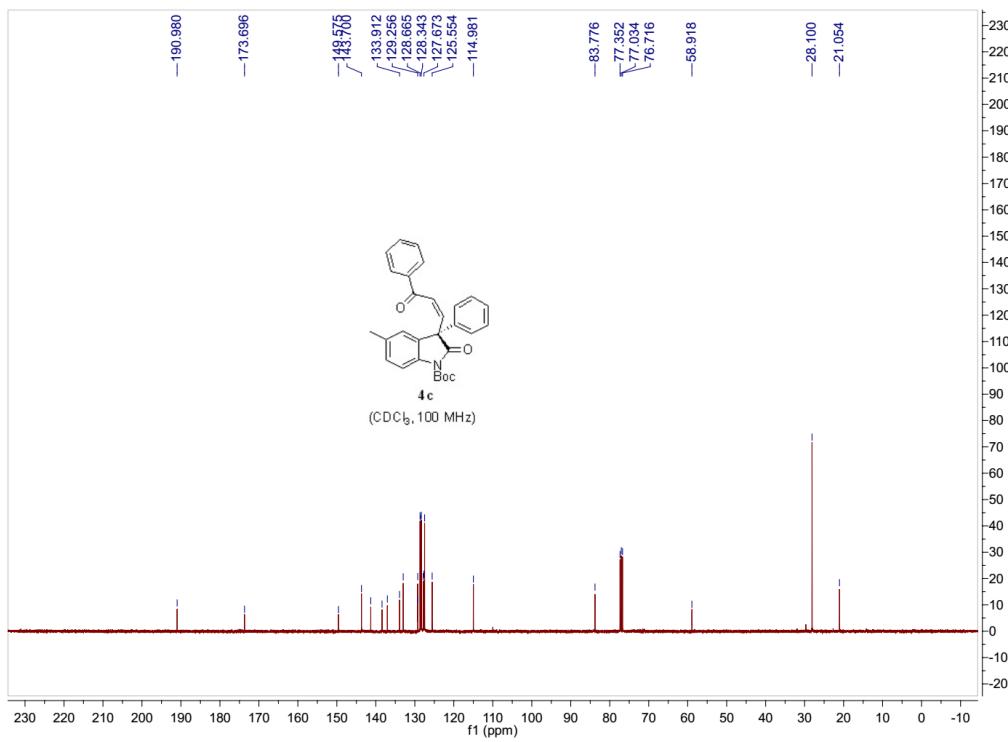
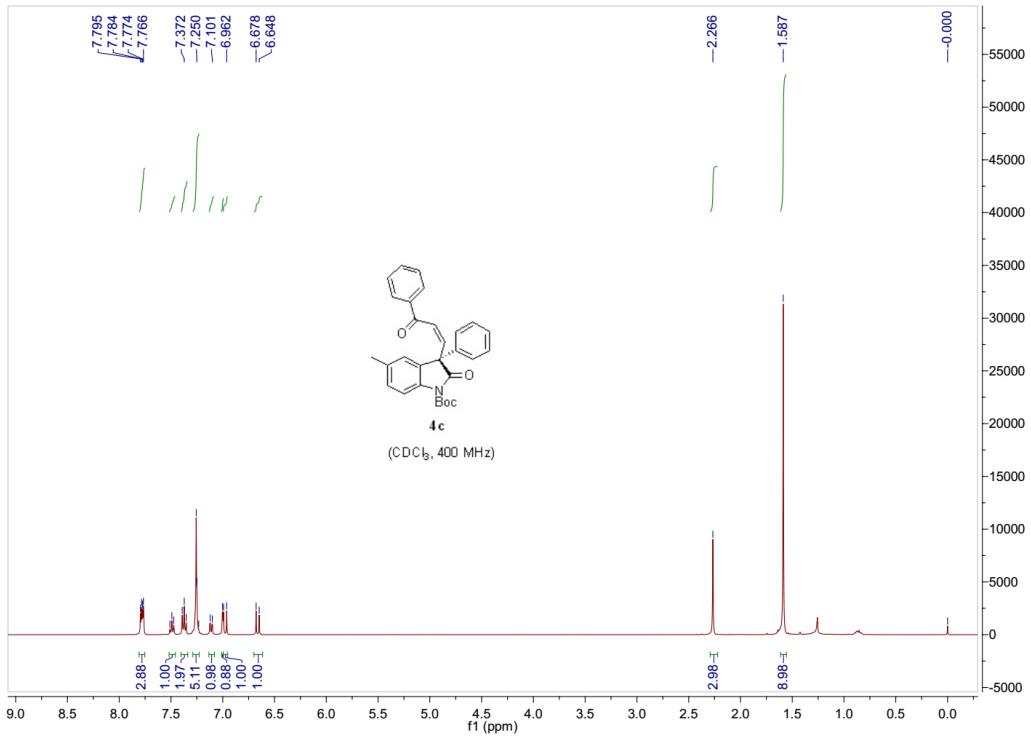


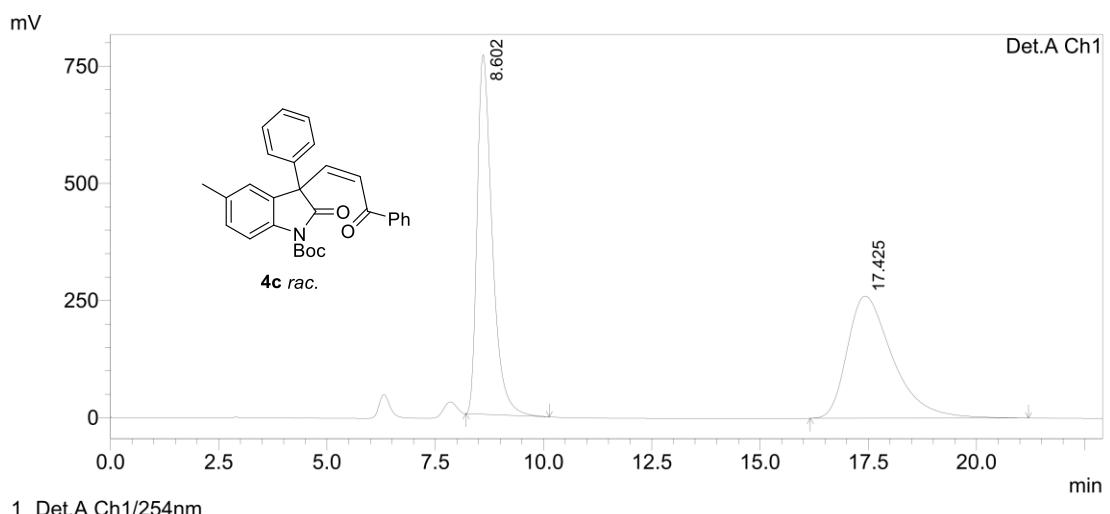
1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.484	39965872	1282353	94.720	97.321
2	21.601	2227623	35306	5.280	2.679
Total		42193496	1317659	100.000	100.000

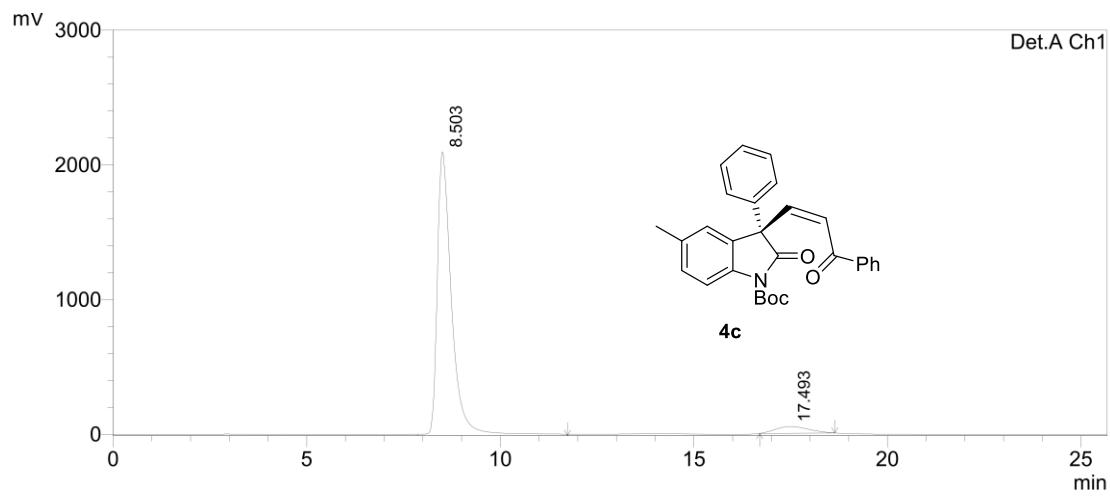




PeakTable

Detector A Ch1 254nm

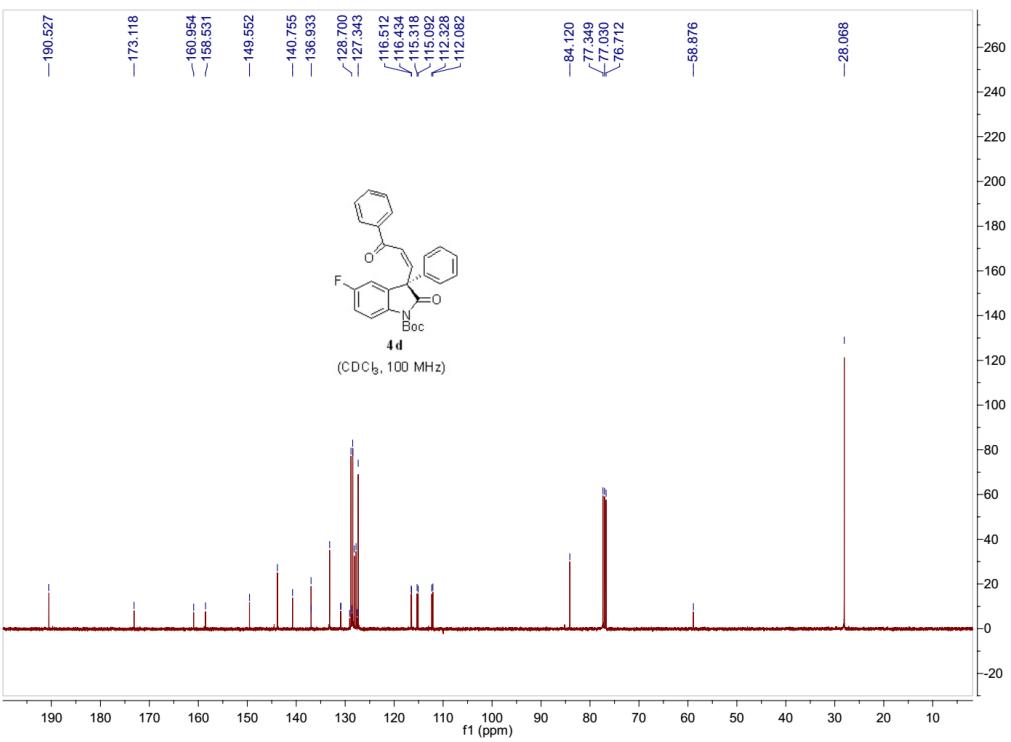
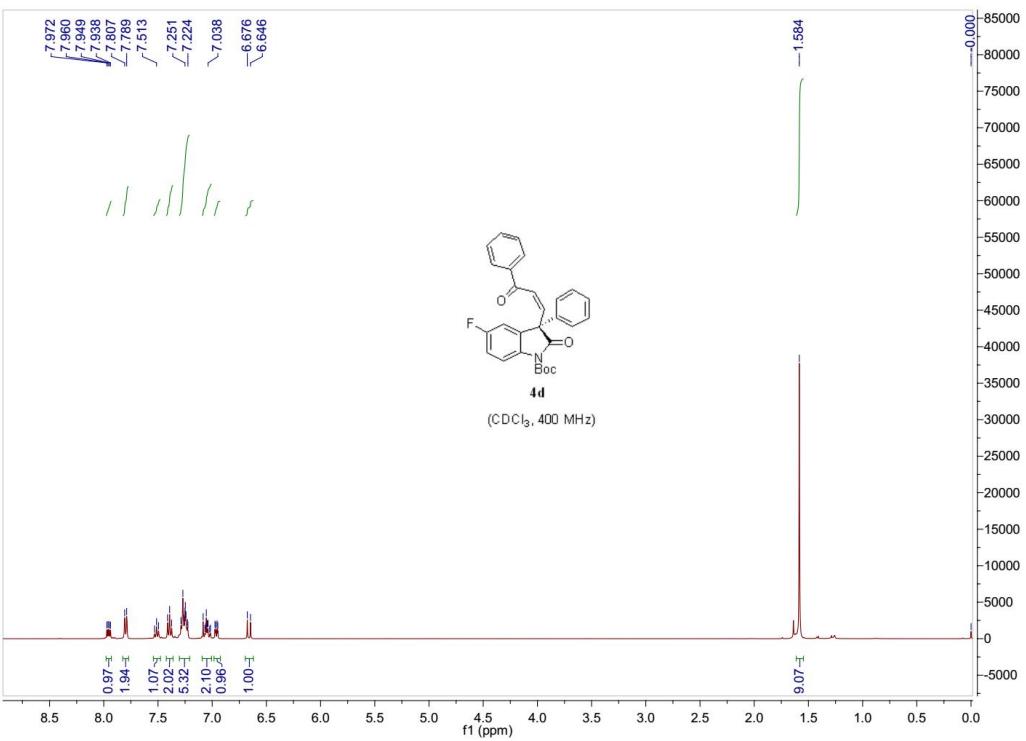
Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.602	18535624	767598	49.370	74.657
2	17.425	19008623	260572	50.630	25.343
Total		37544247	1028170	100.000	100.000

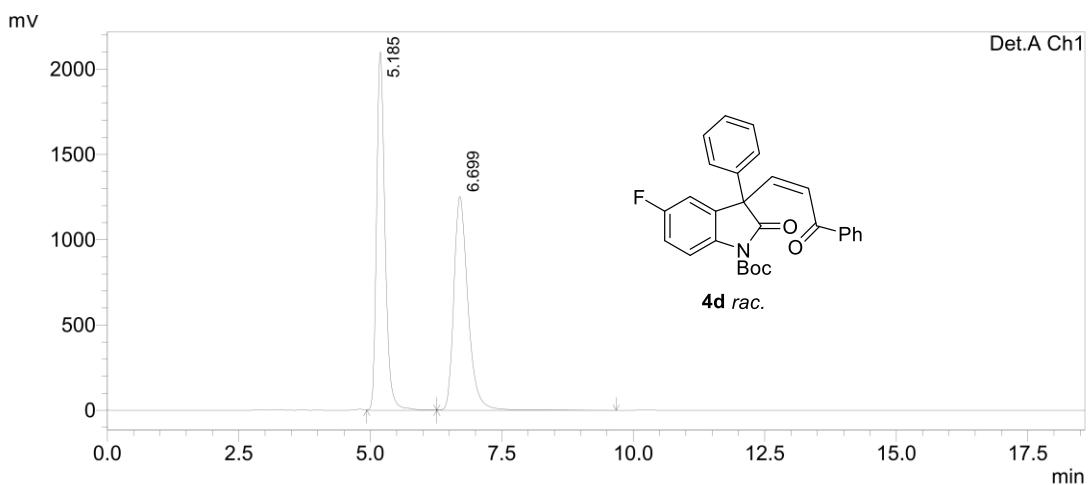
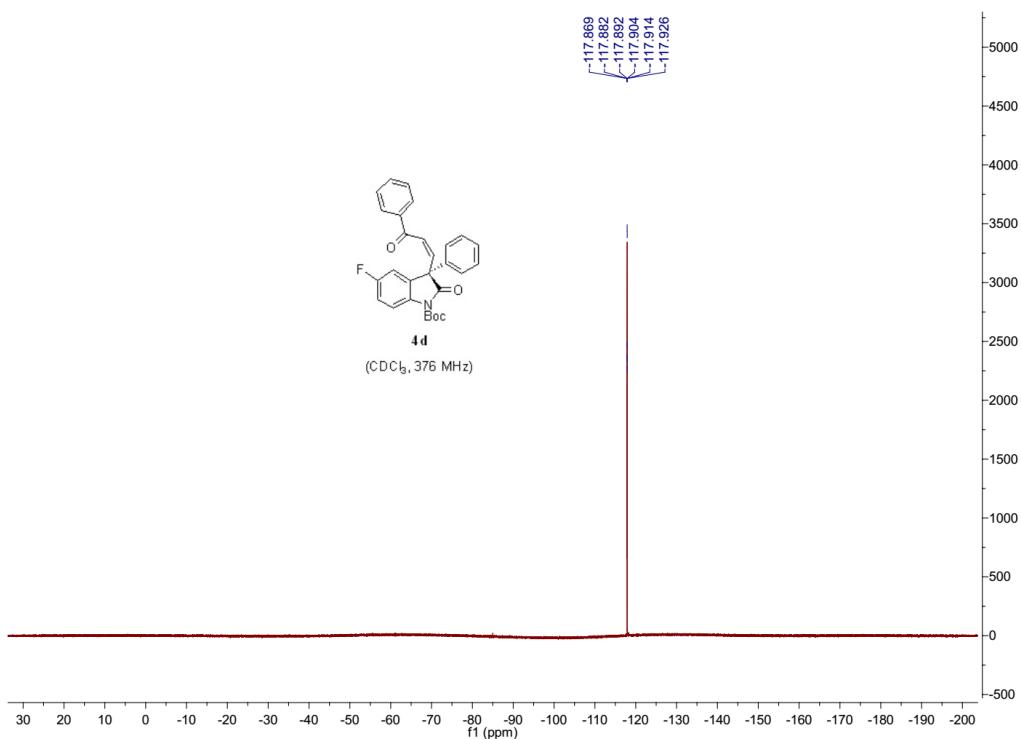


PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.503	55351492	2110634	94.928	97.699
2	17.493	2957380	49706	5.072	2.301
Total		58308872	2160340	100.000	100.000



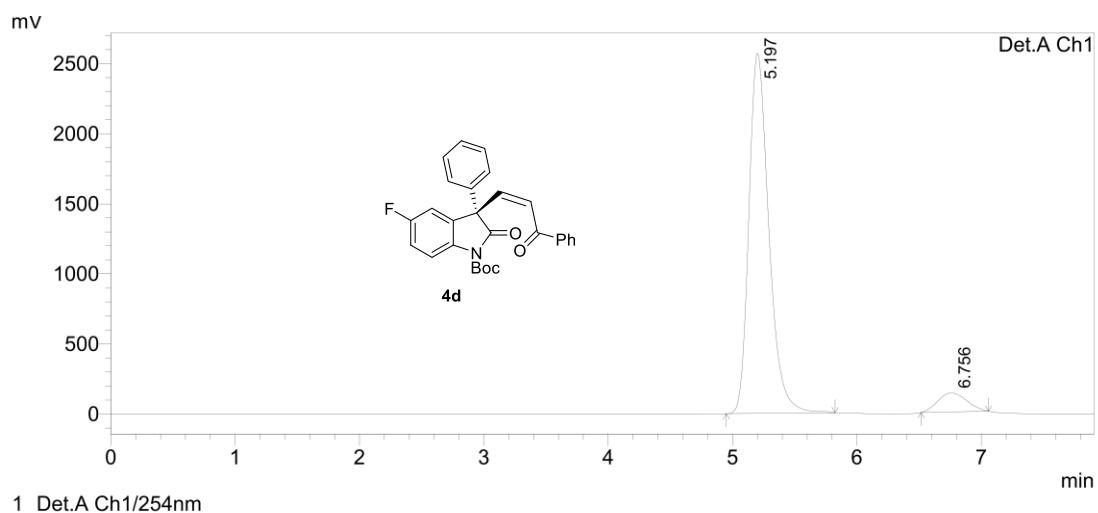


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

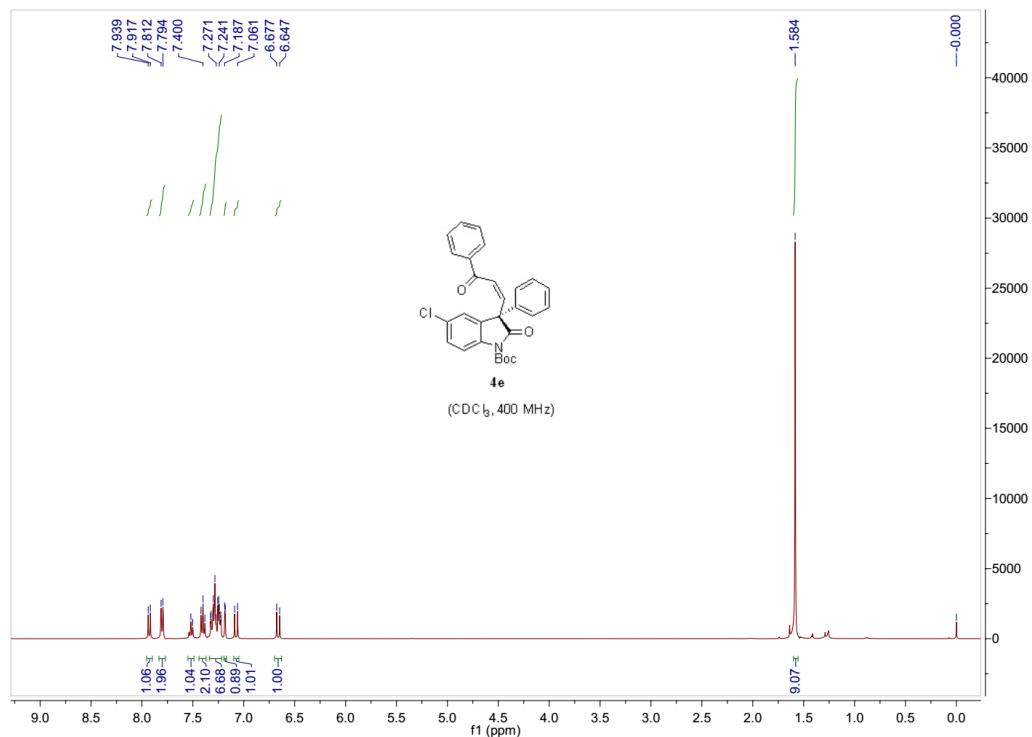
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1	5.185	23441957	2101675	49.983	62.641
2	6.699	23457711	1253449	50.017	37.359
Total		46899668	3355124	100.000	100.000

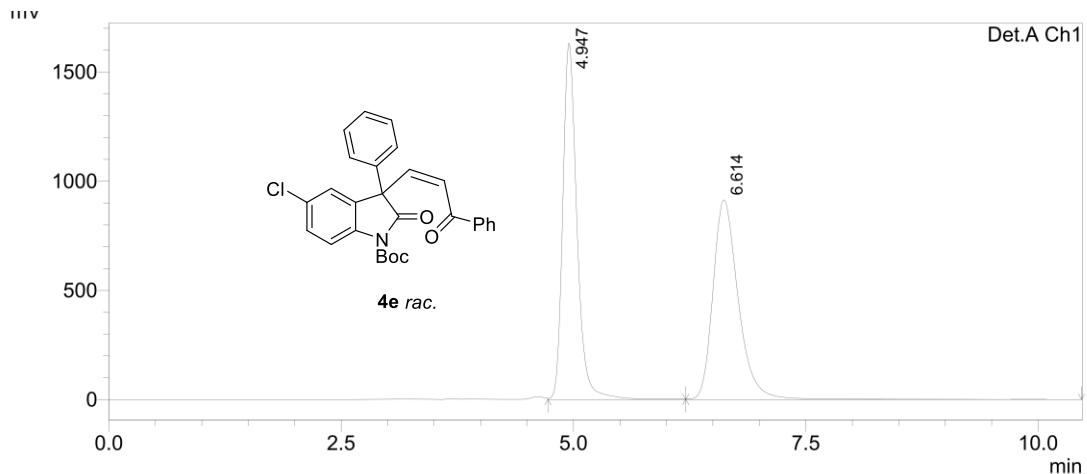
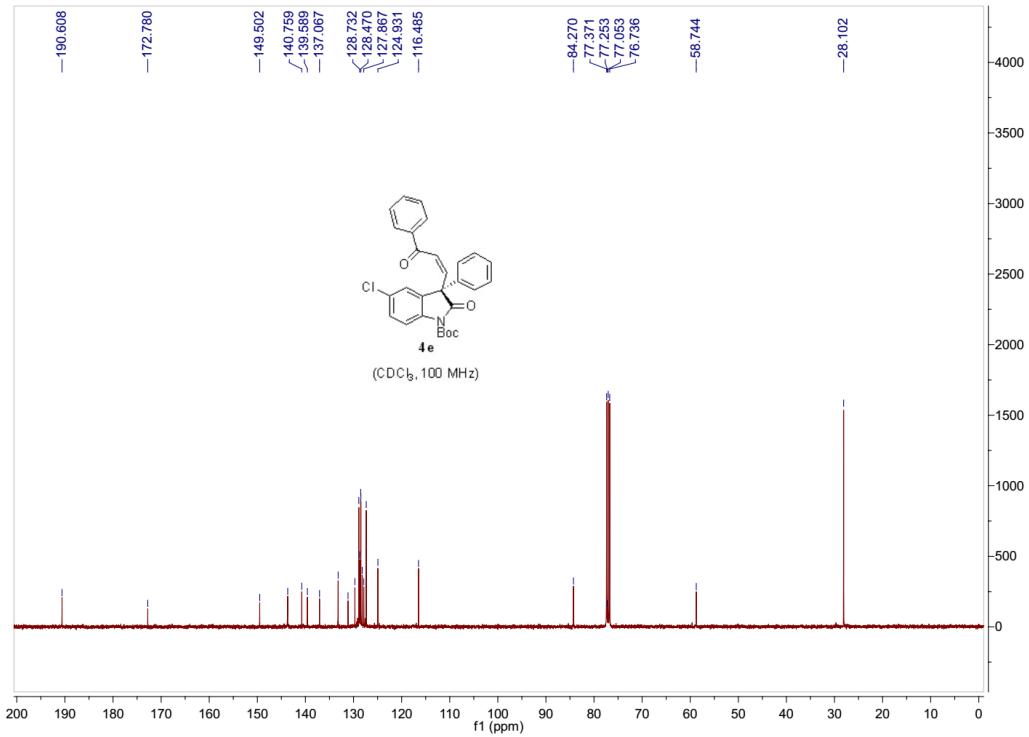


PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.197	28716219	2570385	92.932	94.988
2	6.756	2183889	135623	7.068	5.012
Total		30900108	2706008	100.000	100.000



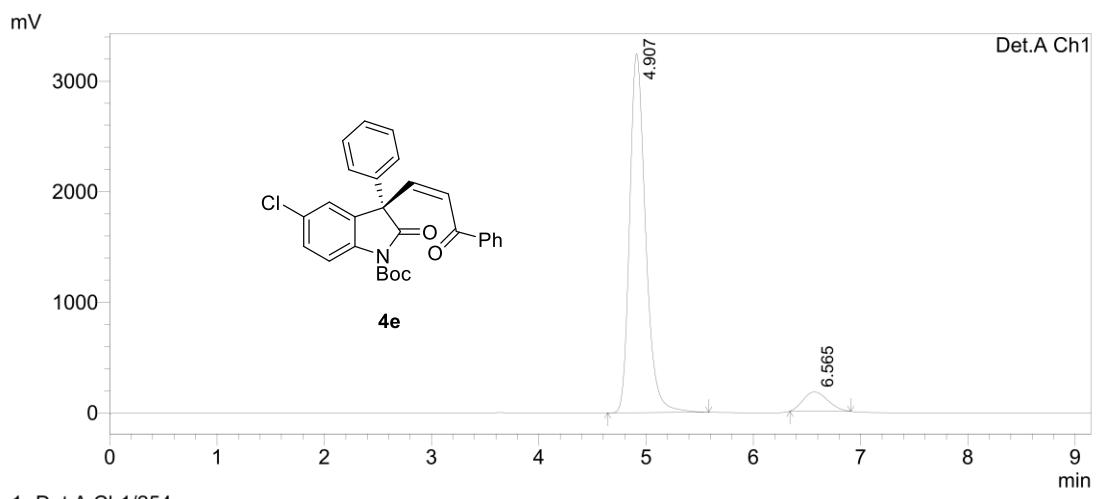


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.947	17364250	1632827	50.065	64.099
2	6.614	17319123	914512	49.935	35.901
Total		34683374	2547338	100.000	100.000

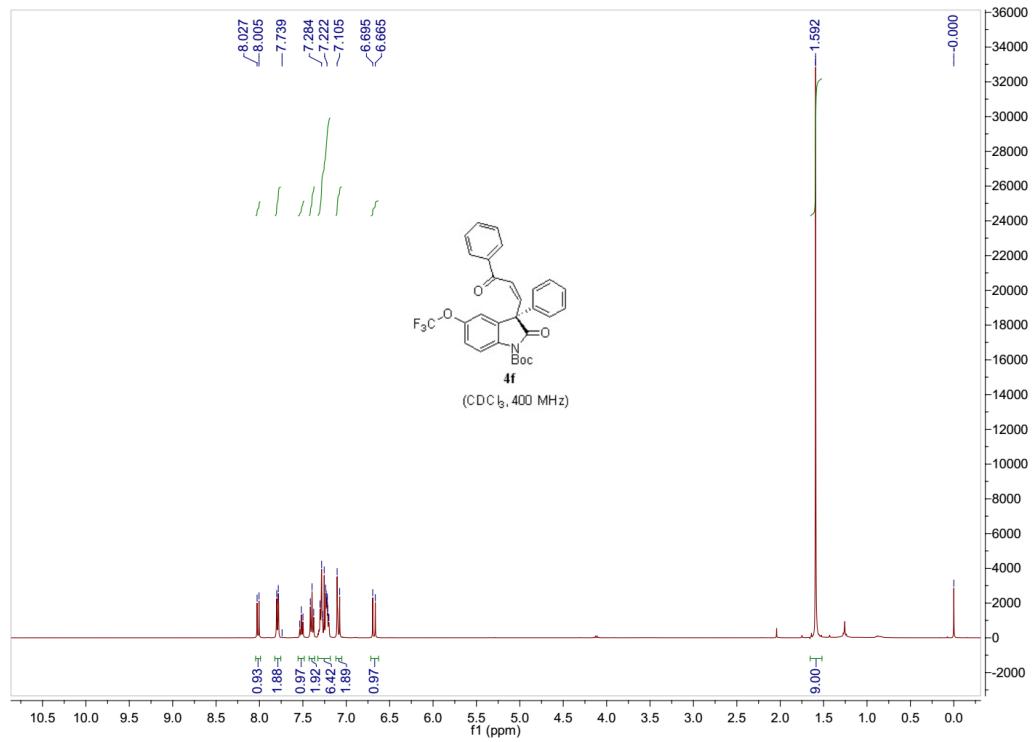


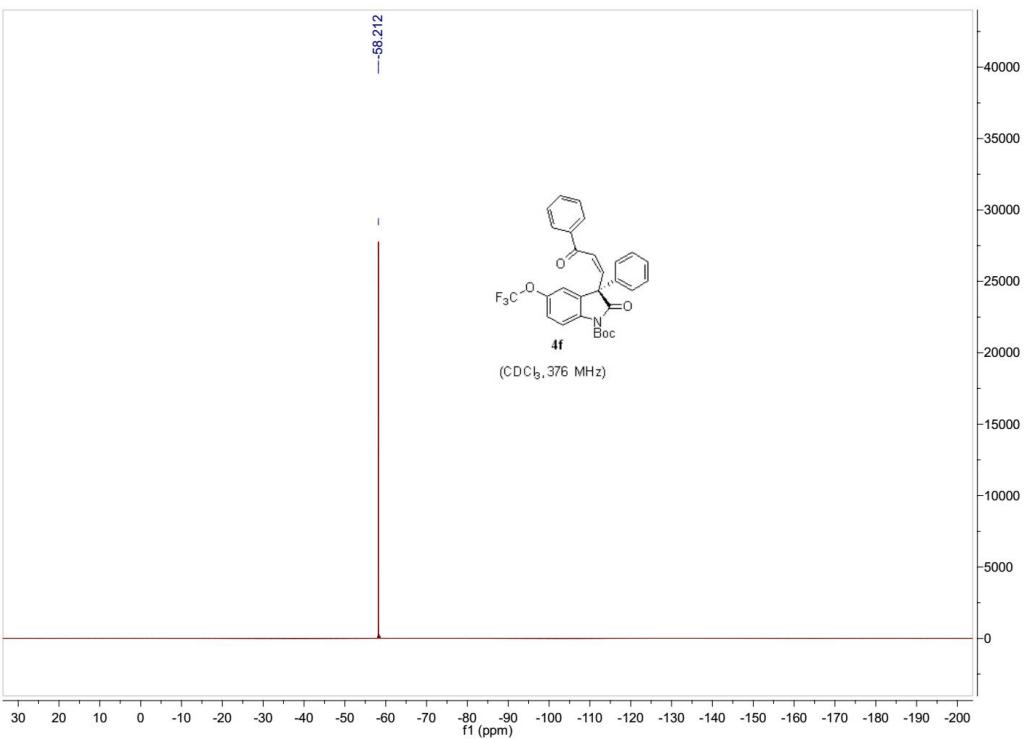
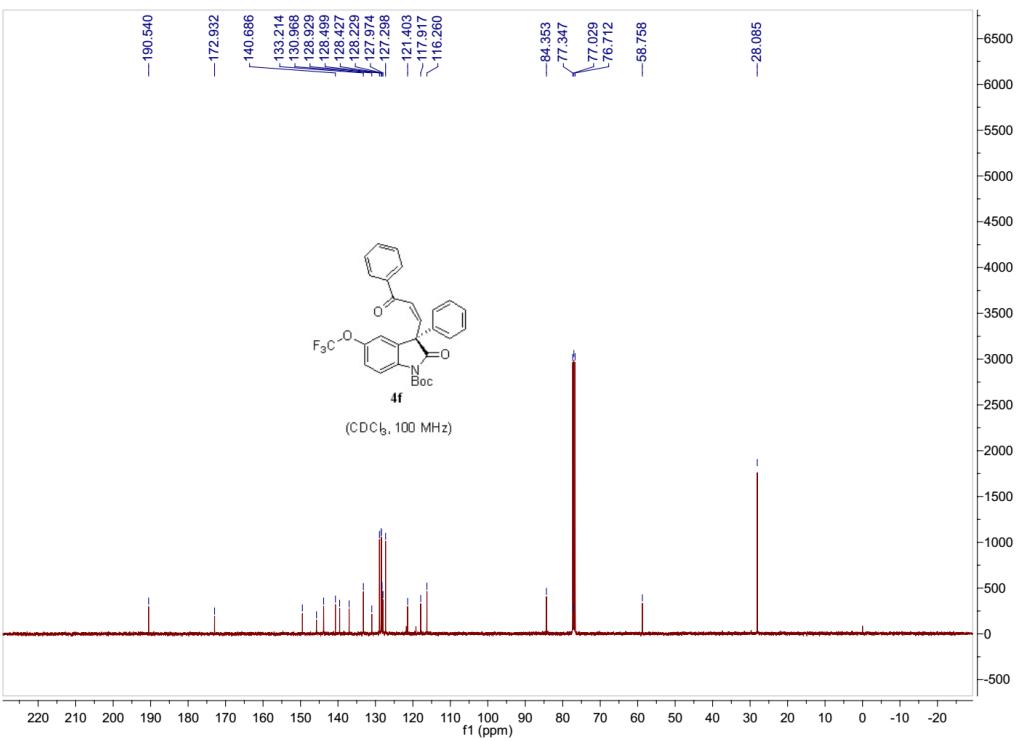
1 Det.A Ch1/254nm

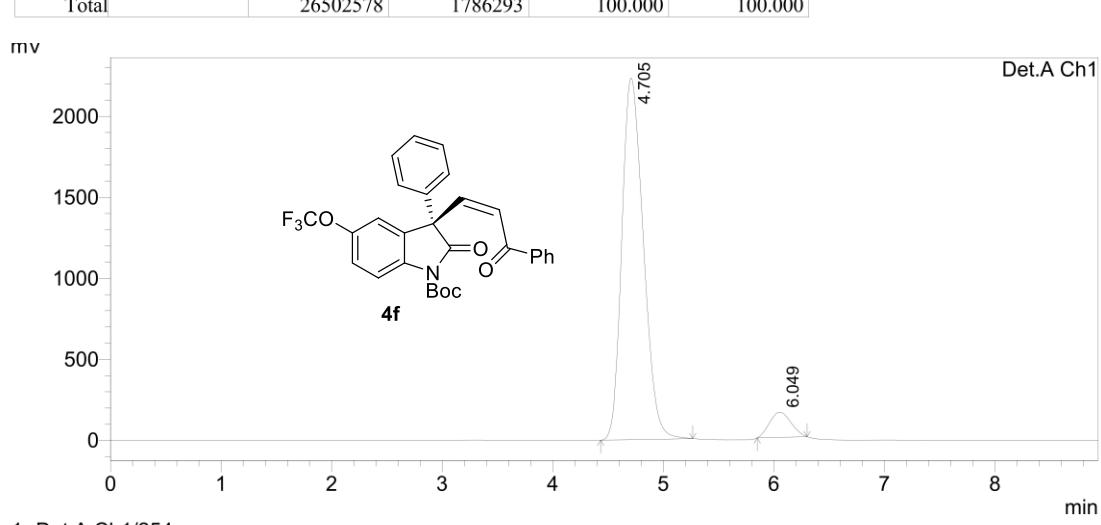
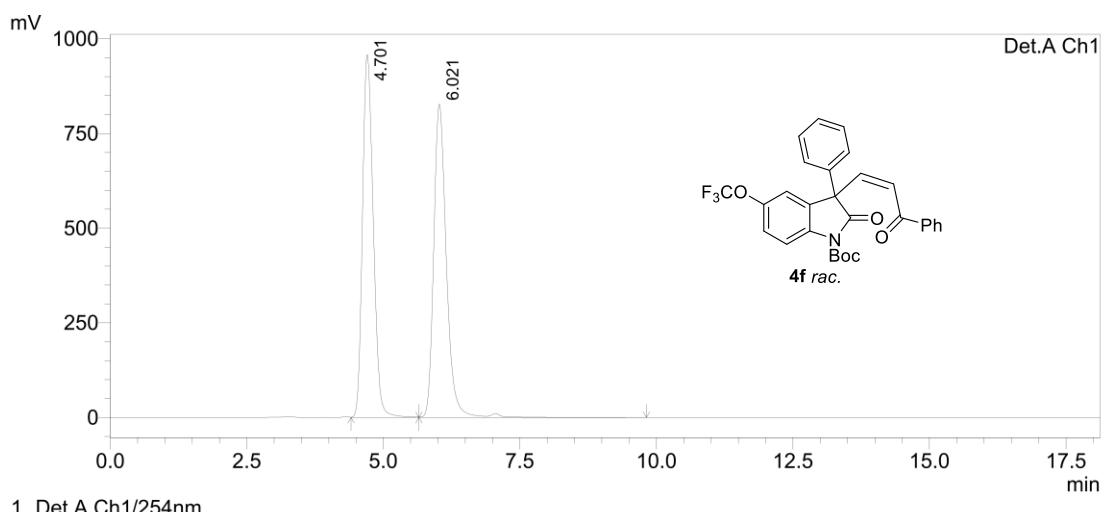
PeakTable

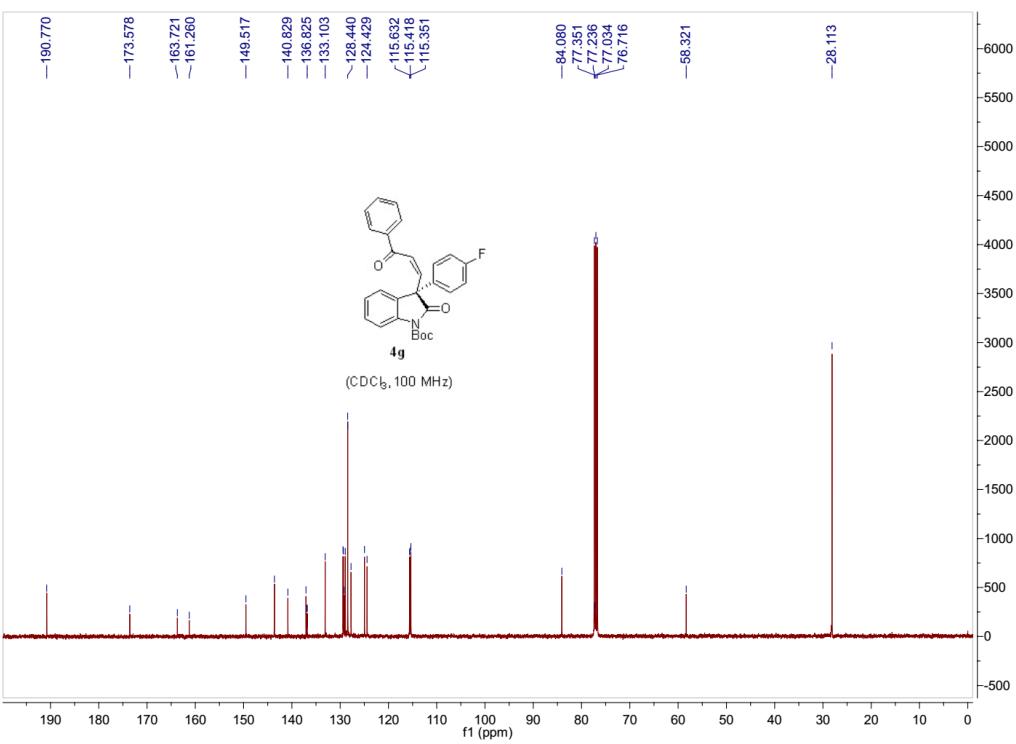
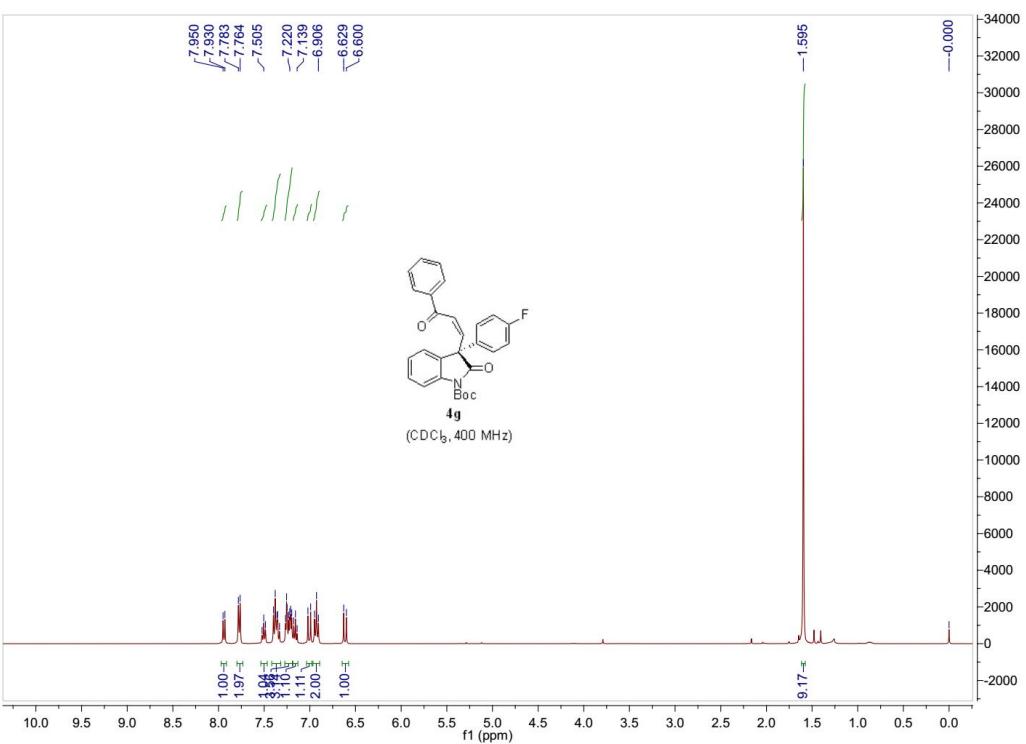
Detector A Ch1 254nm

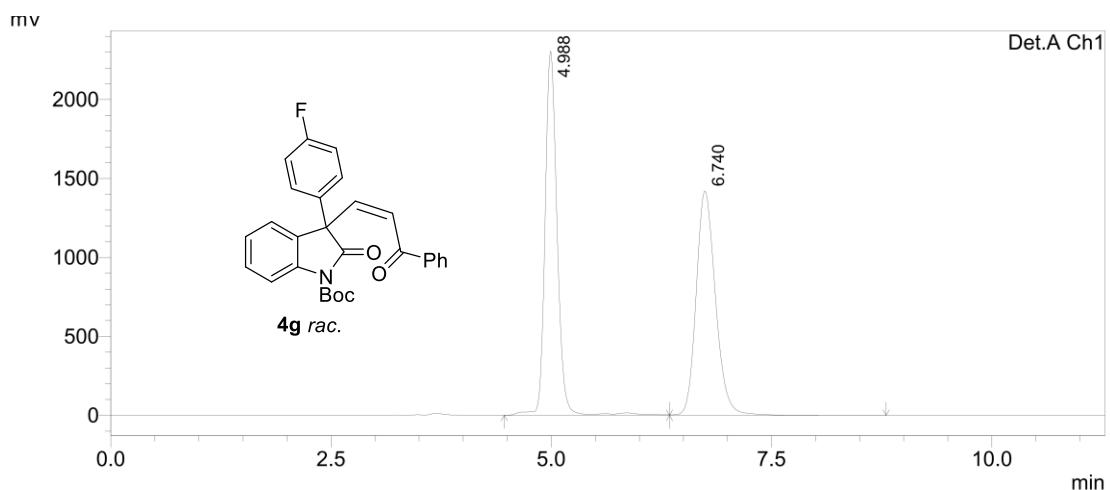
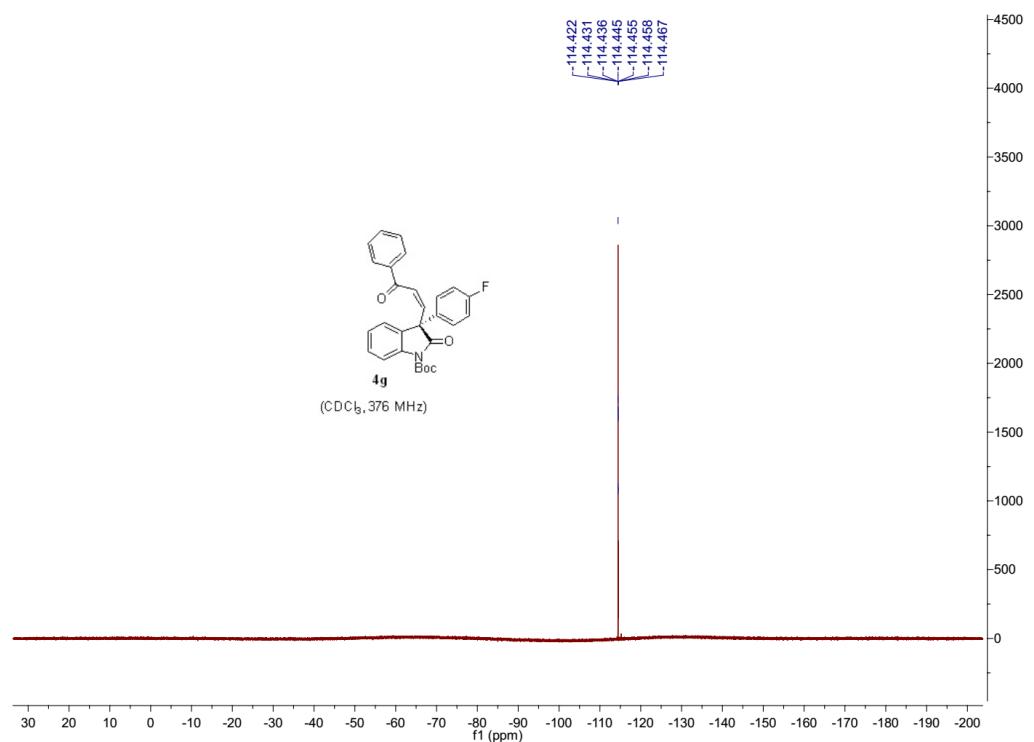
Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.907	33478427	3247059	92.330	94.880
2	6.565	2781139	175203	7.670	5.120
Total		36259567	3422262	100.000	100.000









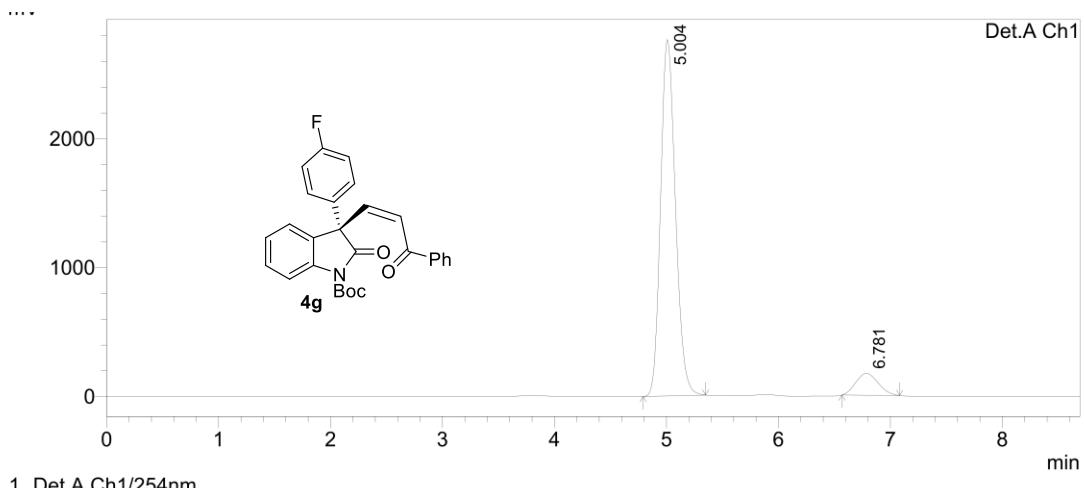


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

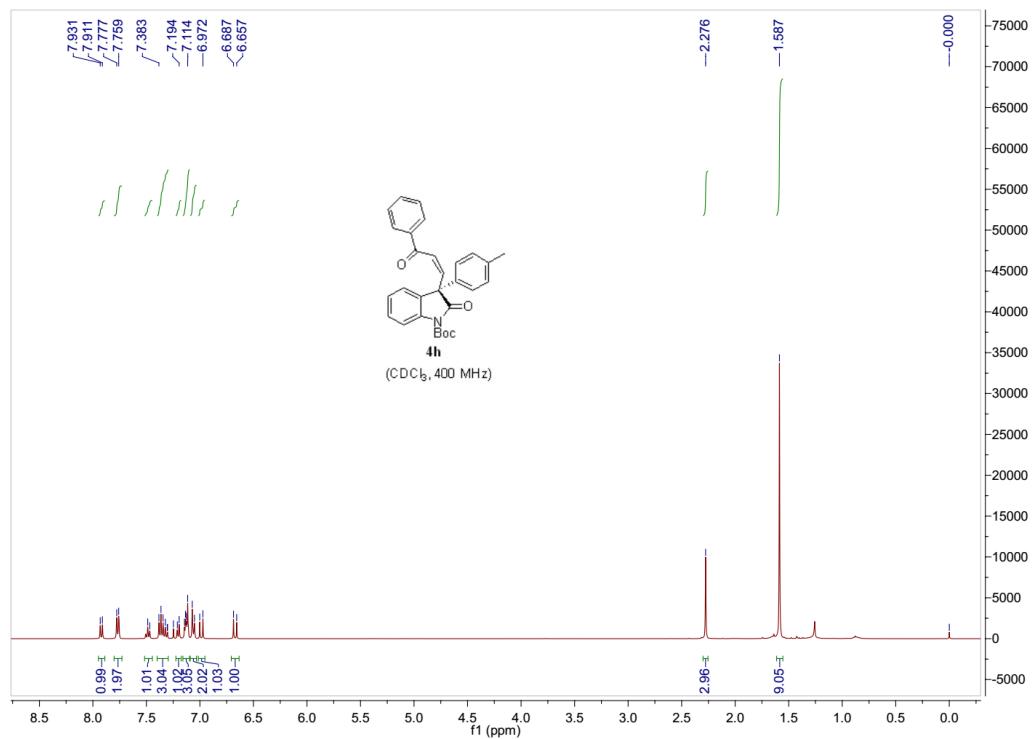
Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.988	22030294	2307491	50.370	61.874
2	6.740	21707001	1421871	49.630	38.126
Total		43737294	3729362	100.000	100.000

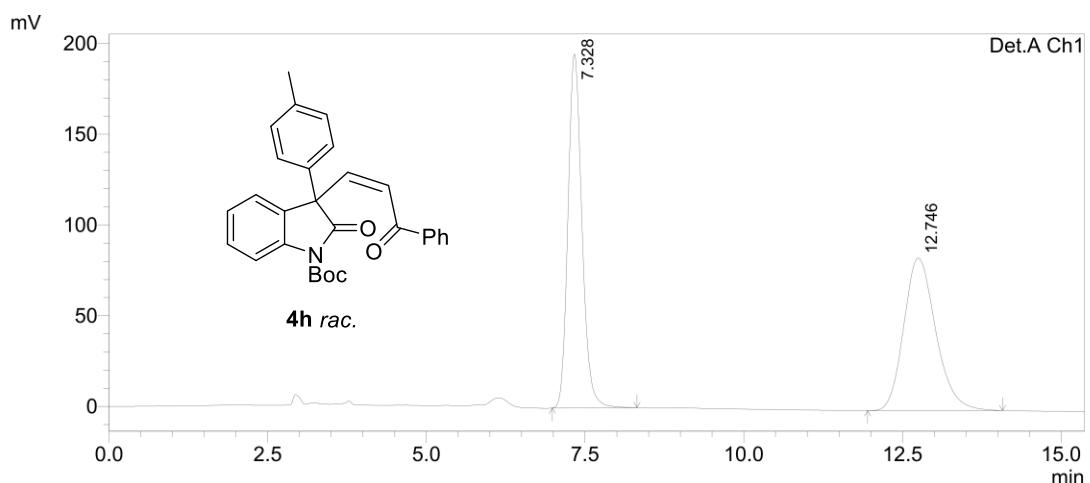
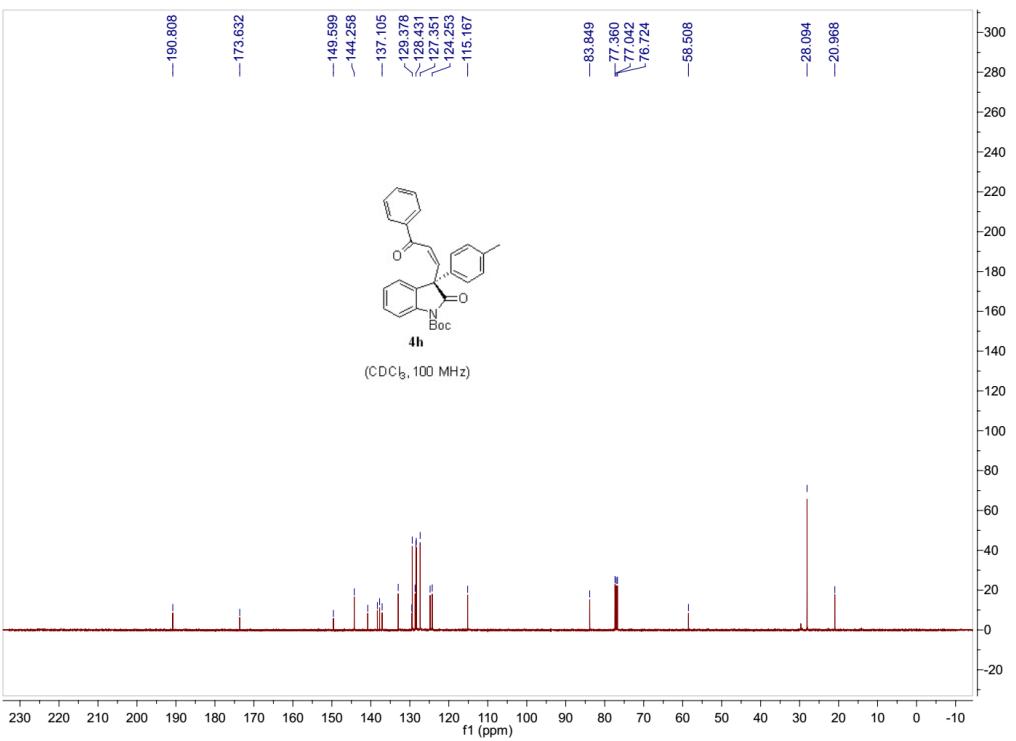


PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.004	25453430	2766307	91.510	94.224
2	6.781	2361540	169590	8.490	5.776
Total		27814970	2935897	100.000	100.000



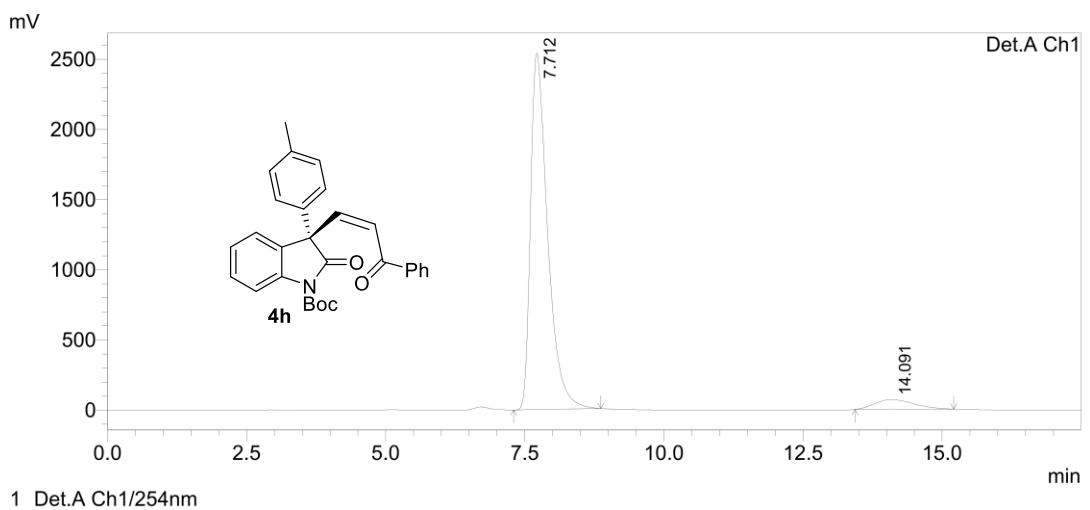


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.328	2984546	195053	50.282	69.867
2	12.746	2951029	84124	49.718	30.133
Total		5935575	279178	100.000	100.000

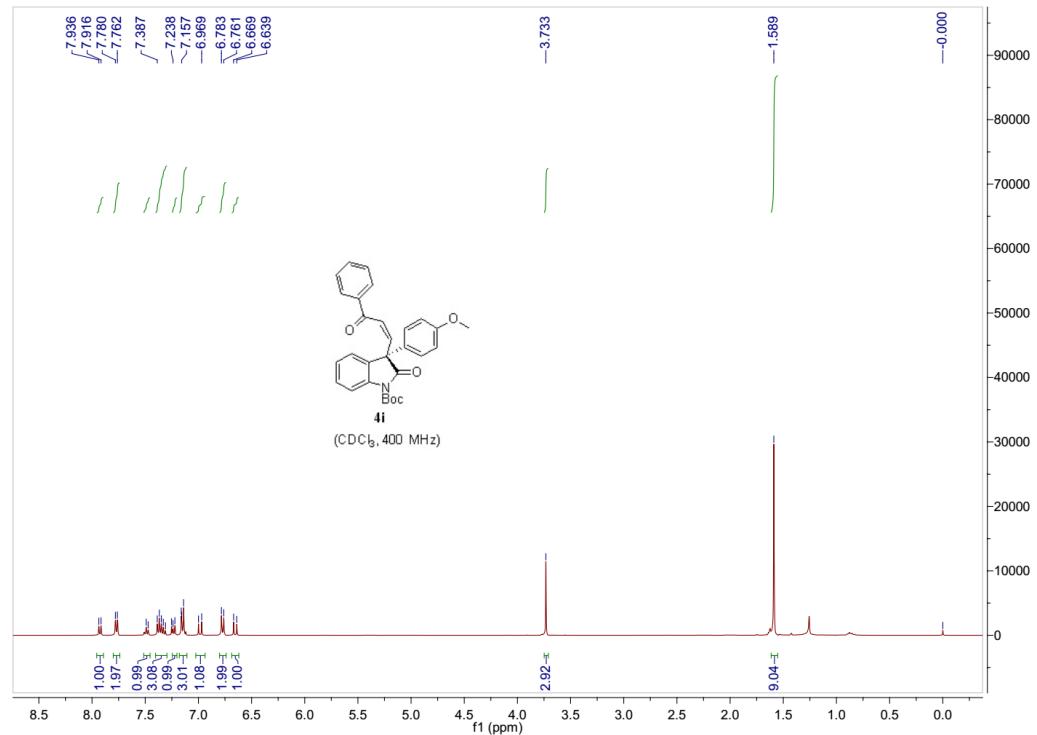


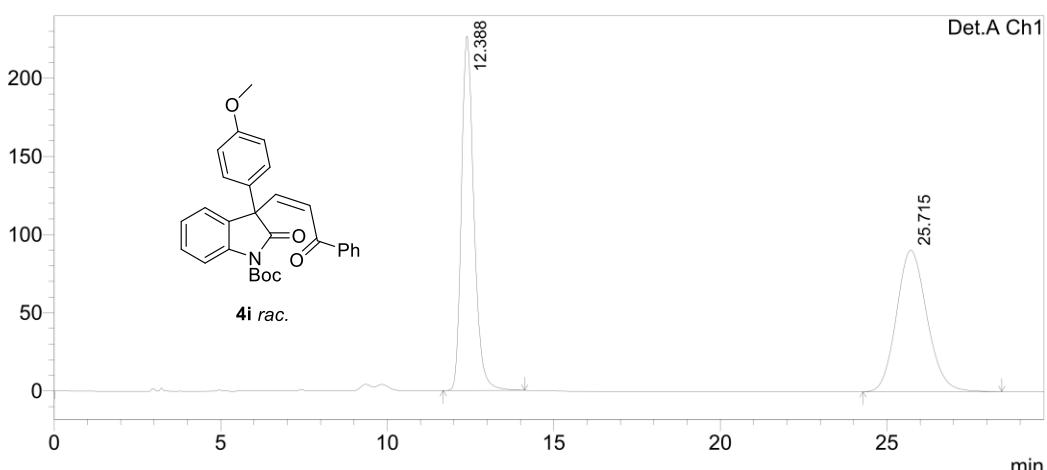
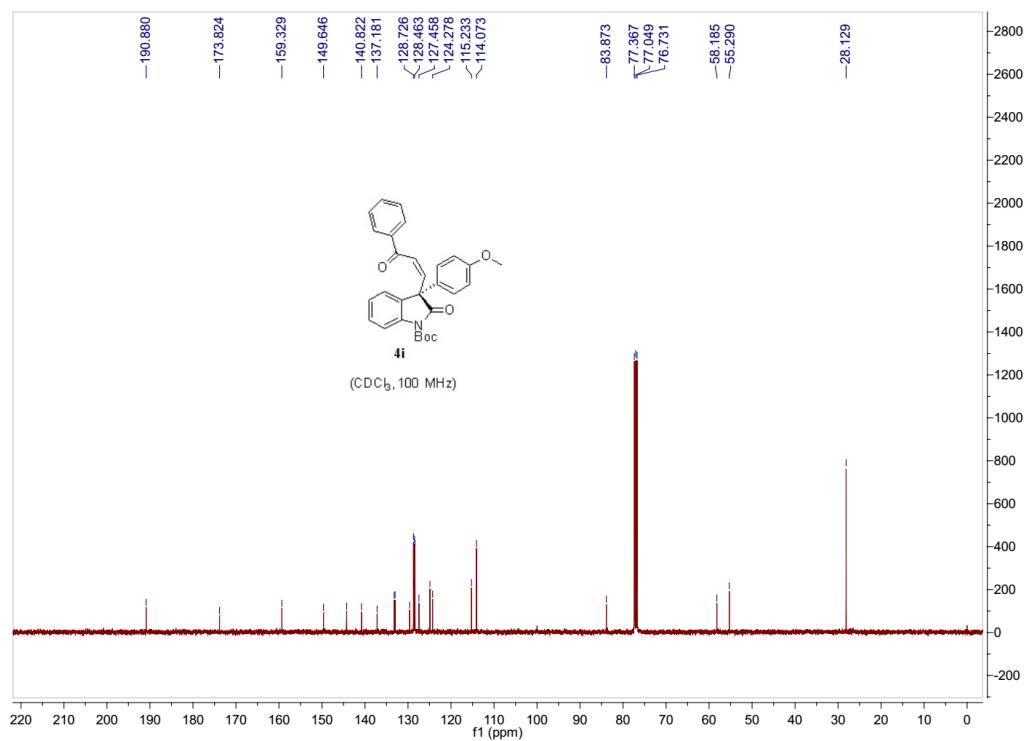
1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.712	54266628	2541542	94.053	97.316
2	14.091	3431436	70084	5.947	2.684
Total		57698064	2611626	100.000	100.000



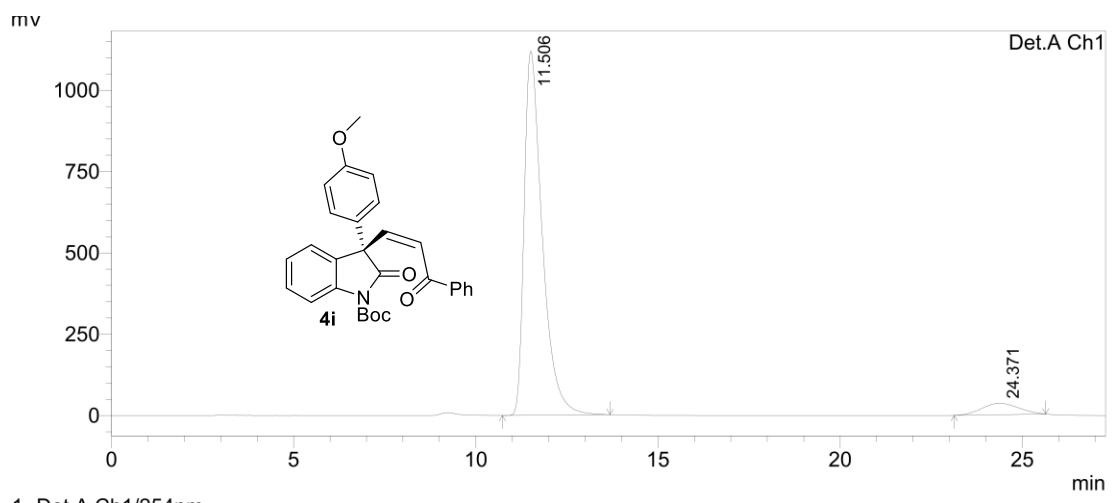


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PeakTable

Detector A Ch1 254nm

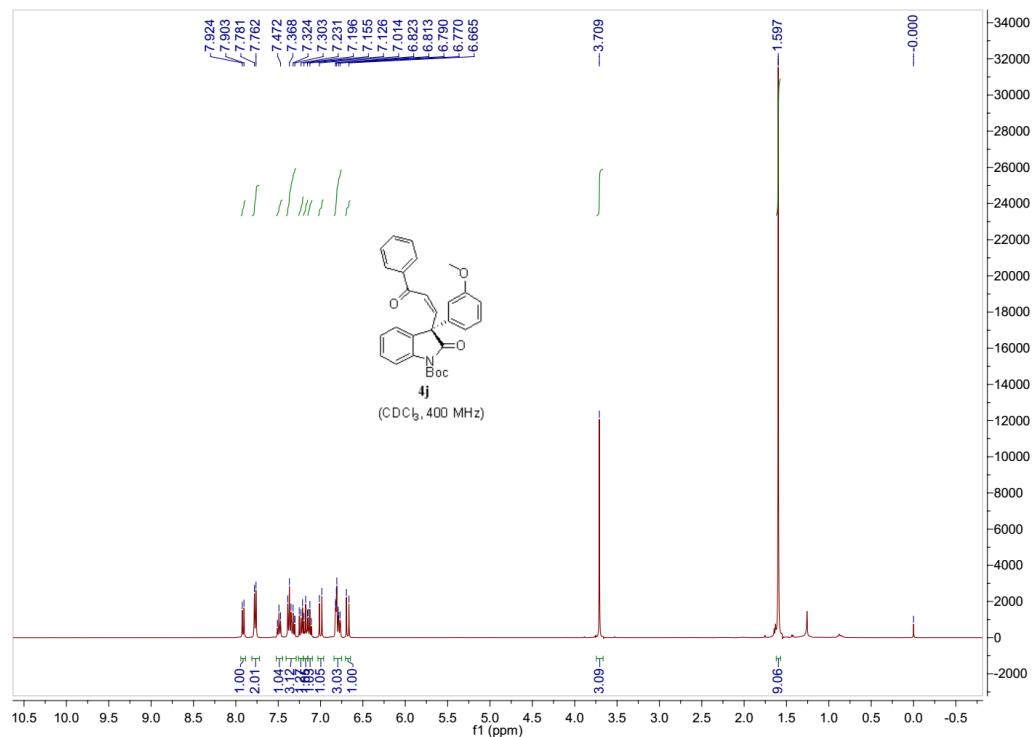
Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.388	5879870	226622	50.588	71.480
2	25.715	5743287	90422	49.412	28.520
Total		11623157	317044	100.000	100.000

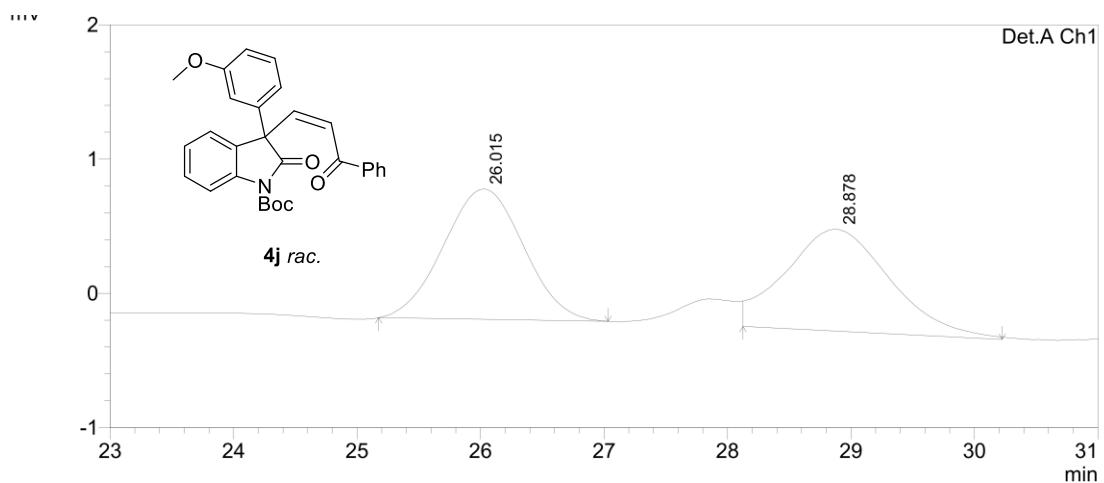
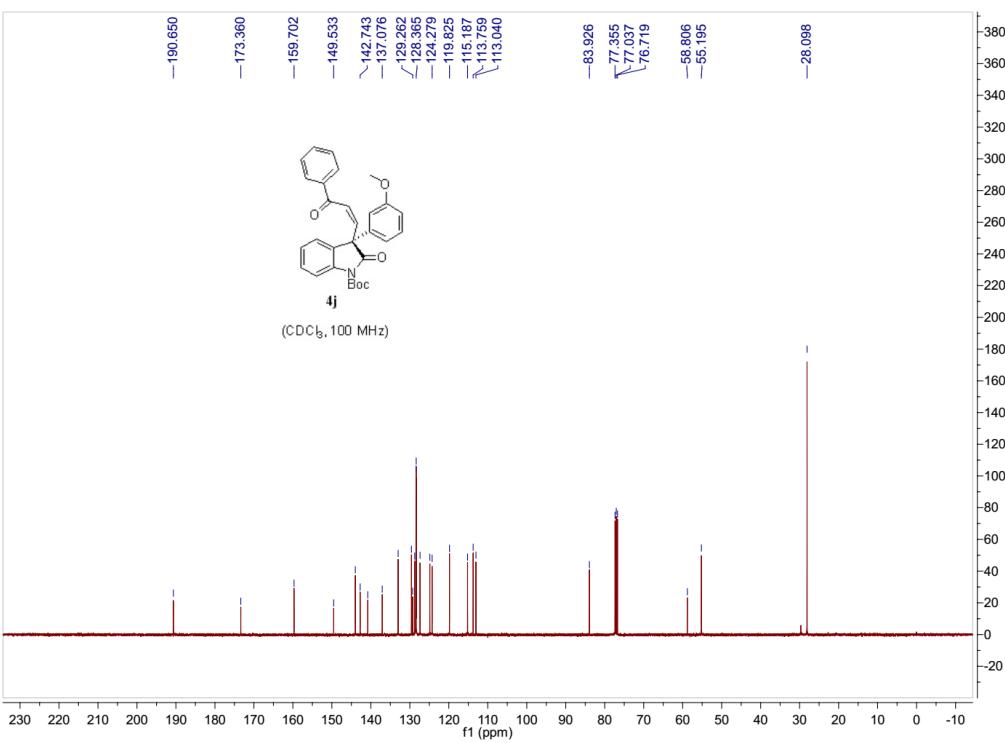


PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.506	38604775	1119500	94.004	96.970
2	24.371	2462462	34978	5.996	3.030
Total		41067237	1154477	100.000	100.000



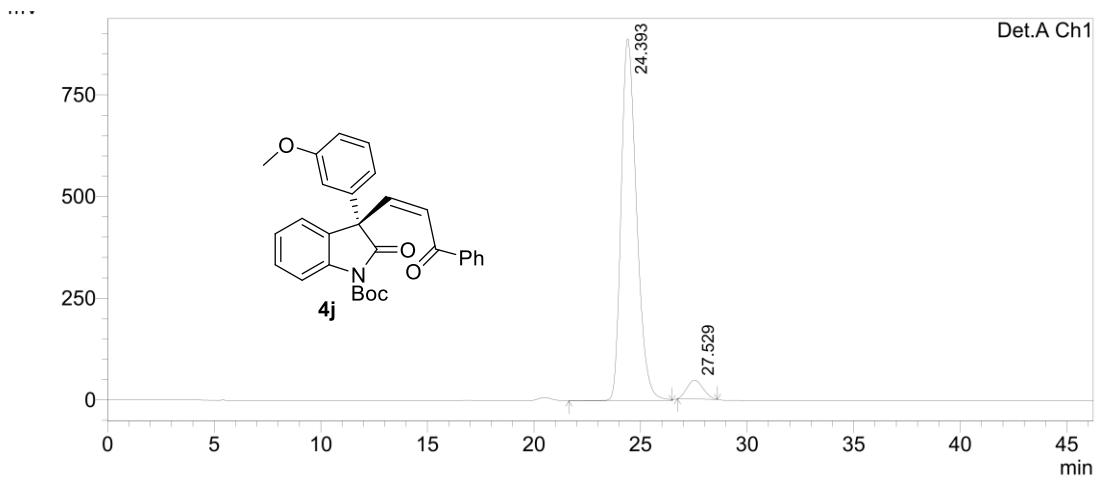


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	26.015	43693	970	49.523	56.113
2	28.878	44534	759	50.477	43.887
Total		88227	1729	100.000	100.000

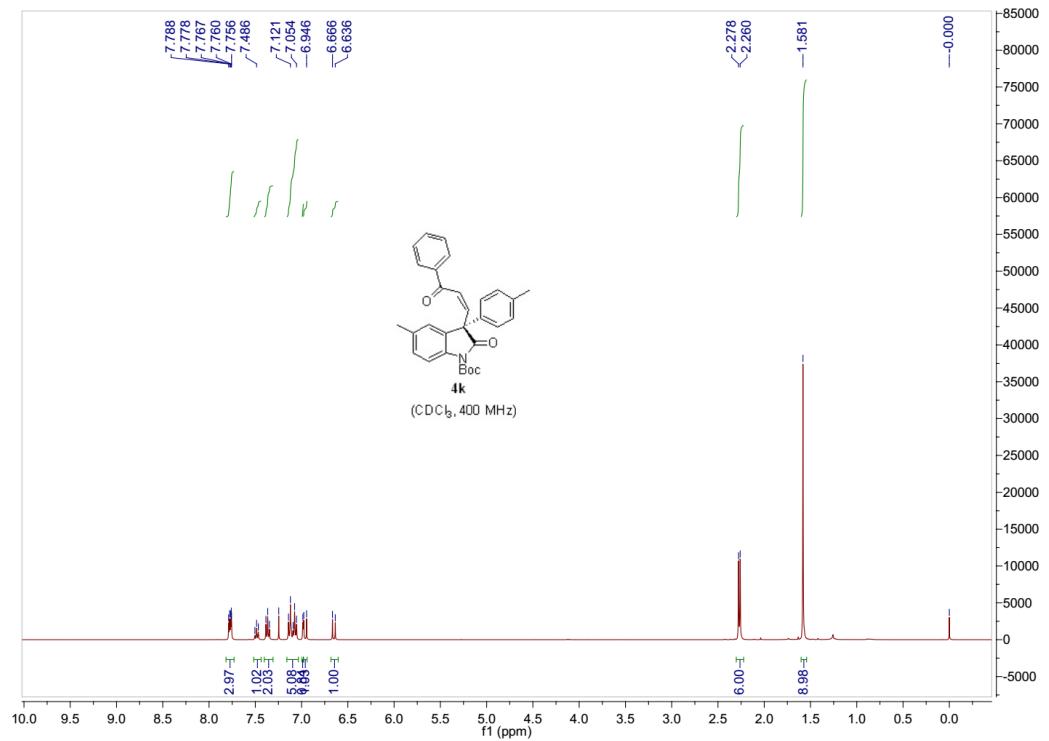


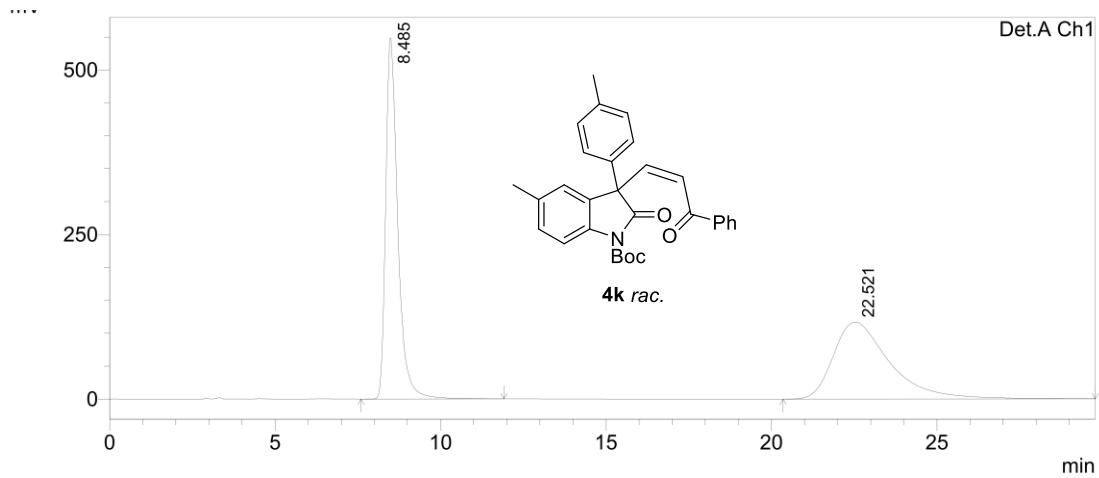
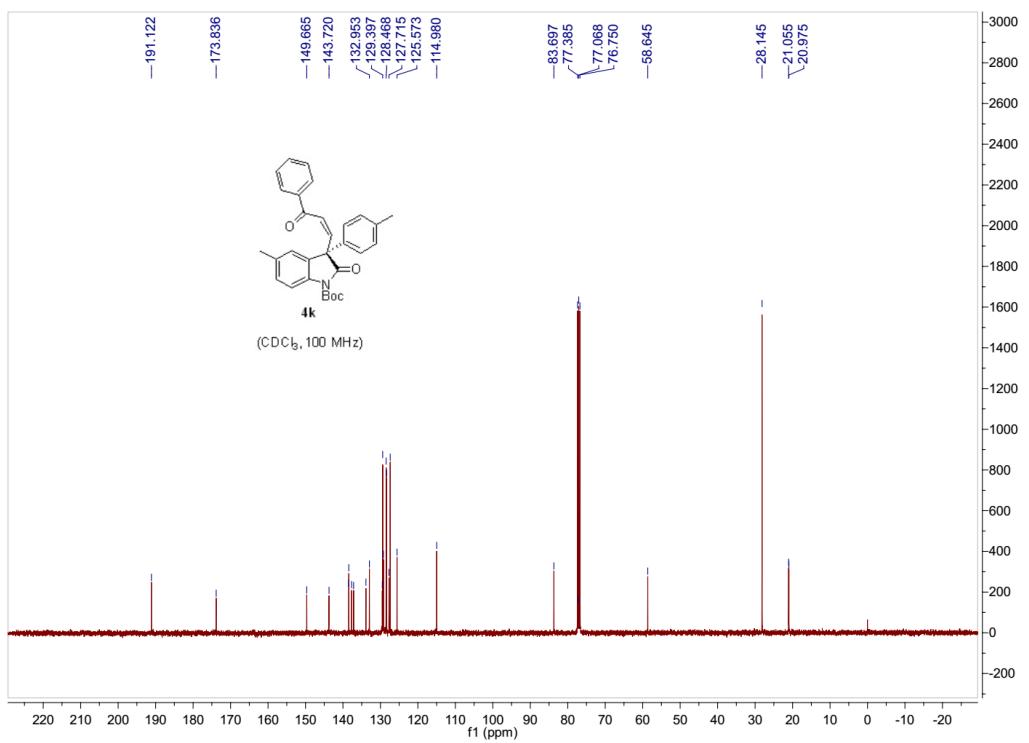
1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	24.393	44932123	889580	94.897	95.072
2	27.529	2416207	46108	5.103	4.928
Total		47348330	935687	100.000	100.000

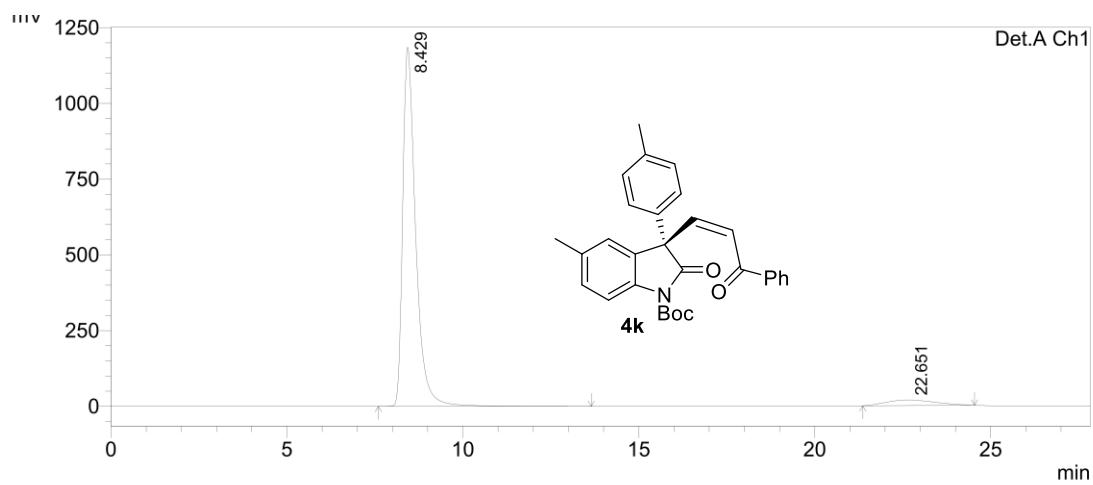




PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.485	13971179	548863	50.288	82.434
2	22.521	13810944	116956	49.712	17.566
Total		27782123	665818	100.000	100.000

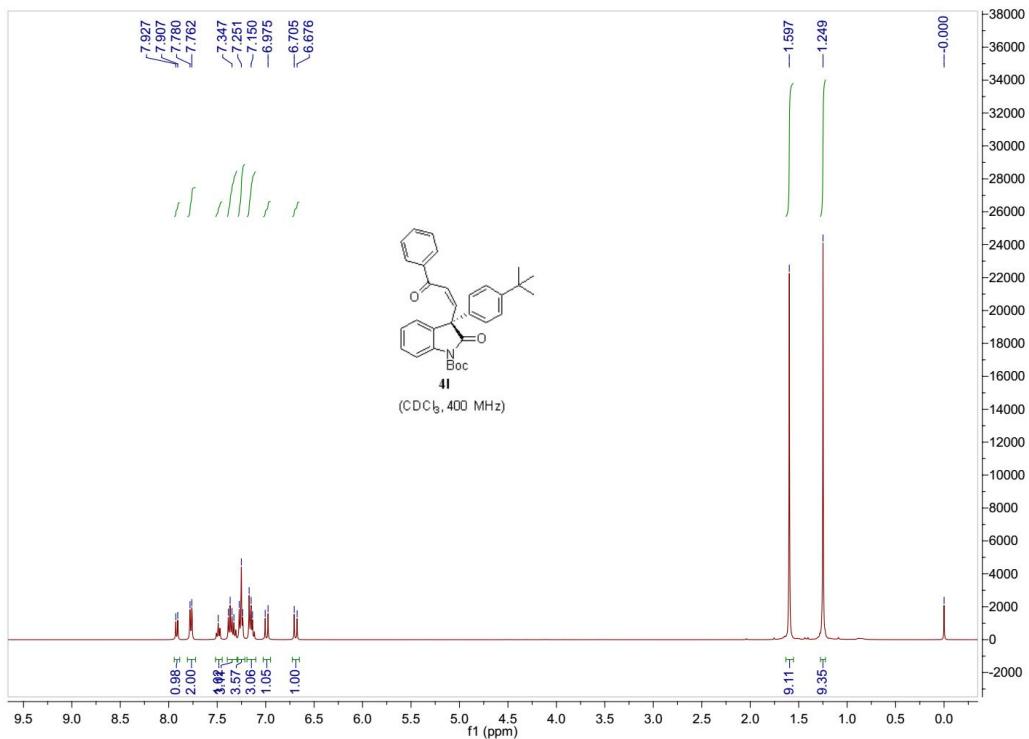


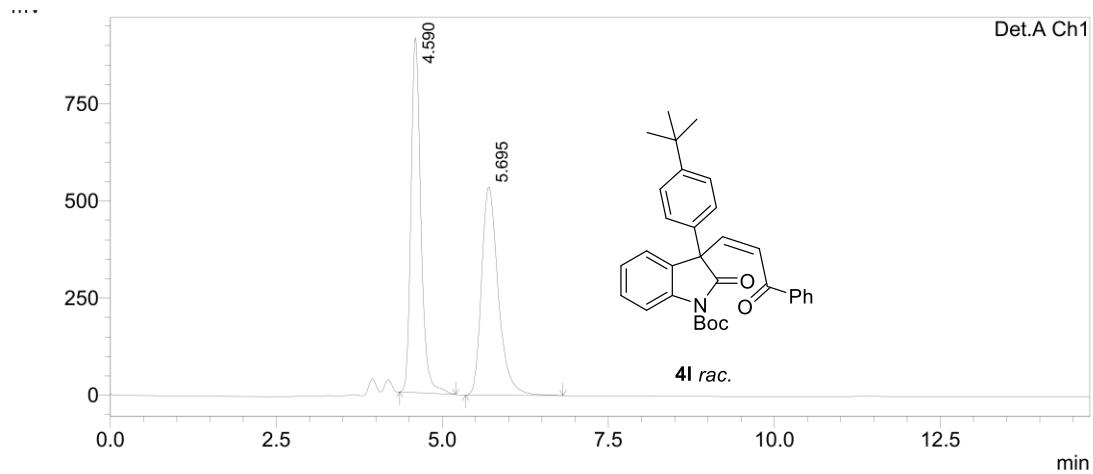
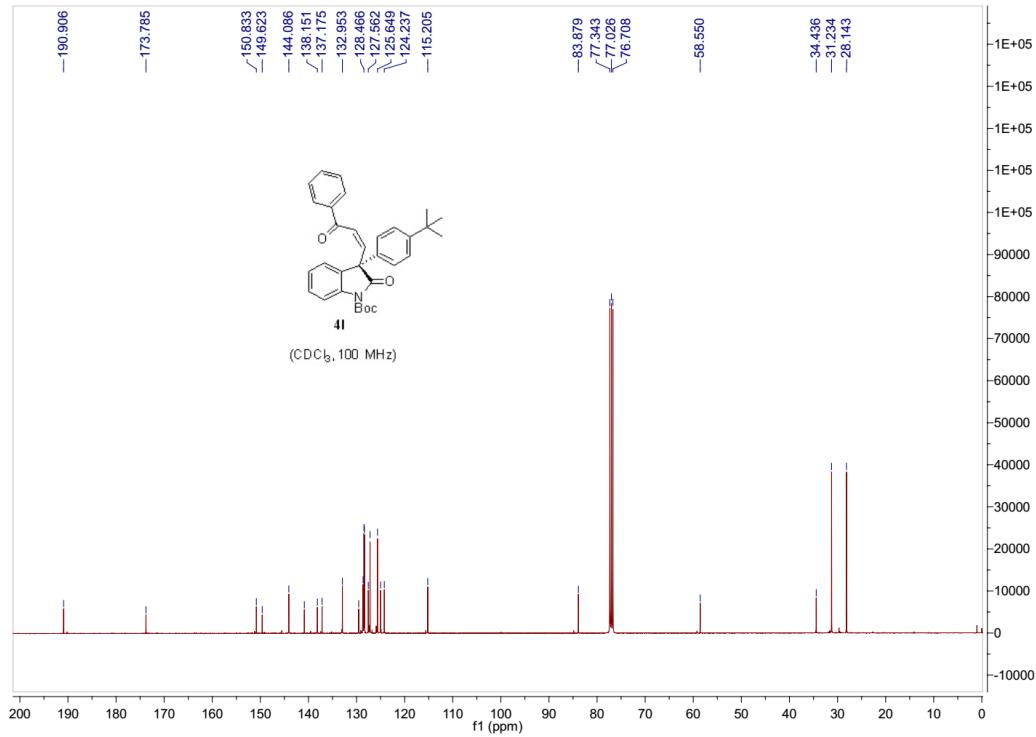
1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.429	30306641	1186017	94.442	98.464
2	22.651	1783467	18504	5.558	1.536
Total		32090108	1204520	100.000	100.000



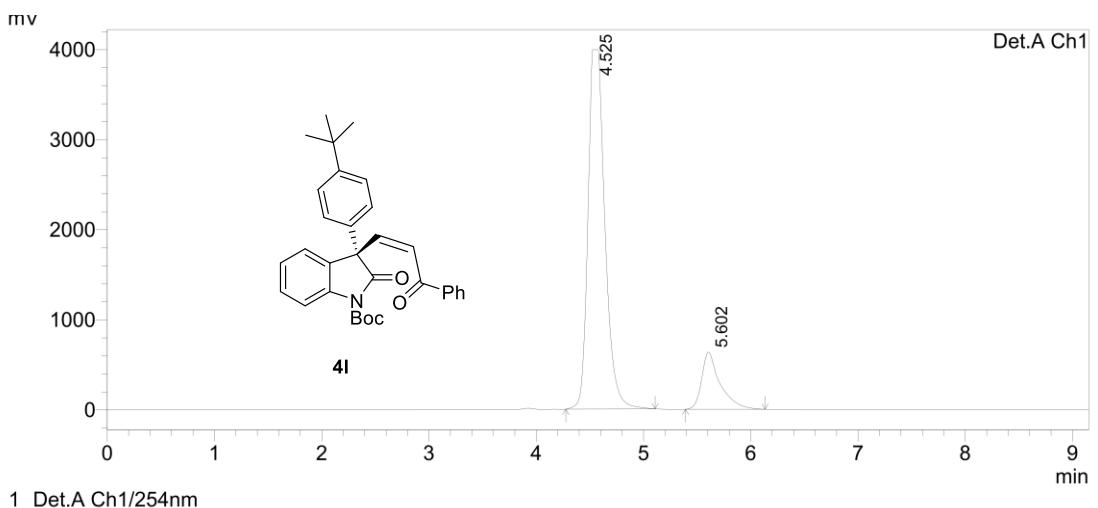


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.590	9506964	913749	50.350	63.013
2	5.695	9374703	536352	49.650	36.987
Total		18881668	1450101	100.000	100.000

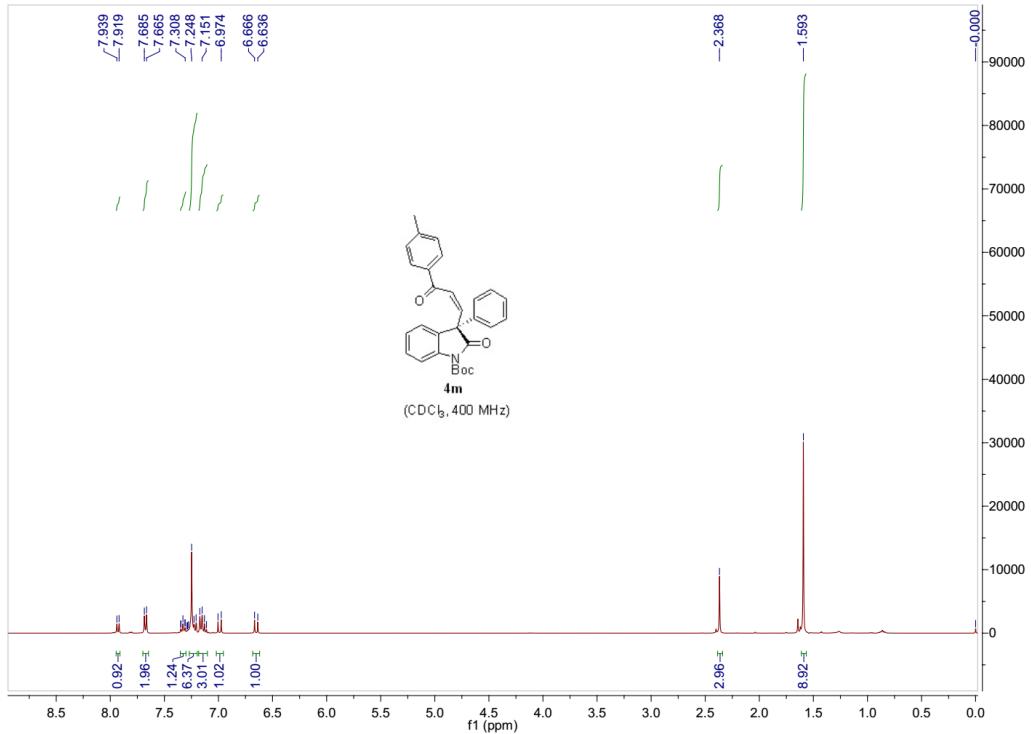


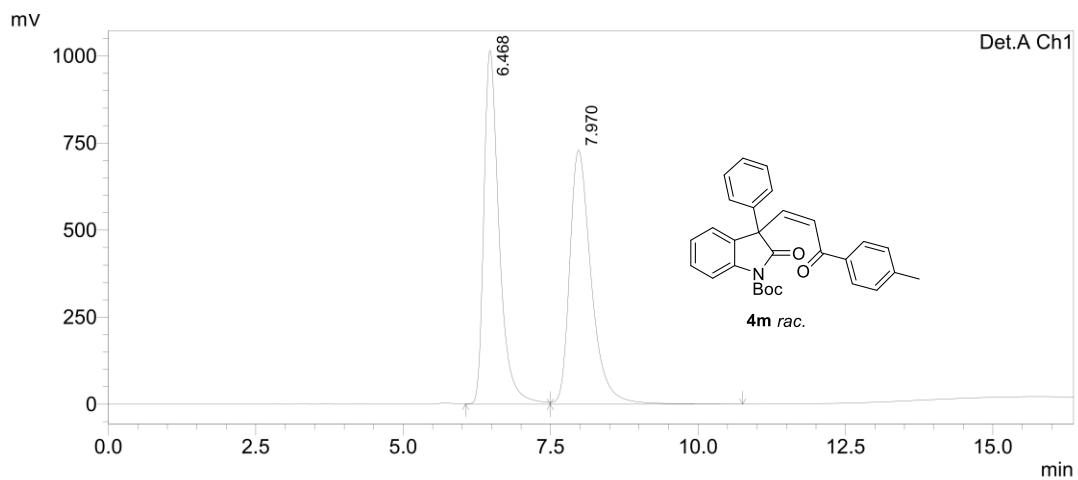
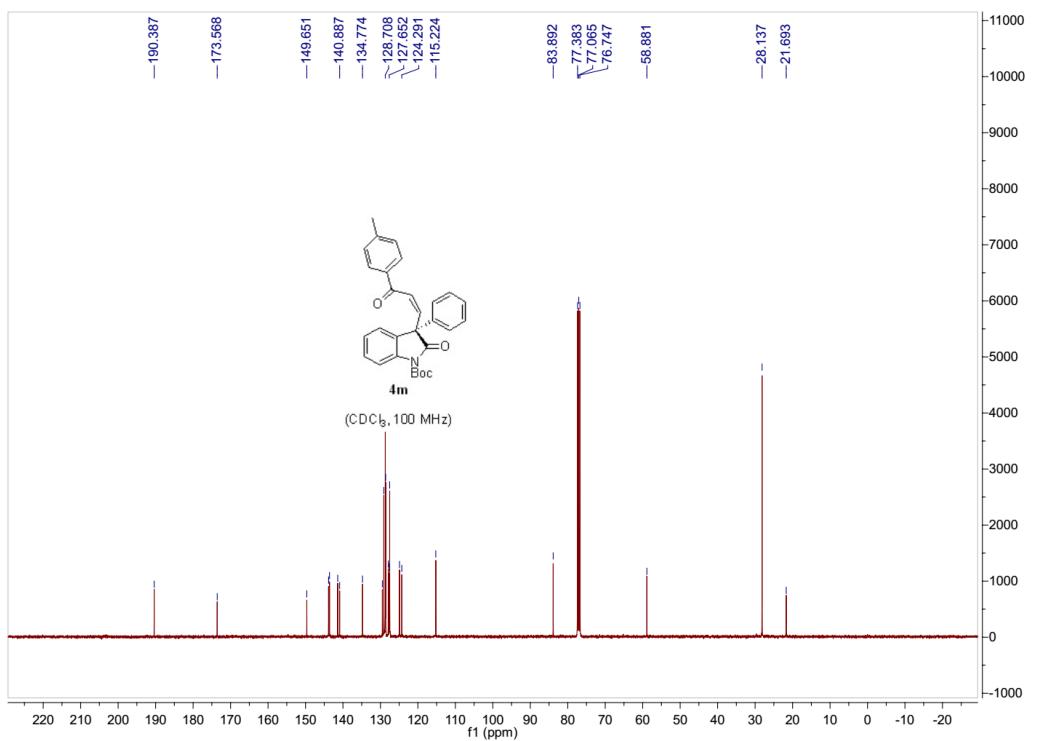
1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.525	43705174	3989798	85.311	86.285
2	5.602	7525407	634196	14.689	13.715
Total		51230581	4623994	100.000	100.000



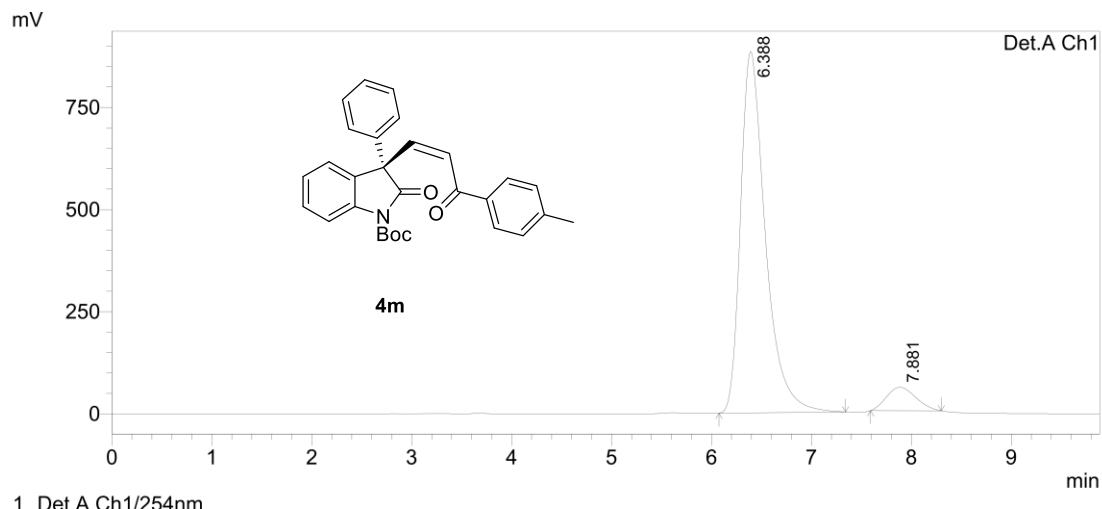


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

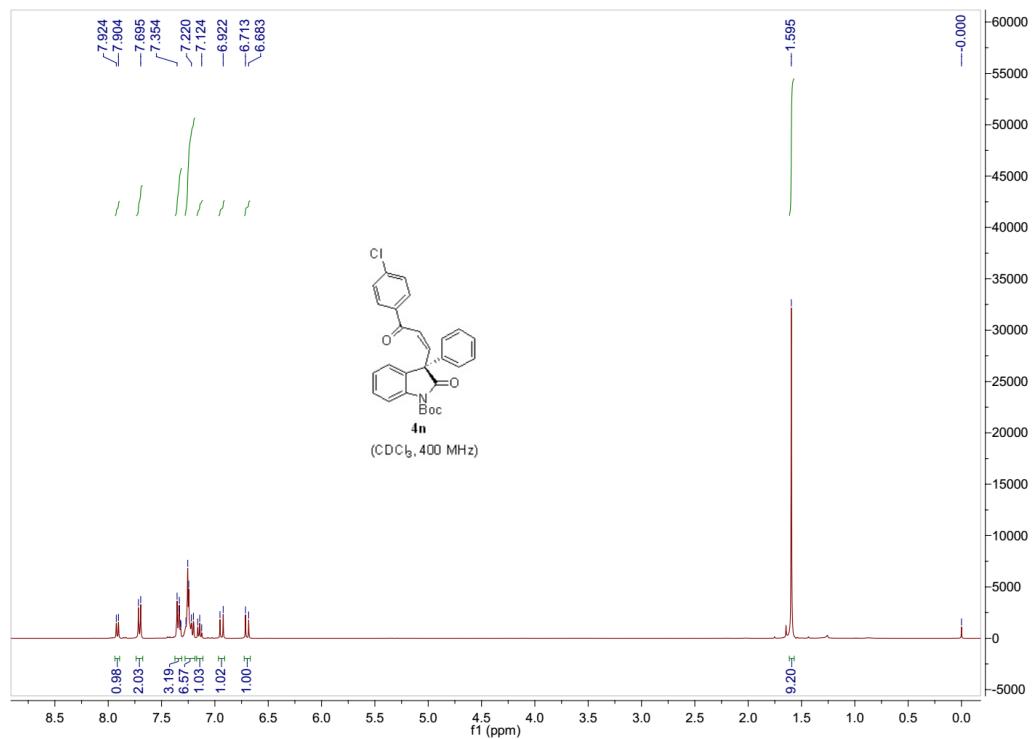
Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.468	18348144	1015913	49.741	58.210
2	7.970	18538860	729331	50.259	41.790
Total		36887004	1745244	100.000	100.000

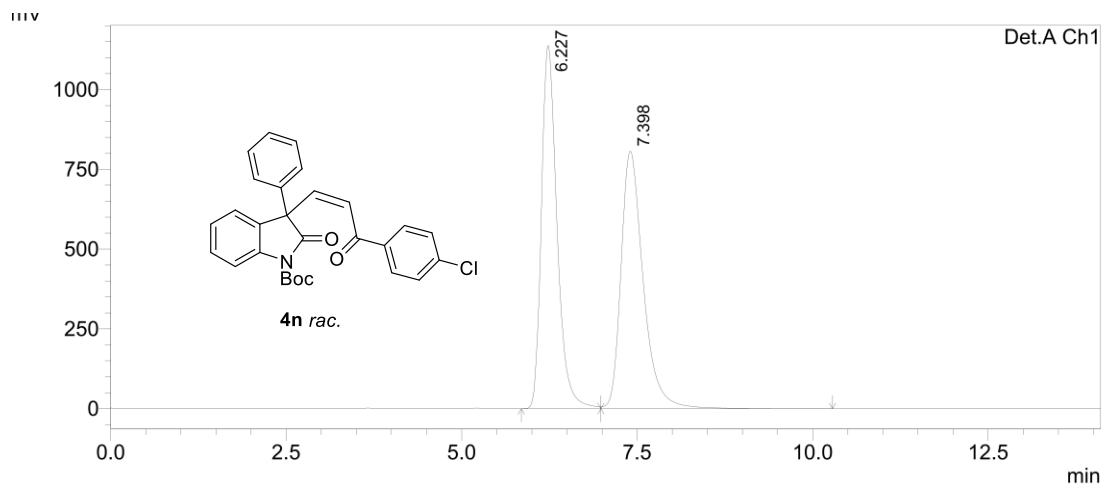
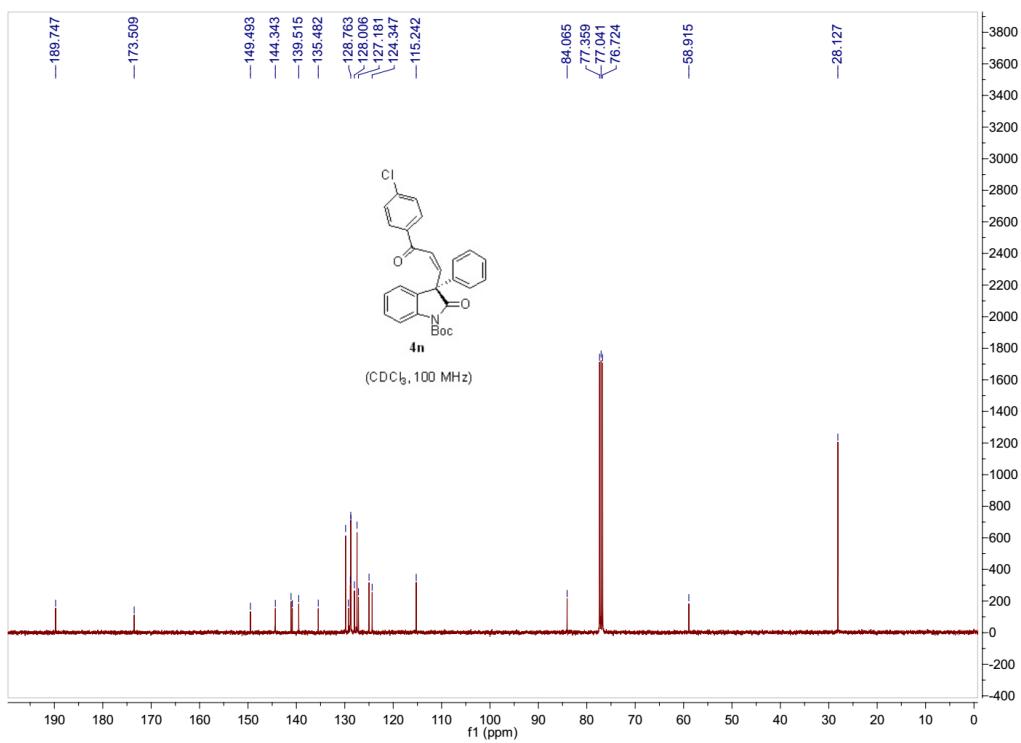


PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.388	15302657	884706	92.885	93.911
2	7.881	1172105	57359	7.115	6.089
Total		16474761	942065	100.000	100.000



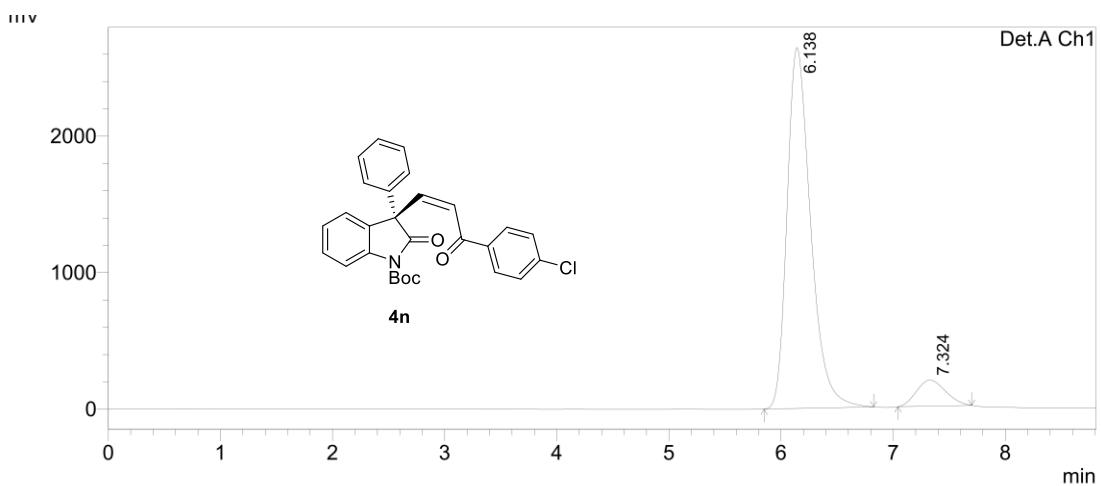


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.227	17608842	1138185	49.741	58.502
2	7.398	17792123	807380	50.259	41.498
Total		35400966	1945565	100.000	100.000

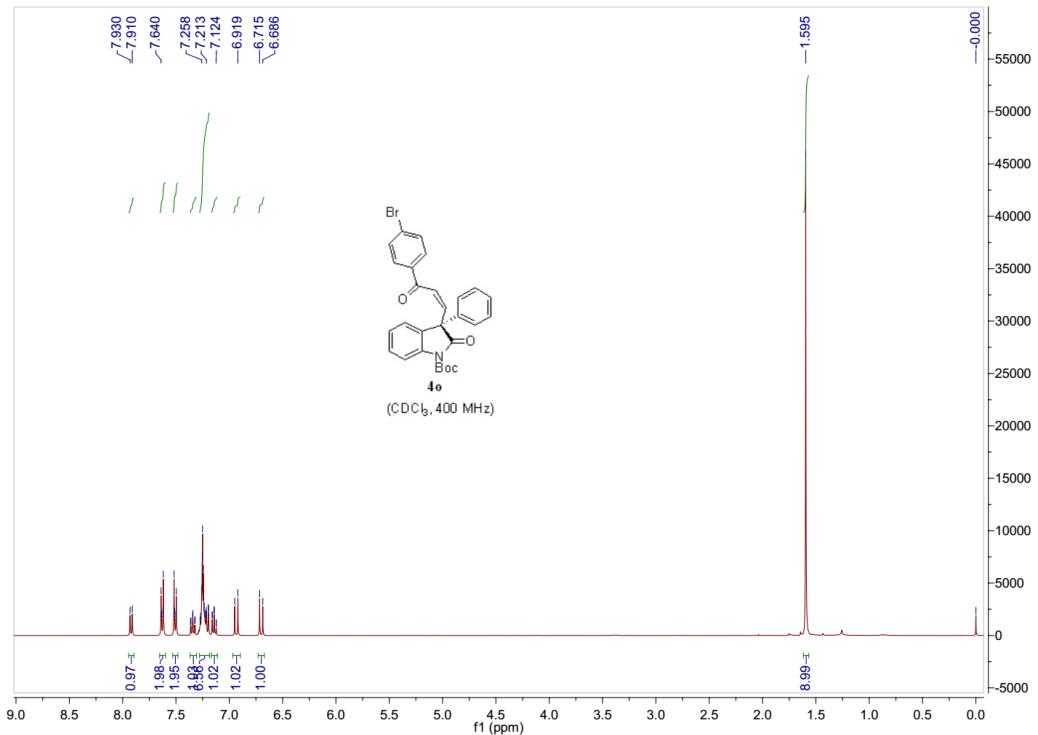


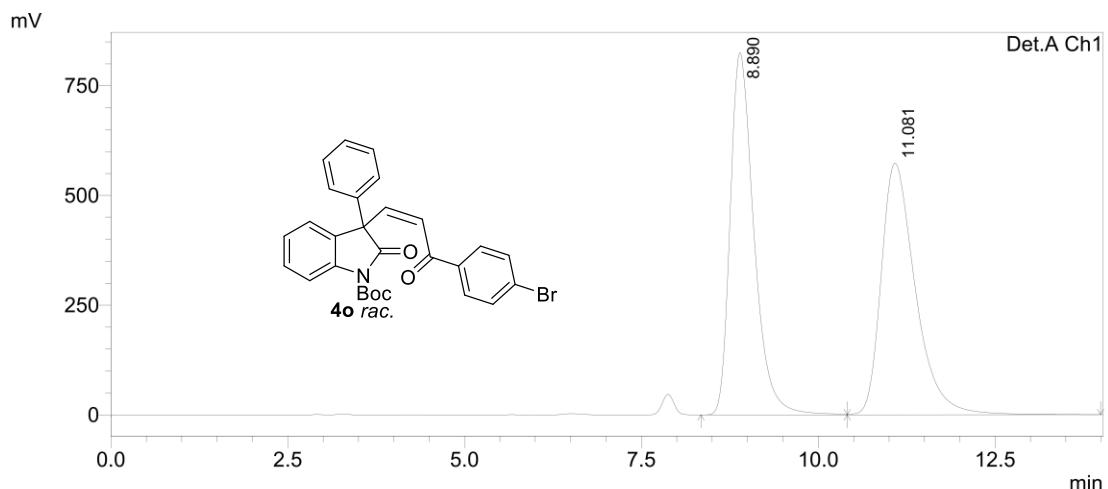
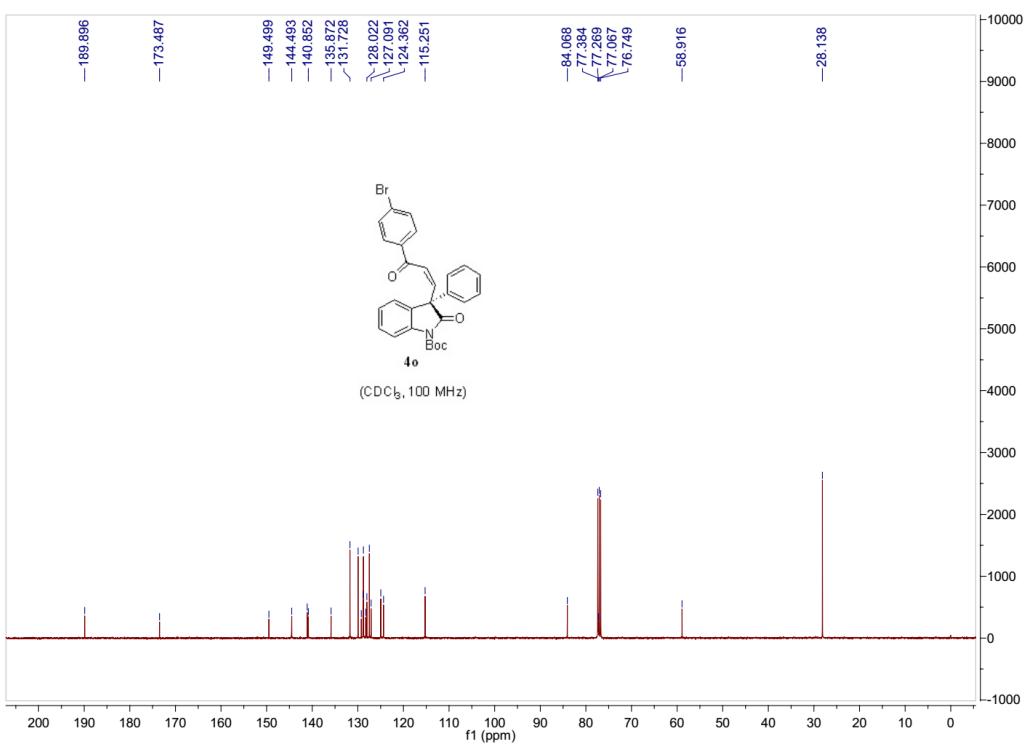
1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.138	38659204	2643997	91.797	93.275
2	7.324	3454750	190618	8.203	6.725
Total		42113954	2834614	100.000	100.000



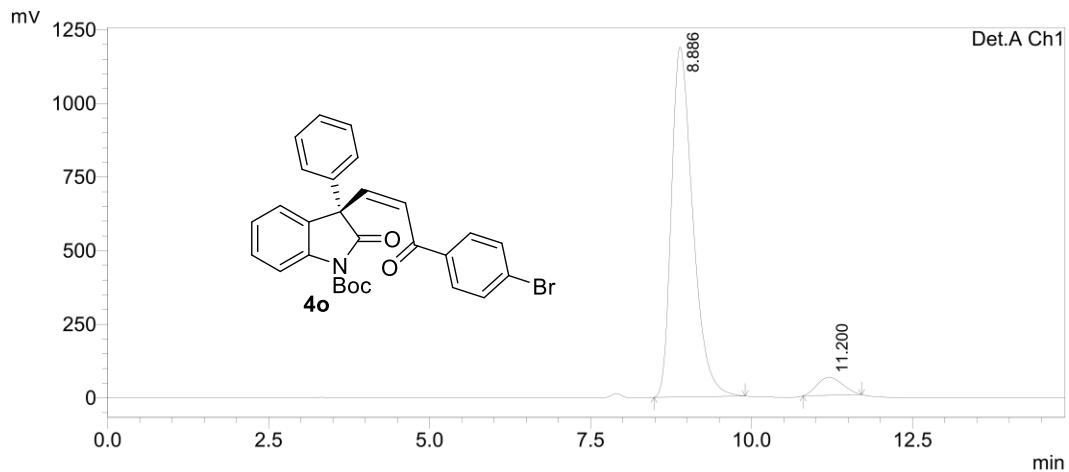


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.890	19323042	825598	50.042	59.011
2	11.081	19290421	573455	49.958	40.989
Total		38613463	1399053	100.000	100.000

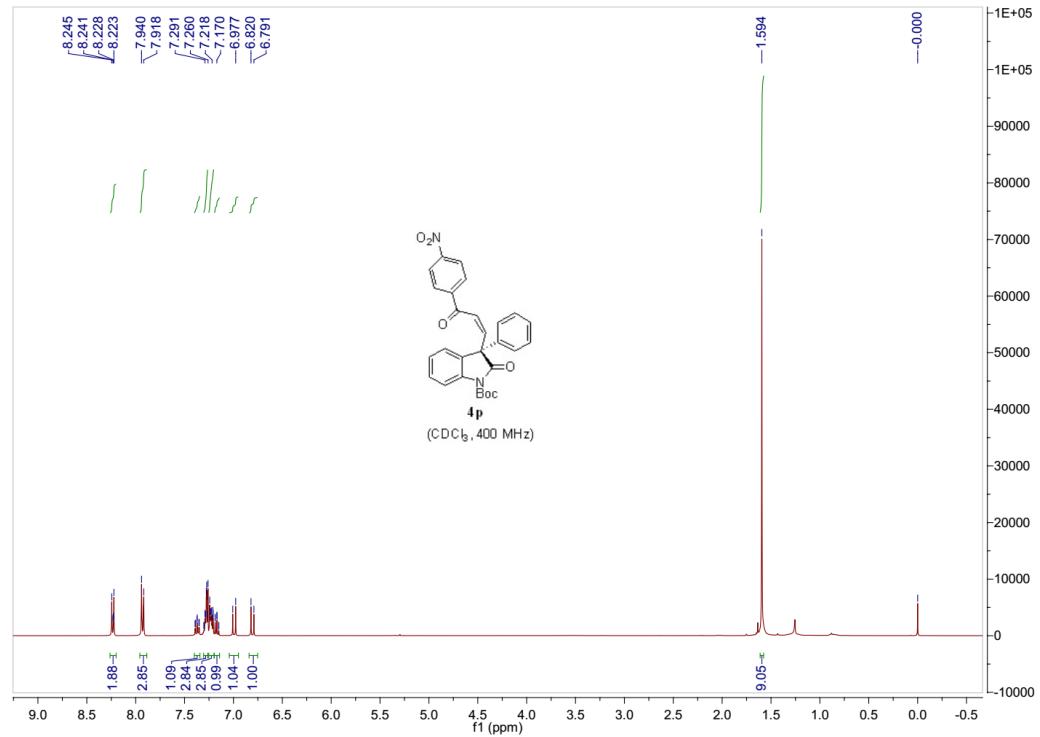


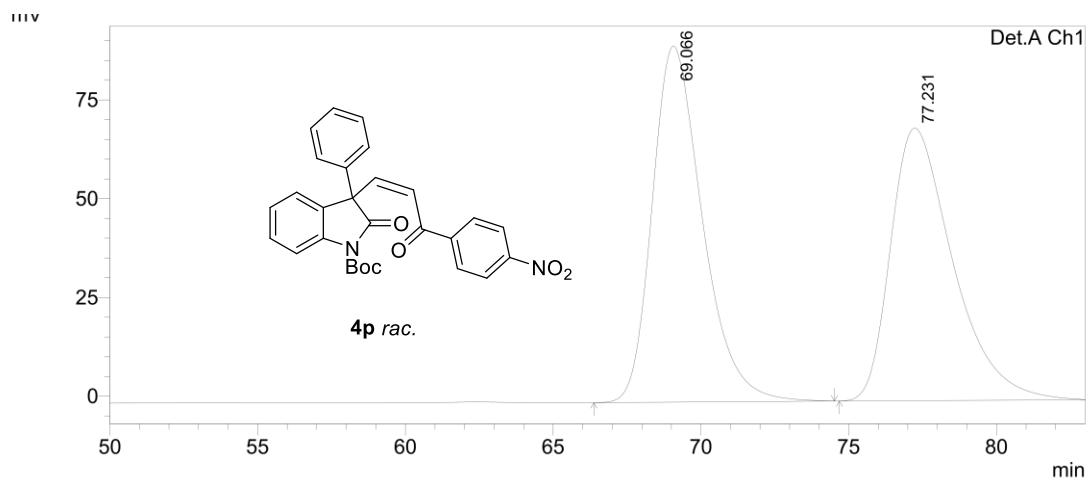
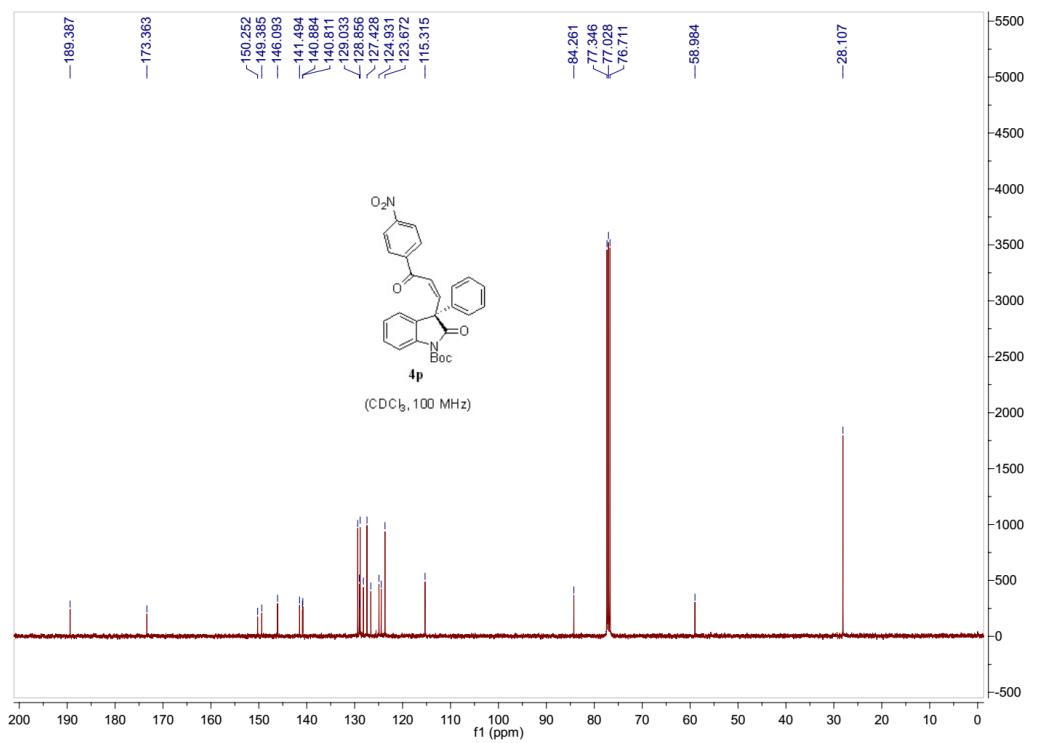
1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.886	27501416	1188000	94.217	95.102
2	11.200	1688112	61180	5.783	4.898
Total		29189528	1249180	100.000	100.000



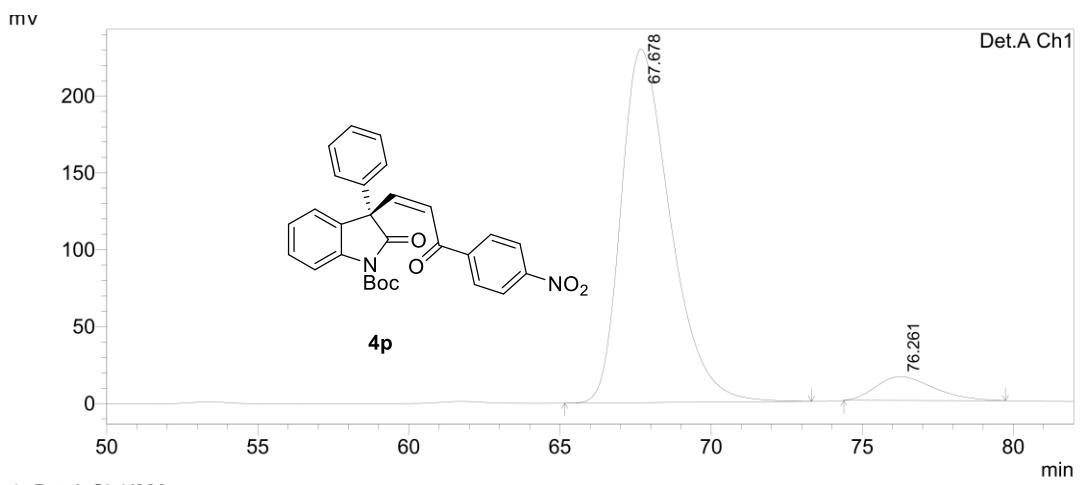


1 Det.A Ch1/220nm

PeakTable

Detector A Ch1 220nm

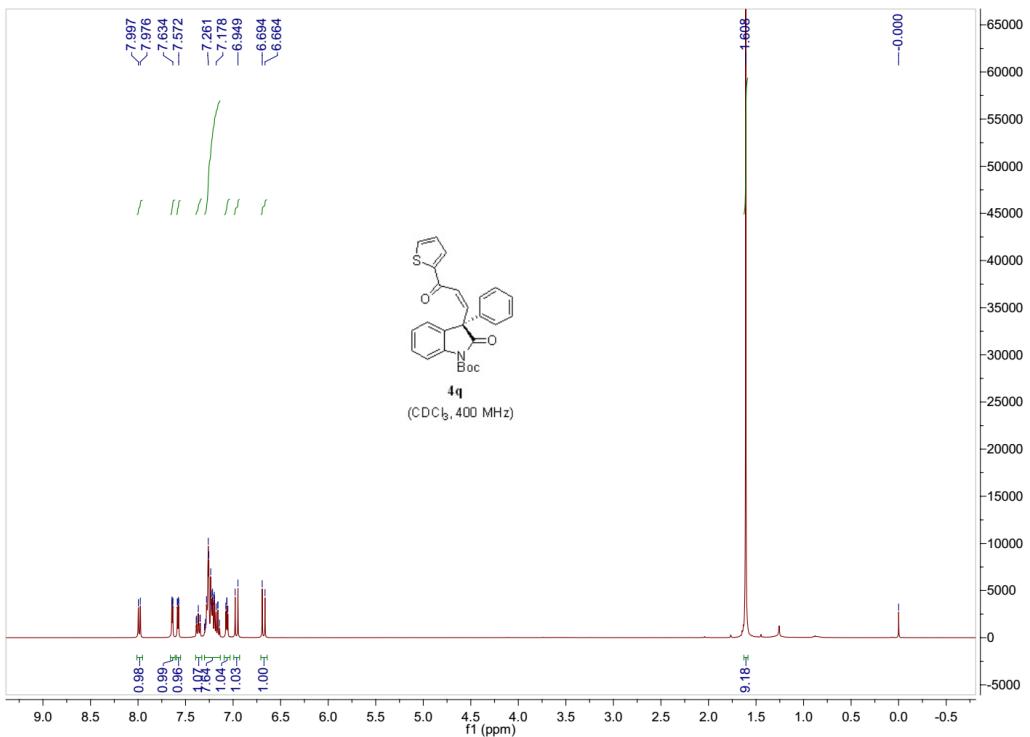
Peak#	Ret. Time	Area	Height	Area %	Height %
1	69.066	10637735	90136	51.257	56.651
2	77.231	10116119	68971	48.743	43.349
Total		20753854	159106	100.000	100.000

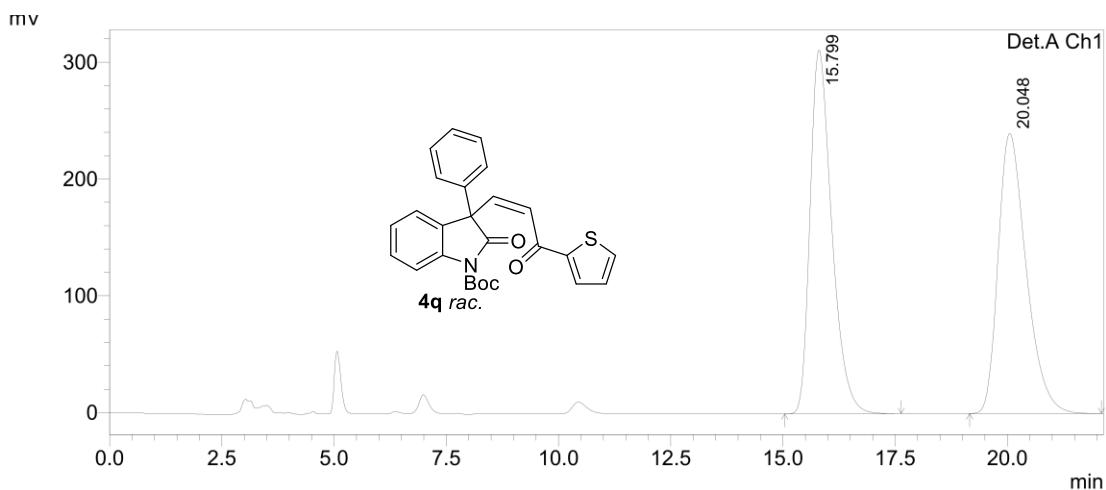
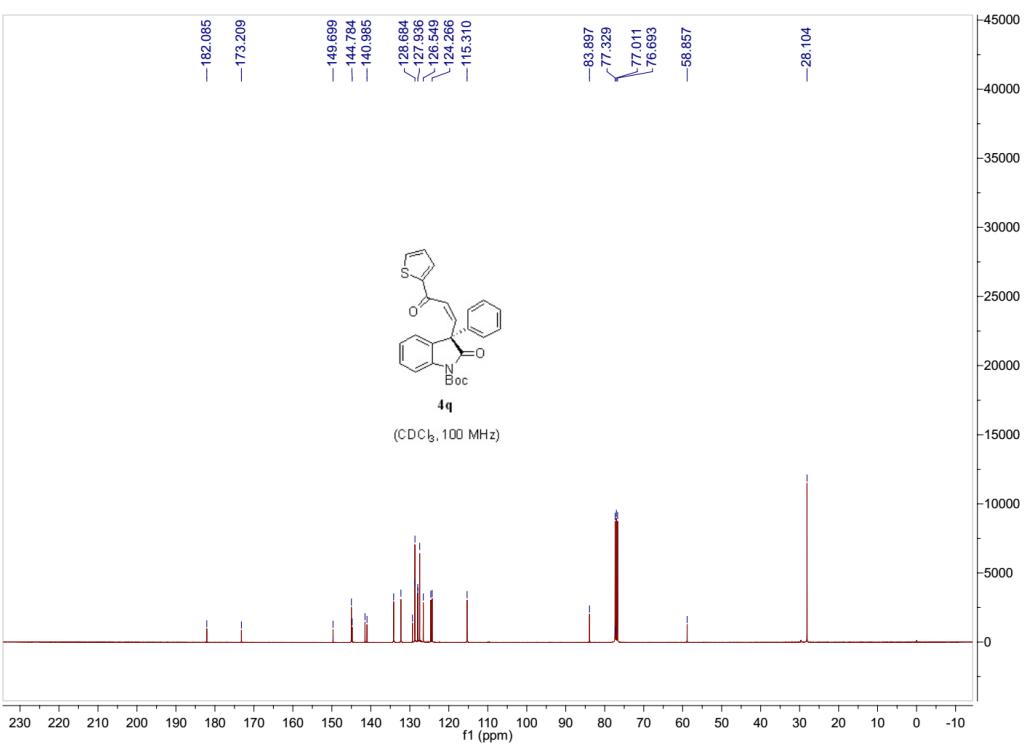


PeakTable

Detector A Ch1 220nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	67.678	2612999	229898	92.728	93.688
2	76.261	2048993	15489	7.272	6.312
Total		28178292	245387	100.000	100.000



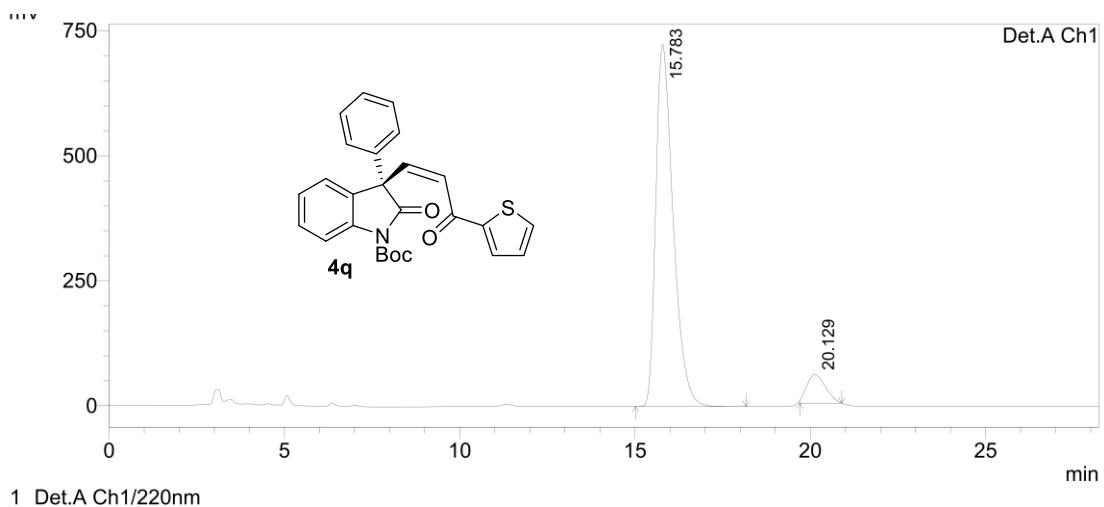


1 Det.A Ch1/220nm

PeakTable

Detector A Ch1 220nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	15.799	10457727	311356	50.085	56.491
2	20.048	10422319	239802	49.915	43.509
Total		20880046	551159	100.000	100.000

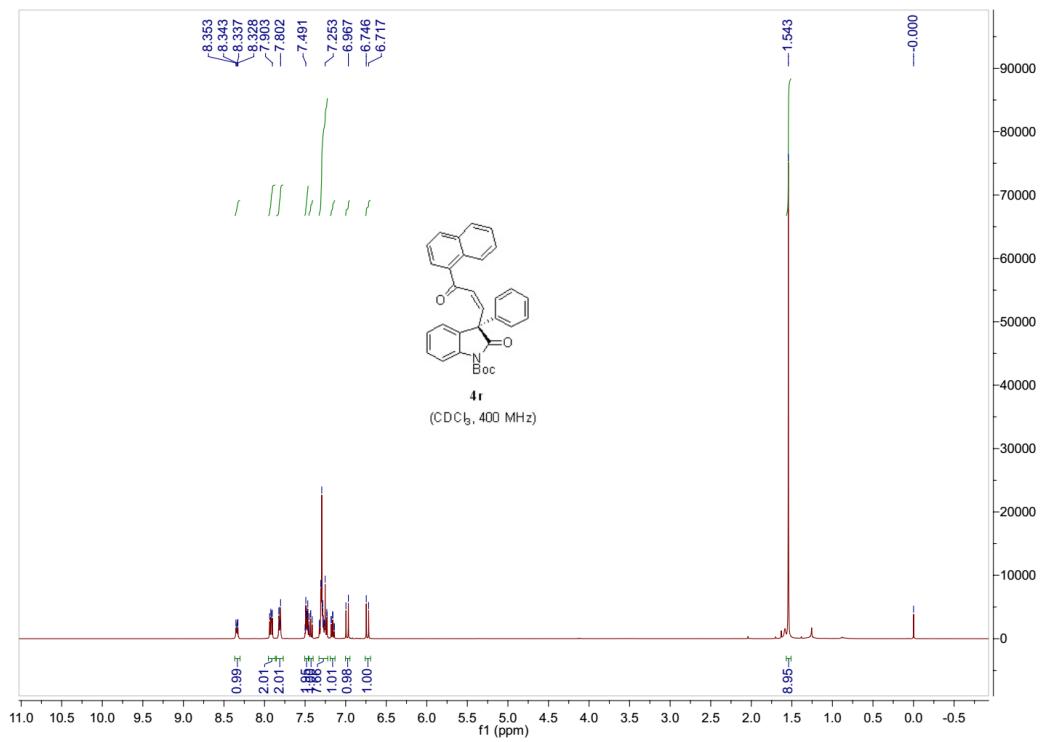


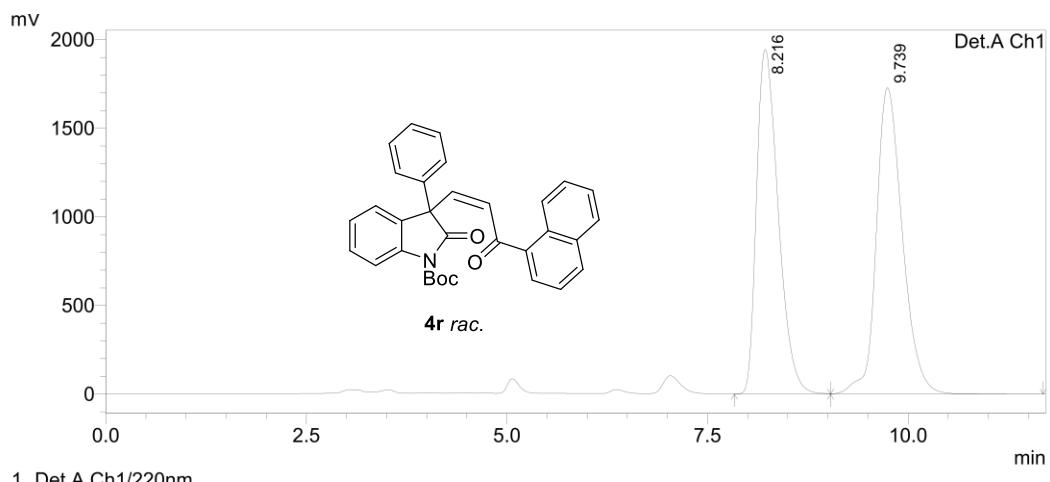
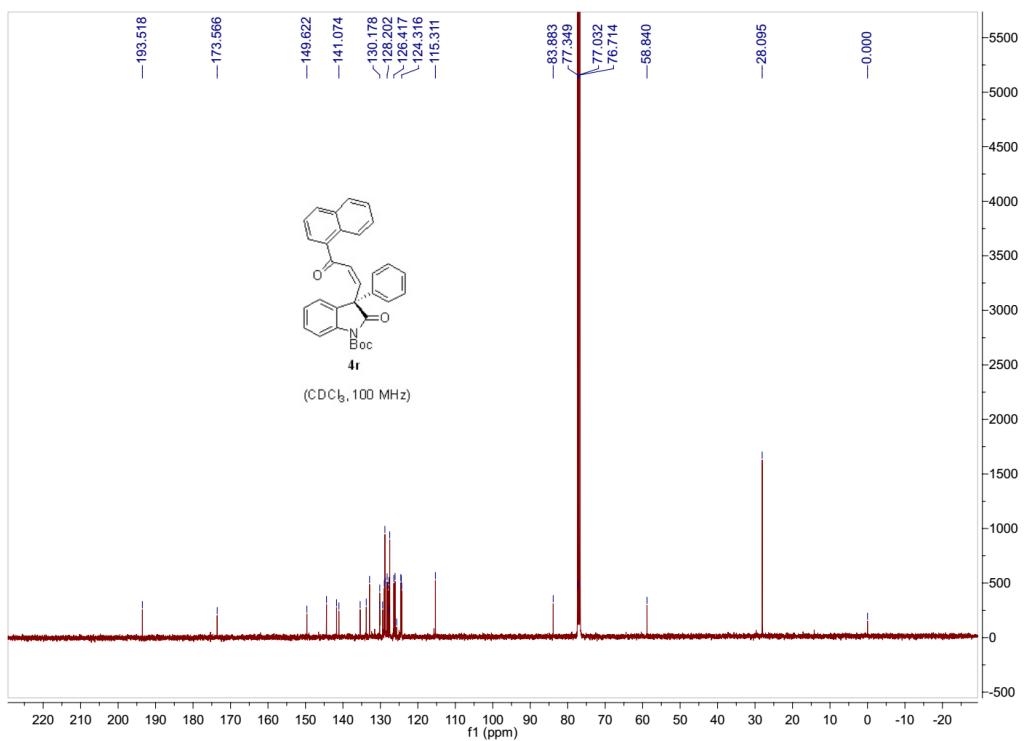
1 Det.A Ch1/220nm

PeakTable

Detector A Ch1 220nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	15.783	24934679	724599	92.206	92.726
2	20.129	2107708	56840	7.794	7.274
Total		27042387	781438	100.000	100.000



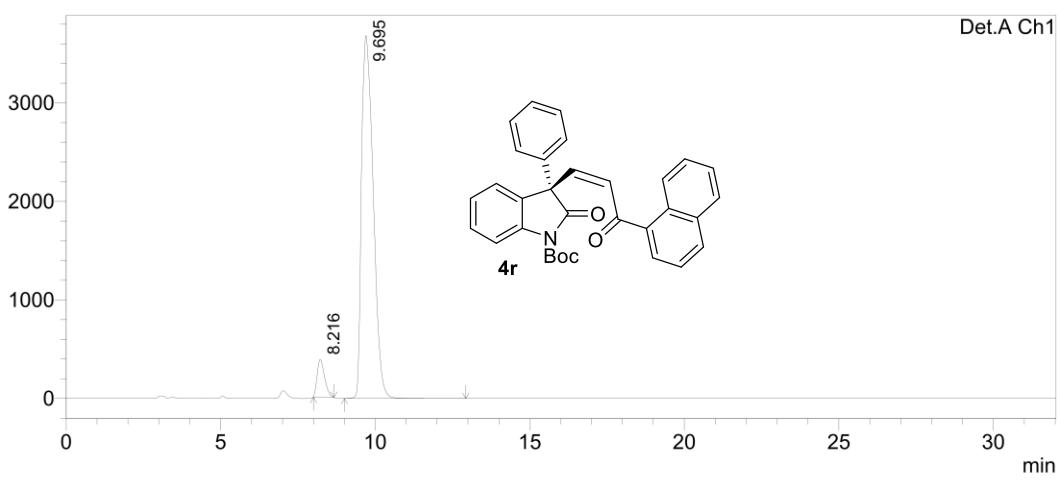


1 Det.A Ch1/220nm

PeakTable

Detector A Ch1 220nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.216	36762625	1945273	48.446	52.936
2	9.739	39121539	1729497	51.554	47.064
Total		75884163	3674770	100.000	100.000

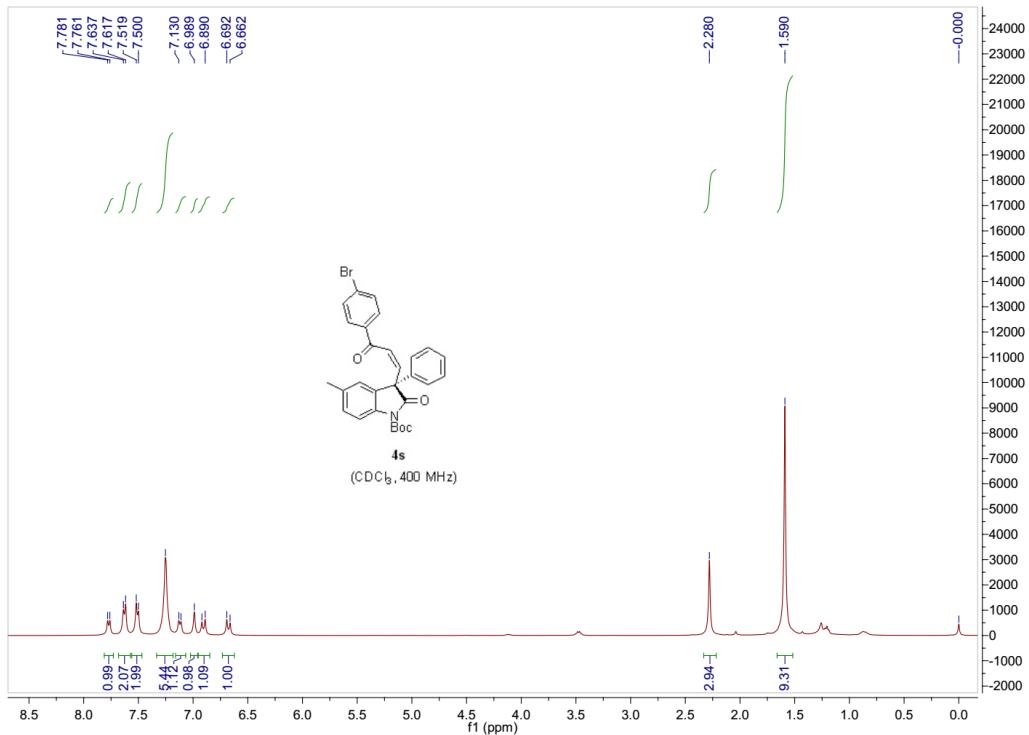


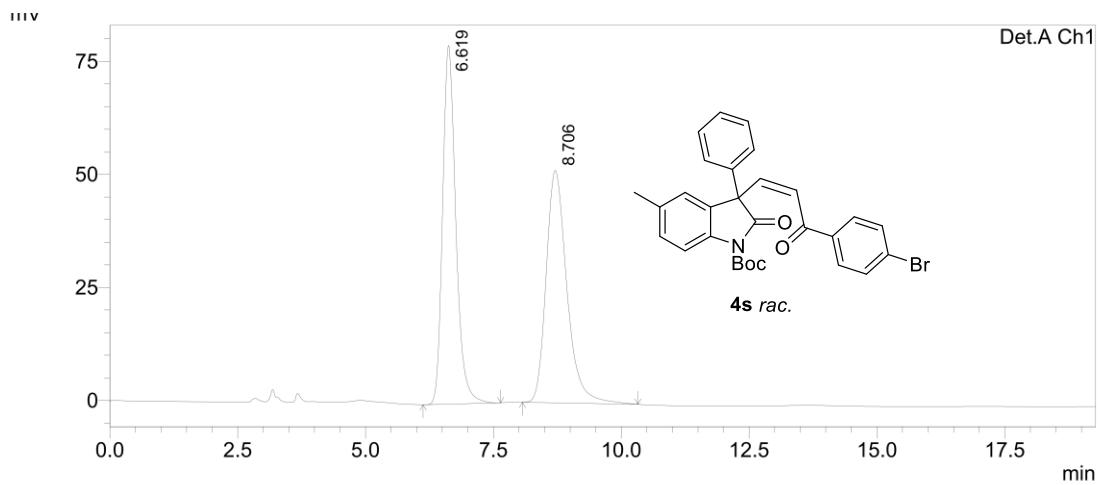
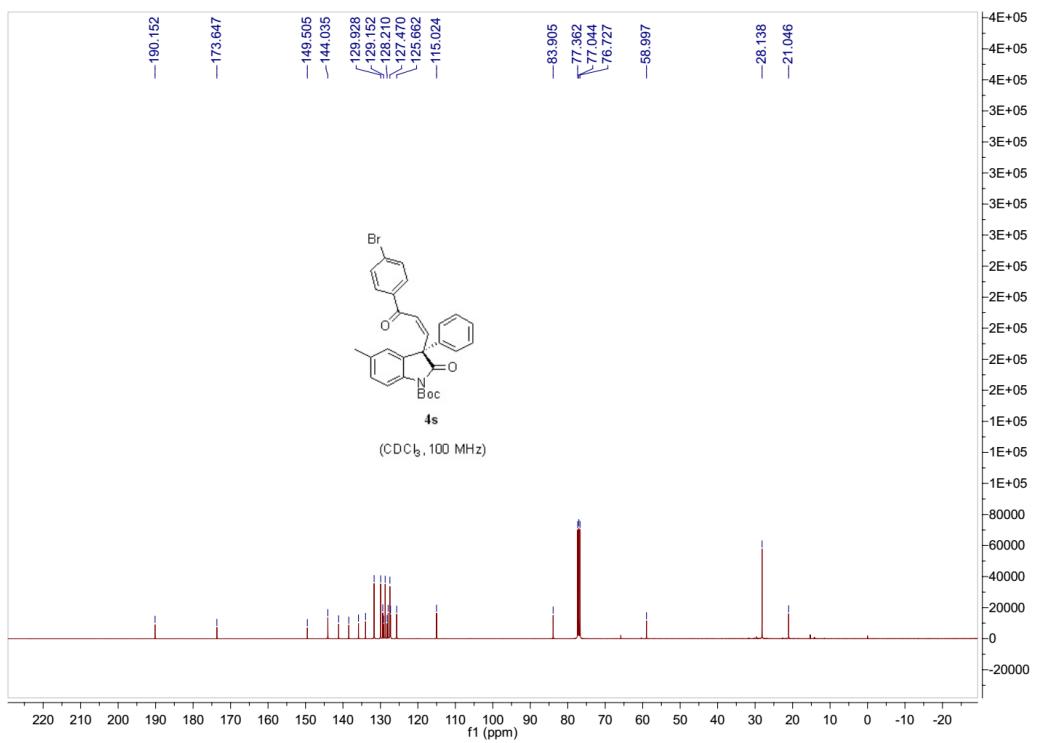
1 Det.A Ch1/220nm

PeakTable

Detector A Ch1 220nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.216	6473647	386427	6.232	9.490
2	9.695	97399347	3685422	93.768	90.510
Total		103872995	4071849	100.000	100.000



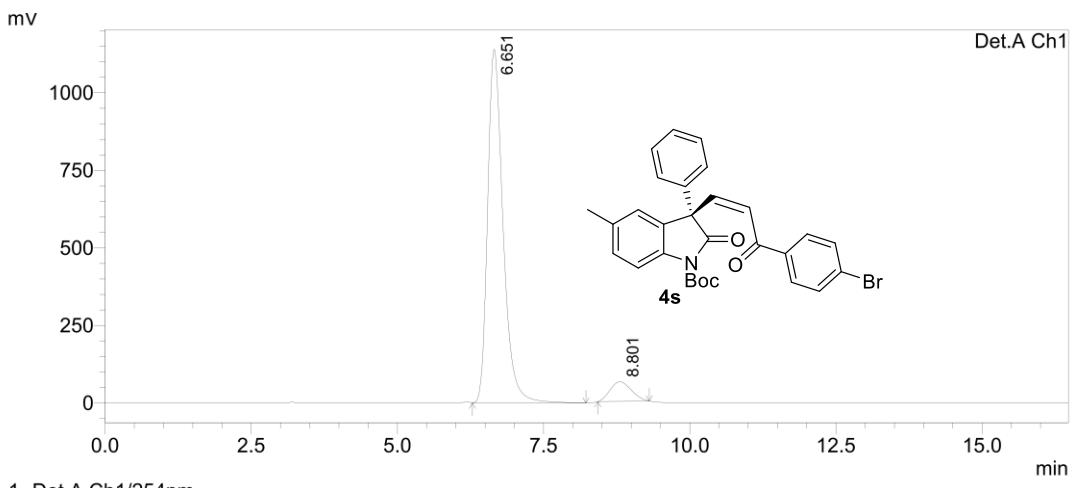


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.619	1426244	79346	49.569	60.688
2	8.706	1451031	51399	50.431	39.312
Total		2877274	130745	100.000	100.000

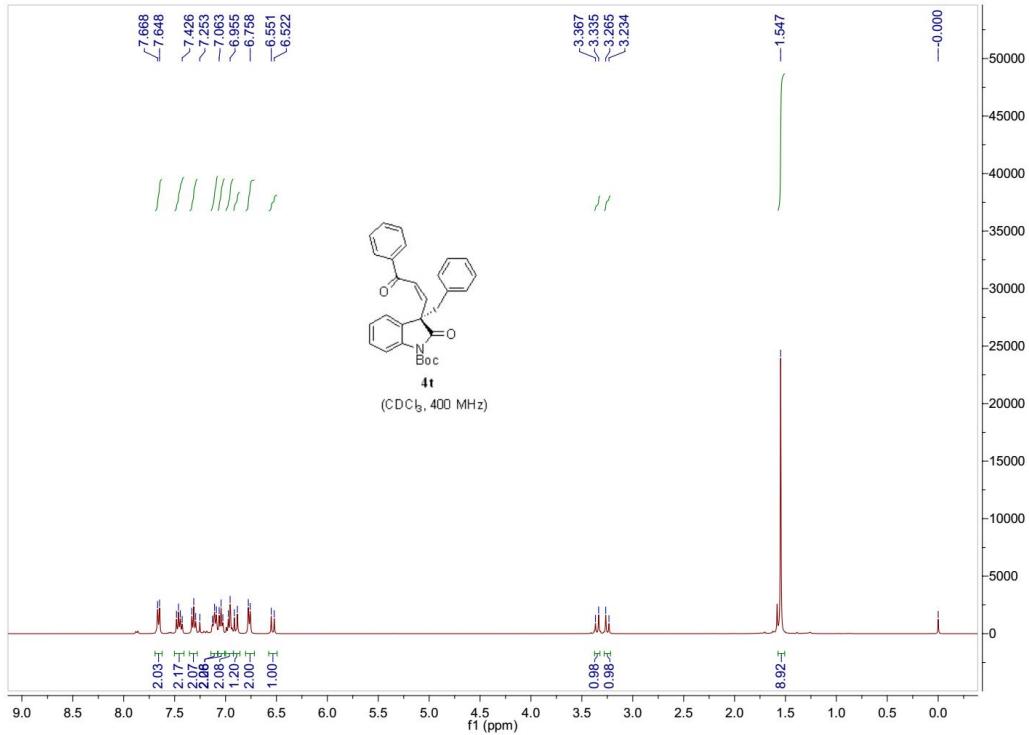


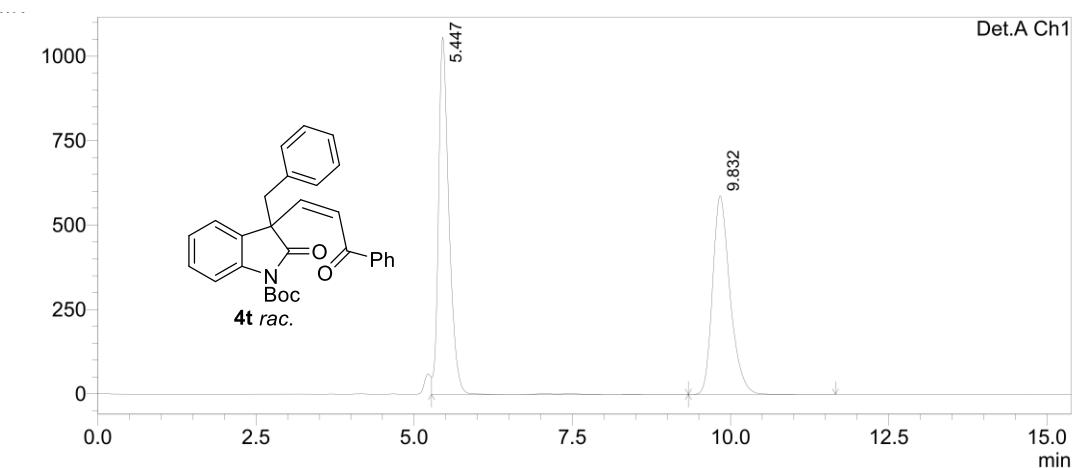
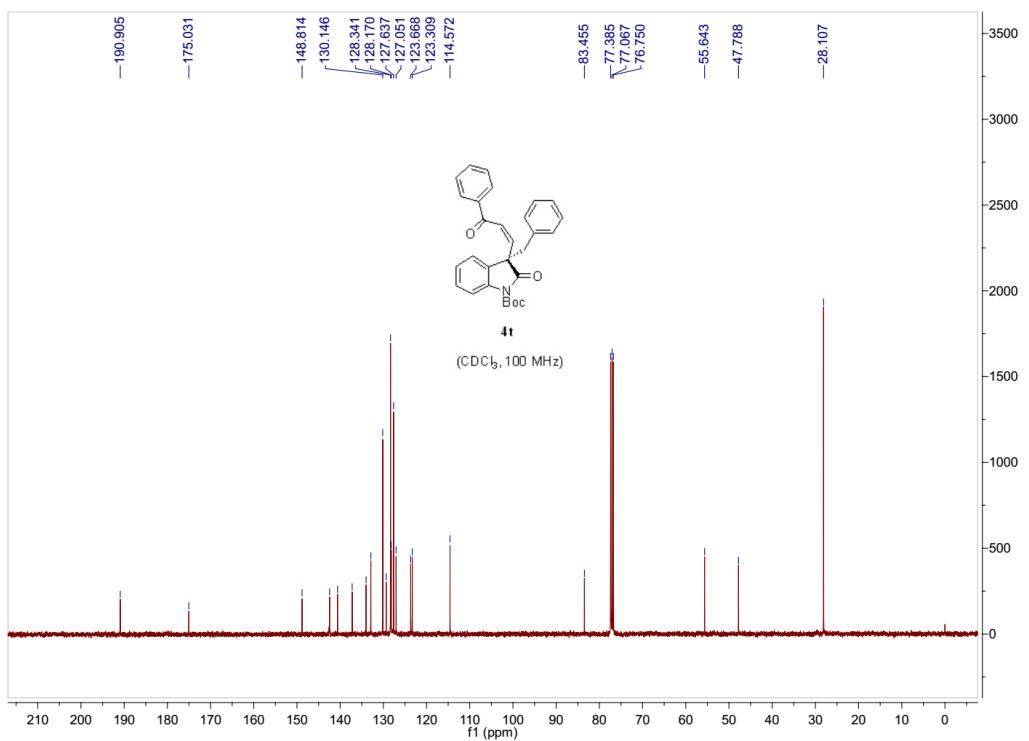
1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.651	21002793	1140236	92.958	94.743
2	8.801	1591021	63268	7.042	5.257
Total		22593814	1203504	100.000	100.000



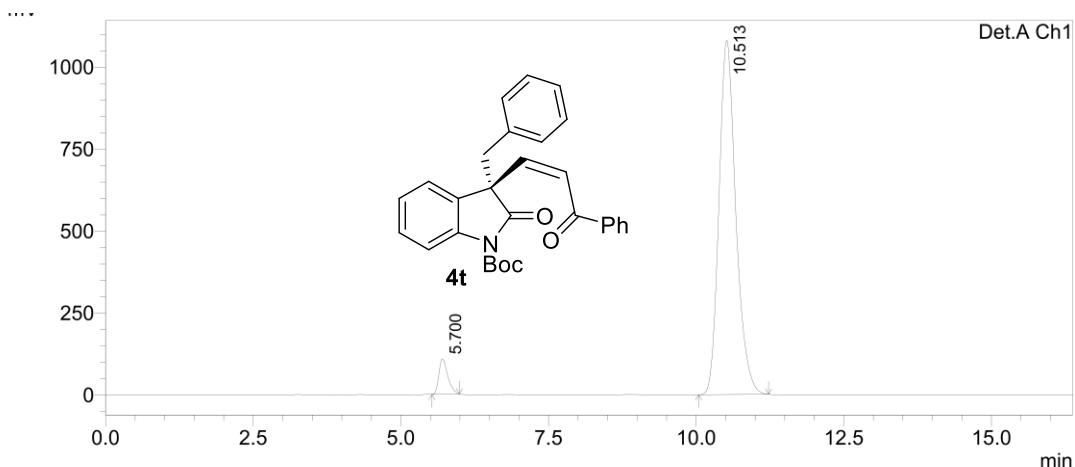


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.447	12077107	1058120	51.725	64.289
2	9.832	11271494	587757	48.275	35.711
Total		23348601	1645877	100.000	100.000

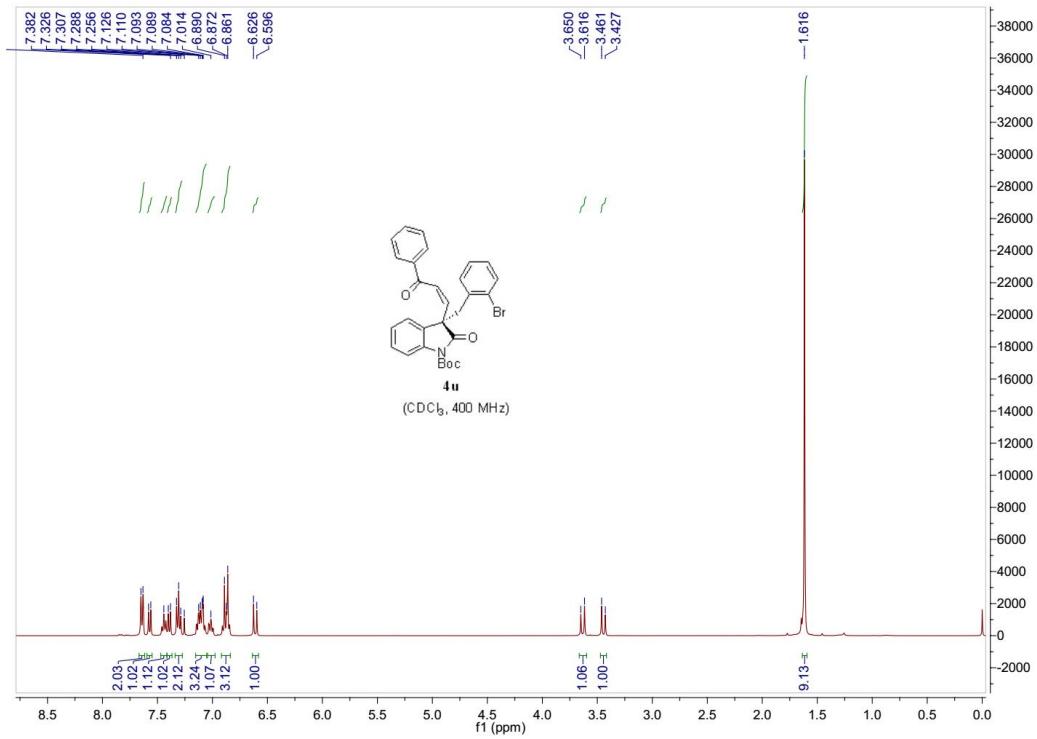


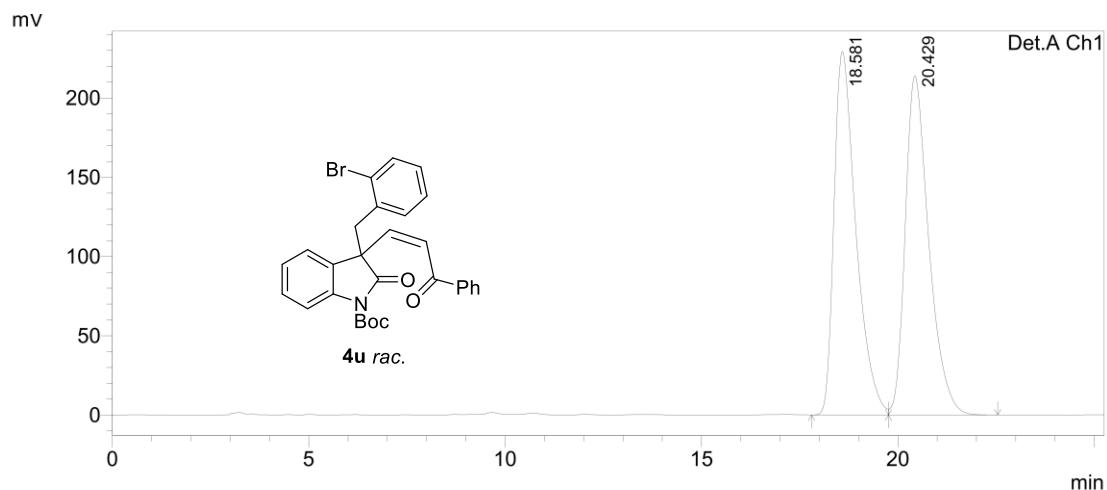
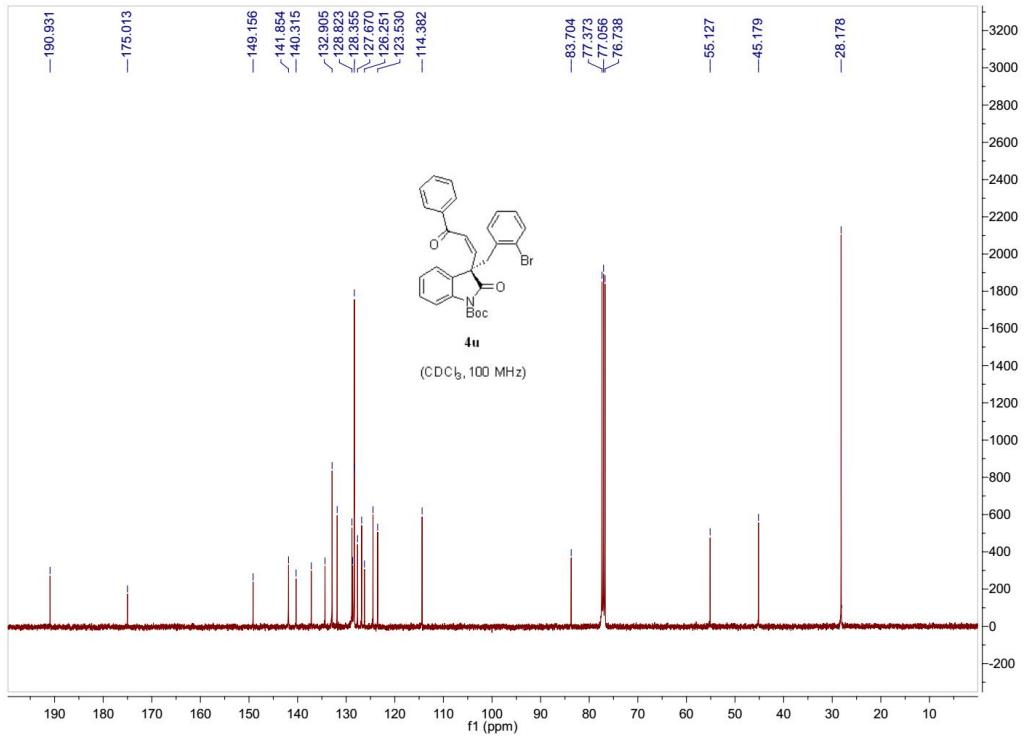
1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.700	1122470	107566	4.962	9.058
2	10.513	21496695	1080013	95.038	90.942
Total		22619165	1187579	100.000	100.000



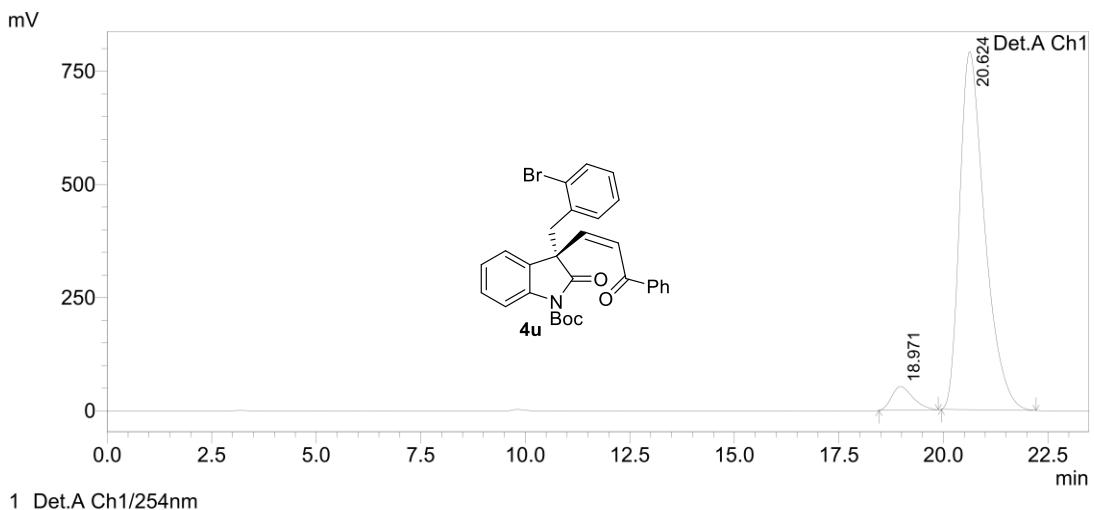


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

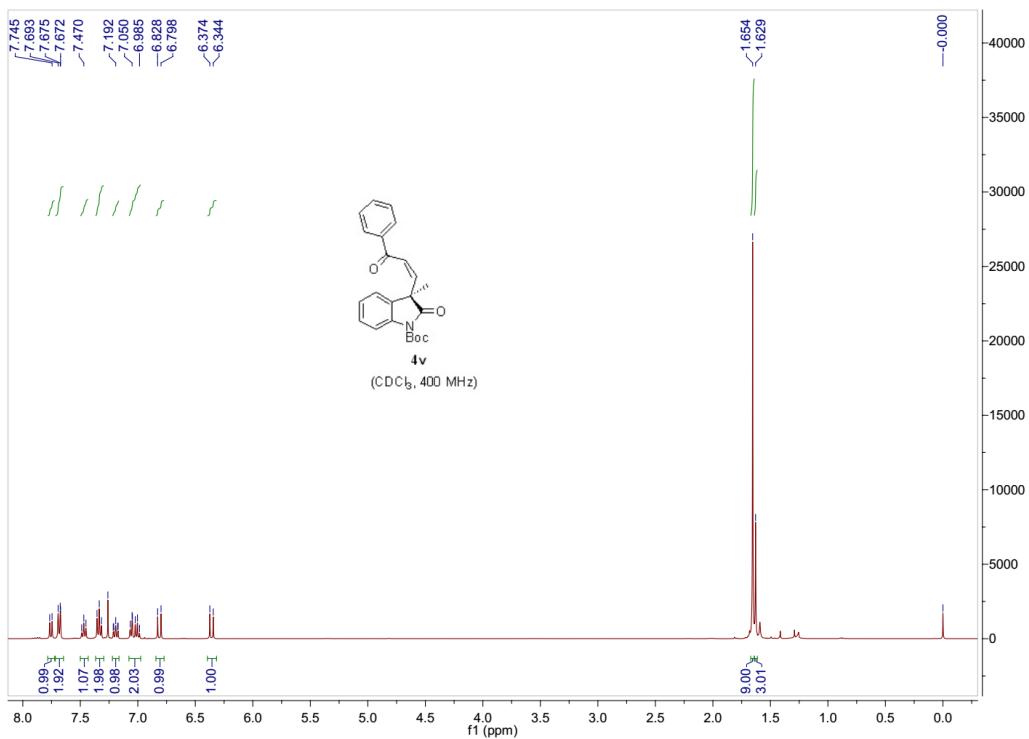
Peak#	Ret. Time	Area	Height	Area %	Height %
1	18.581	8914368	229405	49.884	51.740
2	20.429	8955859	213977	50.116	48.260
Total		17870227	443383	100.000	100.000

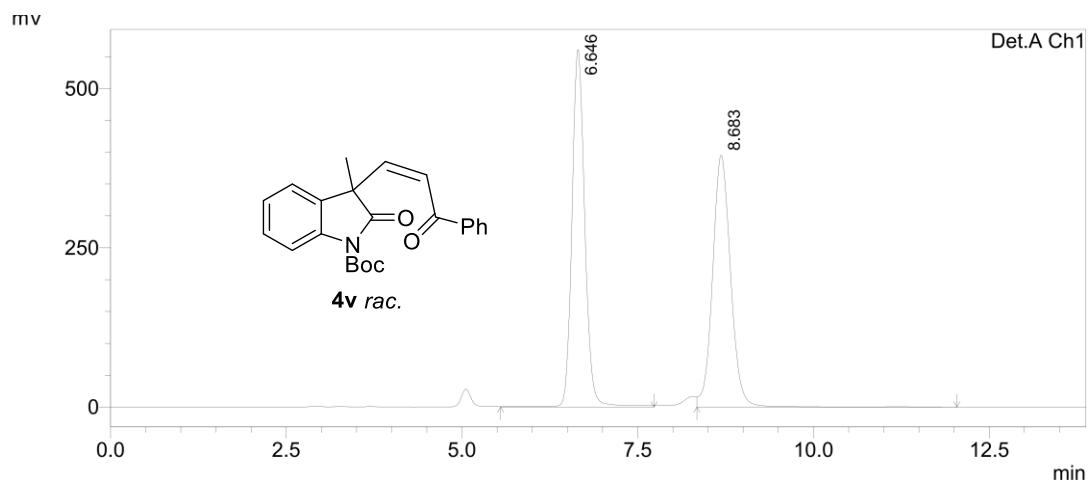
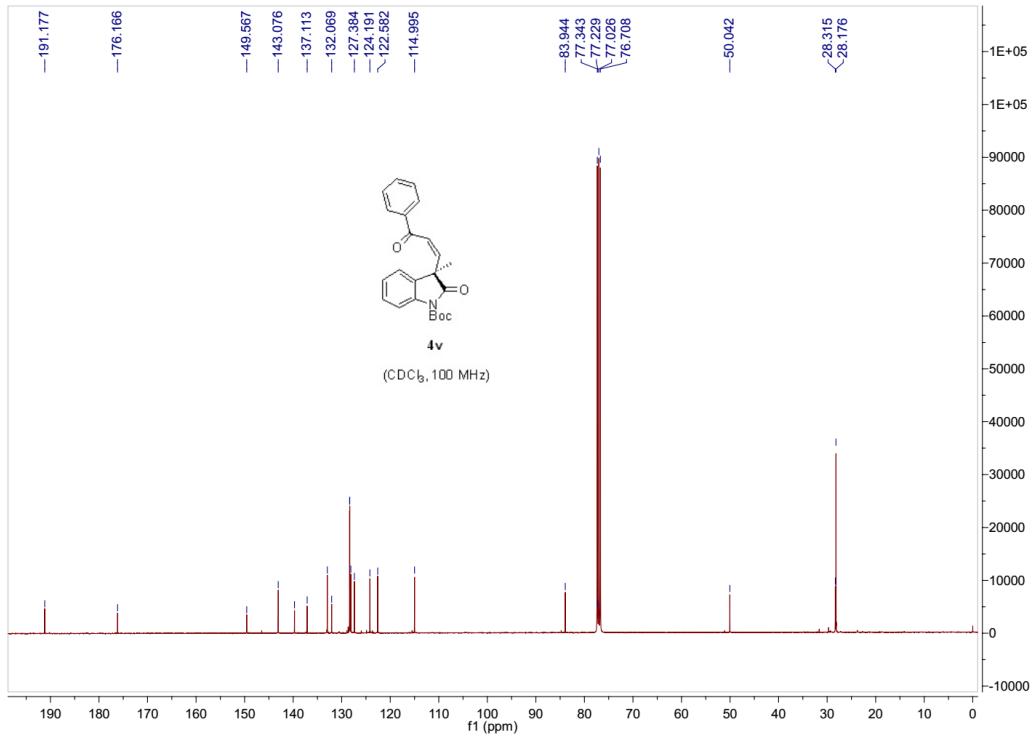


PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	18.971	1844448	52204	5.297	6.193
2	20.624	32977666	790729	94.703	93.807
Total		34822114	842933	100.000	100.000



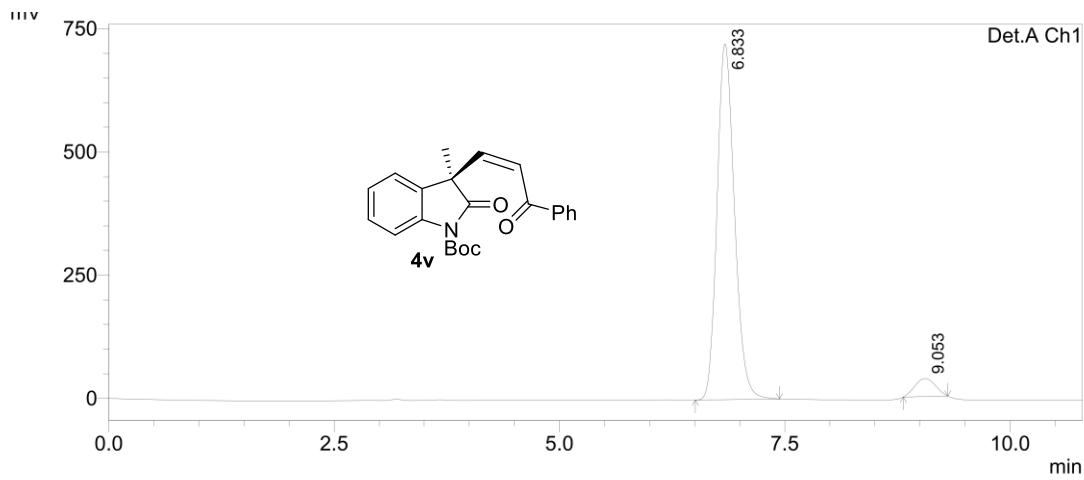


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.646	7157069	561504	50.411	58.680
2	8.683	7040317	395390	49.589	41.320
Total		14197386	956894	100.000	100.000

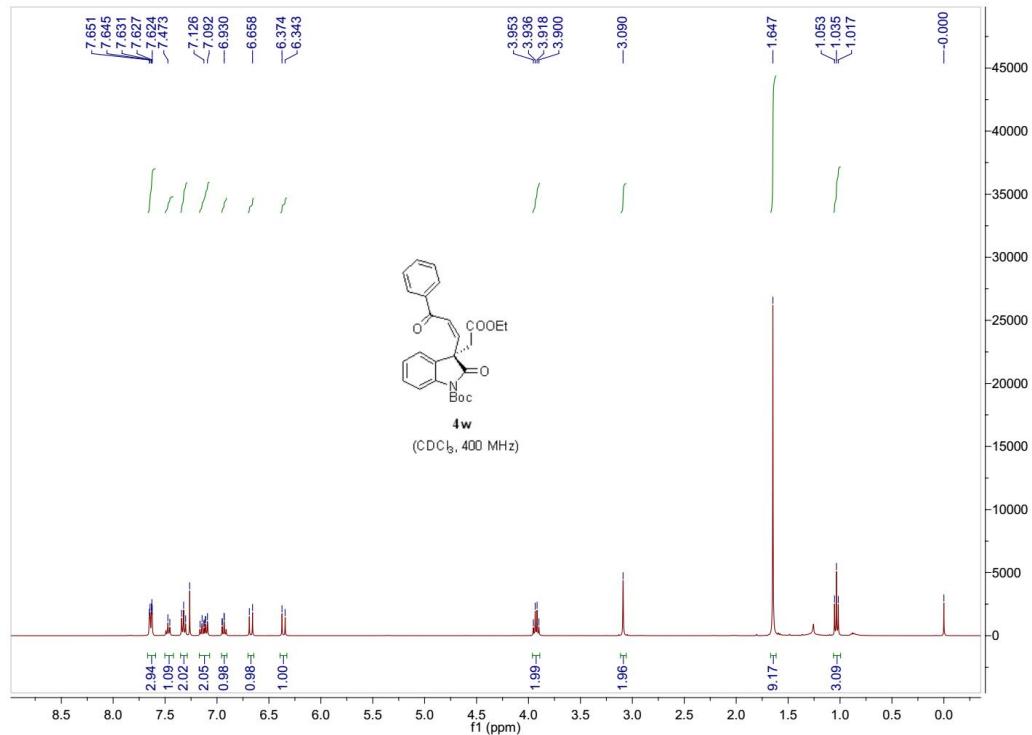


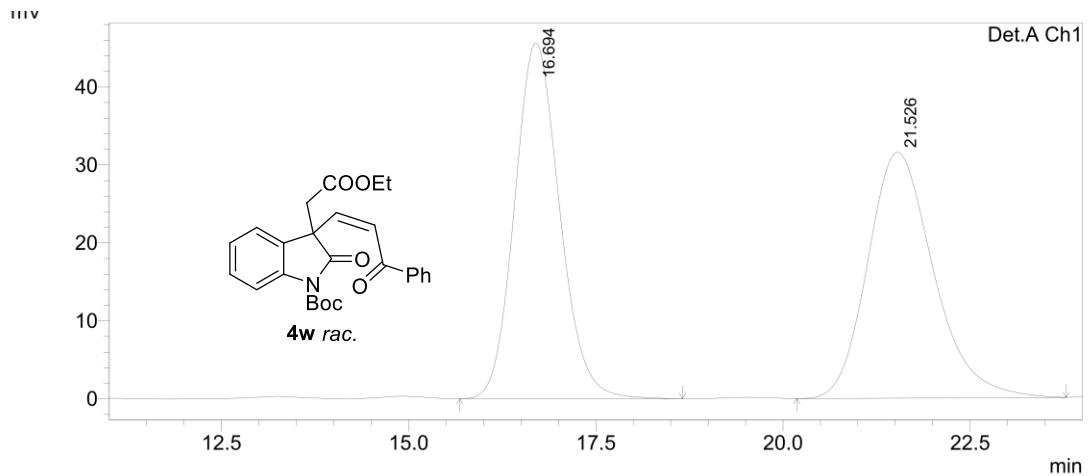
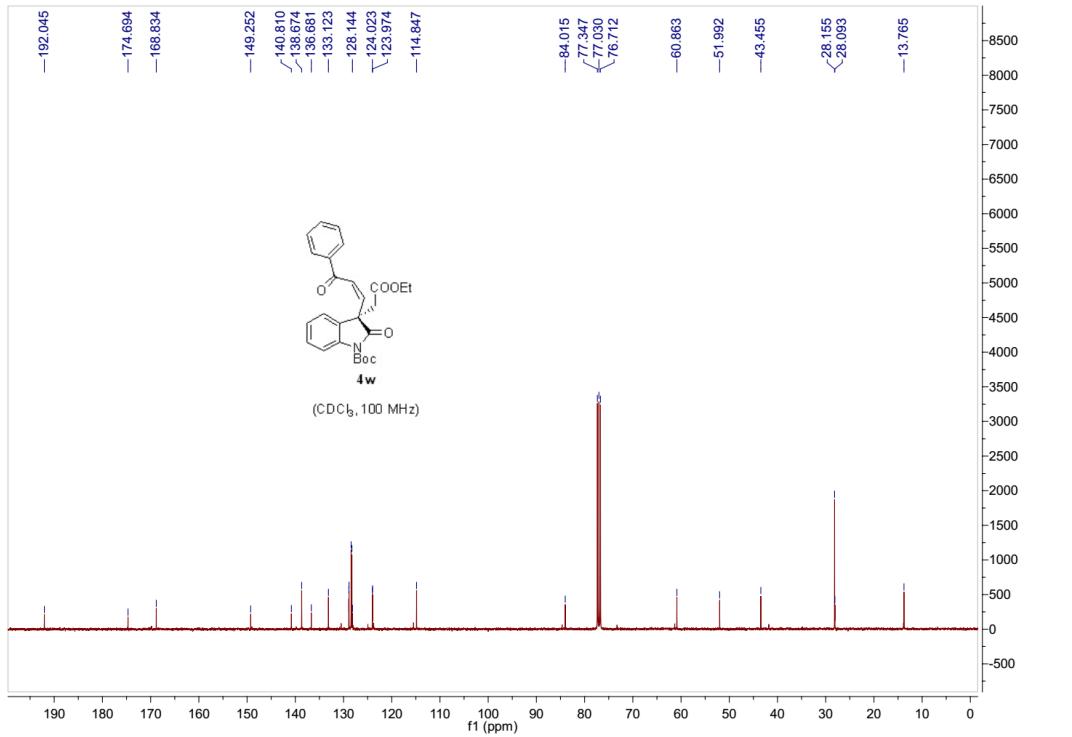
1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.833	9710152	721360	94.350	95.168
2	9.053	581523	36629	5.650	4.832
Total		10291675	757989	100.000	100.000



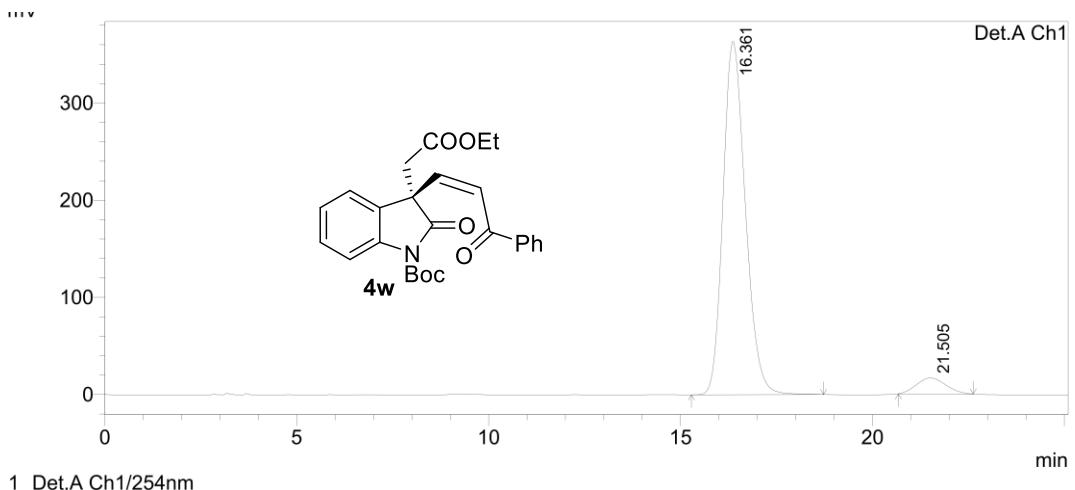


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

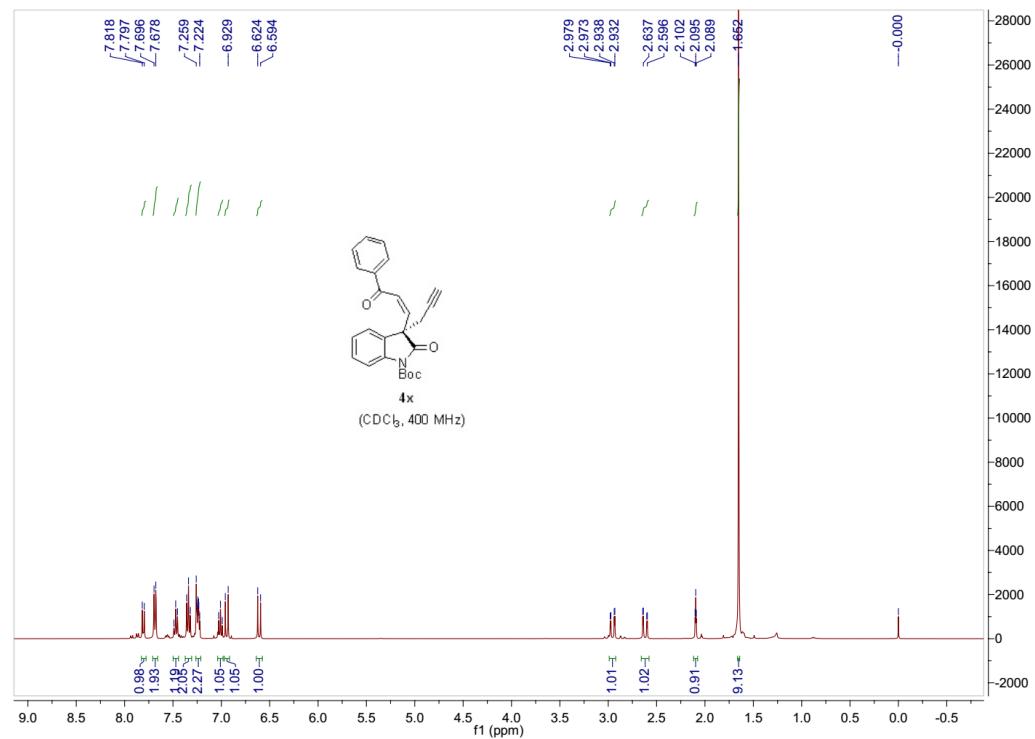
Peak#	Ret. Time	Area	Height	Area %	Height %
1	16.694	1910006	45625	49.729	59.129
2	21.526	1930814	31537	50.271	40.871
Total		3840820	77162	100.000	100.000

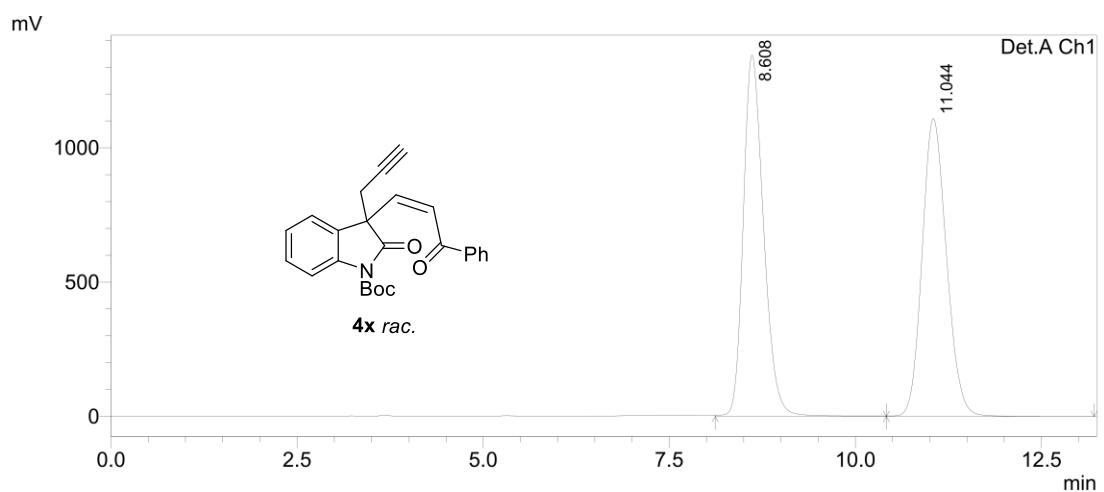
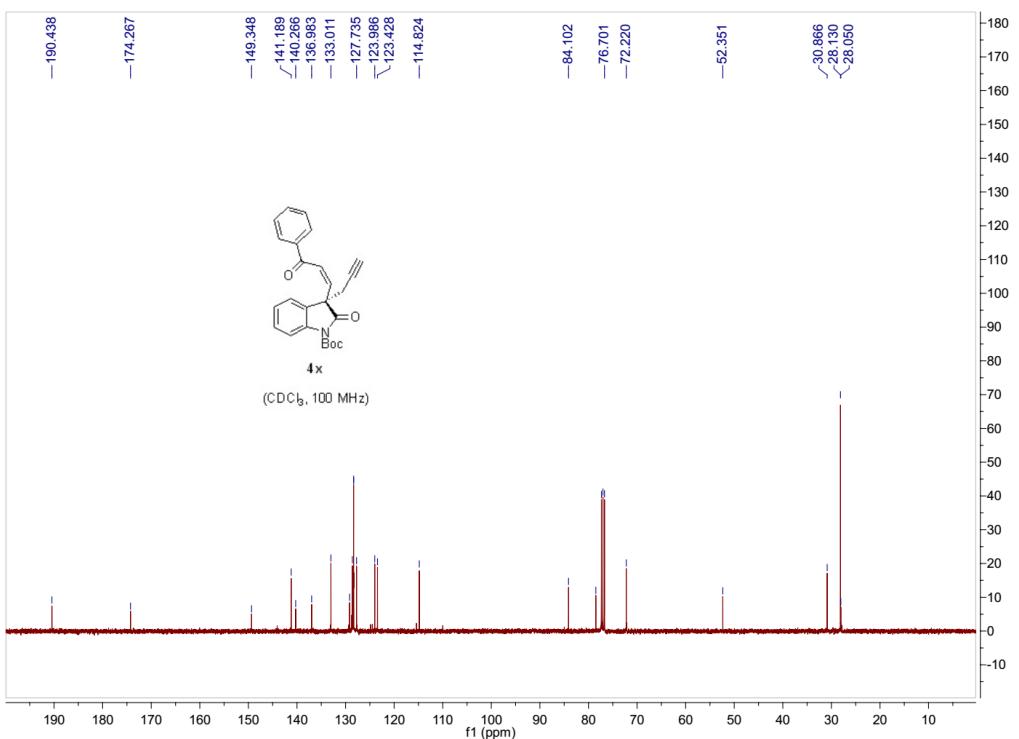


PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	16.361	14715594	363669	94.396	95.685
2	21.505	873643	16398	5.604	4.315
Total		15589237	380067	100.000	100.000

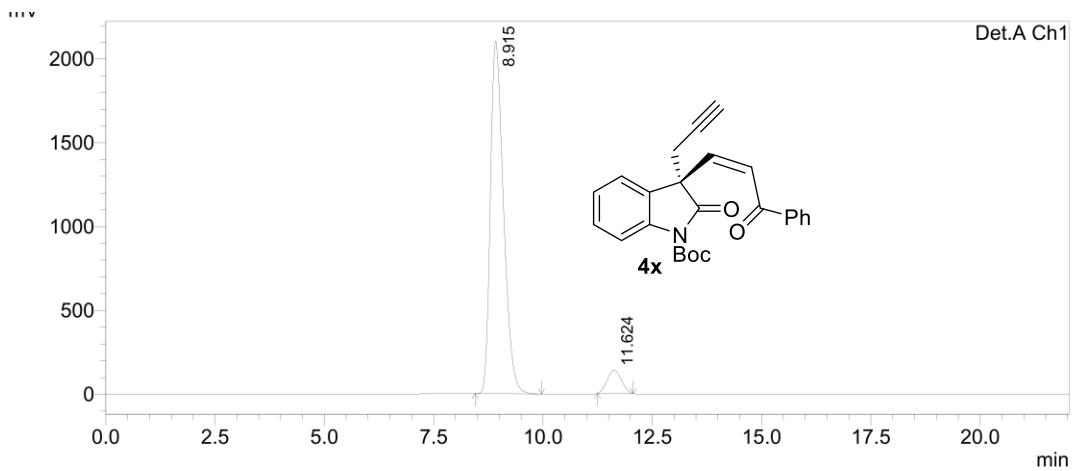




1 Det.A Ch1/254nm

PeakTable

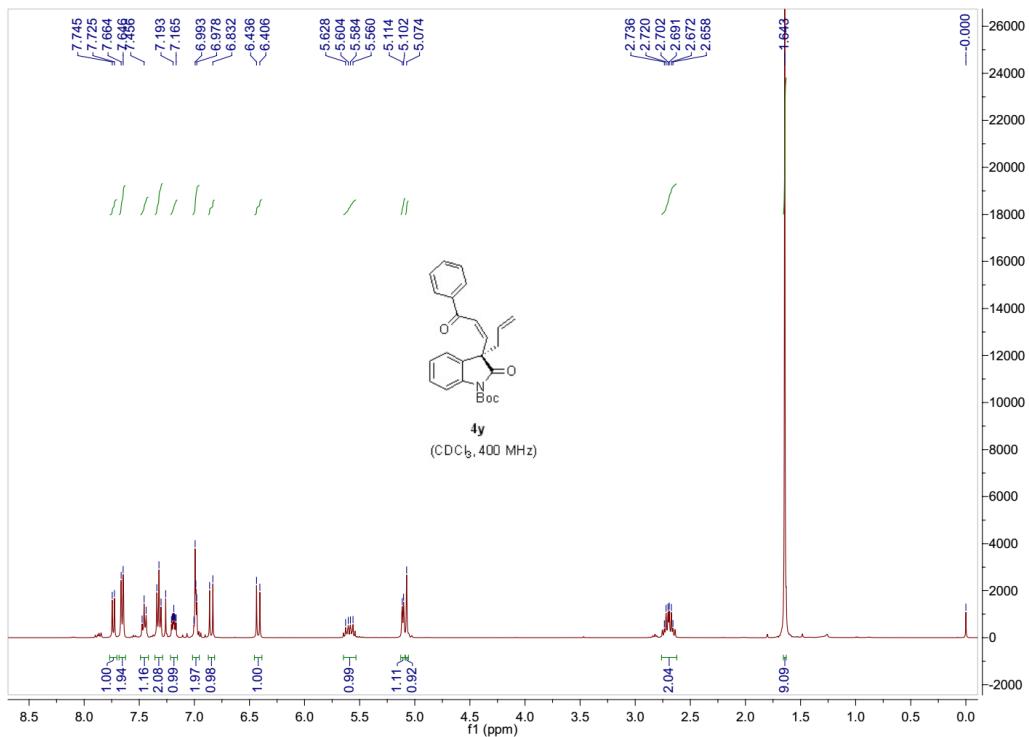
Detector A Ch1 254nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.608	25585389	1344161	50.317	54.790
2	11.044	25263408	1109152	49.683	45.210
Total		50848797	2453313	100.000	100.000

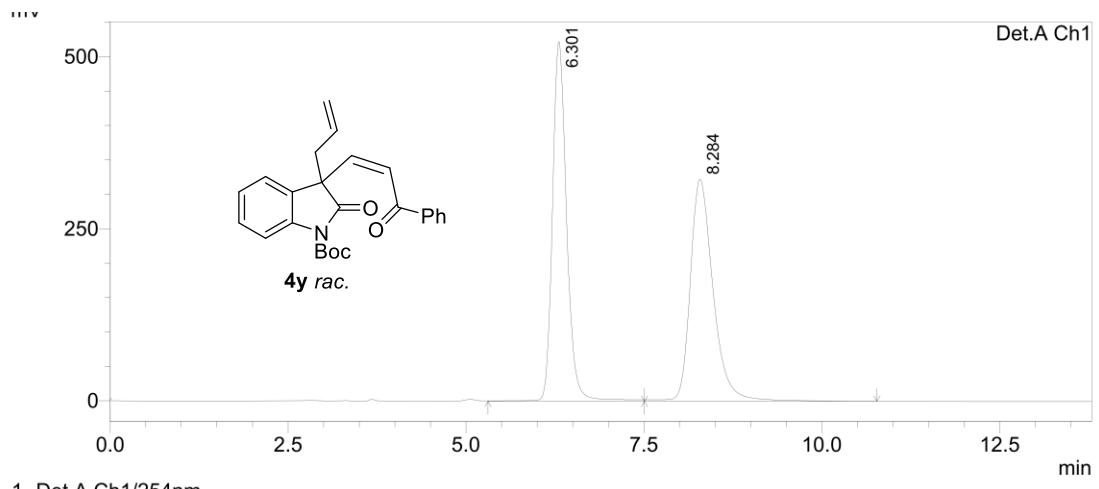
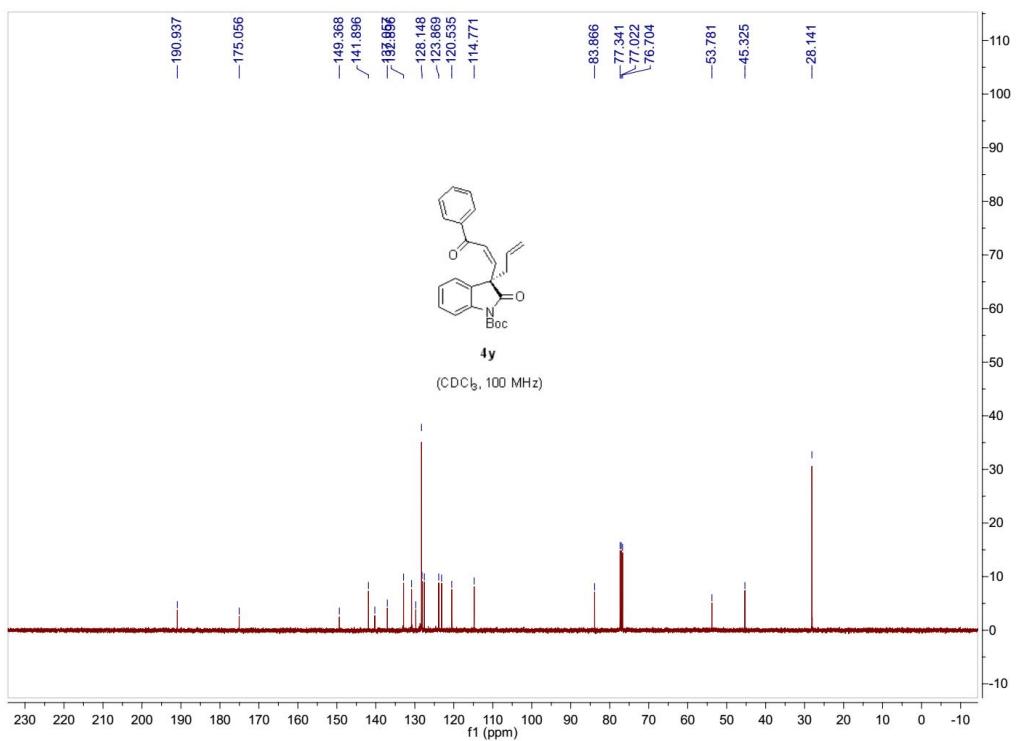


PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.915	43961273	2102039	93.385	93.828
2	11.624	3113966	138265	6.615	6.172
Total		47075238	2240305	100.000	100.000



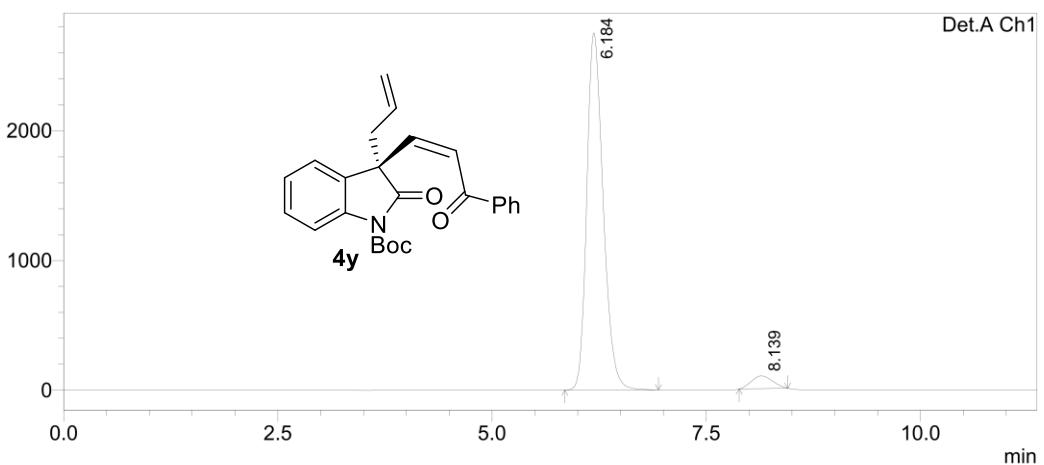


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

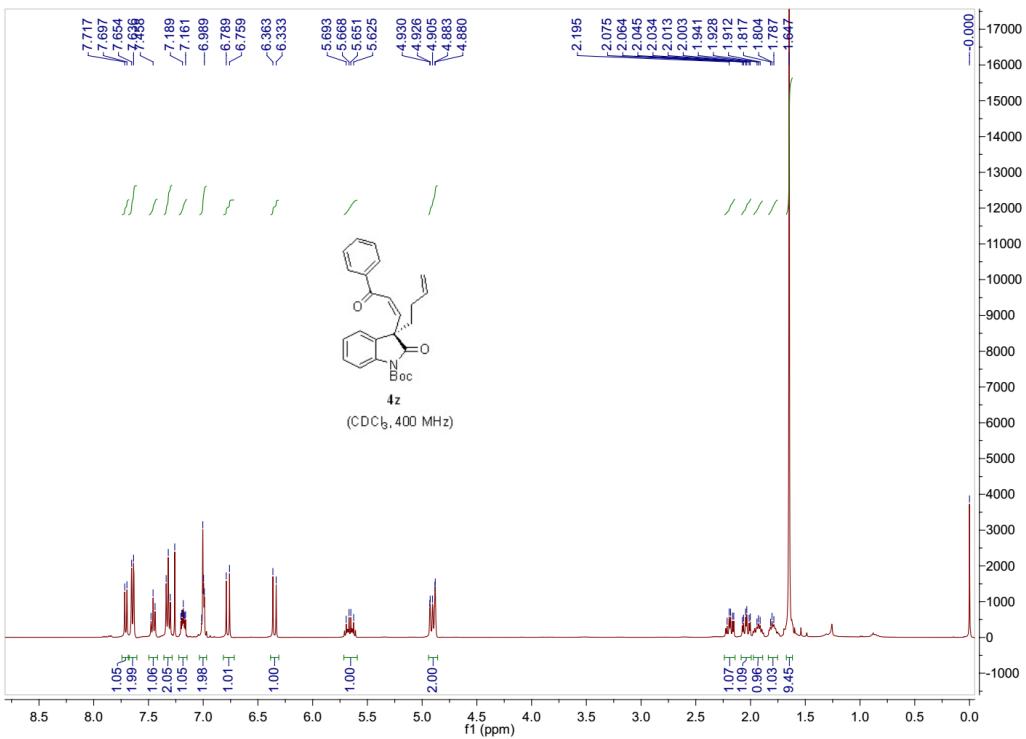
Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.301	7253988	522351	50.037	61.810
2	8.284	7243159	322736	49.963	38.190
Total		14497146	845087	100.000	100.000

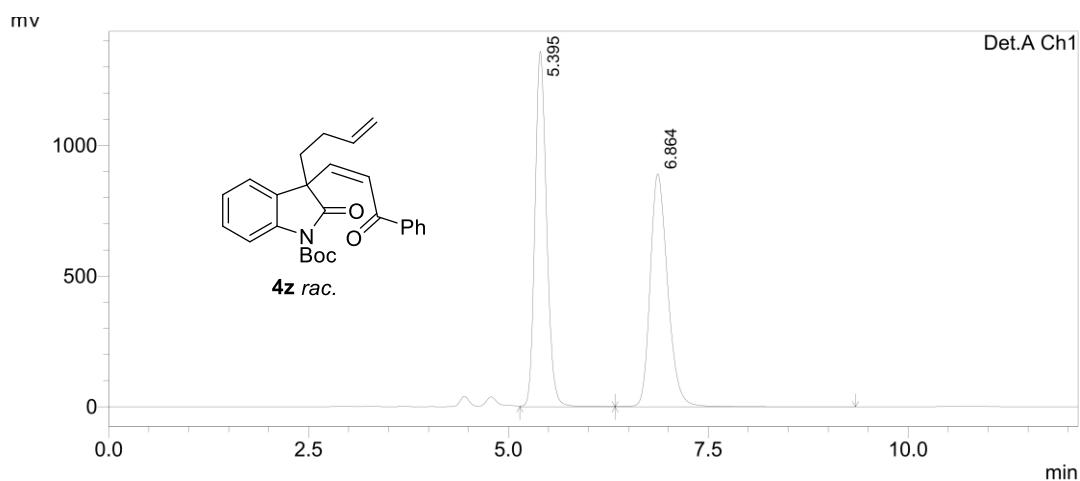
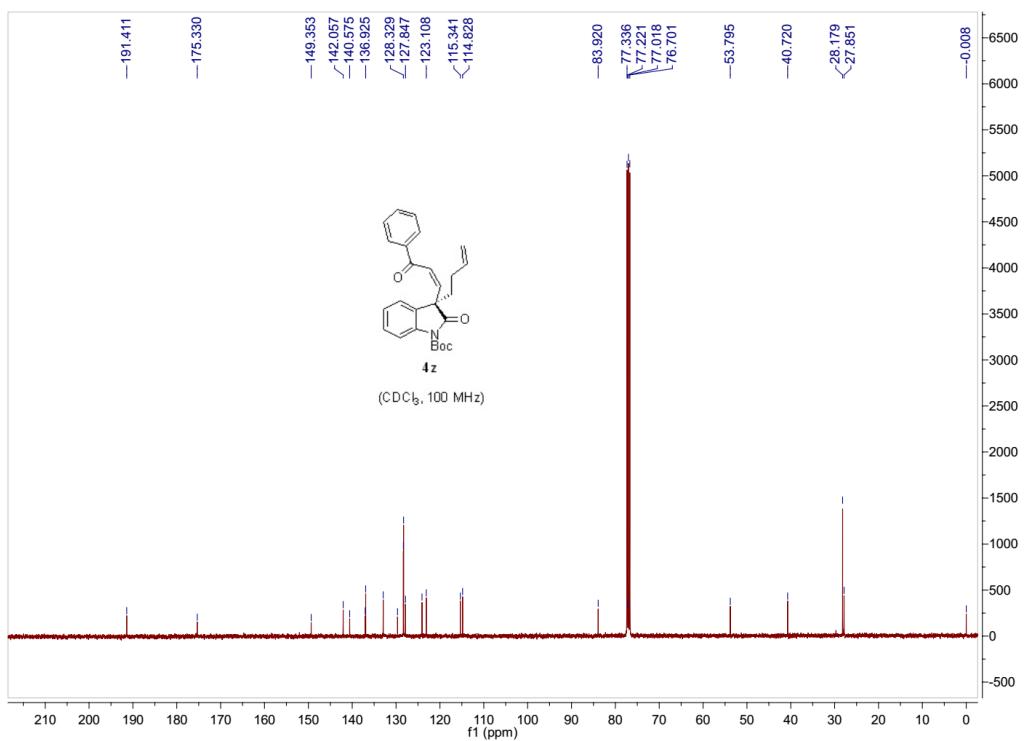


PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.184	36672089	2750143	95.603	96.566
2	8.139	1686823	97799	4.397	3.434
Total		38358913	2847942	100.000	100.000



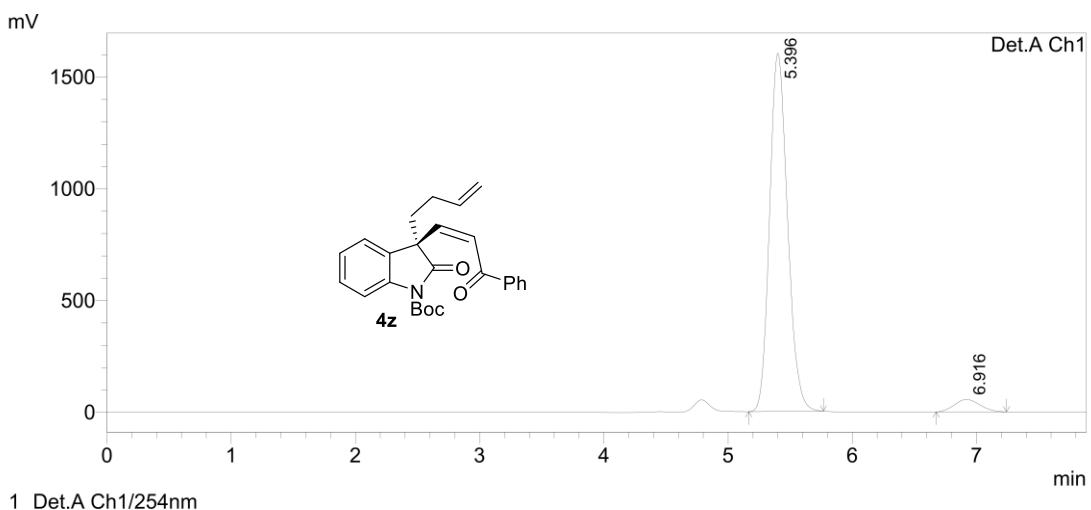


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

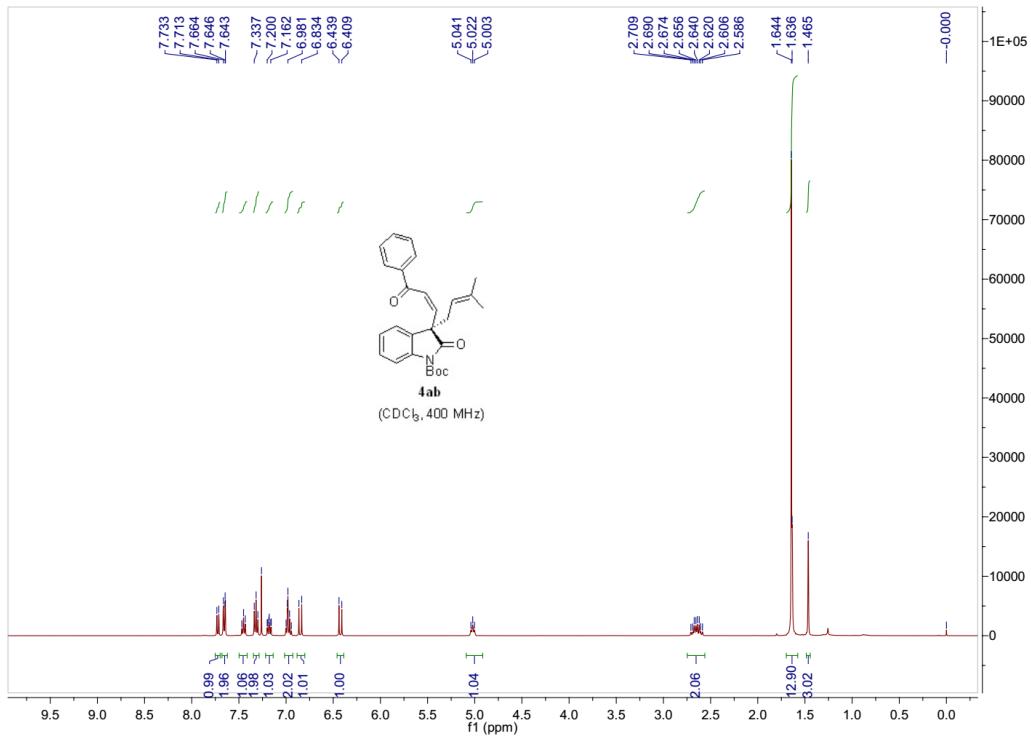
Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.395	13772926	1360370	50.332	60.403
2	6.864	13591364	891804	49.668	39.597
Total		27364290	2252174	100.000	100.000

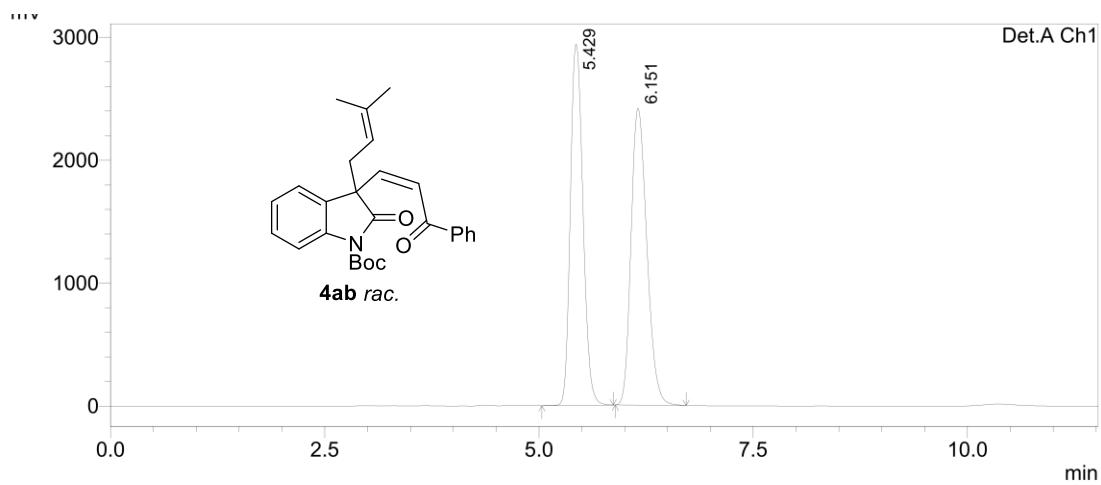
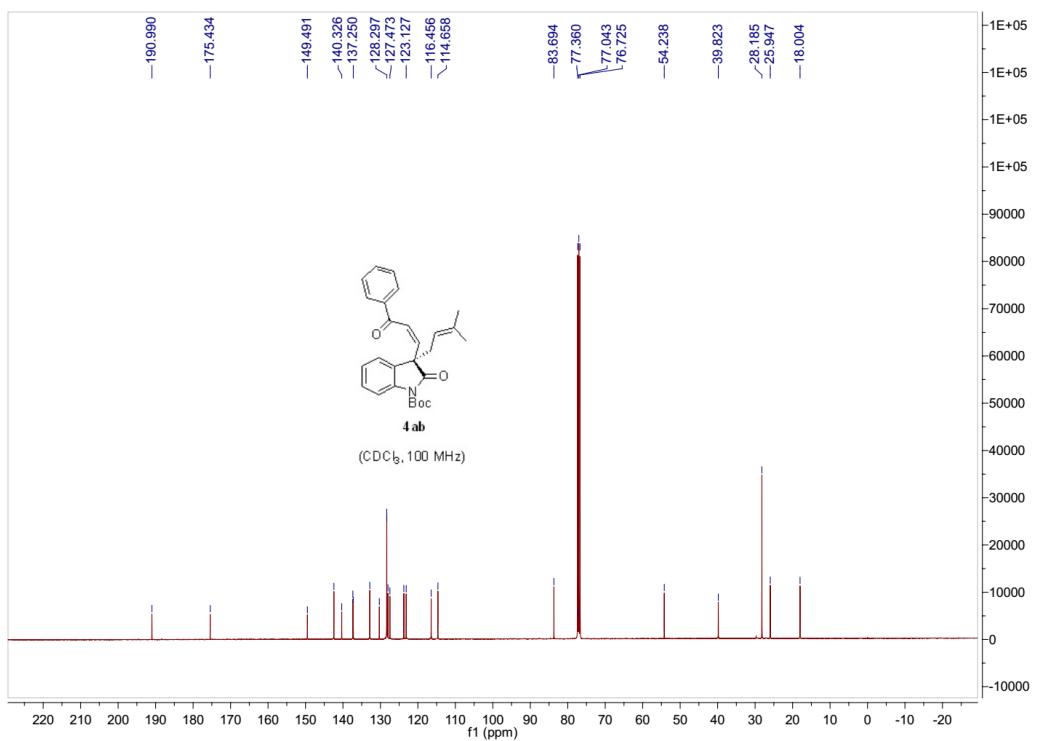


PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.396	16135794	1603273	95.300	96.663
2	6.916	795850	55357	4.700	3.337
Total		16931644	1658629	100.000	100.000

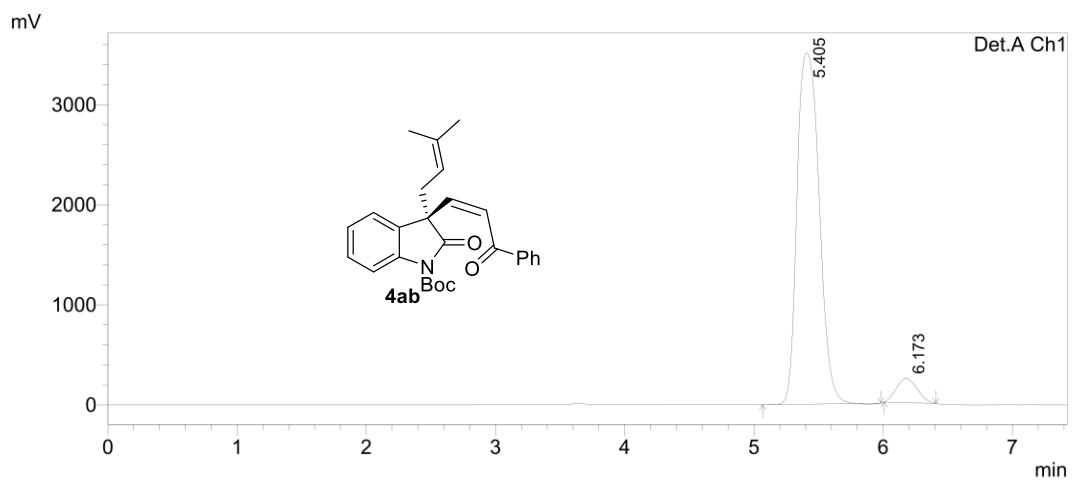




PeakTable

Detector A Ch1 254nm

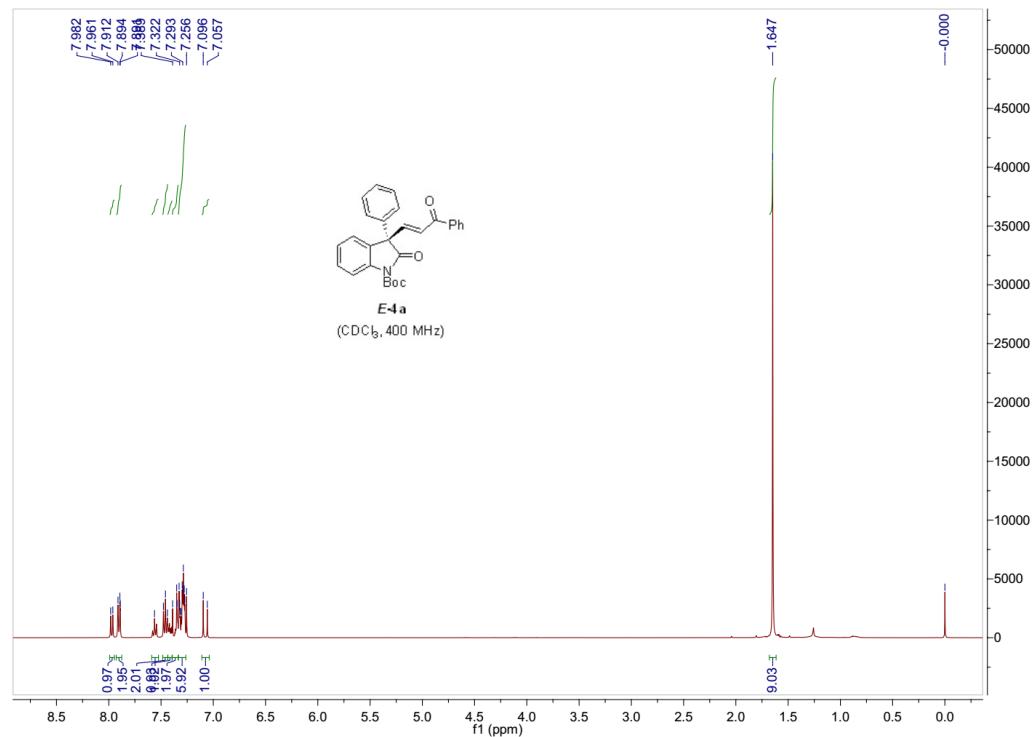
Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.429	30078940	2940142	49.196	54.902
2	6.151	31061873	2415107	50.804	45.098
Total		61140813	5355248	100.000	100.000

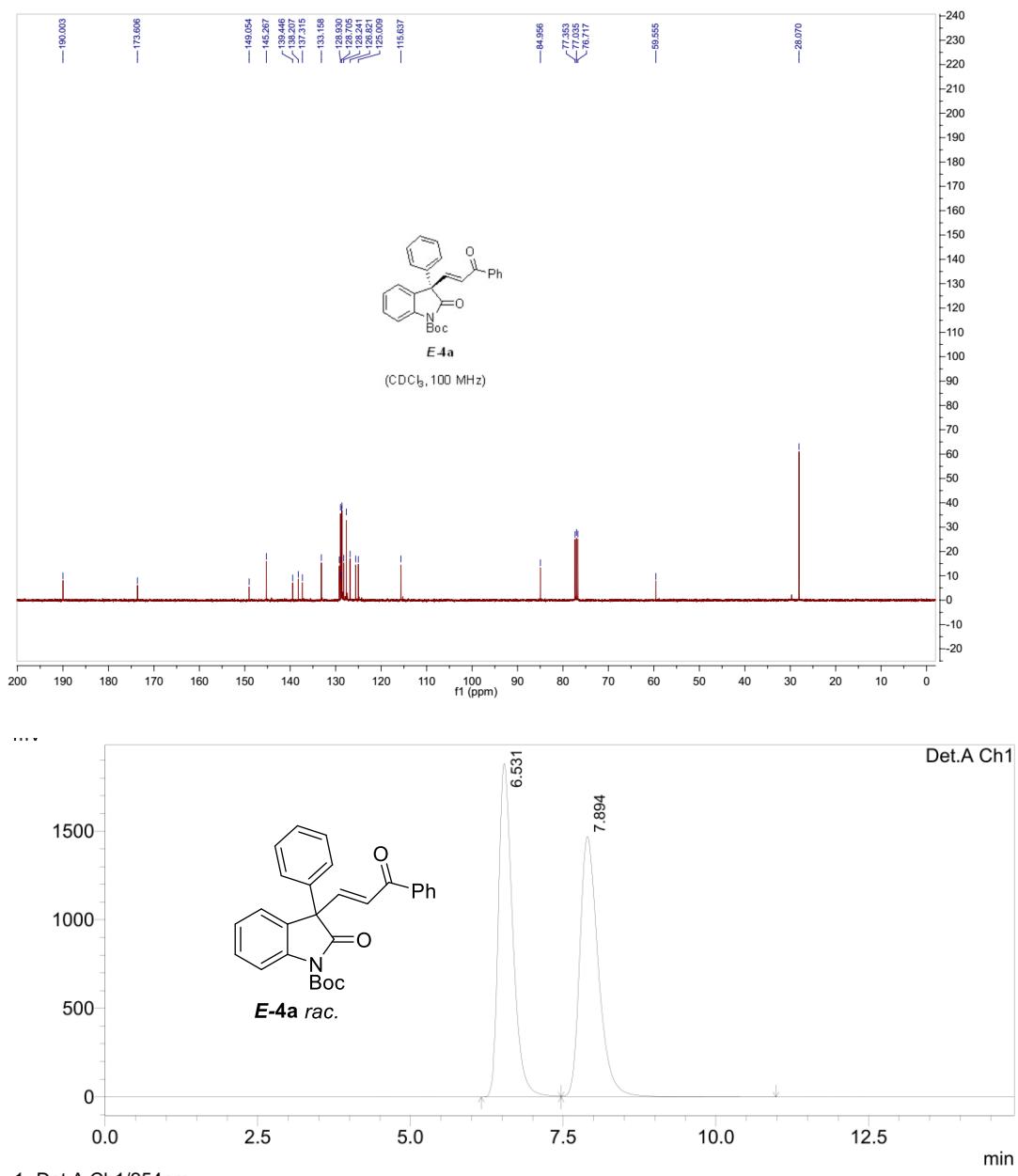


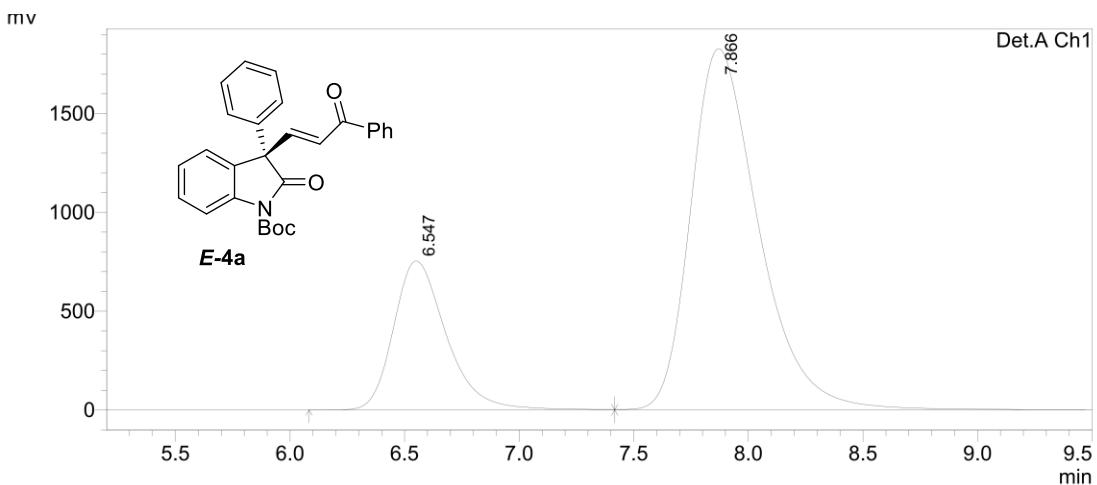
PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.405	41800662	3512064	93.909	93.570
2	6.173	2711395	241329	6.091	6.430
Total		44512057	3753392	100.000	100.000



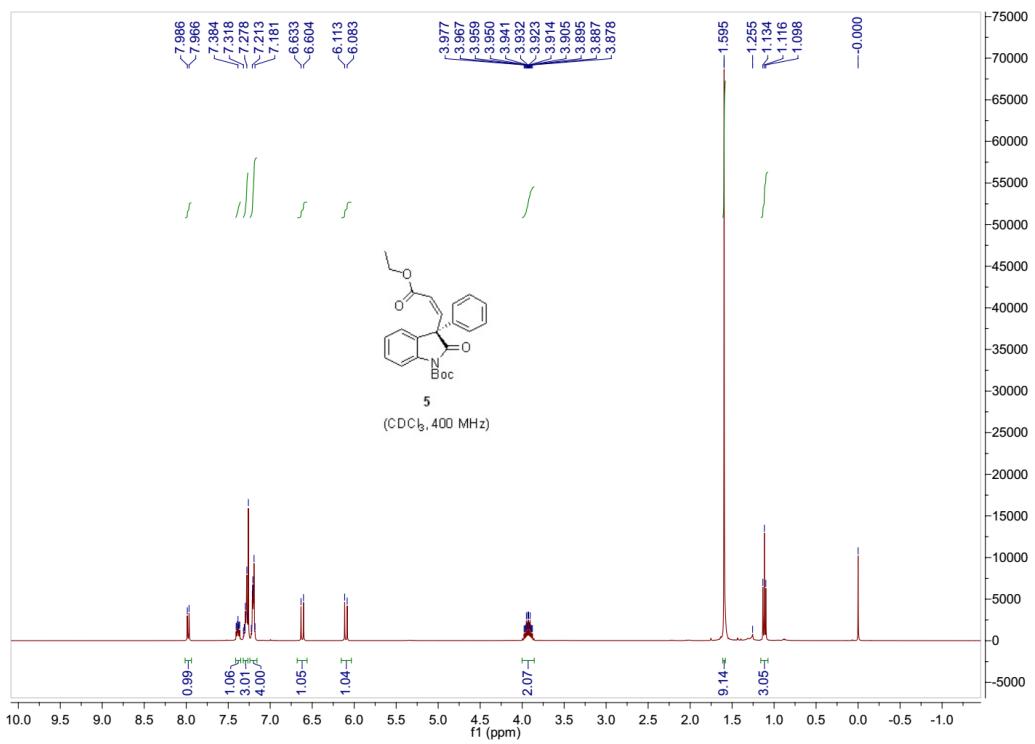


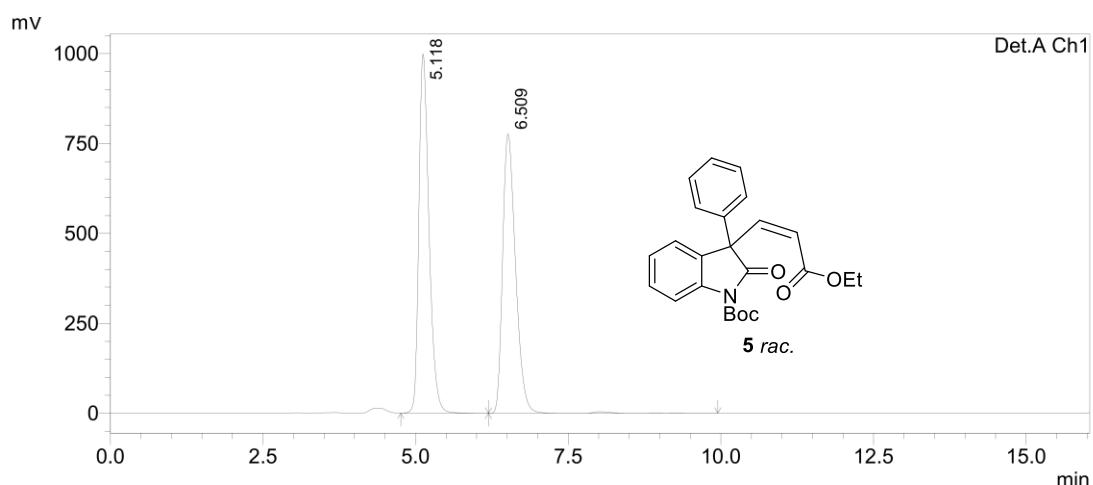
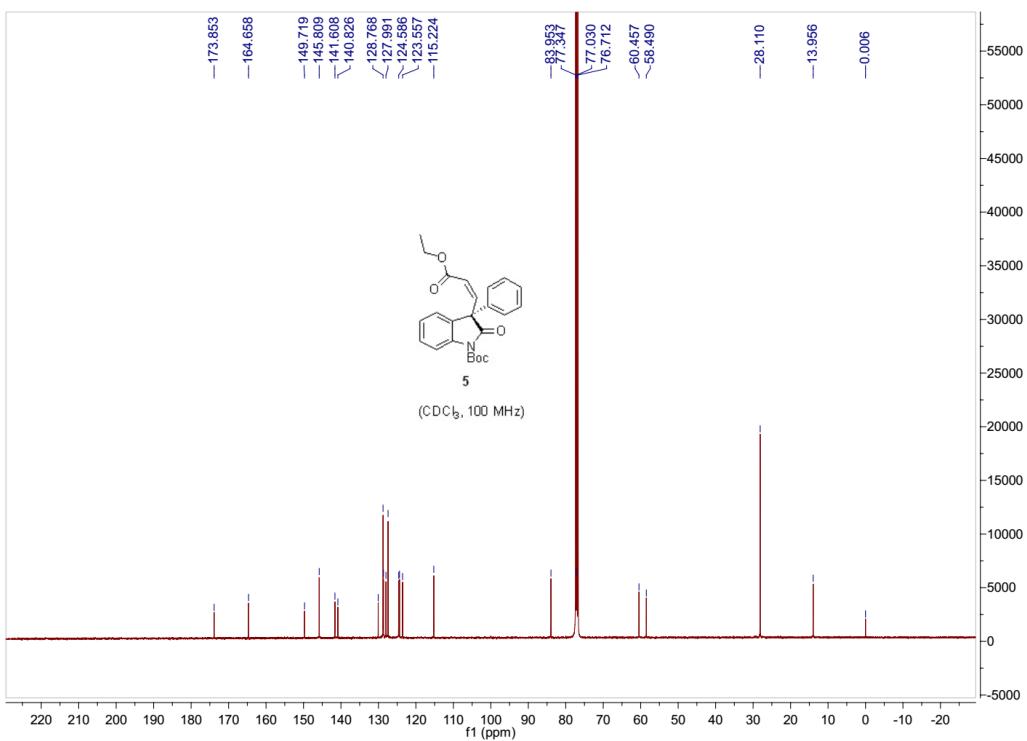


1 Det.A Ch1/254nm

PeakTable

Peak Table					
Detector A Ch1 254nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.547	12057782	753368	24.233	29.202
2	7.866	37699878	1826495	75.767	70.798
Total		49757660	2579863	100.000	100.000



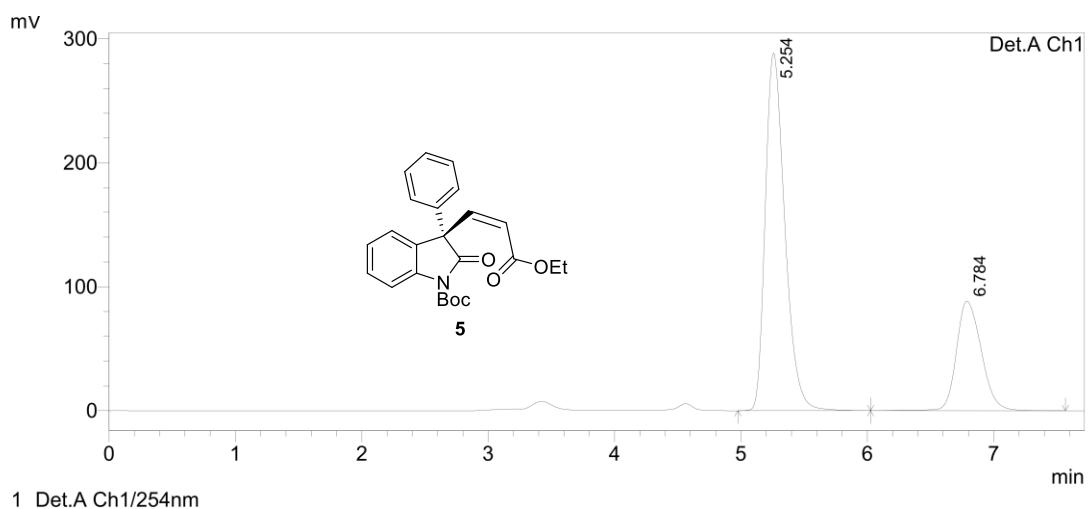


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

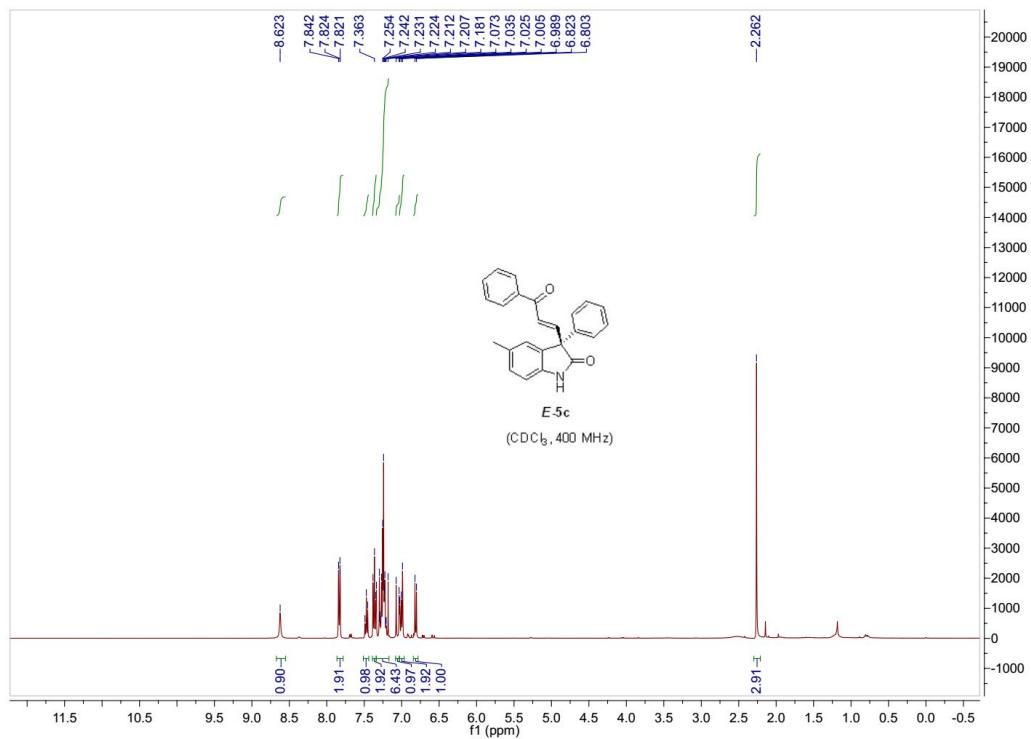
Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.118	11552349	998607	50.343	56.264
2	6.509	11394867	776246	49.657	43.736
Total		22947216	1774853	100.000	100.000

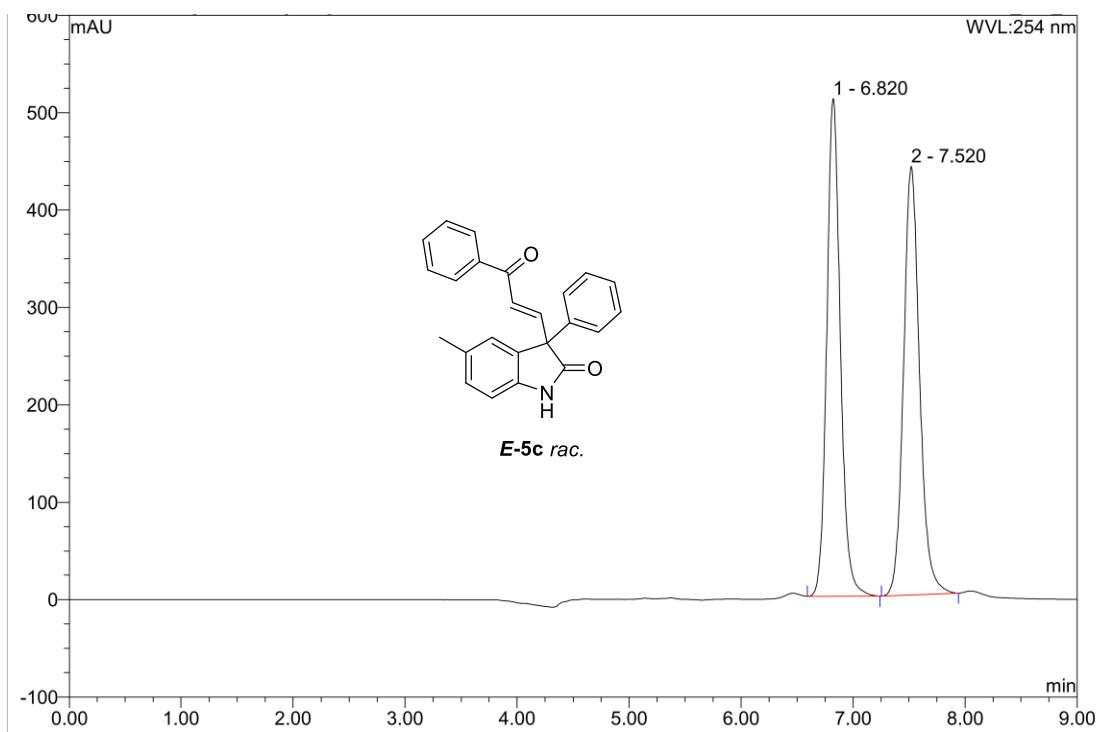
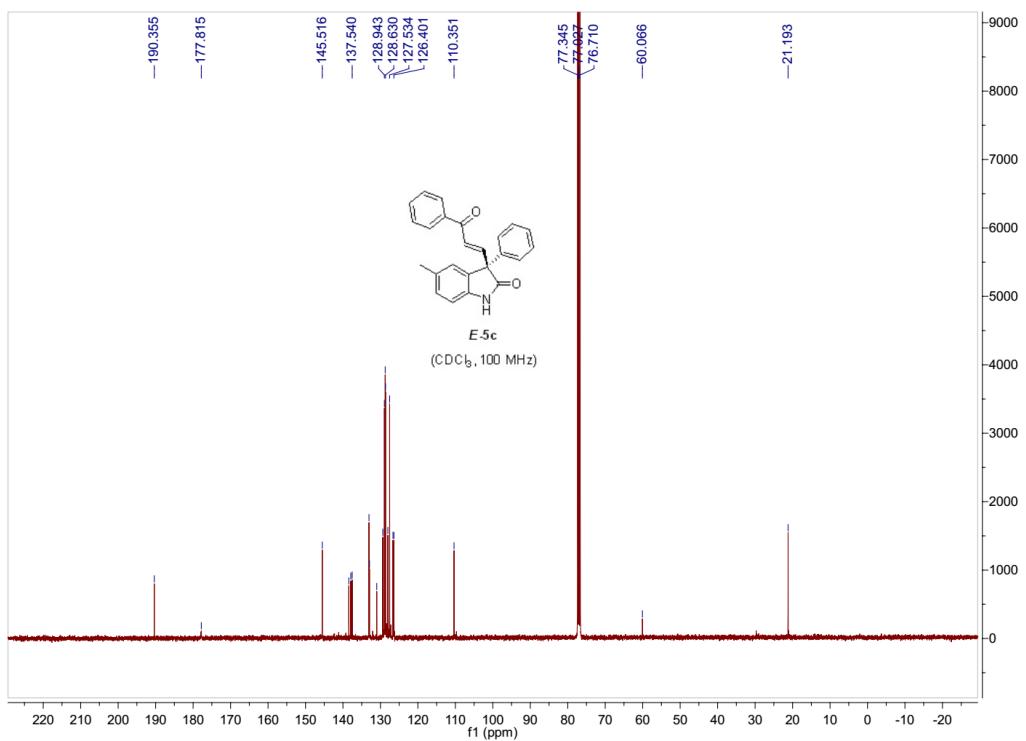


PeakTable

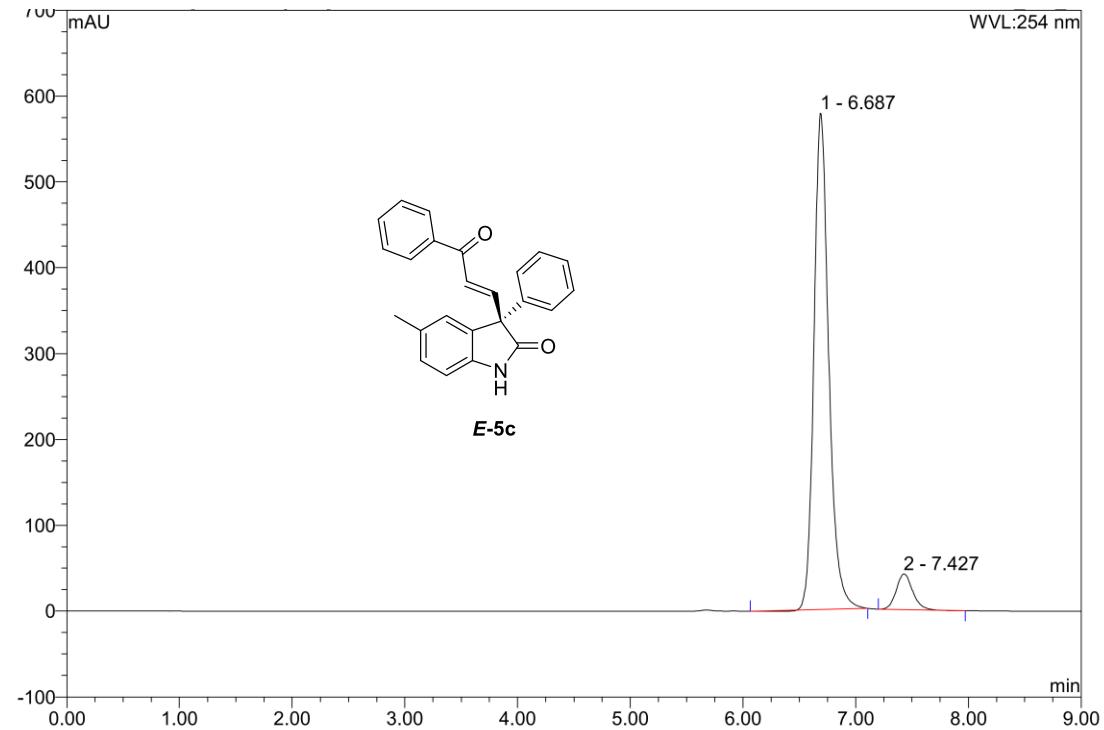
Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.254	3105509	288800	71.917	76.559
2	6.784	1212687	88426	28.083	23.441
Total		4318196	377225	100.000	100.000

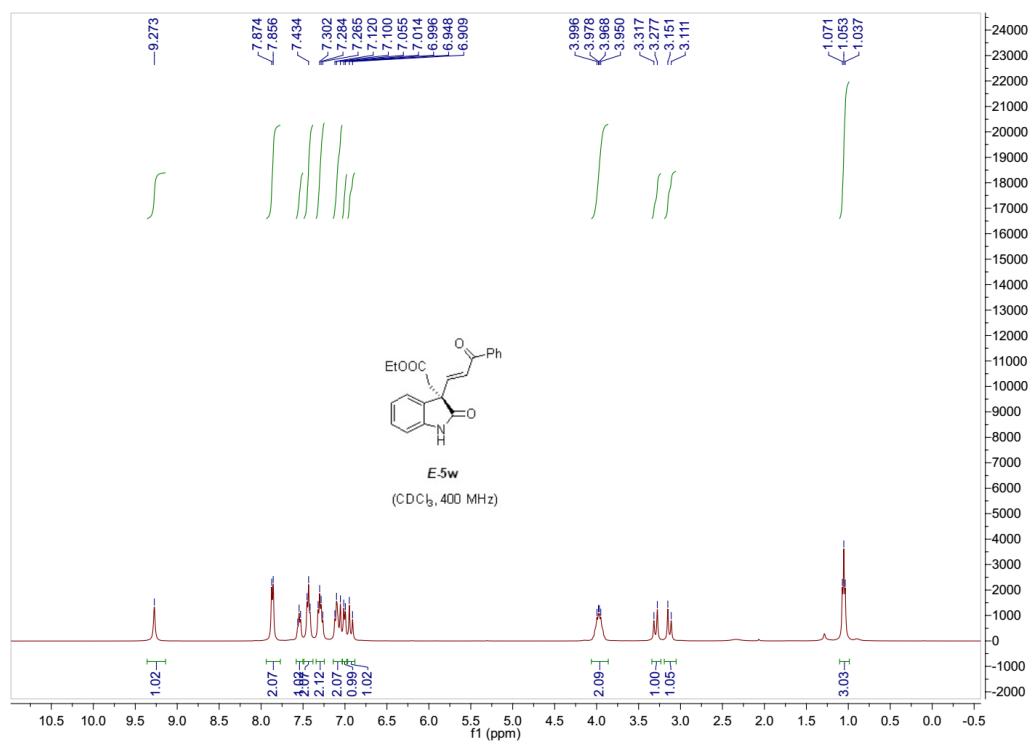


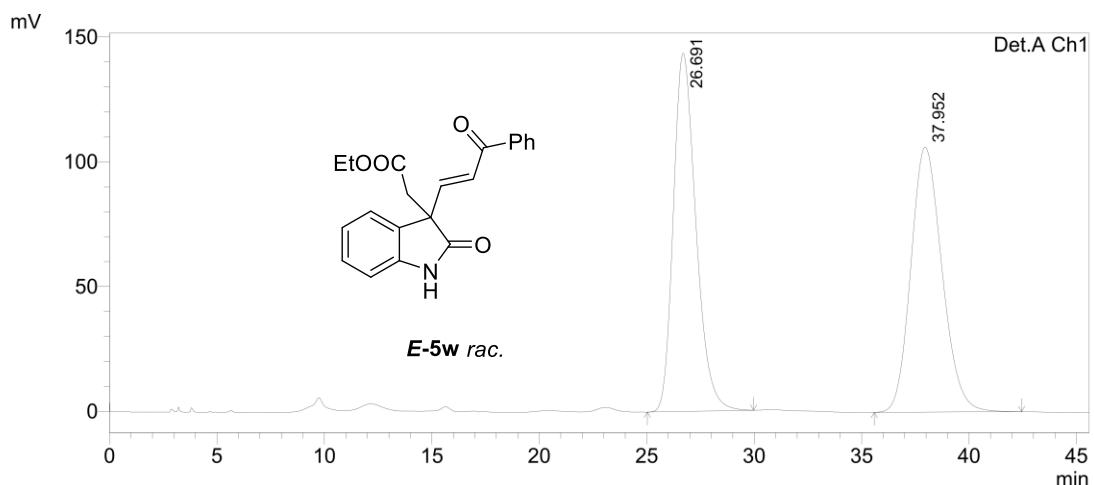
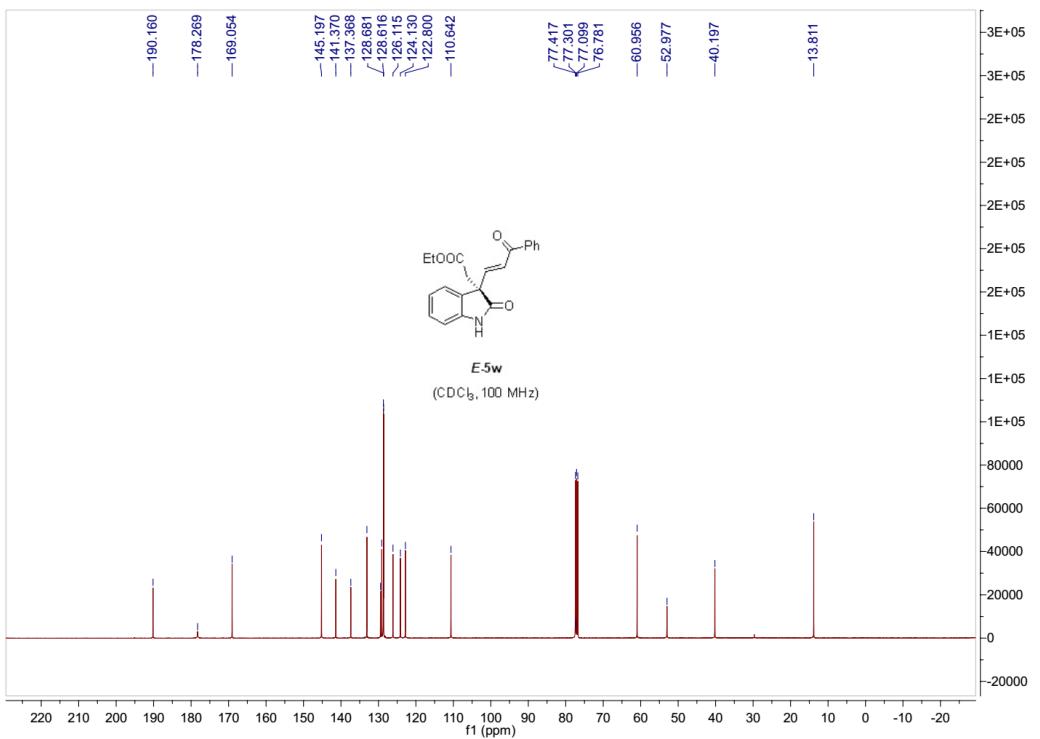


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	6.82	n.a.	511.102	71.936	49.56	n.a.	BMB
2	7.52	n.a.	440.449	73.207	50.44	n.a.	BMB
Total:			951.551	145.143	100.00	0.000	



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	6.69	n.a.	578.235	87.671	92.64	n.a.	BMB*
2	7.43	n.a.	41.614	6.966	7.36	n.a.	BMB*
Total:			619.849	94.637	100.00	0.000	



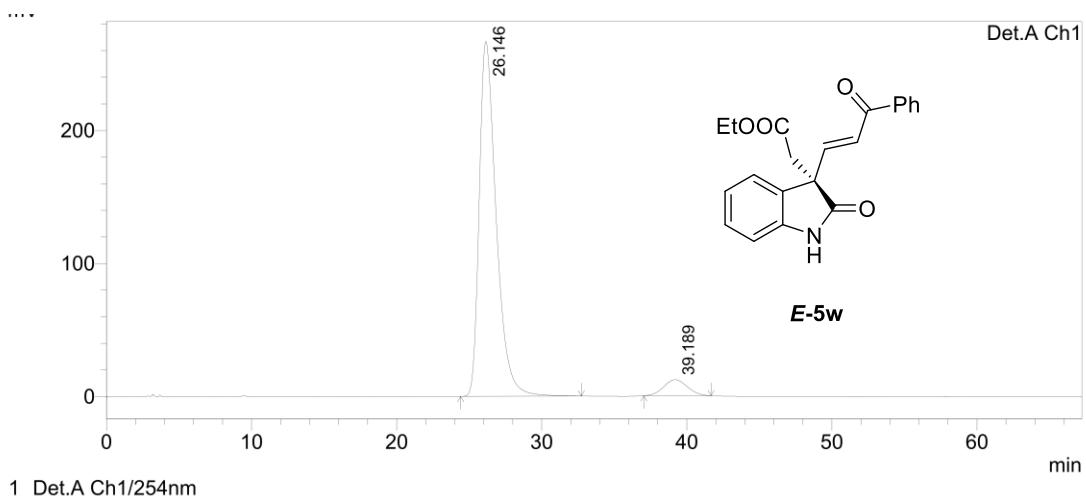


1 Det.A Ch1/254nm

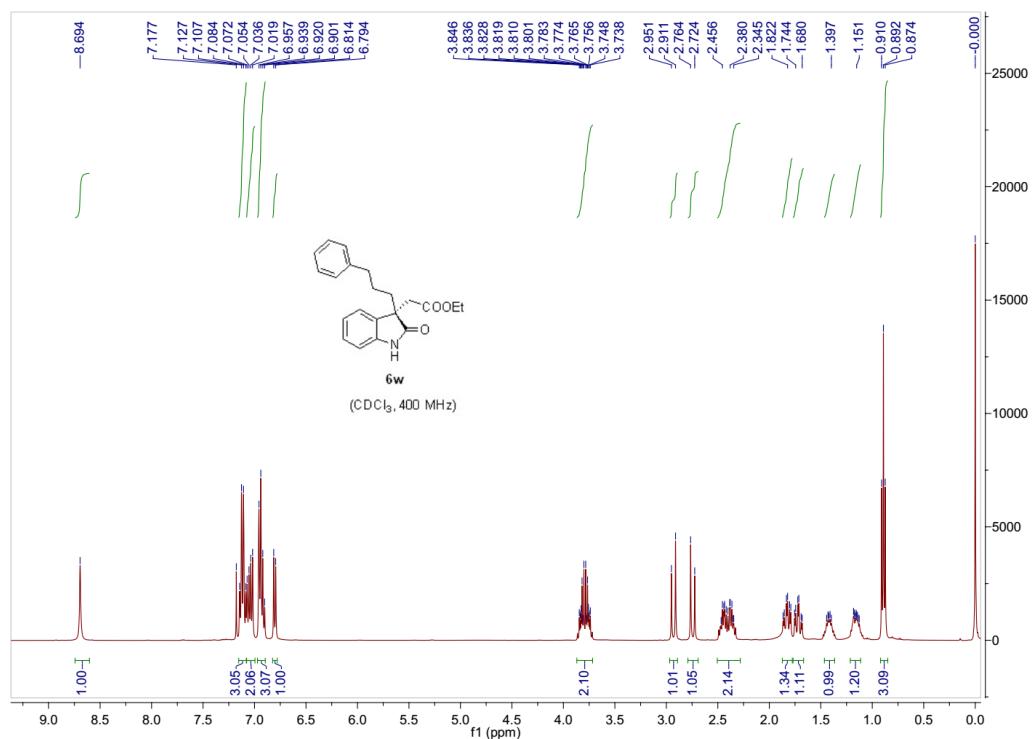
PeakTable

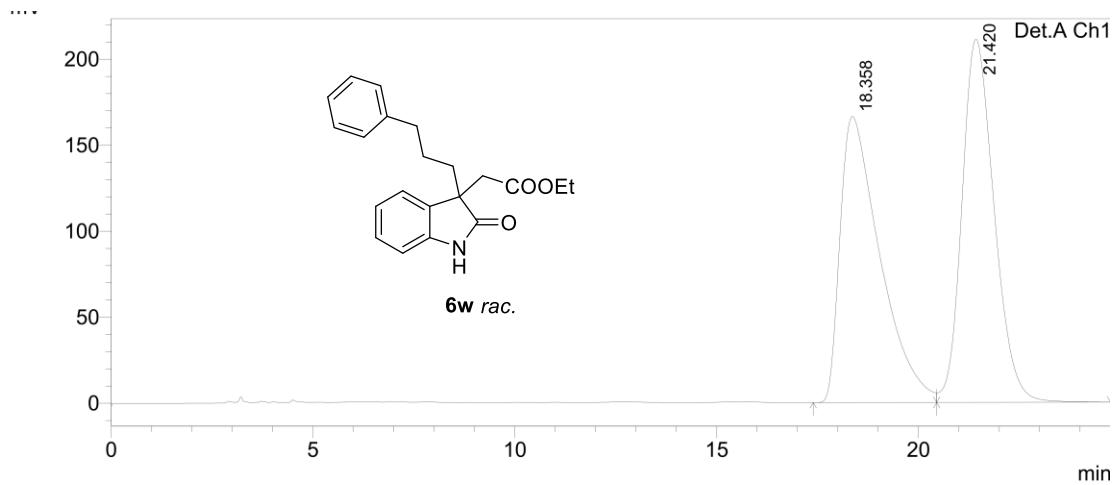
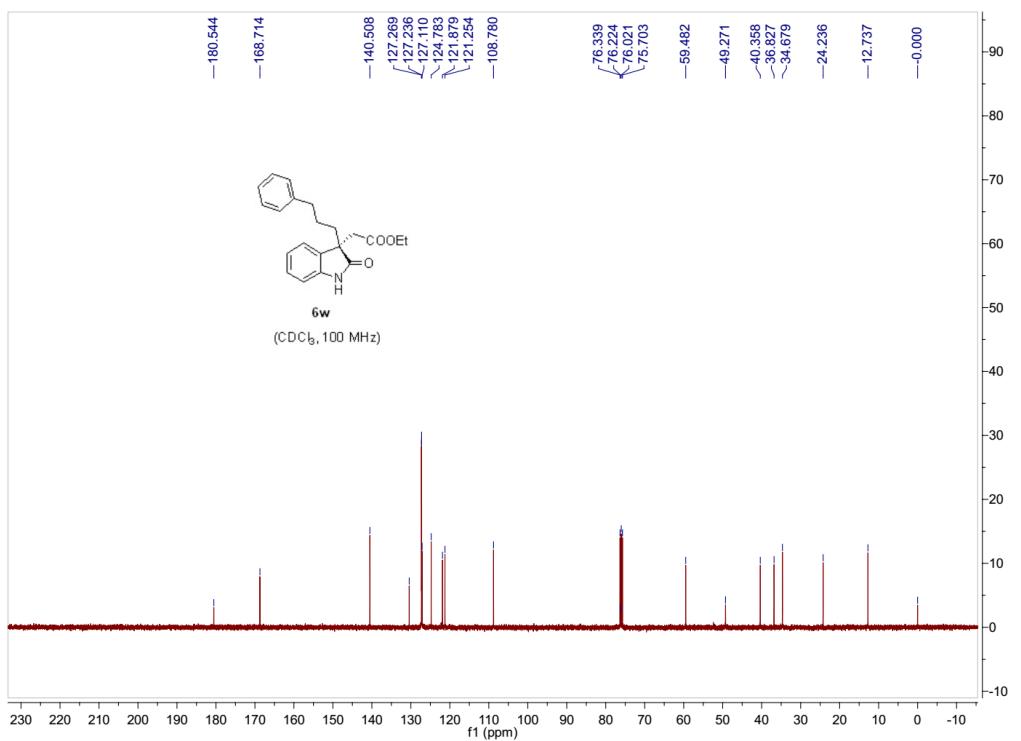
Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	26.691	10500426	143593	49.507	57.491
2	37.952	10709533	106174	50.493	42.509
Total		21209959	249768	100.000	100.000



PeakTable					
Detector A Ch1 254nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	26.146	21690559	266632	94.086	95.668
2	39.189	1363485	12073	5.914	4.332
Total		23054045	278705	100.000	100.000



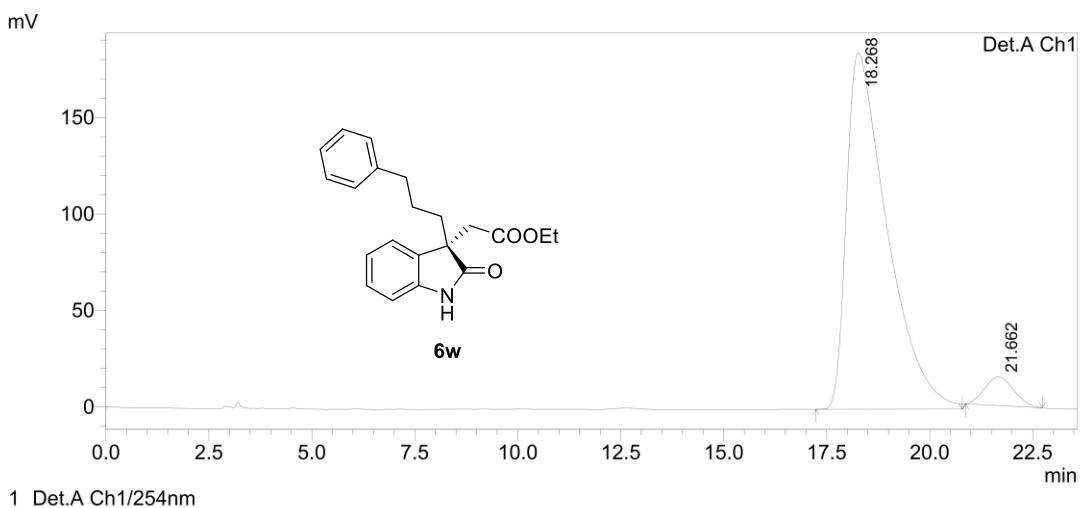


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

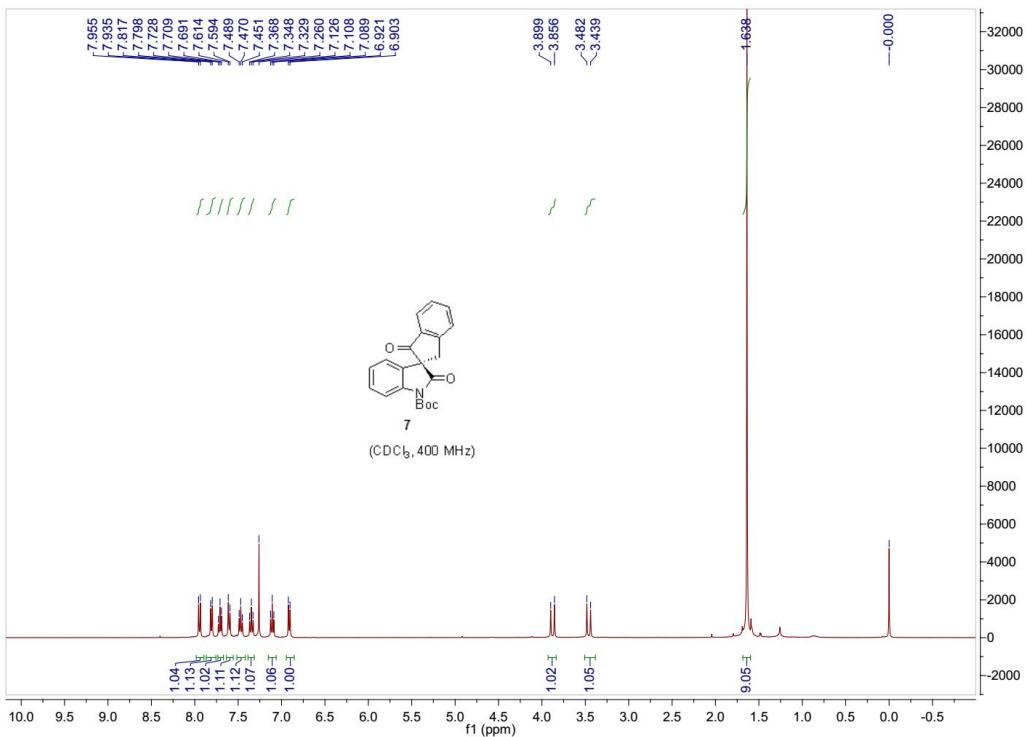
Peak#	Ret. Time	Area	Height	Area %	Height %
1	18.358	11400439	166266	49.343	44.064
2	21.420	11704187	211060	50.657	55.936
Total		23104626	377326	100.000	100.000

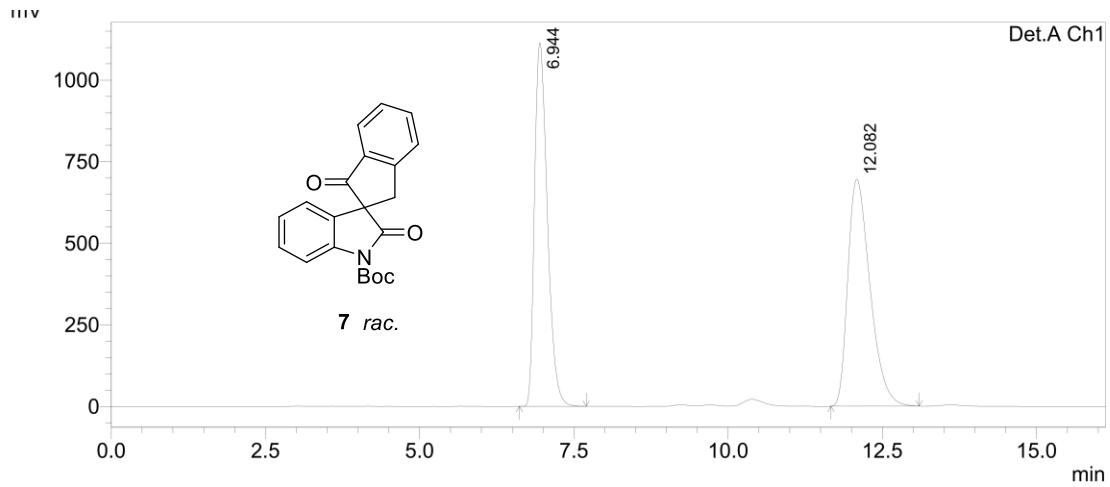
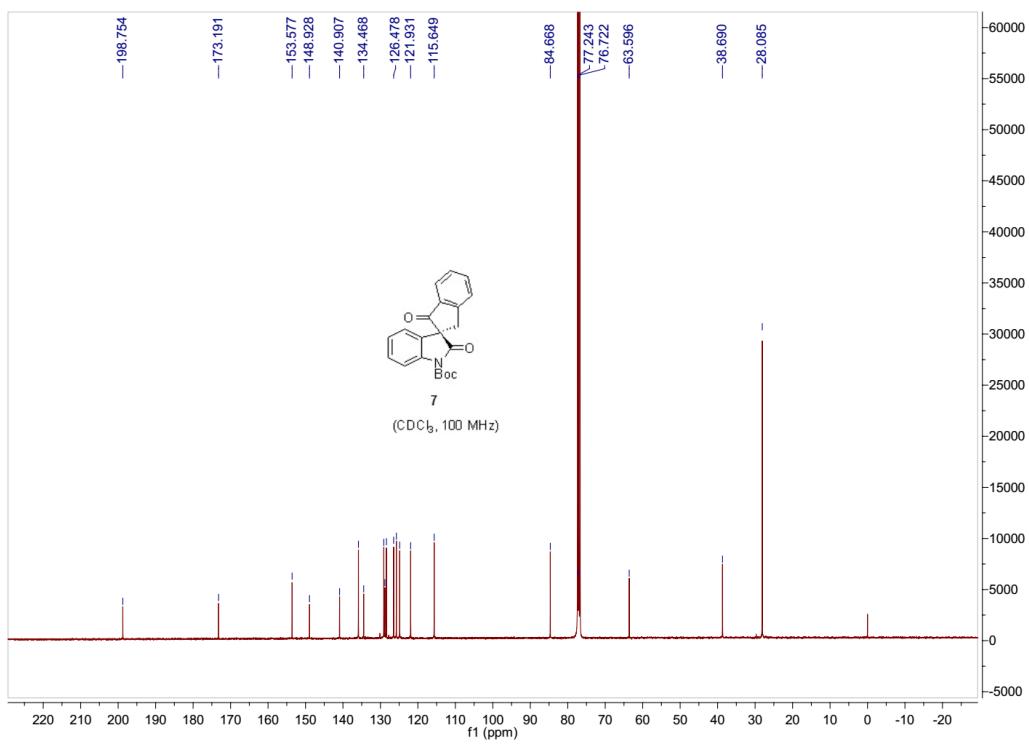


PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	18.268	12689231	184733	94.546	92.578
2	21.662	732030	14811	5.454	7.422
Total		13421261	199543	100.000	100.000



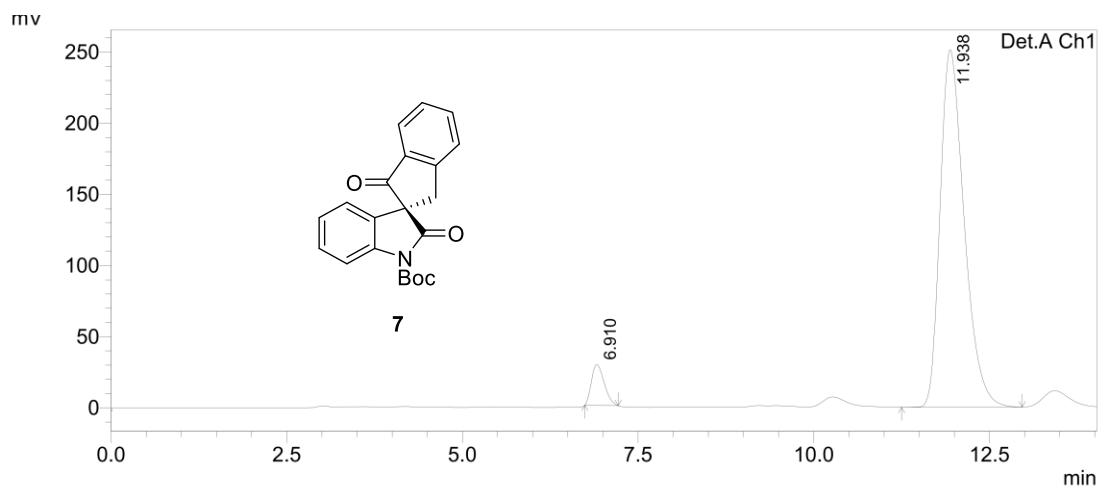


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.944	16179783	1114444	48.164	61.565
2	12.082	17413204	695739	51.836	38.435
Total		33592987	1810183	100.000	100.000



PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.910	362480	28770	5.711	10.278
2	11.938	5984271	251140	94.289	89.722
Total		6346752	279910	100.000	100.000

Part III. X-ray crystal structure for **3h** (CCDC 1524645) showing the thermal ellipsoids at 50% probability level.

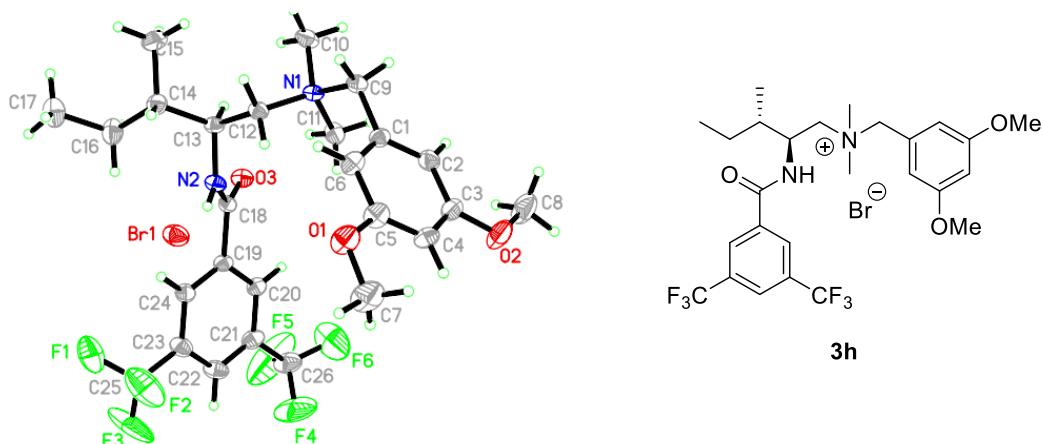


Table S1. Crystal data and structure refinement for **3h**.

Identification code	3h	
Empirical formula	$C_{27} H_{34} Br Cl_3 F_6 N_2 O$	
Formula weight	734.82	
Temperature	173(2) K	
Wavelength	1.54178 Å	
Crystal system, space group	Orthorhombic, P 21 21 21	
Unit cell dimensions	$a = 8.9751(4)$ Å	alpha = 90 deg.
	$b = 17.1860(7)$ Å	beta = 90 deg.
	$c = 21.3036(8)$ Å	gamma = 90 deg.
Volume	3286.0(2) Å ³	
Z, Calculated density	4, 1.485 Mg/m ³	
Absorption coefficient	4.530 mm ⁻¹	
F(000)	1496	
Crystal size	0.24 x 0.18 x 0.15 mm	
Theta range for data collection	3.30 to 68.40 deg.	
Limiting indices	$-10 \leq h \leq 10, -20 \leq k \leq 20, -25 \leq l \leq 25$	
Reflections collected / unique	25372 / 6036 [R(int) = 0.0572]	
Completeness to theta = 68.40	100.0 %	
Max. and min. transmission	0.5498 and 0.4094	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	6036 / 0 / 385	
Goodness-of-fit on F ²	1.040	
Final R indices [I>2sigma(I)]	R1 = 0.0514, wR2 = 0.1324	
R indices (all data)	R1 = 0.0583, wR2 = 0.1387	
Absolute structure parameter	0.00(2)	
Largest diff. peak and hole	0.829 and -0.307 e.Å ⁻³	