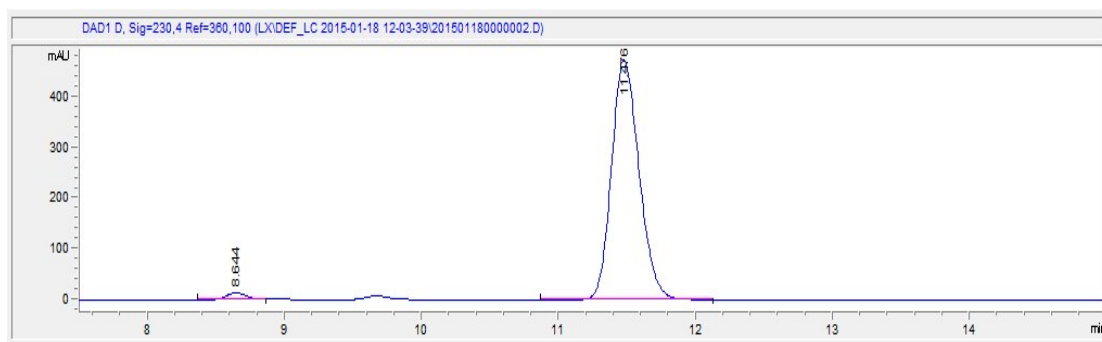
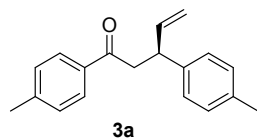
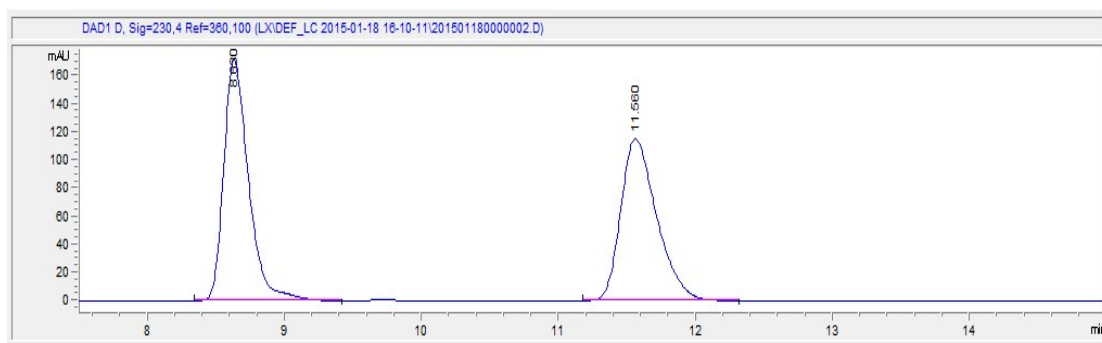


1. Chiral HPLC Data

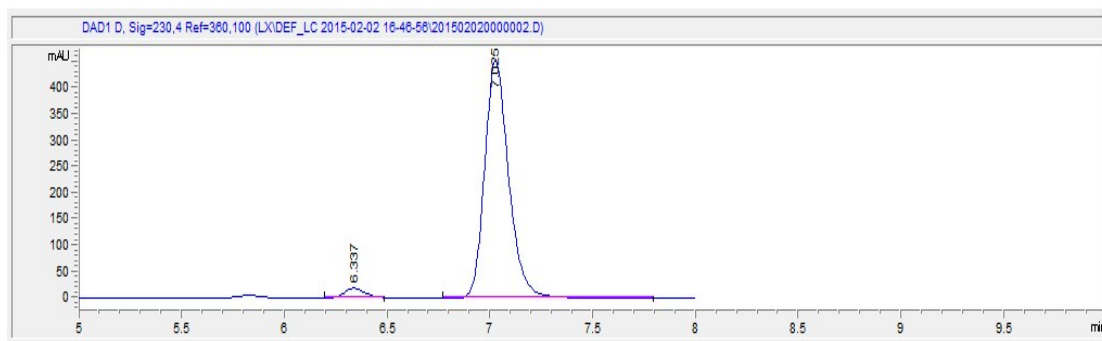
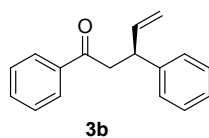


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	8.644	140.2	13.8	0.157	0.842	2.078
2	11.476	6606.6	472.6	0.2151	0.783	97.922

Racemic

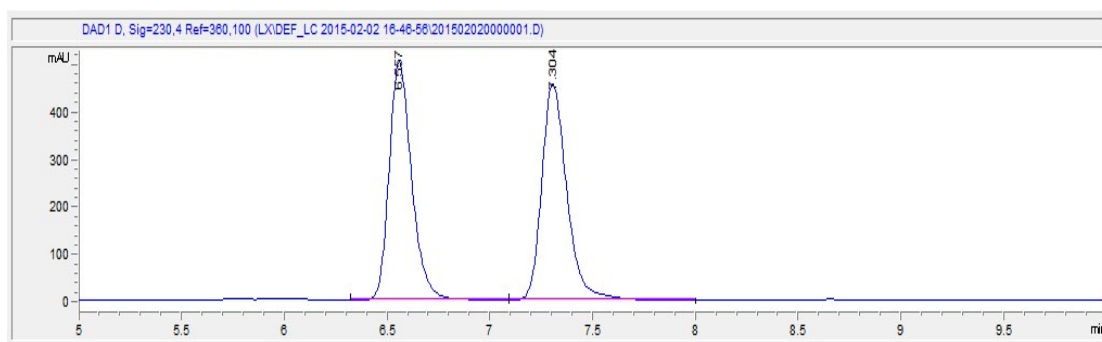


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	8.63	2151.1	171.1	0.1907	0.661	50.761
2	11.56	2086.6	115	0.2757	0.659	49.239

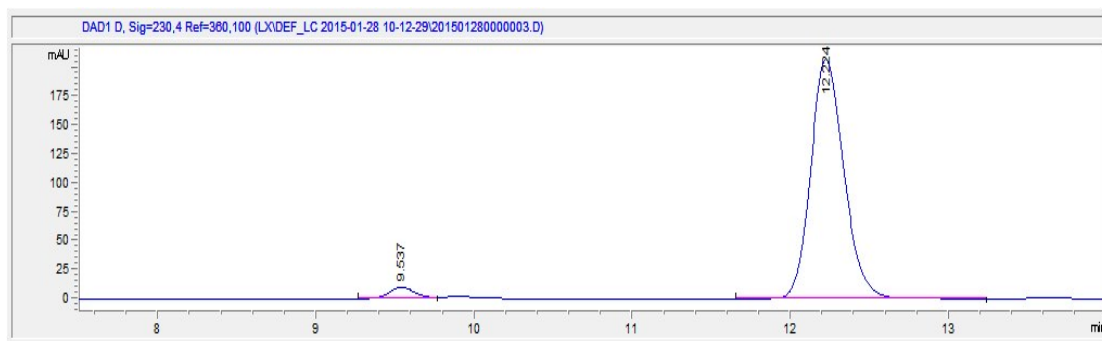
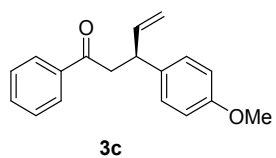


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	6.337	124.8	18.1	0.1152	0.83	3.282
2	7.025	3678	454	0.1245	0.76	96.718

Racemic

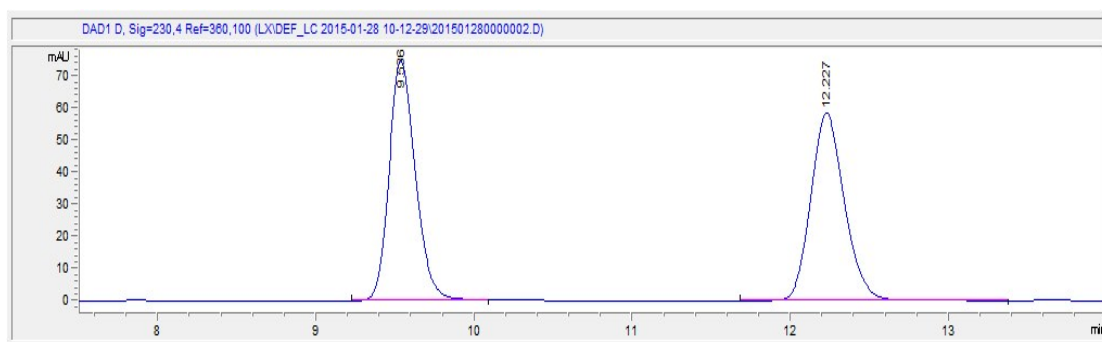


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	6.557	3814	501.5	0.1167	0.737	49.747
2	7.304	3852.8	456	0.1286	0.735	50.253

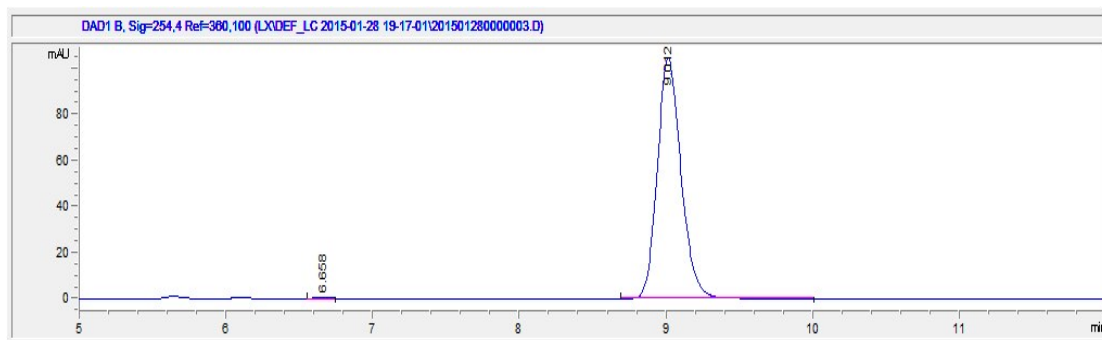
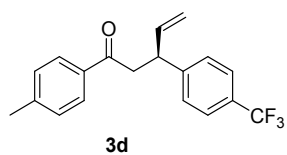


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	9.537	93.9	9.2	0.1707	0.928	3.025
2	12.224	3011.1	207.2	0.2235	0.822	96.975

Racemic

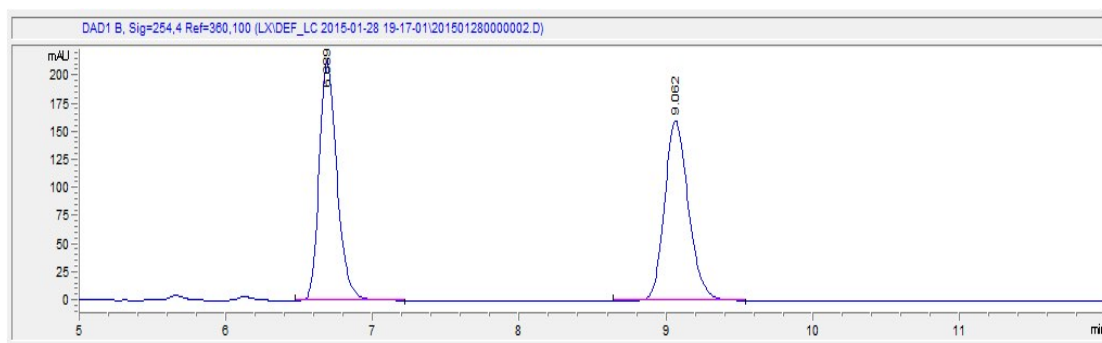


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	9.536	862	74.6	0.1768	0.796	50.026
2	12.227	861	58.3	0.2265	0.824	49.974

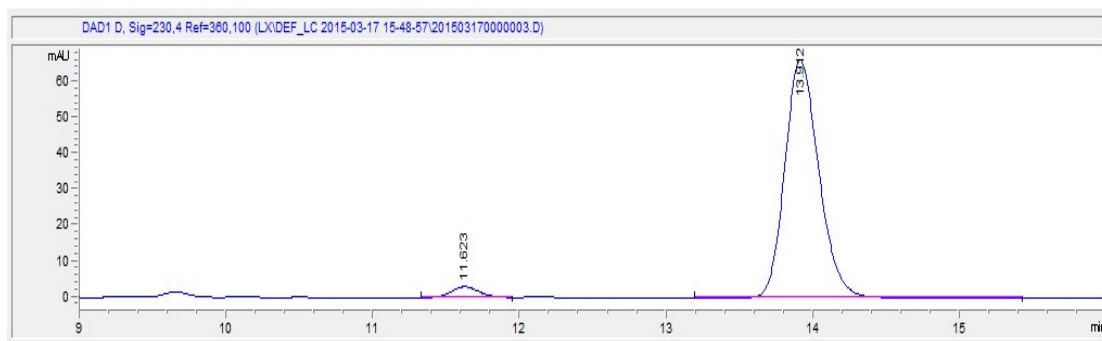
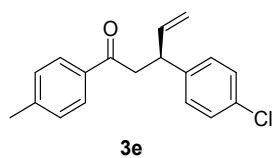


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	6.665	5.6	5.6E-1	0.1668	0.489	0.480
2	9.012	1169.7	104.3	0.1728	0.8	99.520

Racemic

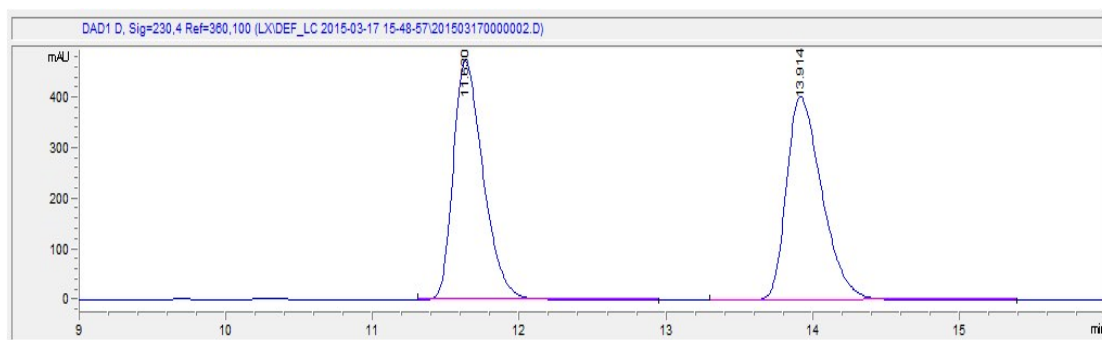


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	6.689	620.2	73.9	0.1279	0.749	49.742
2	9.062	626.7	55.4	0.1739	0.802	50.258

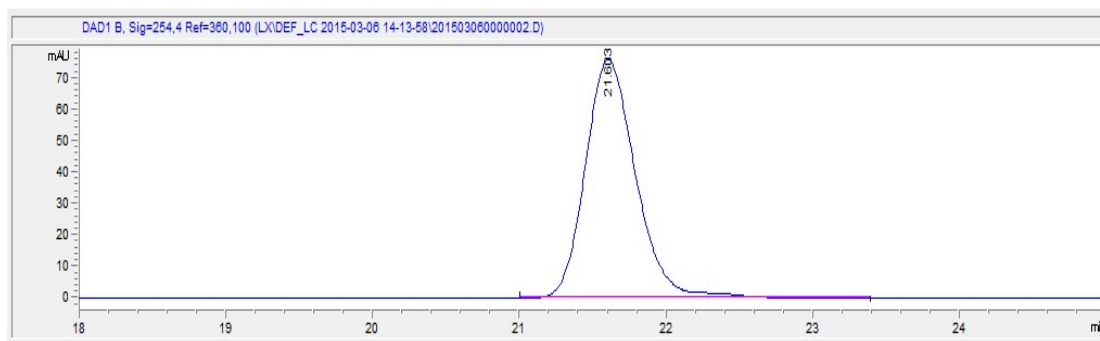
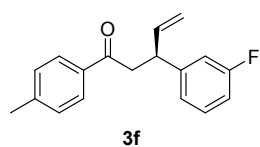


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	11.623	39.7	3	0.2011	0.852	3.575
2	13.912	1070.6	66.4	0.2502	0.794	96.425

Racemic

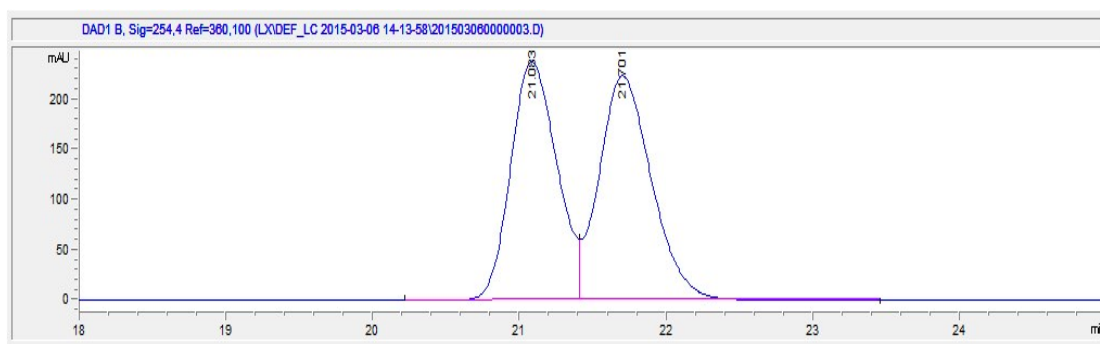


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	11.63	6725.4	472.9	0.2179	0.64	49.910
2	13.914	6749.6	401.7	0.258	0.623	50.090

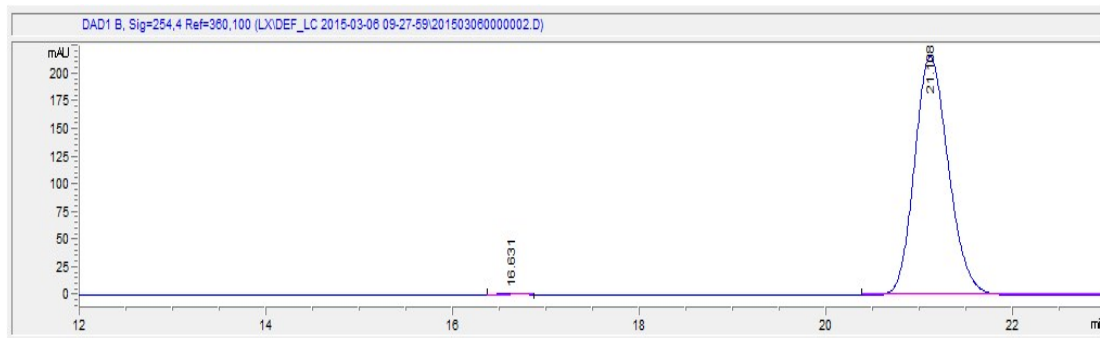
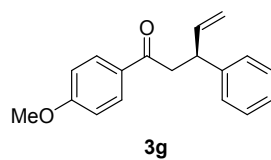


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	21.603	1809.4	75.8	0.3664	0.776	100.000

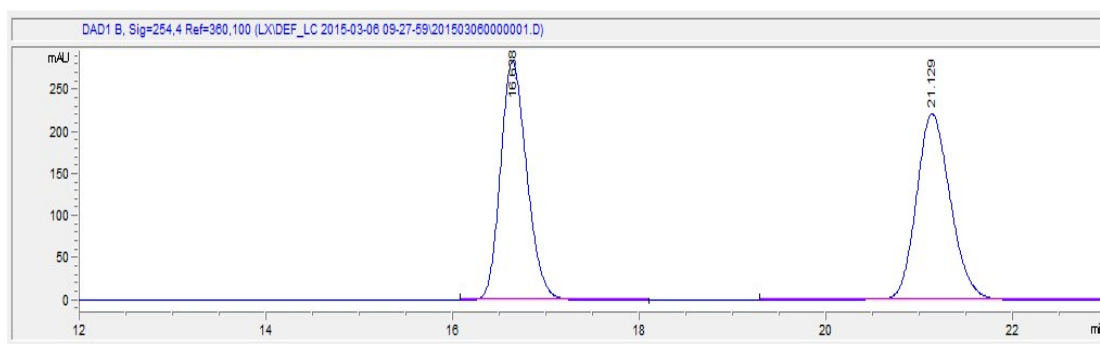
Racemic

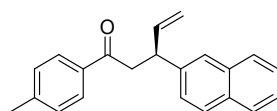


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	21.083	5211.4	237.4	0.3421	0.814	48.424
2	21.701	5550.6	223.5	0.3797	0.76	51.576

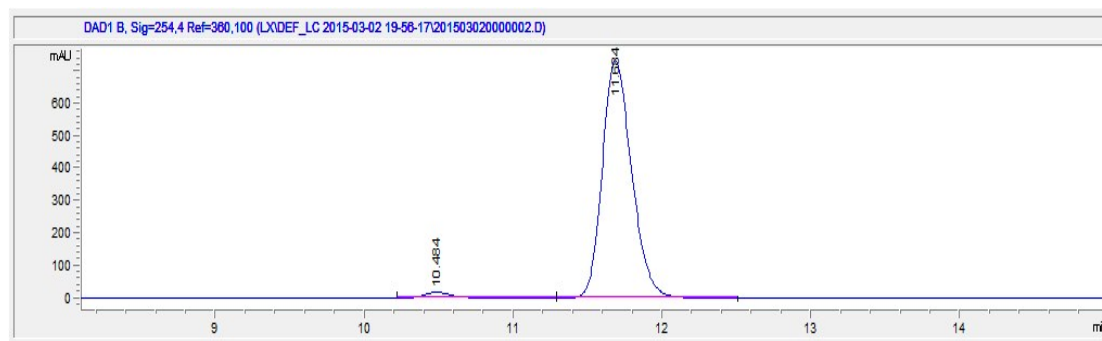


Racemic



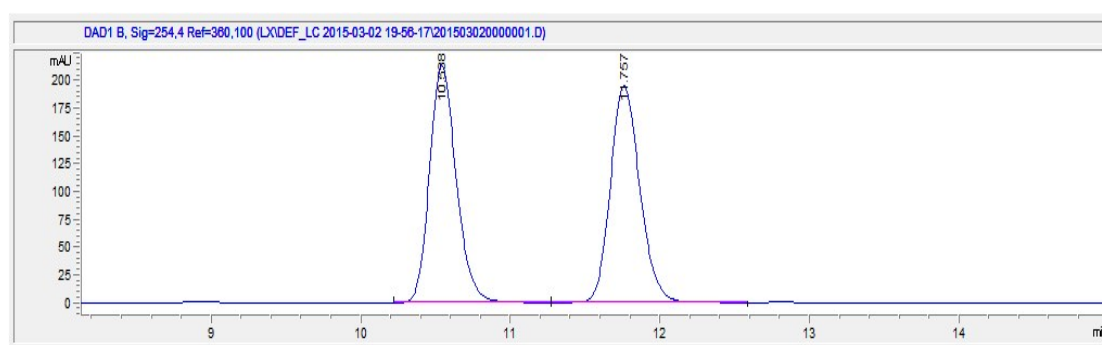


3h

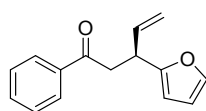


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	10.484	232.4	17.7	0.1969	0.699	2.262
2	11.684	10042.5	735	0.2114	0.751	97.738

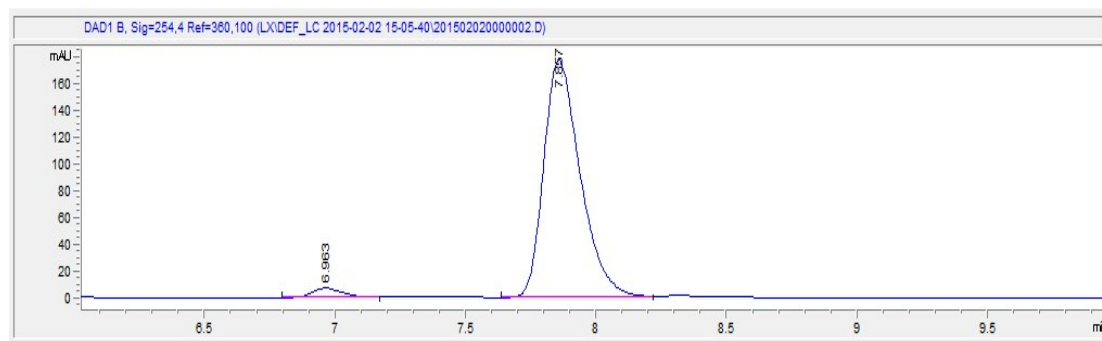
Racemic



#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	10.538	2651	214	0.1905	0.79	49.763
2	11.757	2676.2	195.8	0.2115	0.817	50.237

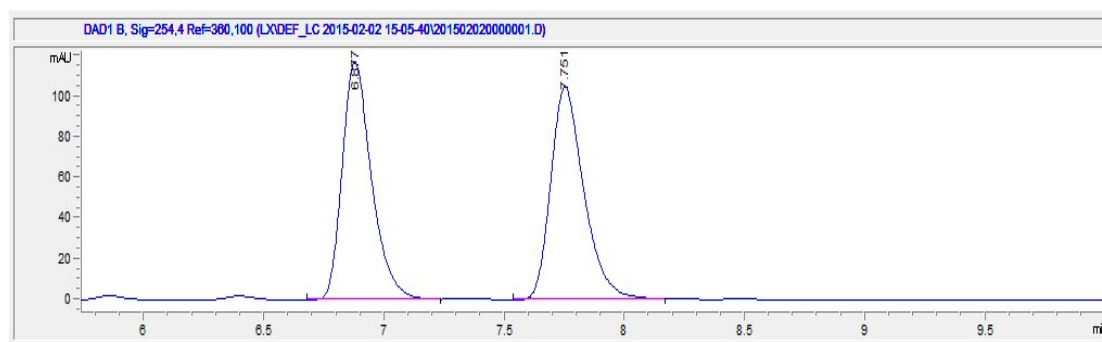


3i

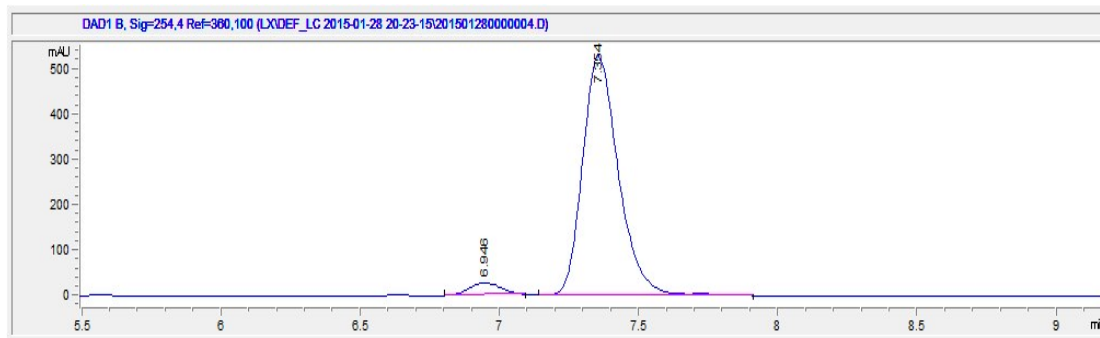
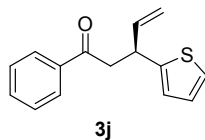


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	6.963	55.4	6.9	0.1235	0.778	3.092
2	7.857	1735.4	177.6	0.148	0.664	96.908

Racemic

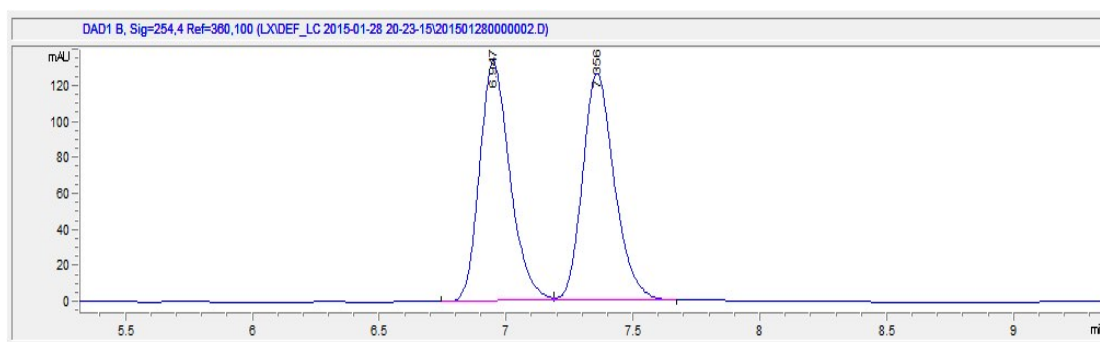


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	6.877	999.3	117.4	0.1293	0.69	49.909
2	7.751	1003	104.7	0.1458	0.695	50.091

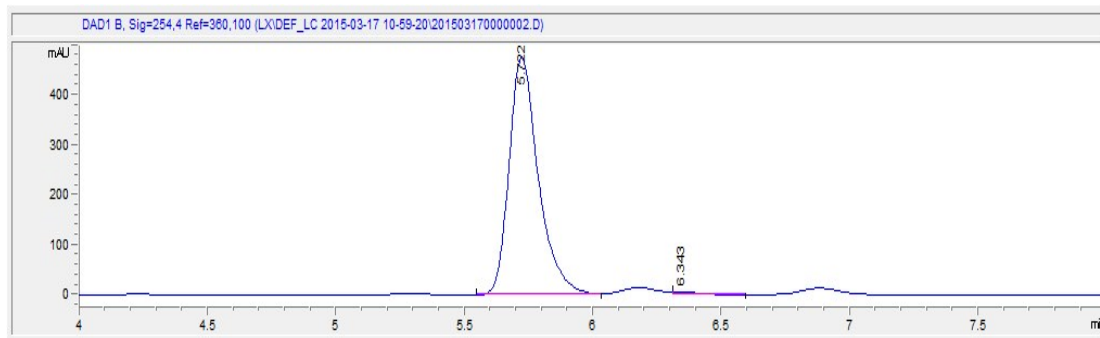
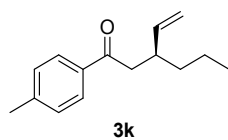


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	6.946	225.4	28.1	0.1335	0.94	4.479
2	7.354	4807.5	529.8	0.1512	0.748	95.521

Racemic

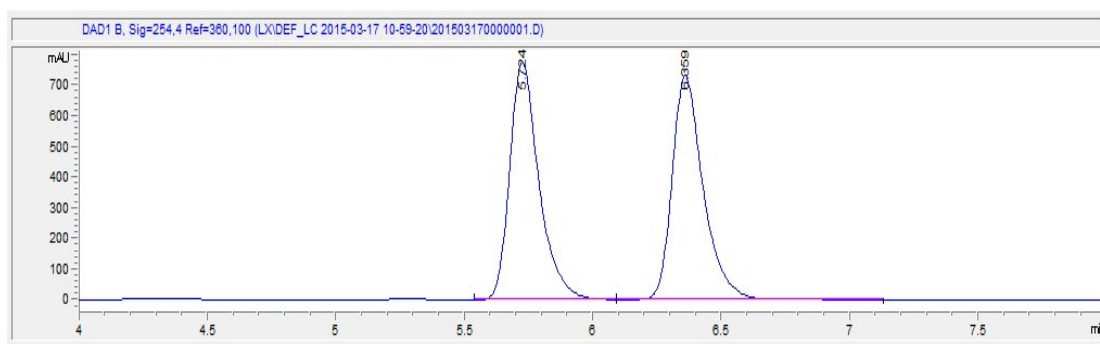


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	6.947	1113.1	133.3	0.1274	0.762	50.173
2	7.356	1105.4	125.9	0.1344	0.777	49.827

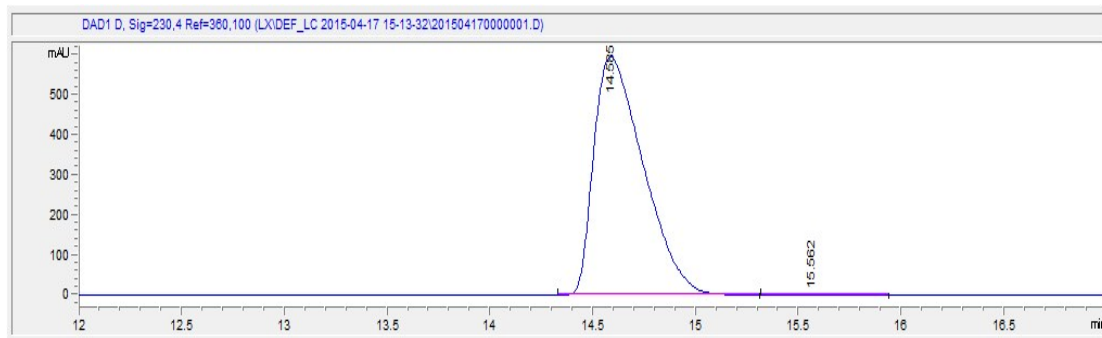
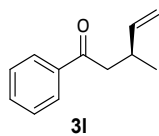


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	5.722	3744.8	476.3	0.1177	0.702	99.205
2	6.343	30	4.6	0.0974	0.346	0.795

Racemic

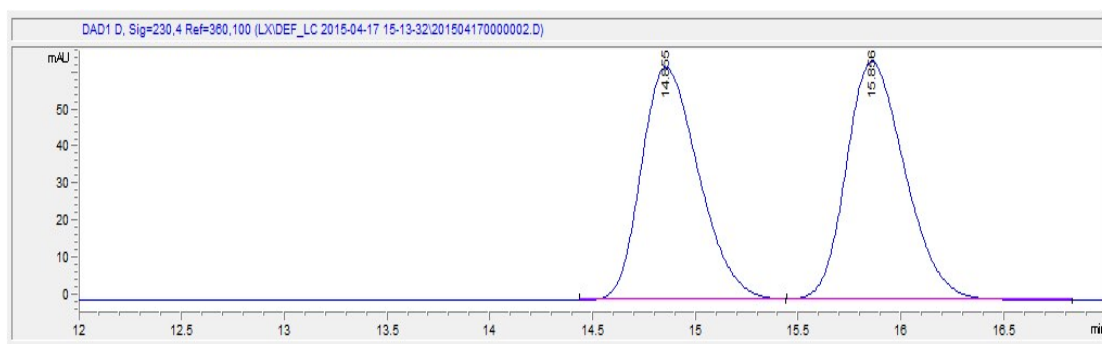


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	5.724	6154.1	777	0.1204	0.691	49.710
2	6.359	6226	733.1	0.1291	0.668	50.290

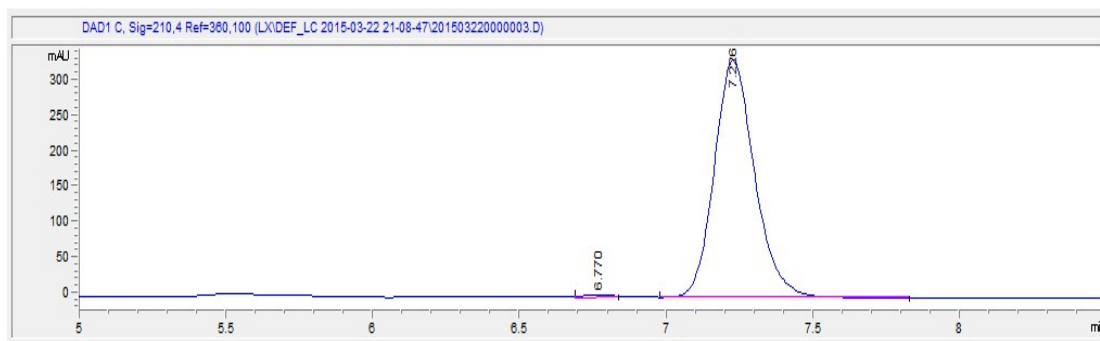
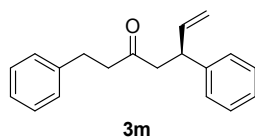


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	14.585	9979.1	595.2	0.2596	0.48	99.809
2	15.562	19.1	1.1	0.2685	0.712	0.191

Racemic

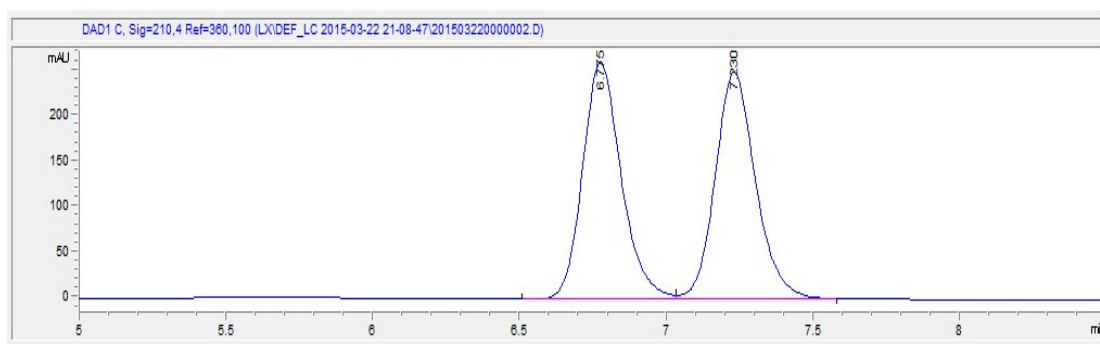


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	14.855	1216.5	63	0.3013	0.718	48.812
2	15.856	1275.7	64.3	0.3074	0.73	51.188

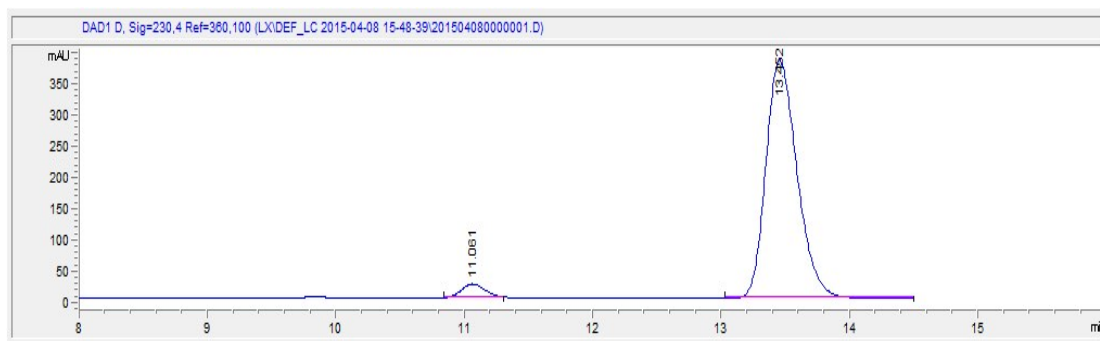
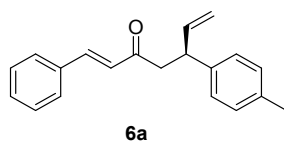


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	6.77	20.9	3	0.1145	1.55	0.649
2	7.226	3199.4	335.1	0.1454	0.813	99.351

Racemic

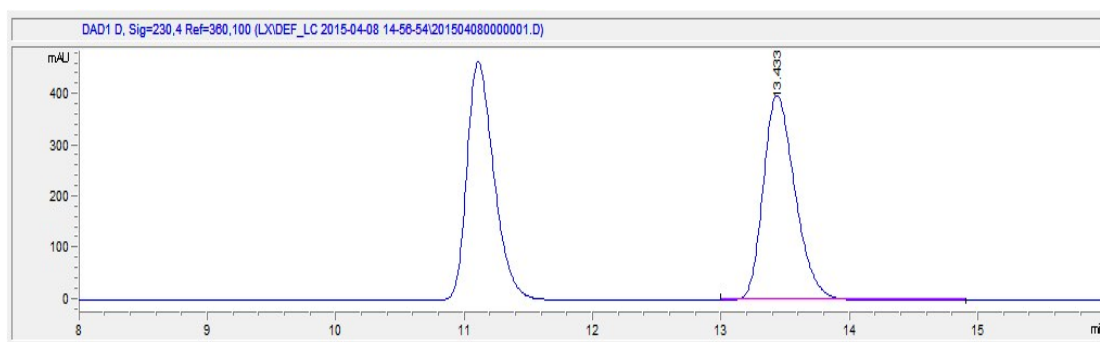


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	6.775	2382.1	261	0.1385	0.807	49.823
2	7.23	2399	249.6	0.1461	0.825	50.177

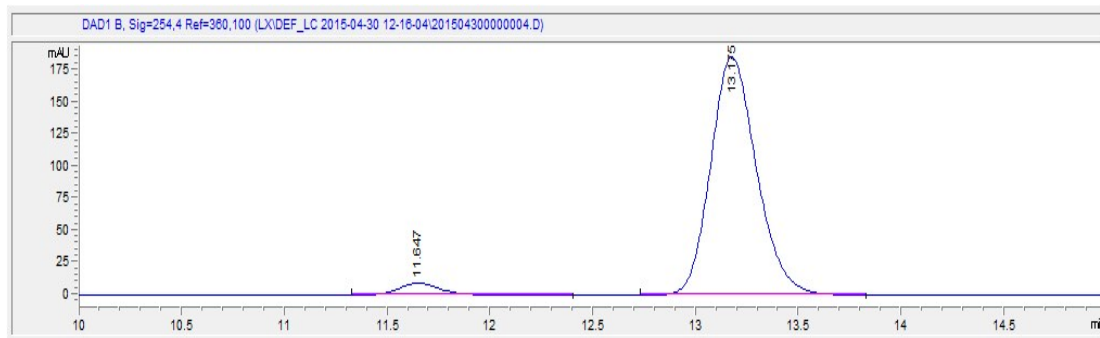
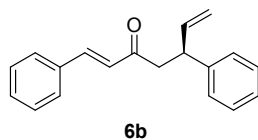


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	11.061	269.5	21.6	0.2083	0.828	4.016
2	13.452	6439.9	381.9	0.2607	0.739	95.984

Racemic

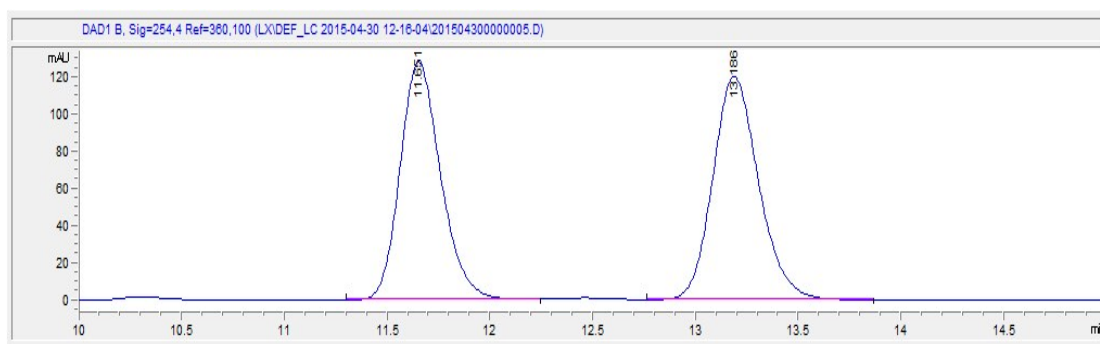


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	11.107	6775.5	465.2	0.2239	0.674	49.633
2	13.433	6875.5	399.6	0.2667	0.722	50.367

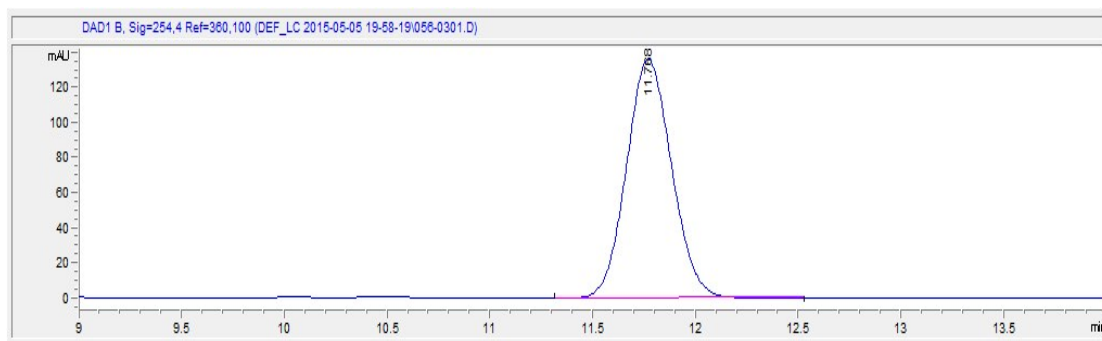
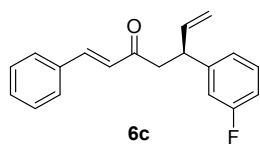


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	11.647	125.2	9.1	0.21	0.807	4.170
2	13.175	2876.4	185.5	0.2389	0.811	95.830

Racemic

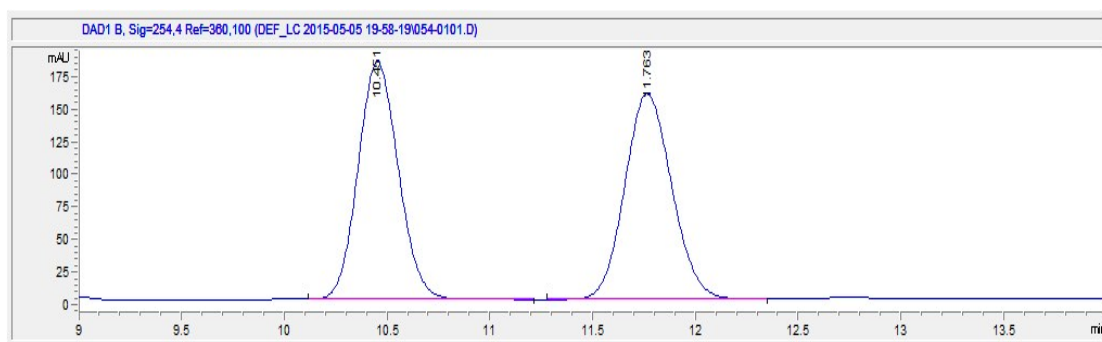


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	11.651	1758.7	128.1	0.2122	0.794	48.538
2	13.186	1864.6	120.2	0.239	0.82	51.462

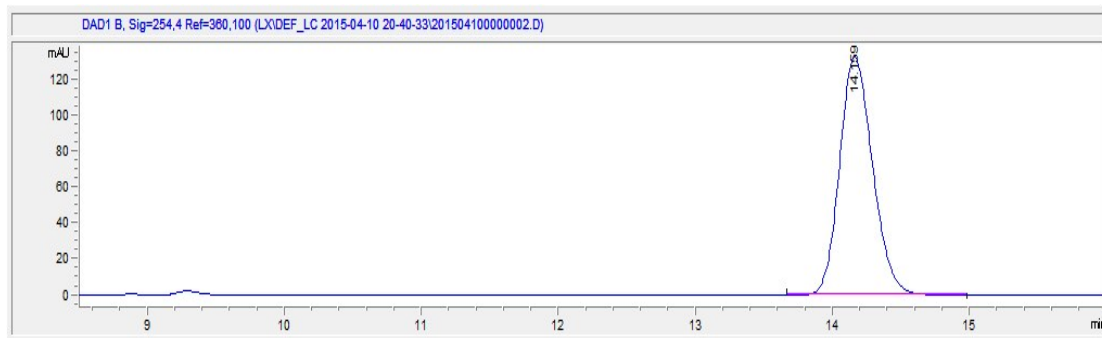
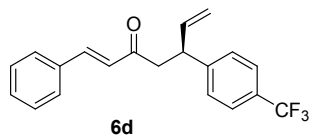


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	11.768	2080.3	135.8	0.2387	0.888	100.000

Racemic

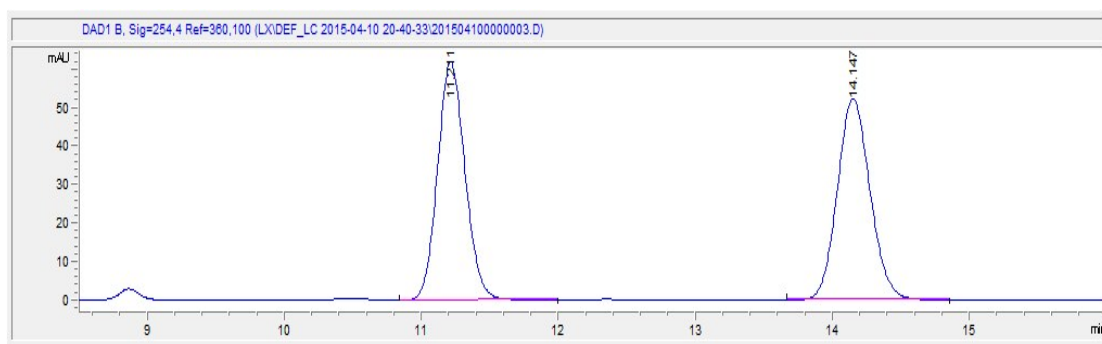


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	10.451	2480.7	182	0.211	0.878	49.727
2	11.763	2508	157.6	0.2477	0.874	50.273

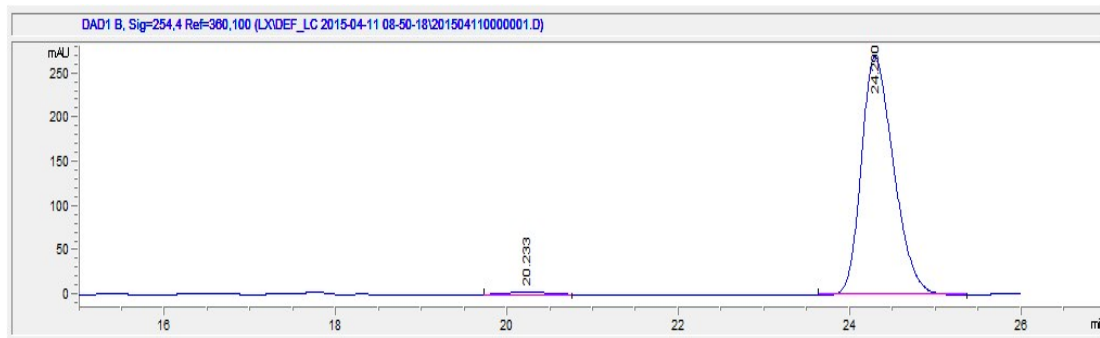
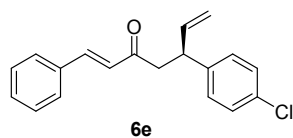


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	14.159	2220.2	132.7	0.2612	0.792	100.000

Racemic

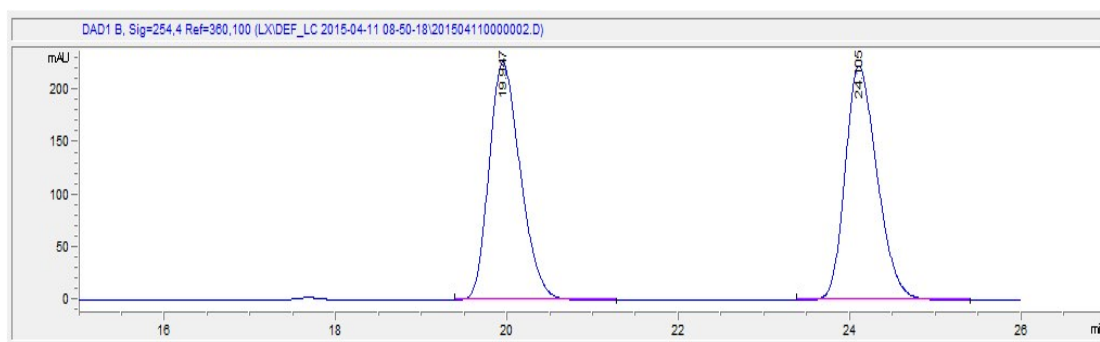


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	11.211	863.8	62	0.2145	0.864	49.802
2	14.147	870.7	52.3	0.2581	0.871	50.198

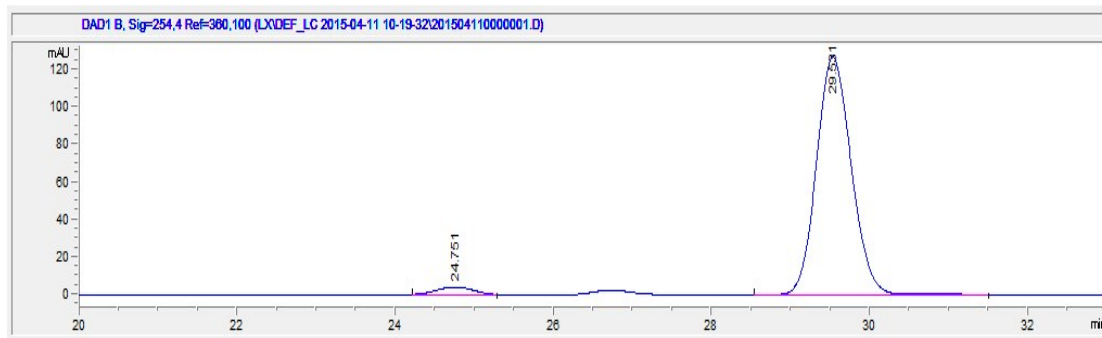
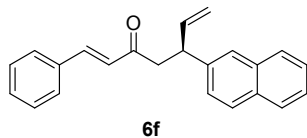


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	20.233	133.3	4.1	0.5437	0.957	1.851
2	24.29	7069.4	269.2	0.4044	0.686	98.149

Racemic

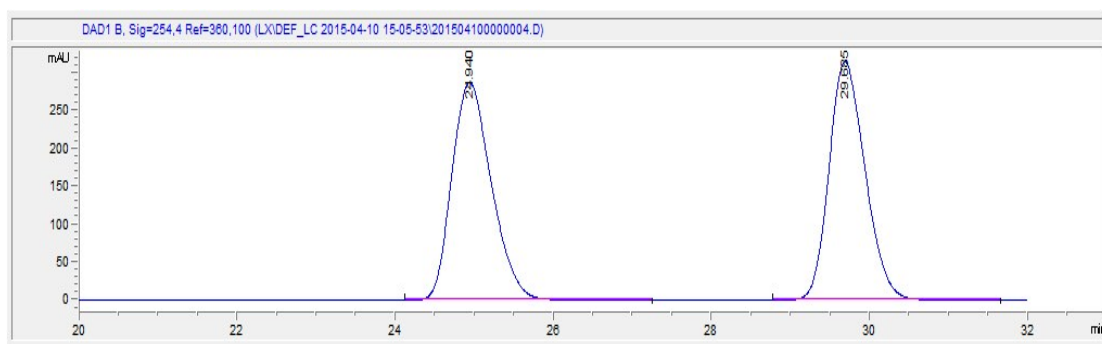


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	19.947	5754	227	0.3917	0.752	49.902
2	24.105	5776.6	223.2	0.3999	0.721	50.098

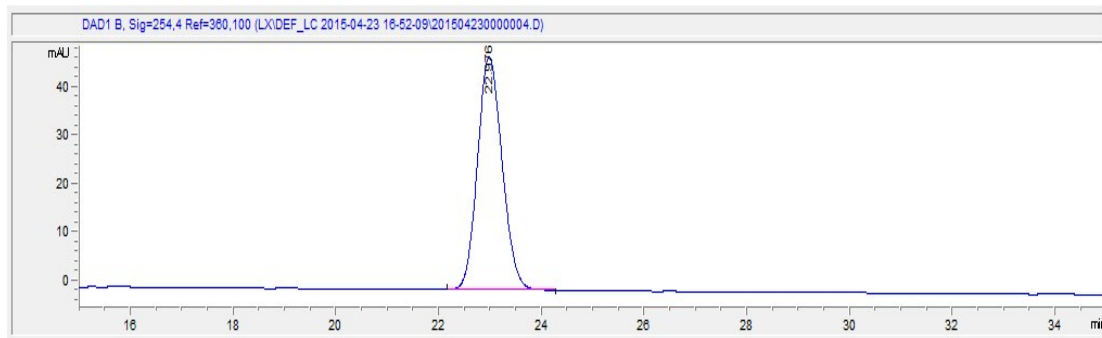
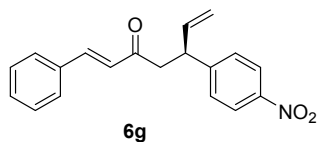


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	24.751	145.8	4.3	0.5588	1.002	3.595
2	29.531	3908.9	127.1	0.5127	0.847	96.405

Racemic

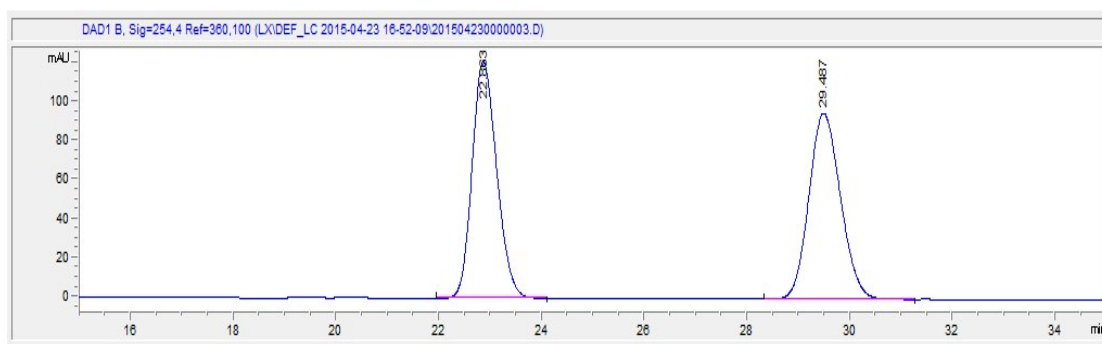


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	24.94	9970.8	286.4	0.5382	0.777	49.959
2	29.685	9987	314.1	0.4929	0.754	50.041

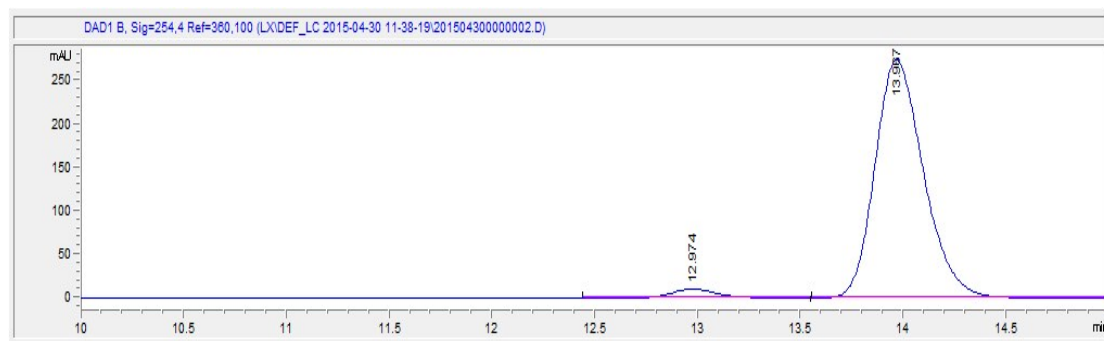
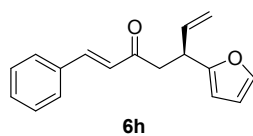


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	22.976	1610.8	48.3	0.5194	0.844	100.000

Racemic

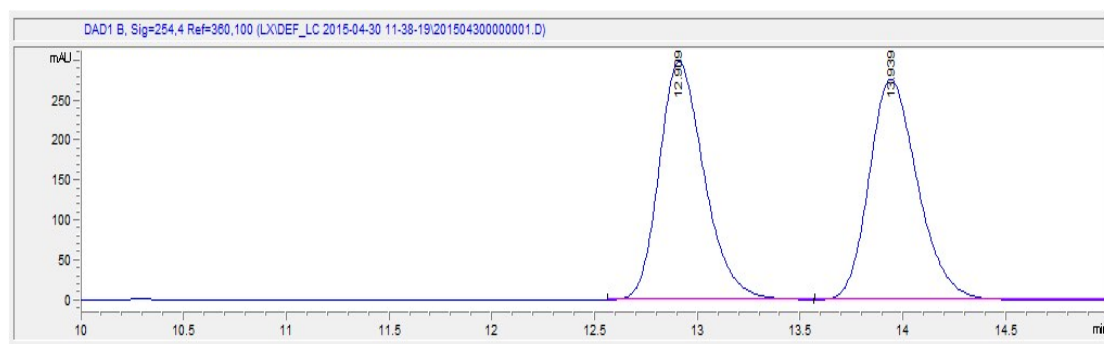


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	22.863	4042.8	121.3	0.519	0.789	49.777
2	29.487	4079	95.4	0.663	0.842	50.223

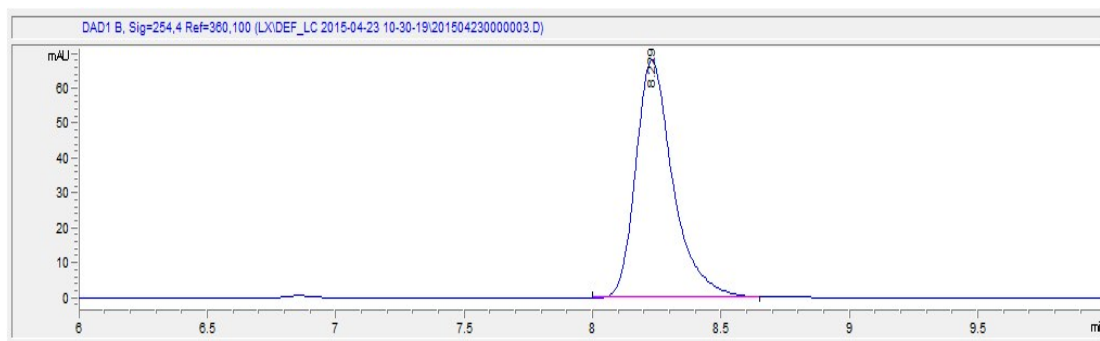
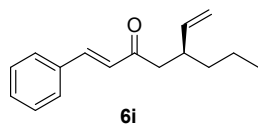


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	12.974	156.9	10.3	0.2334	0.836	3.367
2	13.967	4502.8	274.4	0.2535	0.754	96.633

Racemic

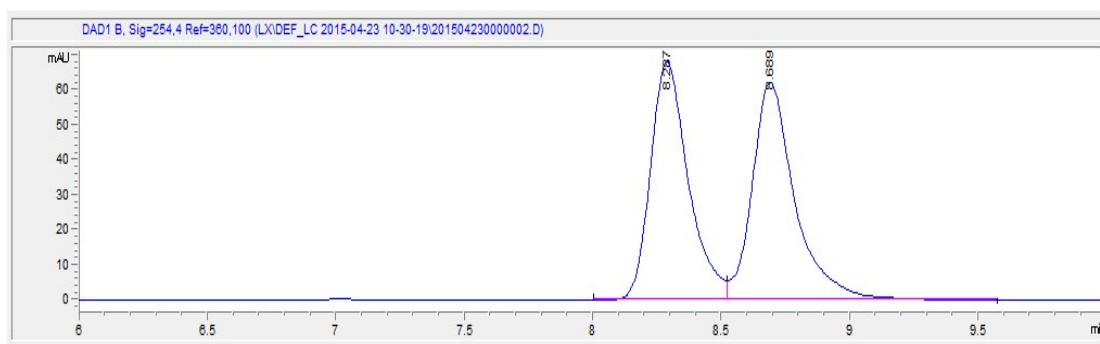


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	12.909	4534.2	297.8	0.2336	0.744	50.067
2	13.939	4522.1	276.5	0.2508	0.765	49.933

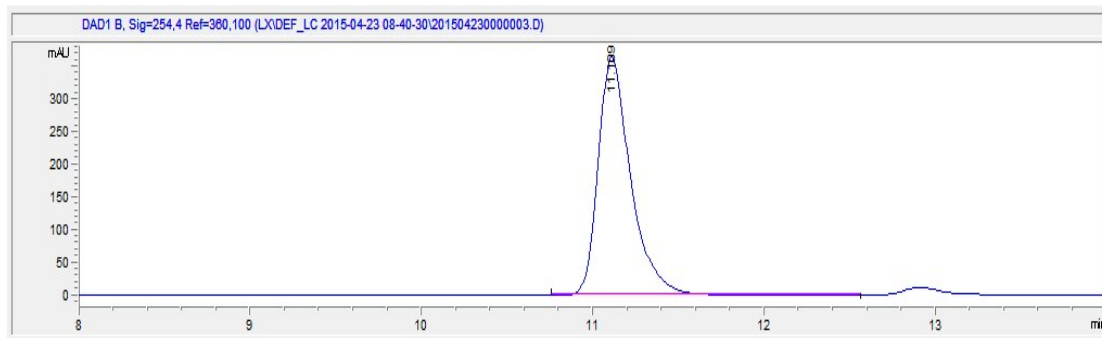
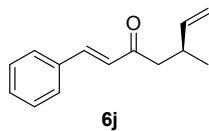


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	8.229	683.6	68.2	0.151	0.707	100.000

Racemic

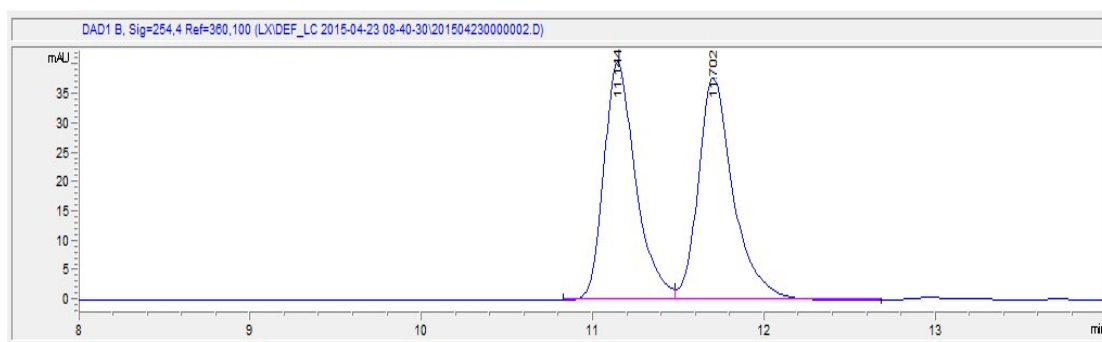


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	8.287	698.1	68.1	0.1536	0.713	49.305
2	8.689	717.8	62.3	0.1705	0.667	50.695

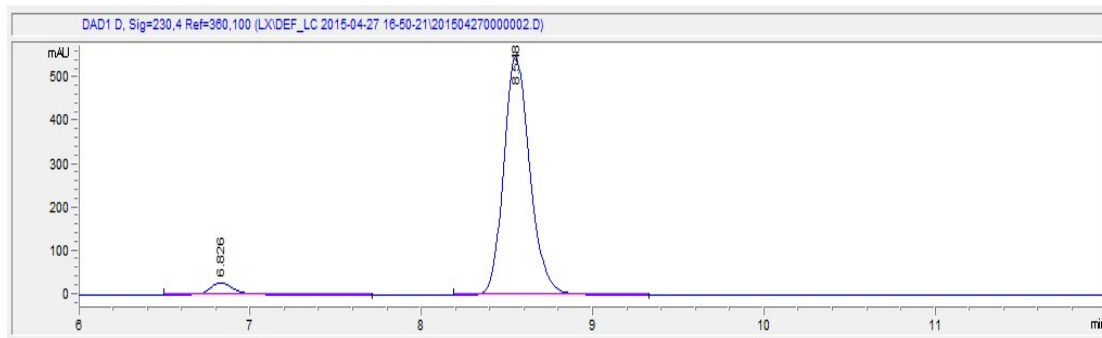
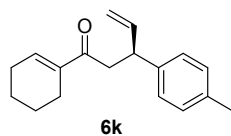


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	11.109	4823.1	365	0.1981	0.653	100.000

Racemic

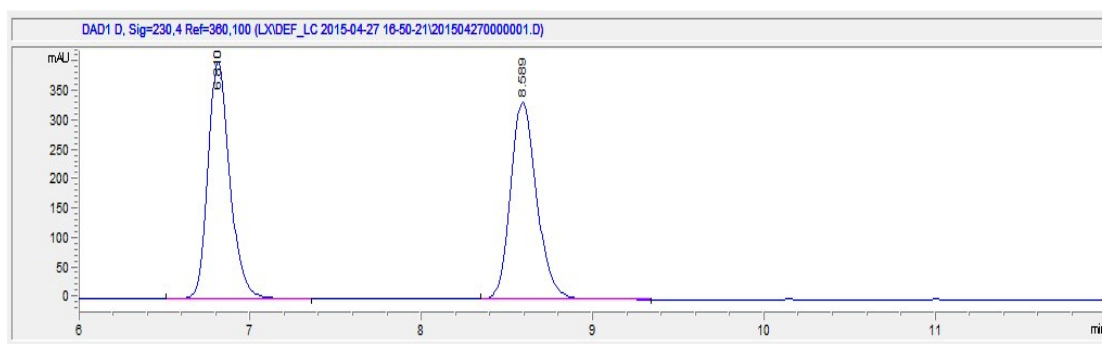


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	11.144	523.8	40.5	0.1947	0.71	49.435
2	11.702	535.8	37.8	0.2113	0.69	50.565

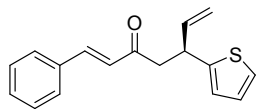


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	6.826	263	27.8	0.1425	0.716	4.306
2	8.548	5844.5	549.8	0.162	0.796	95.694

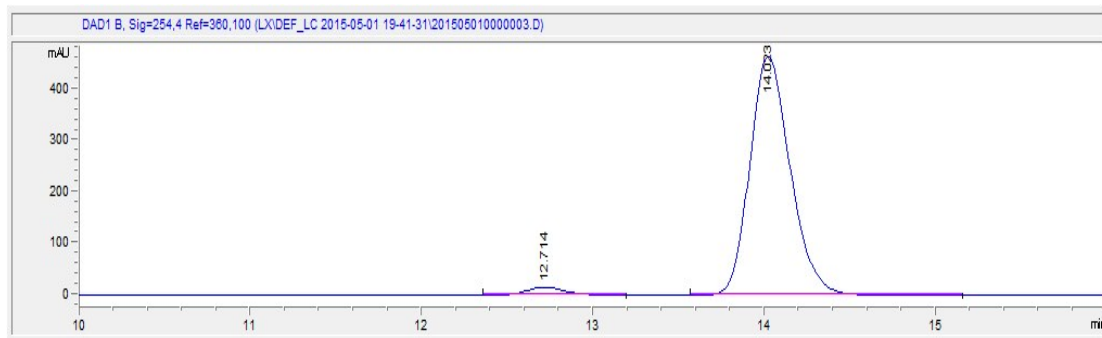
Racemic



#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	6.81	3572.8	403.2	0.1334	0.771	49.951
2	8.589	3579.9	334.5	0.1629	0.793	50.049

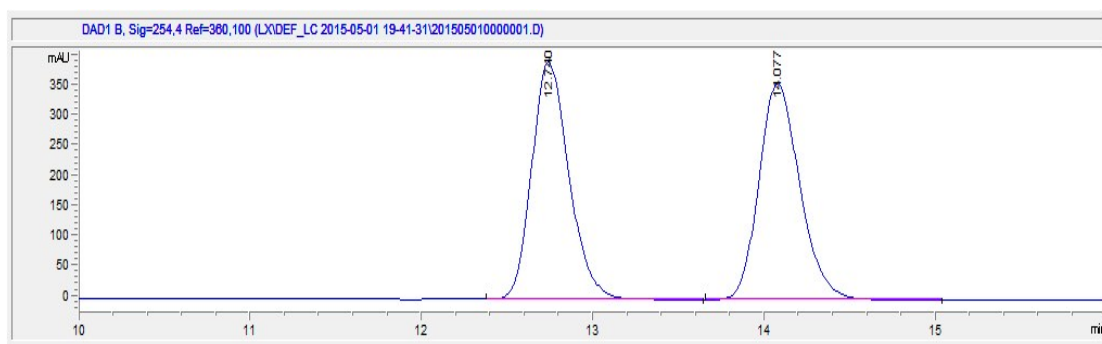


6l



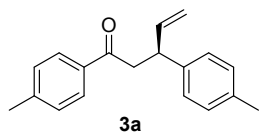
#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	12.714	230	15.5	0.2267	0.82	2.930
2	14.023	7619.6	464.2	0.2515	0.79	97.070

Racemic

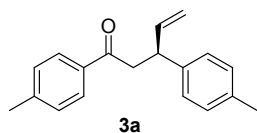
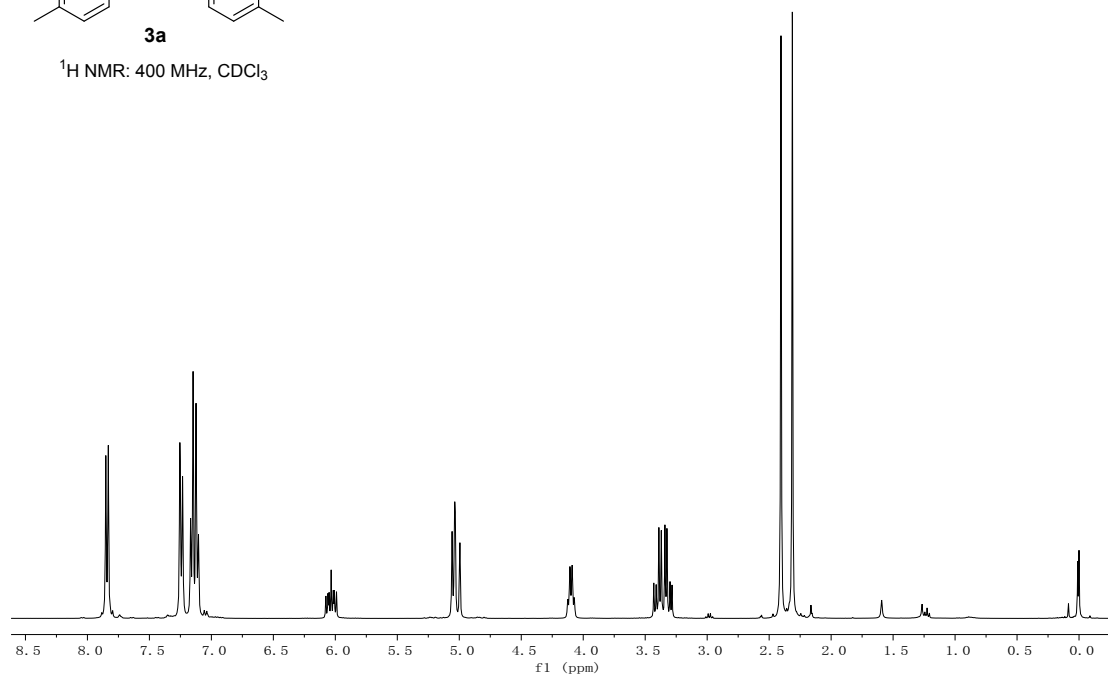


#	时间	峰面积	峰高	峰宽	对称因子	峰面积 %
1	12.74	5957.8	394.3	0.2323	0.781	49.995
2	14.077	5959.1	359.5	0.2554	0.795	50.005

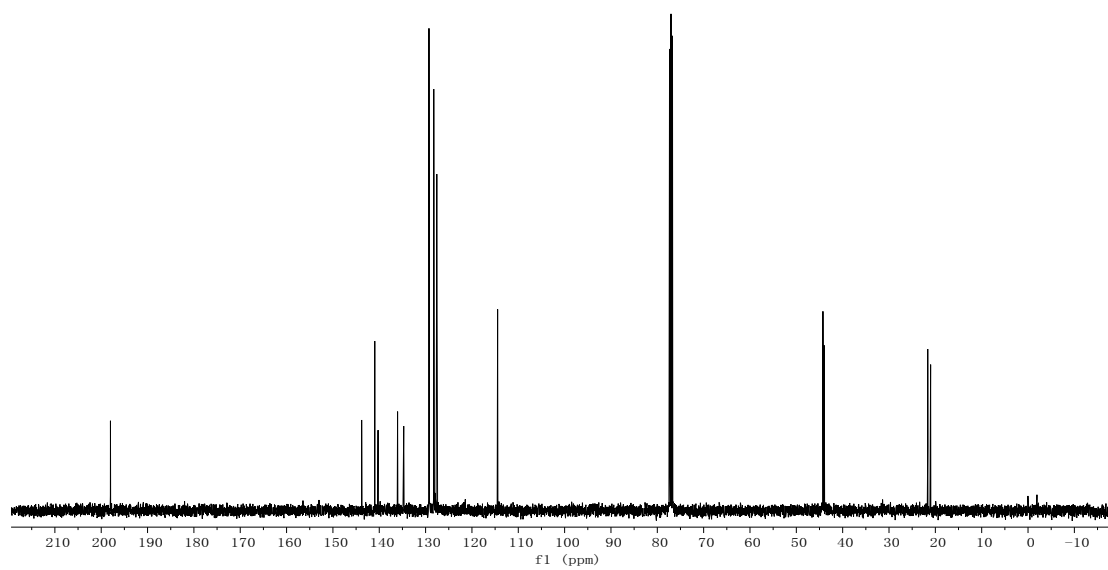
2. NMR Spectral Data

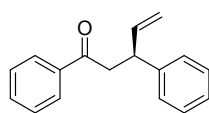


^1H NMR: 400 MHz, CDCl_3



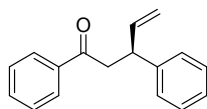
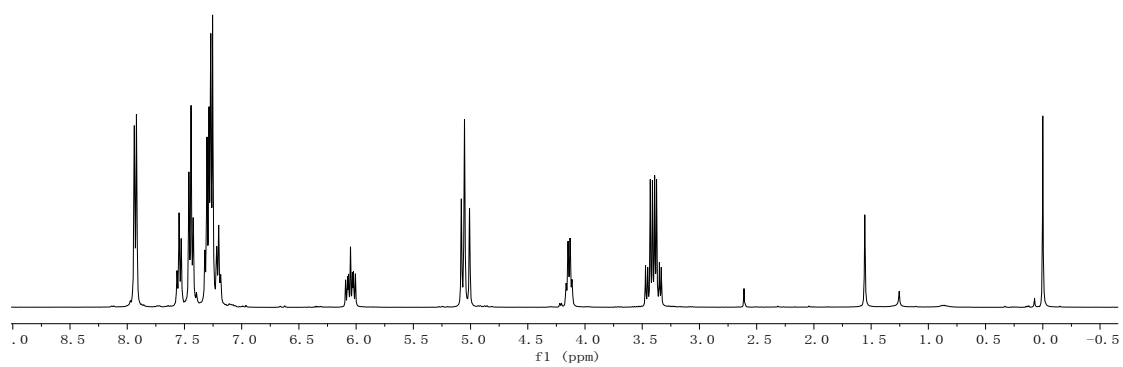
^{13}C NMR: 100 MHz, CDCl_3





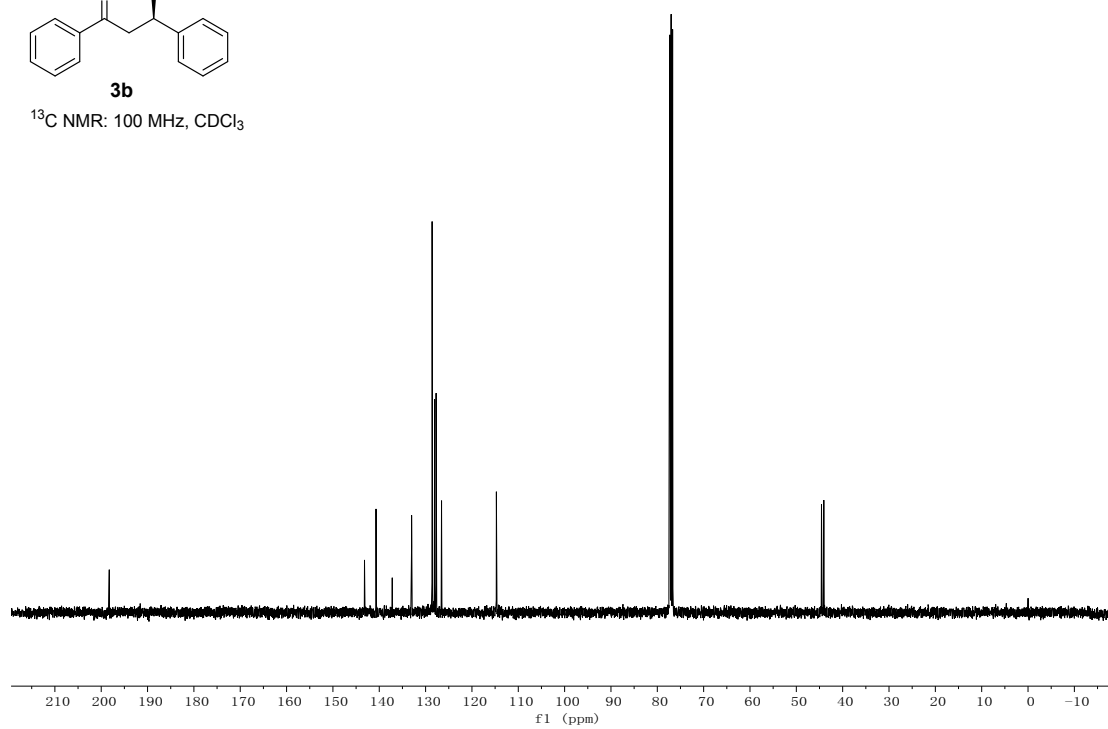
3b

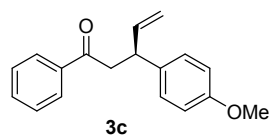
^1H NMR: 400 MHz, CDCl_3



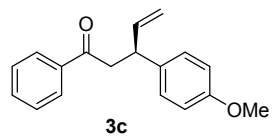
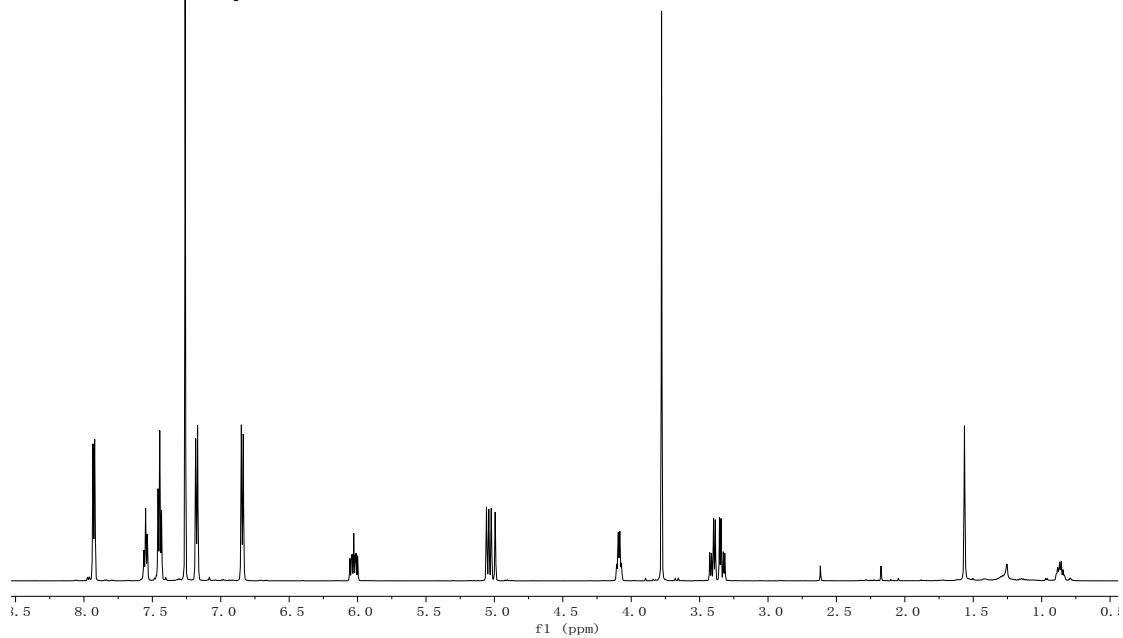
3b

^{13}C NMR: 100 MHz, CDCl_3

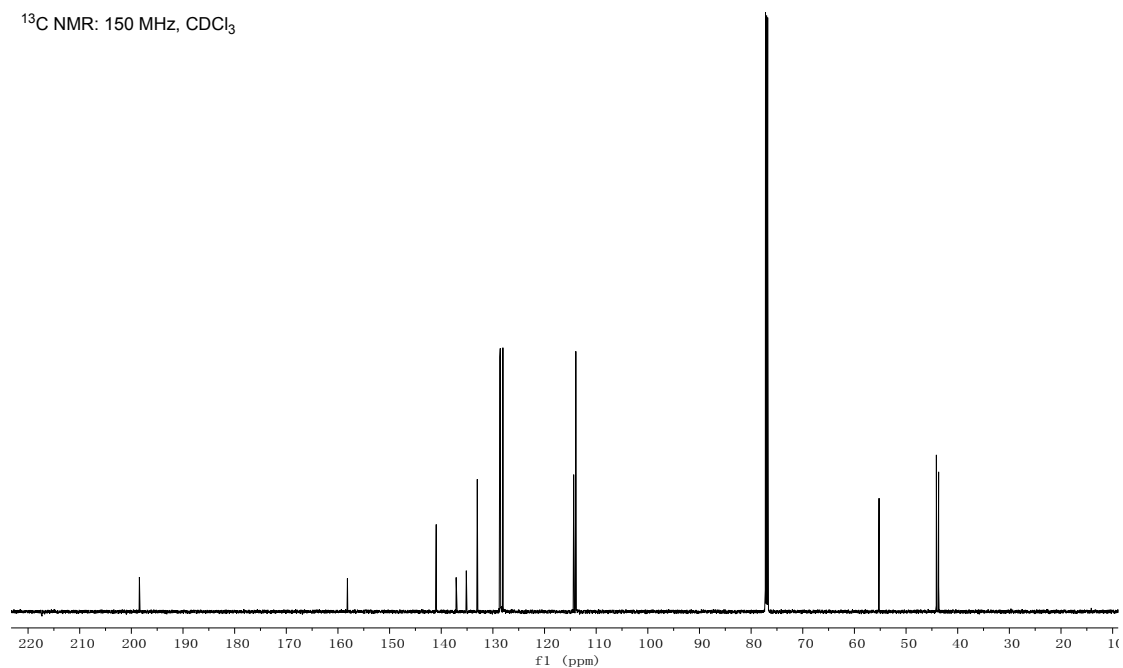


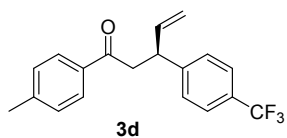


^1H NMR: 600 MHz, CDCl_3

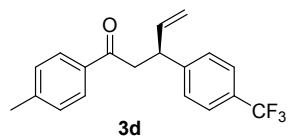
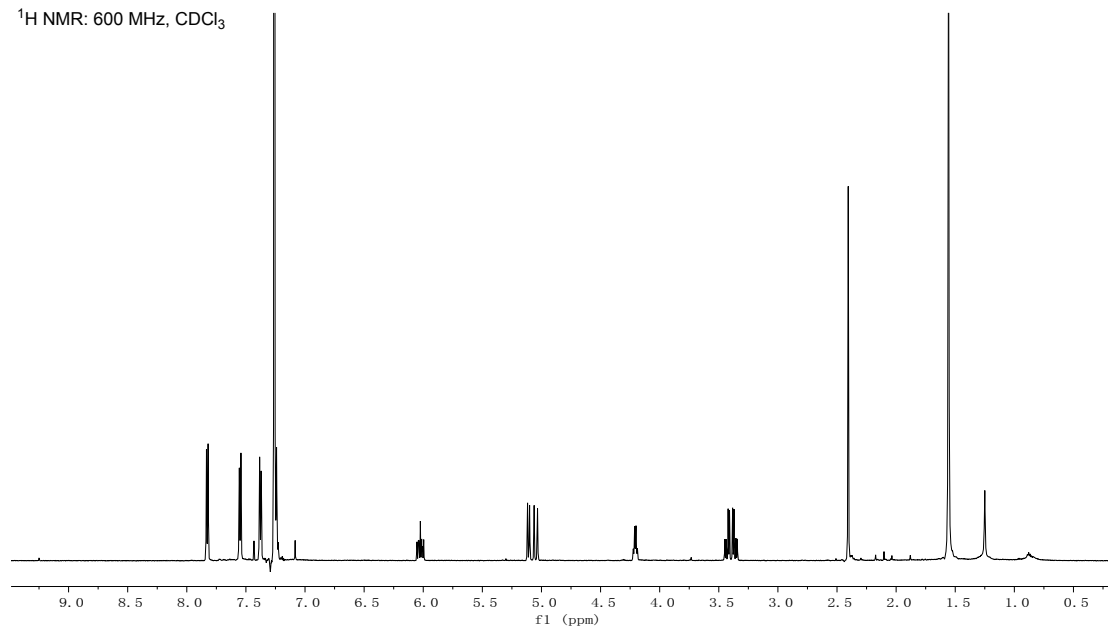


^{13}C NMR: 150 MHz, CDCl_3

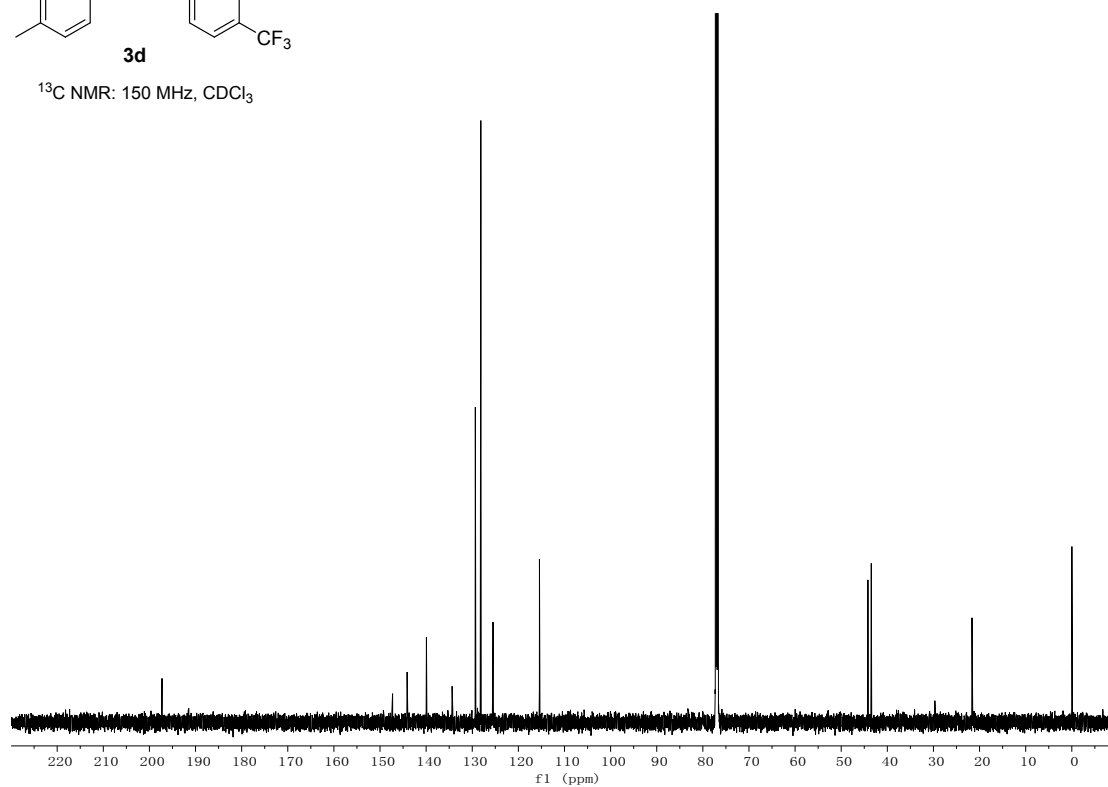


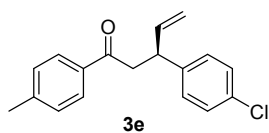


^1H NMR: 600 MHz, CDCl_3

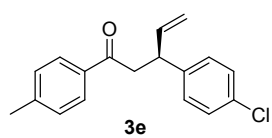
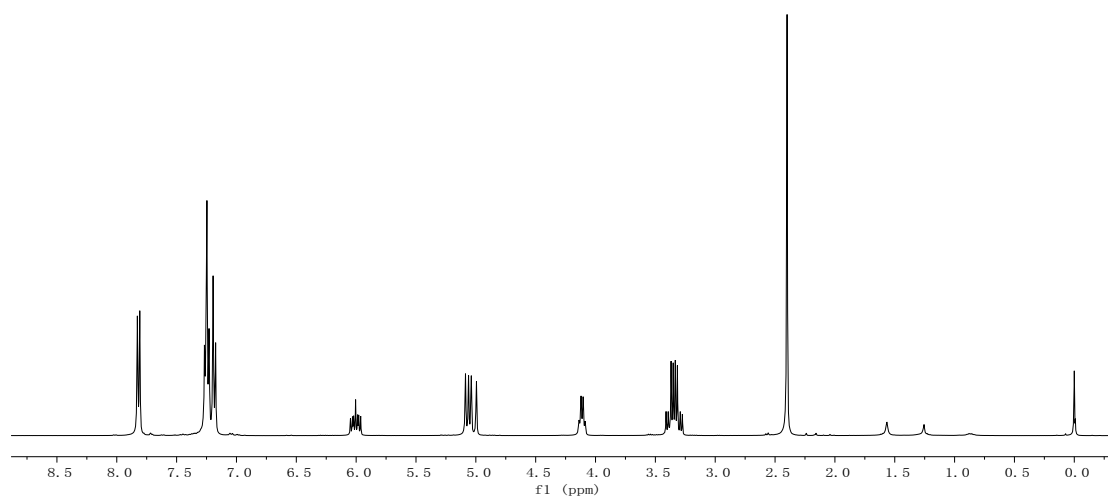


^{13}C NMR: 150 MHz, CDCl_3

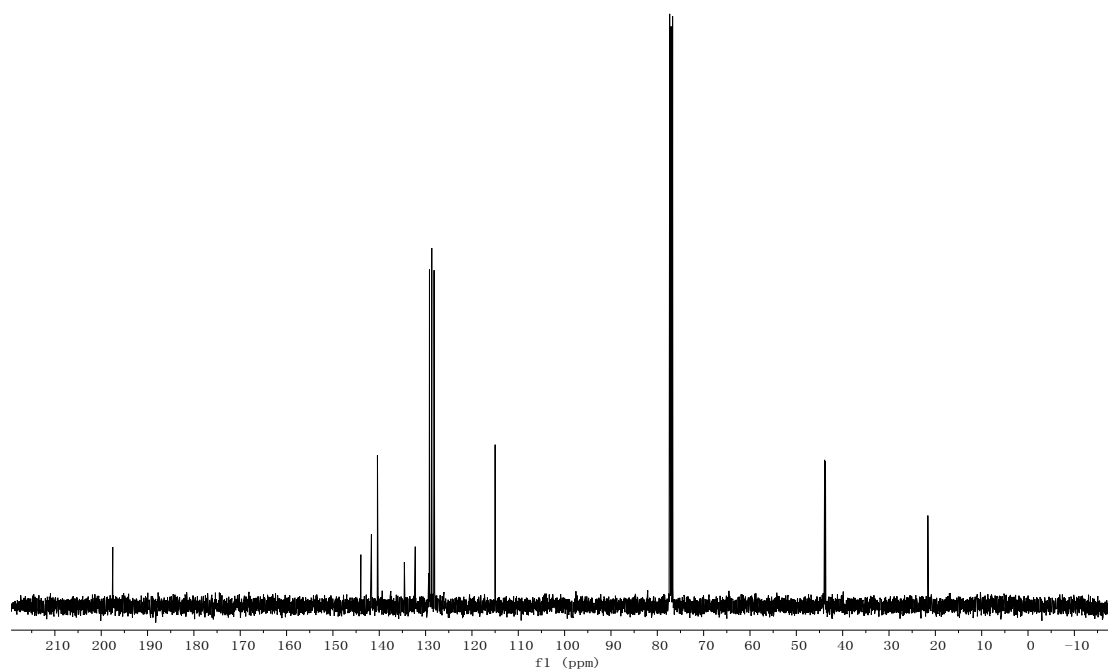


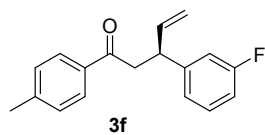


^1H NMR: 400 MHz, CDCl_3

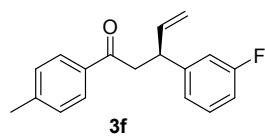
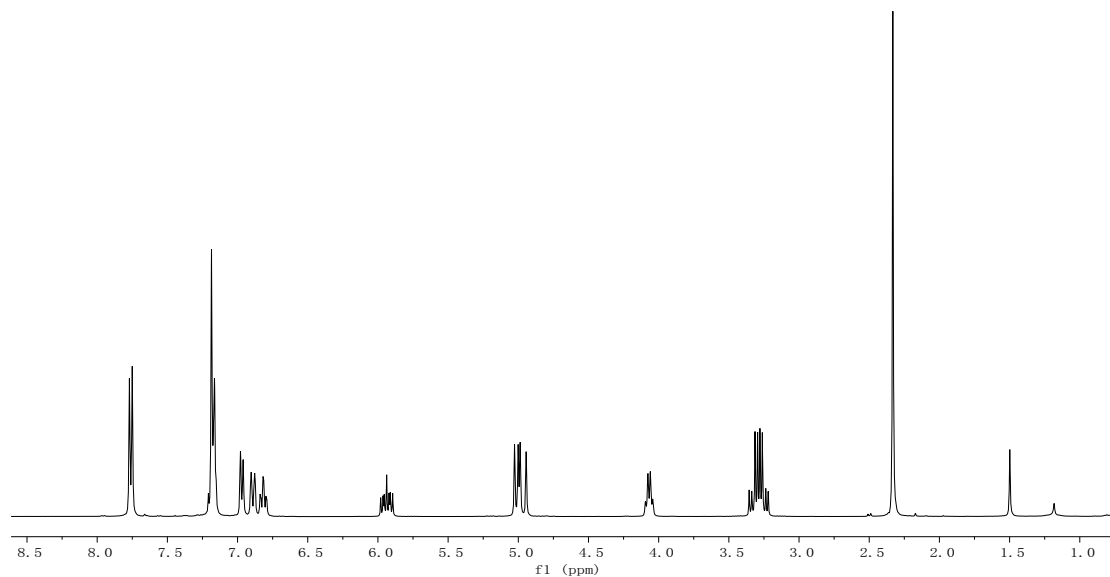


^{13}C NMR: 100 MHz, CDCl_3

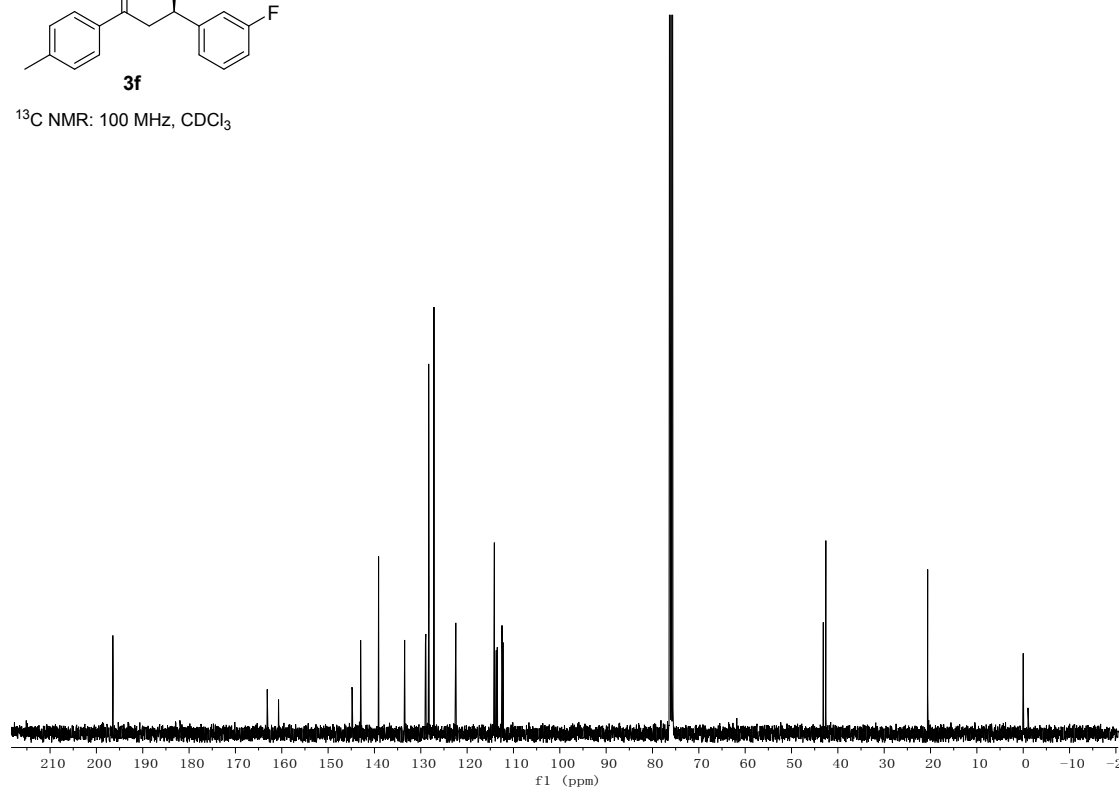


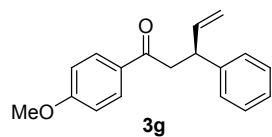


^1H NMR: 400 MHz, CDCl_3

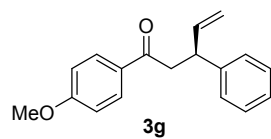
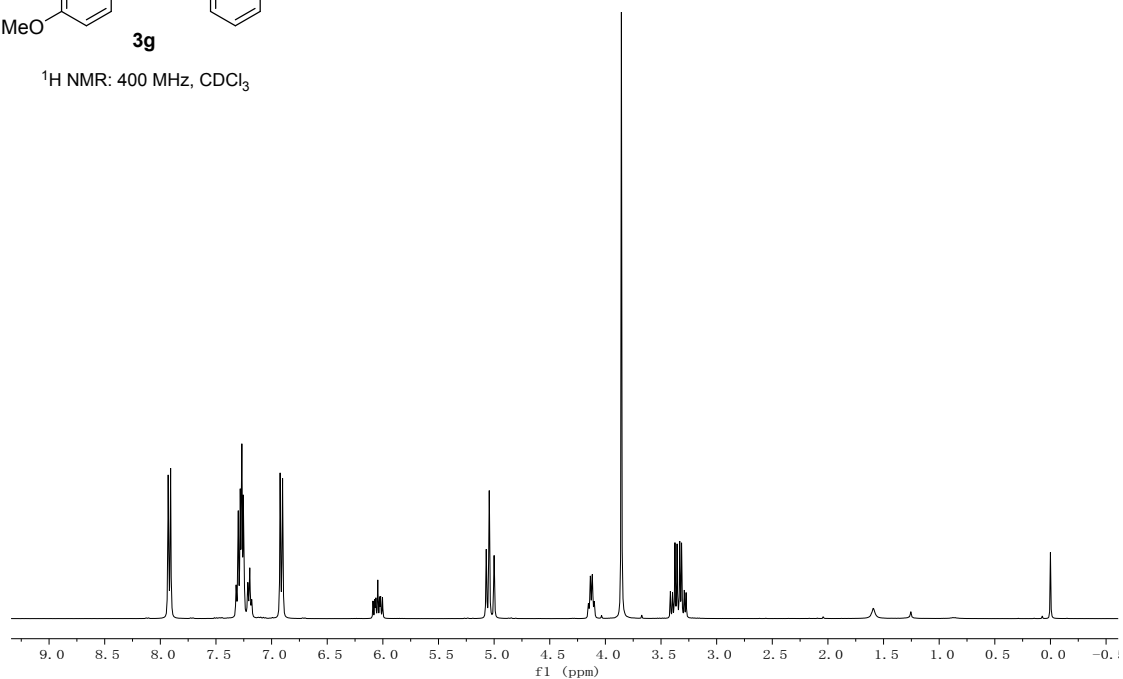


^{13}C NMR: 100 MHz, CDCl_3

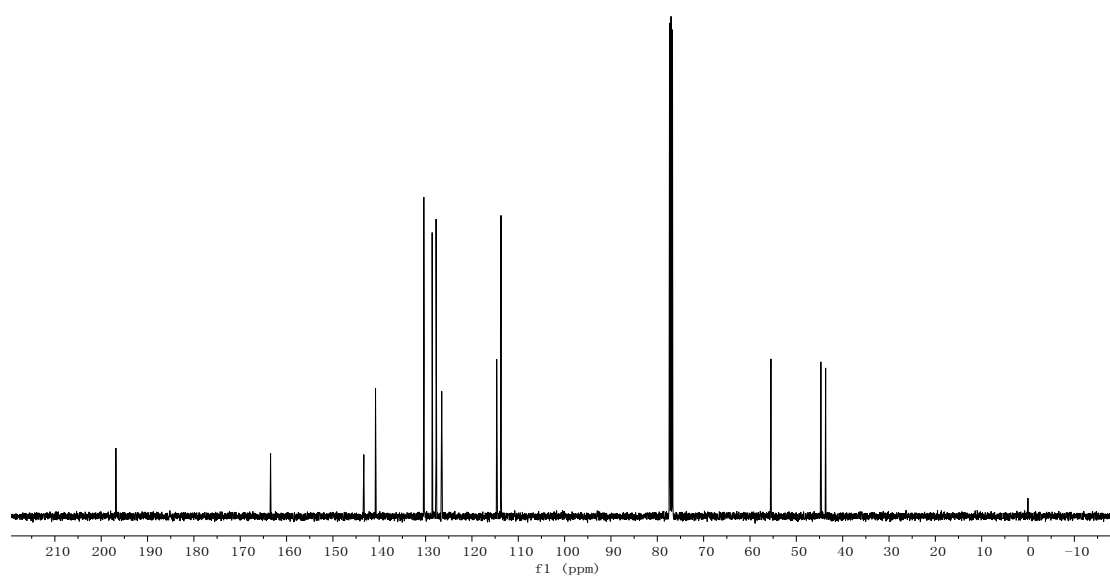


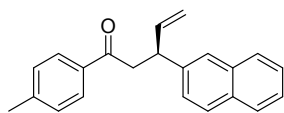


^1H NMR: 400 MHz, CDCl_3



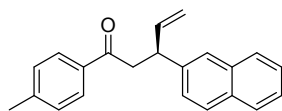
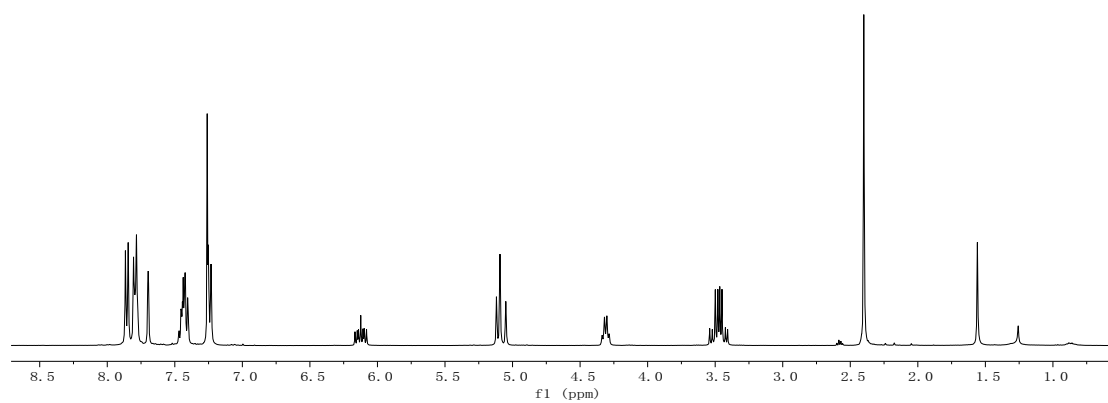
^{13}C NMR: 100 MHz, CDCl_3





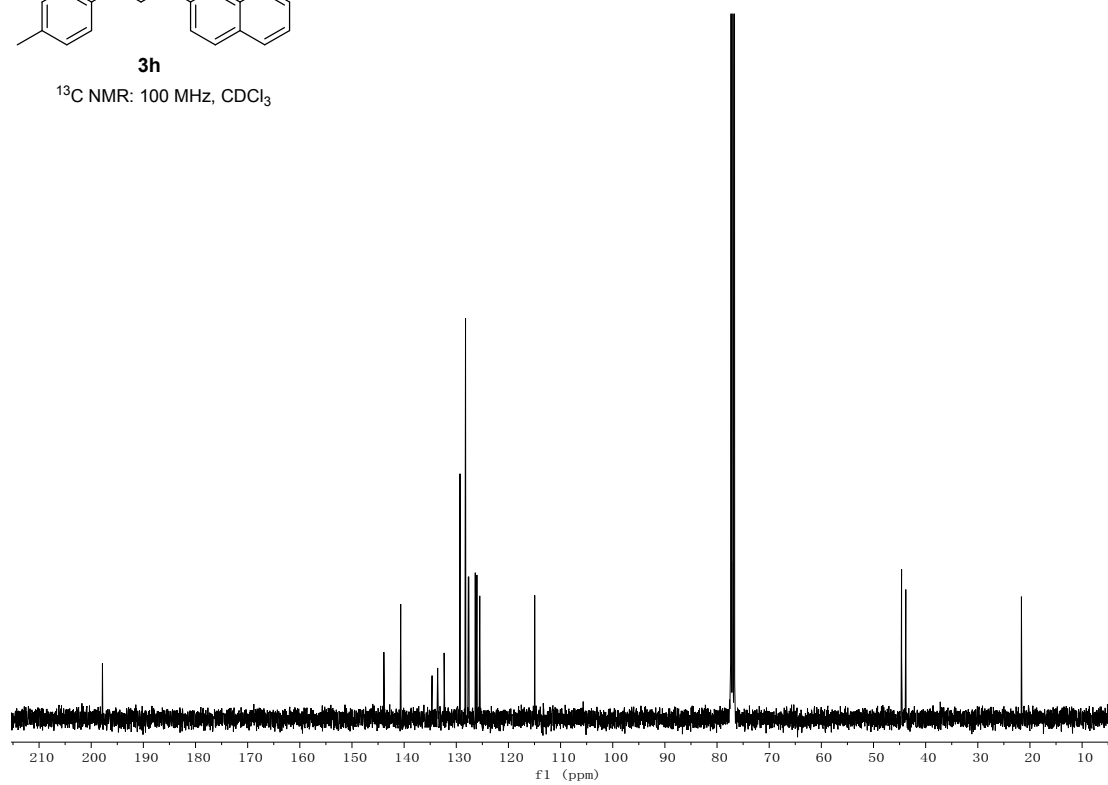
3h

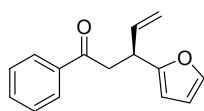
^1H NMR: 400 MHz, CDCl_3



3h

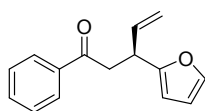
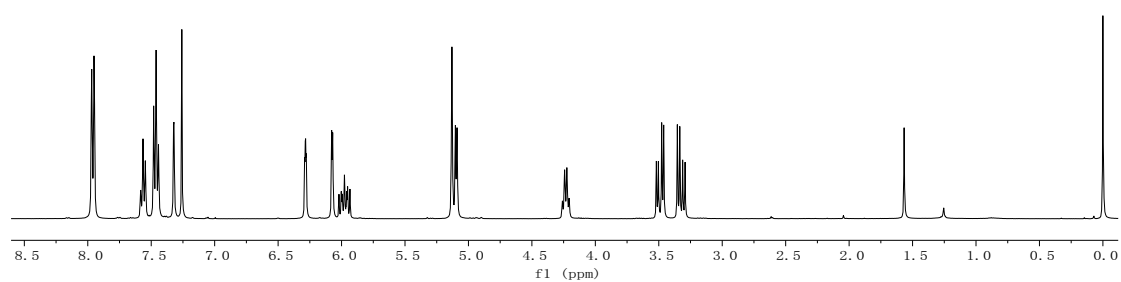
^{13}C NMR: 100 MHz, CDCl_3





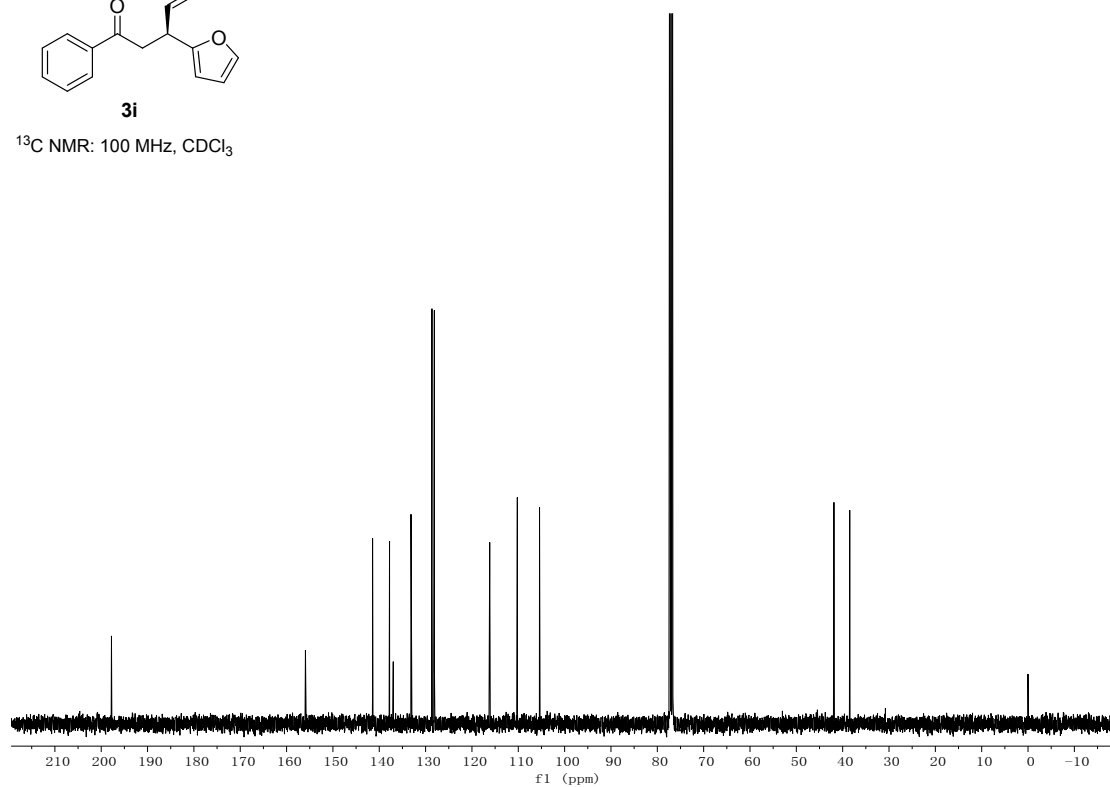
3i

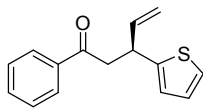
^1H NMR: 400 MHz, CDCl_3



3i

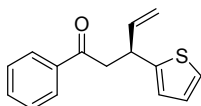
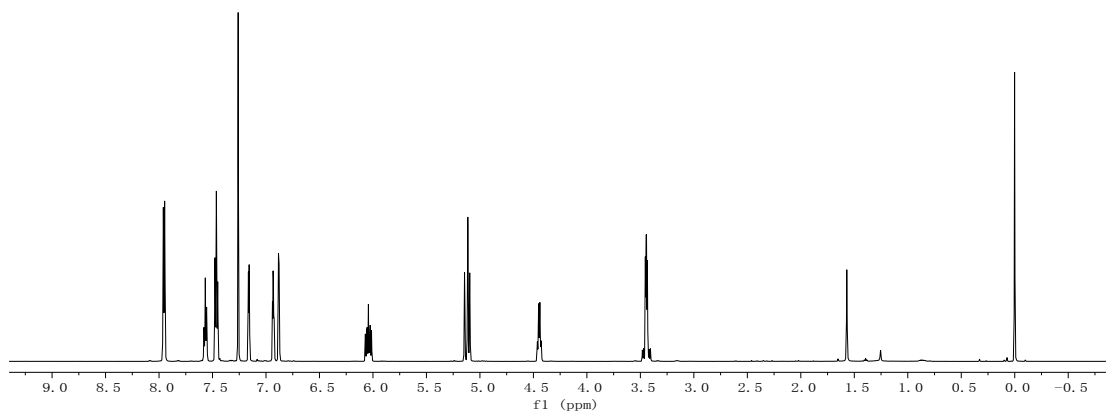
^{13}C NMR: 100 MHz, CDCl_3





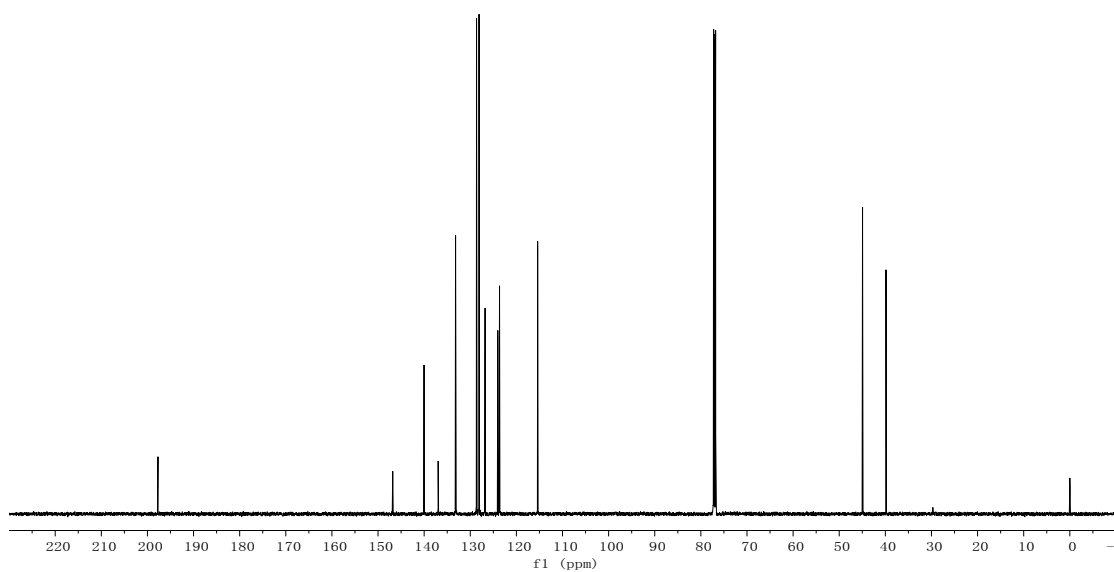
3j

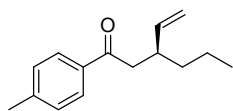
^1H NMR: 600 MHz, CDCl_3



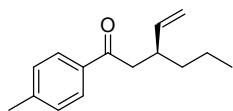
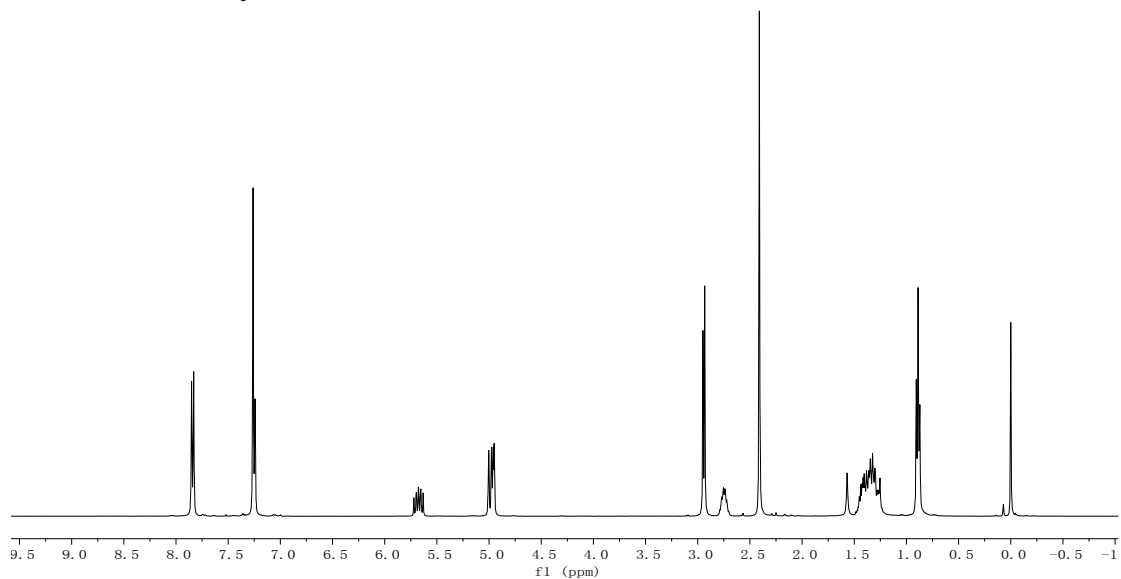
3j

^{13}C NMR: 150 MHz, CDCl_3

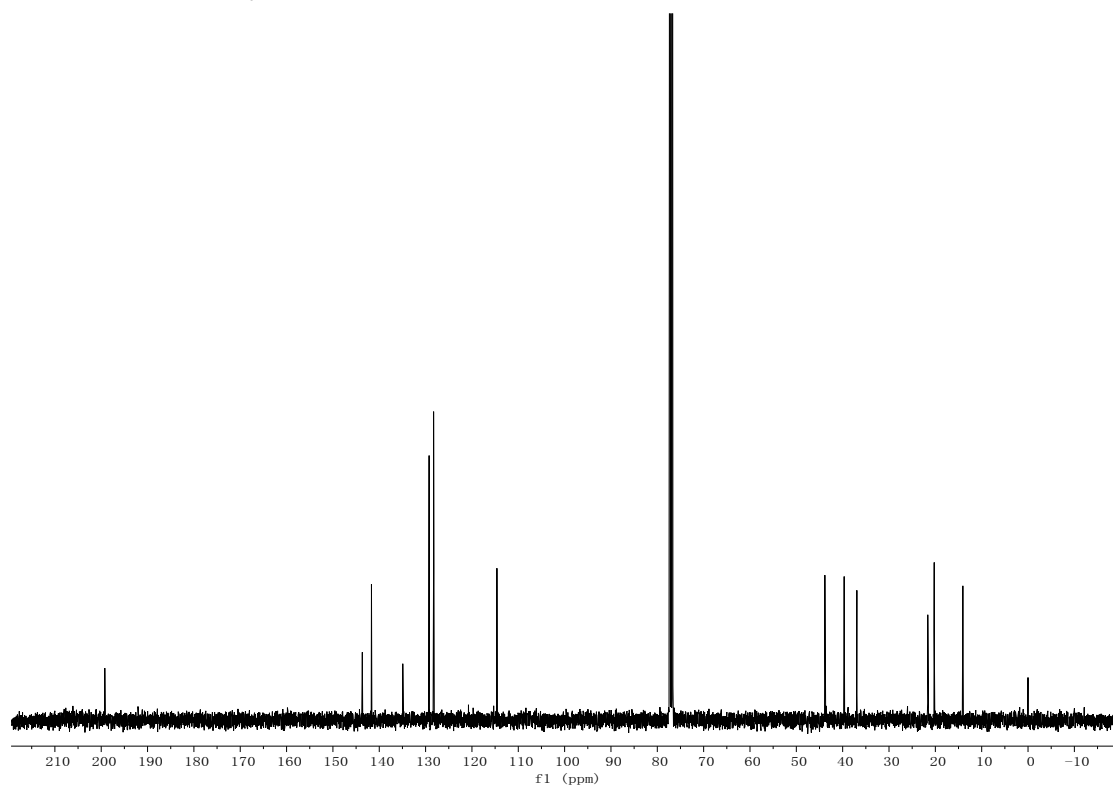


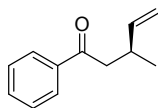


^1H NMR: 400 MHz, CDCl_3



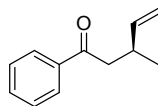
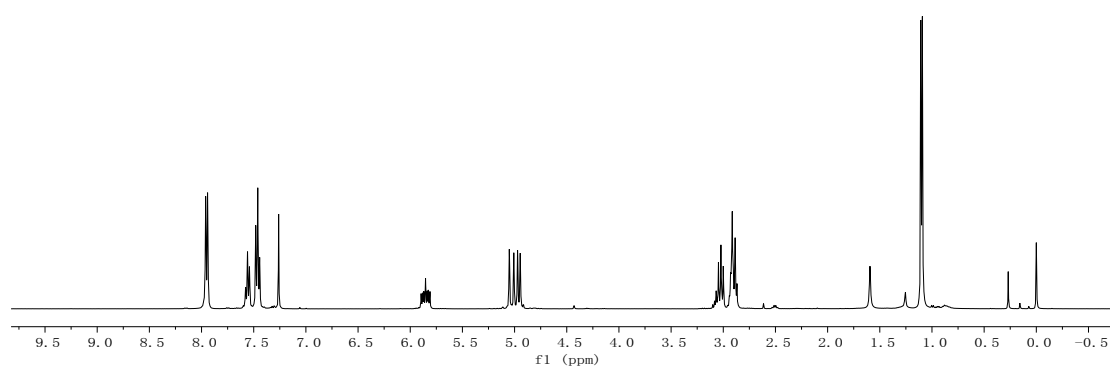
^{13}C NMR: 100 MHz, CDCl_3





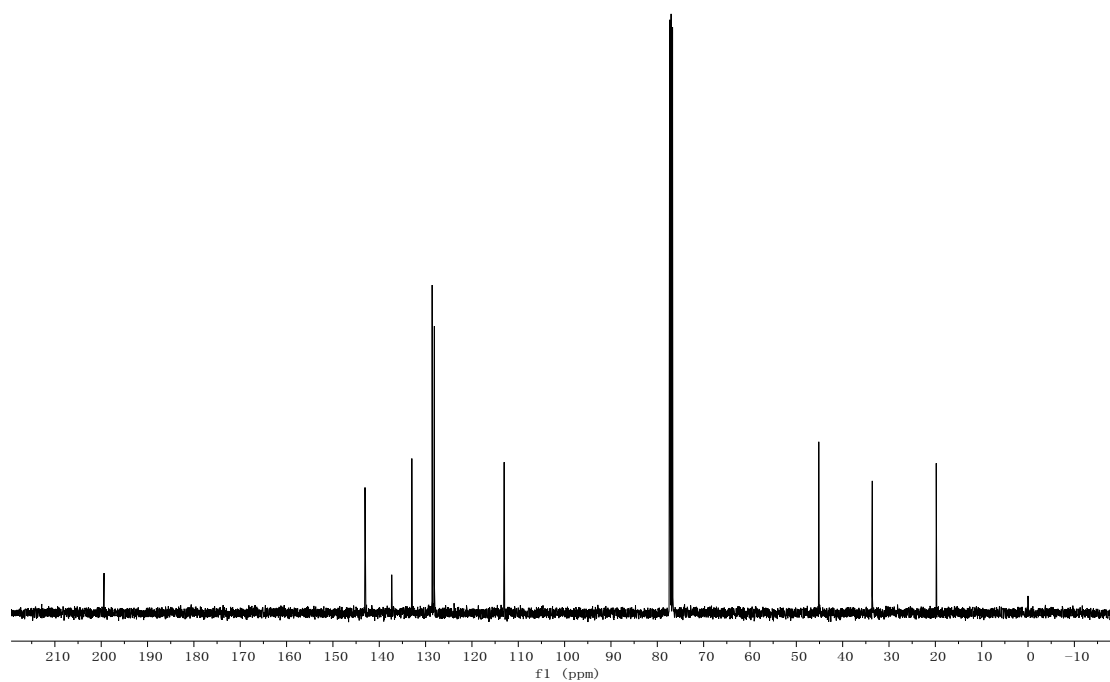
3I

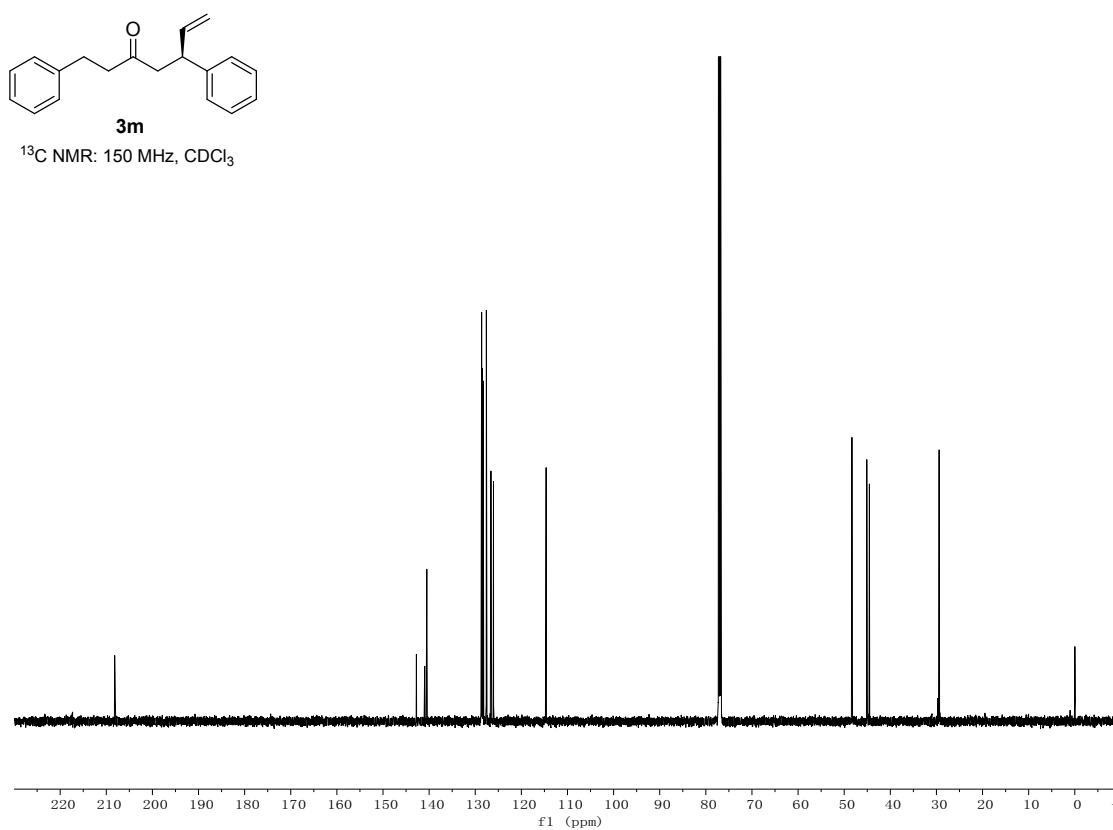
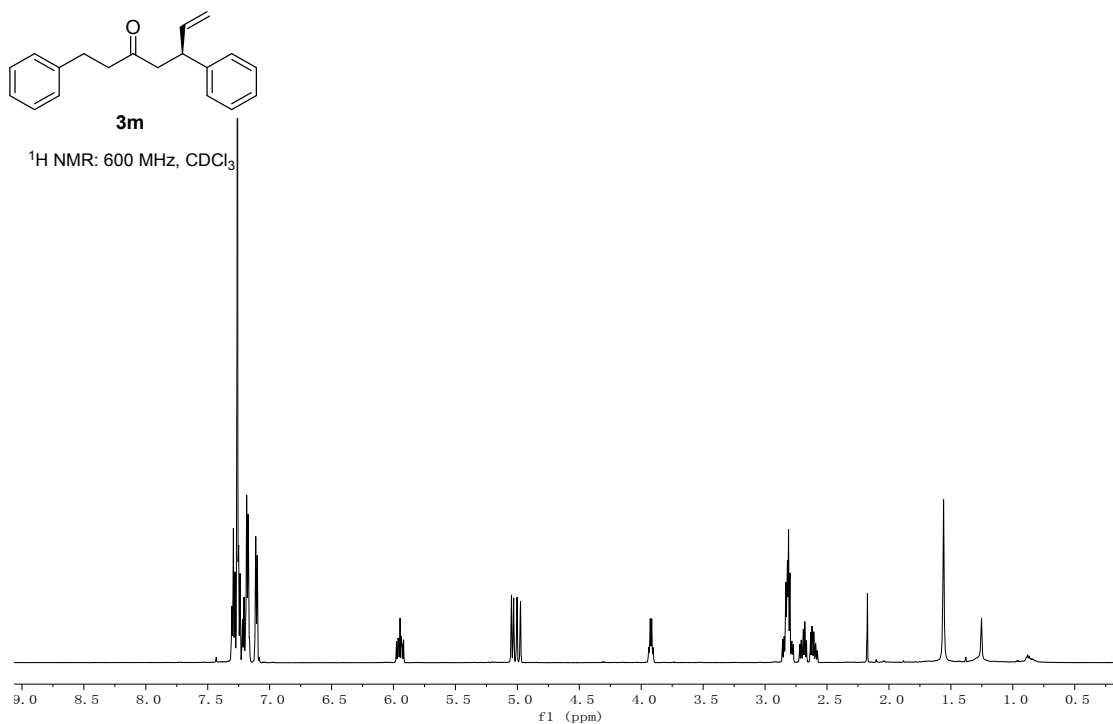
^1H NMR: 400 MHz, CDCl_3

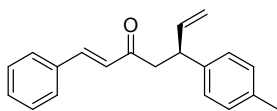


3I

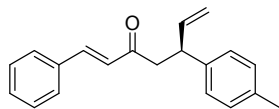
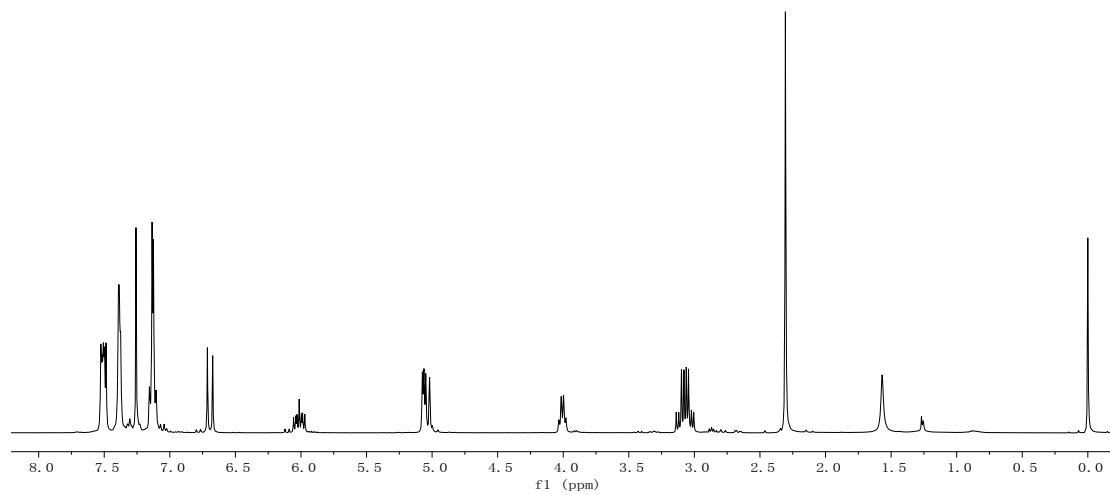
^{13}C NMR: 100 MHz, CDCl_3



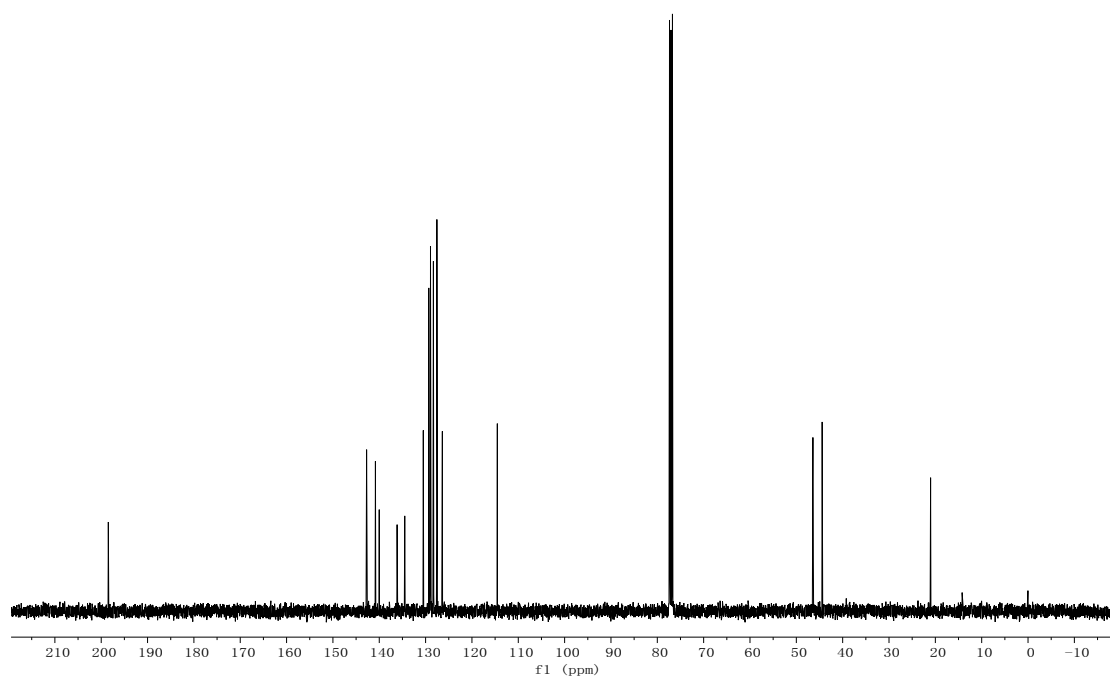


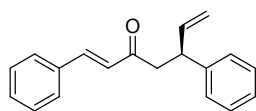


6a
 ^1H NMR: 400 MHz, CDCl_3



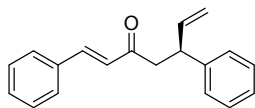
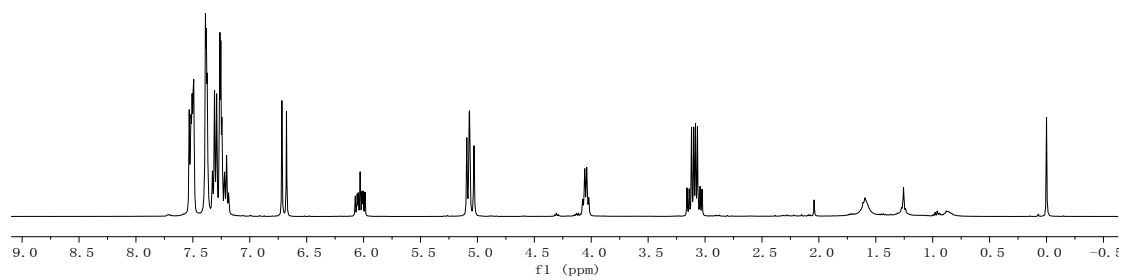
6a
 ^{13}C NMR: 100 MHz, CDCl_3





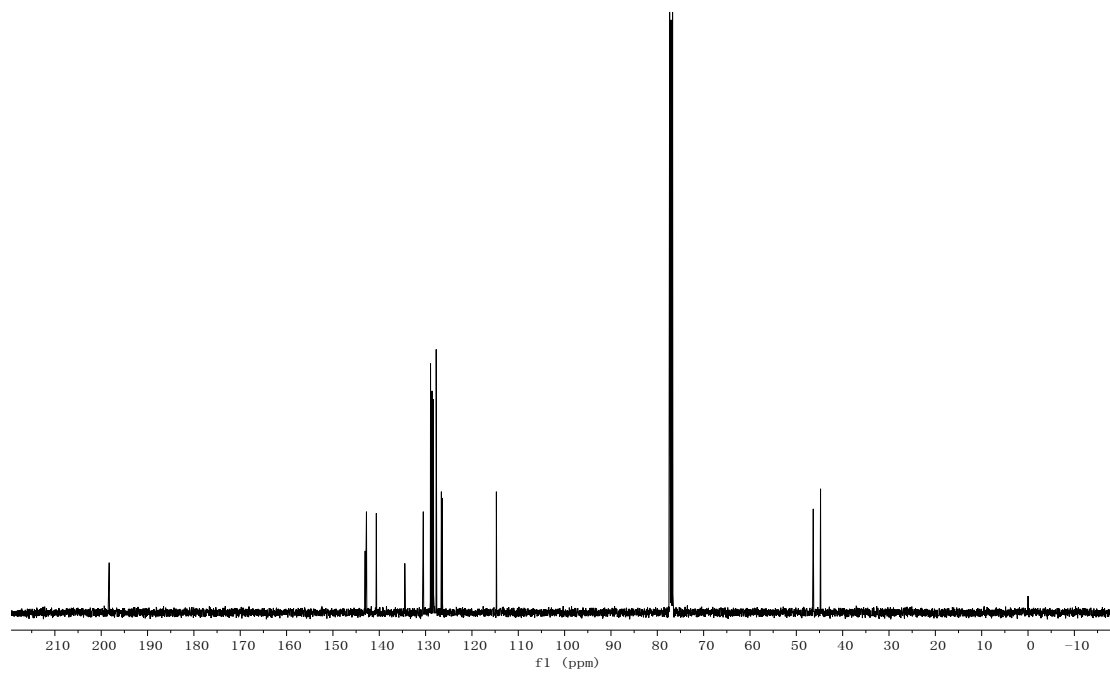
6b

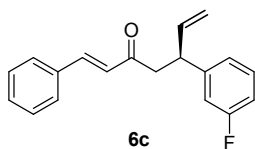
^1H NMR: 400 MHz, CDCl_3



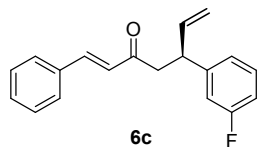
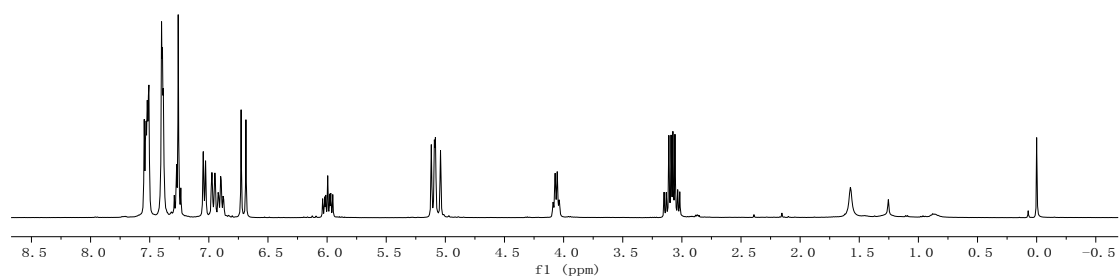
6b

^{13}C NMR: 100 MHz, CDCl_3

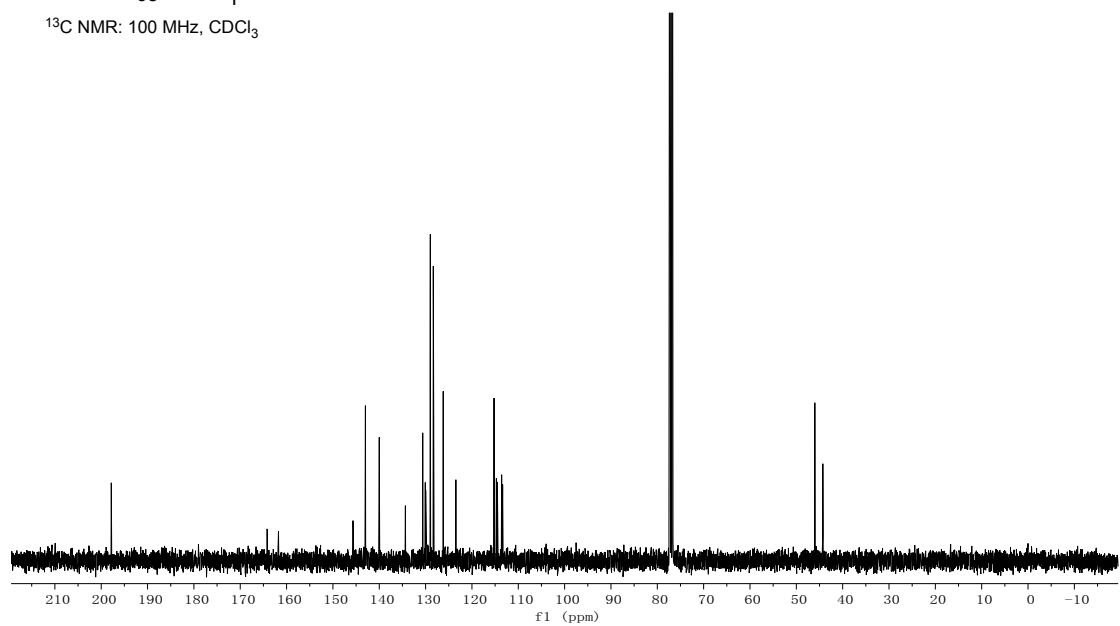


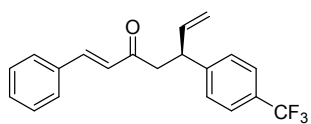


^1H NMR: 400 MHz, CDCl_3



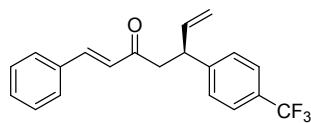
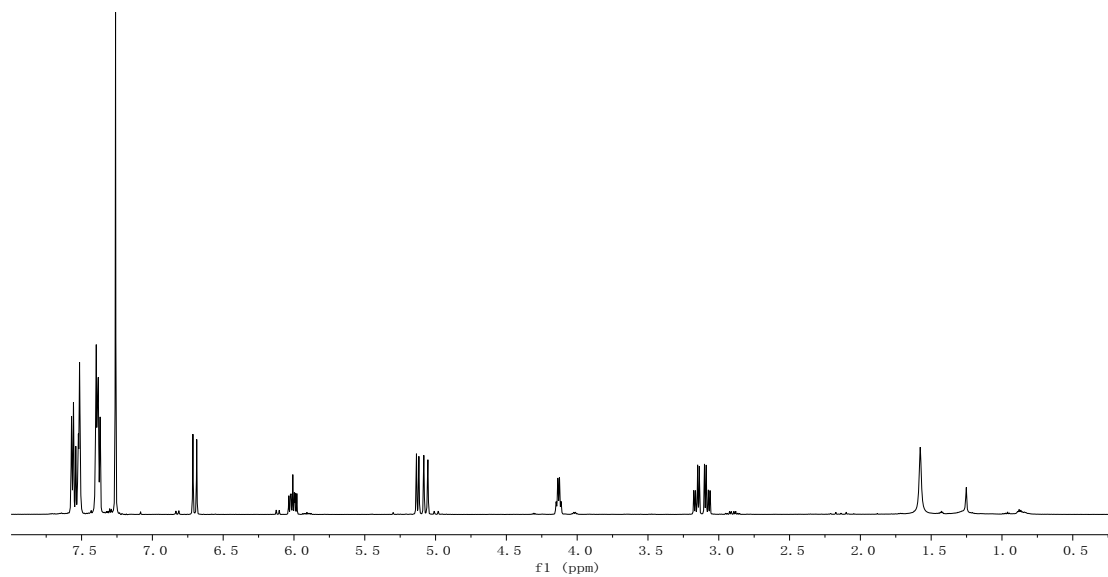
^{13}C NMR: 100 MHz, CDCl_3





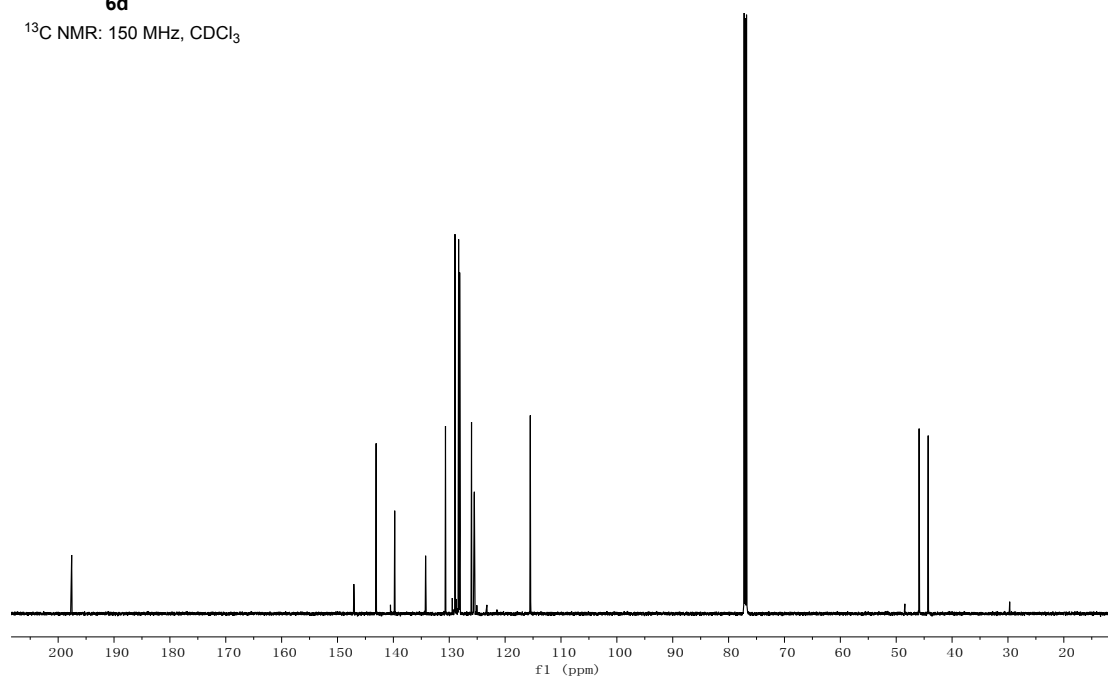
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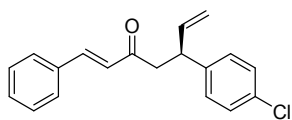
¹H NMR: 400 MHz, CDCl₃



6d

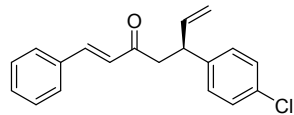
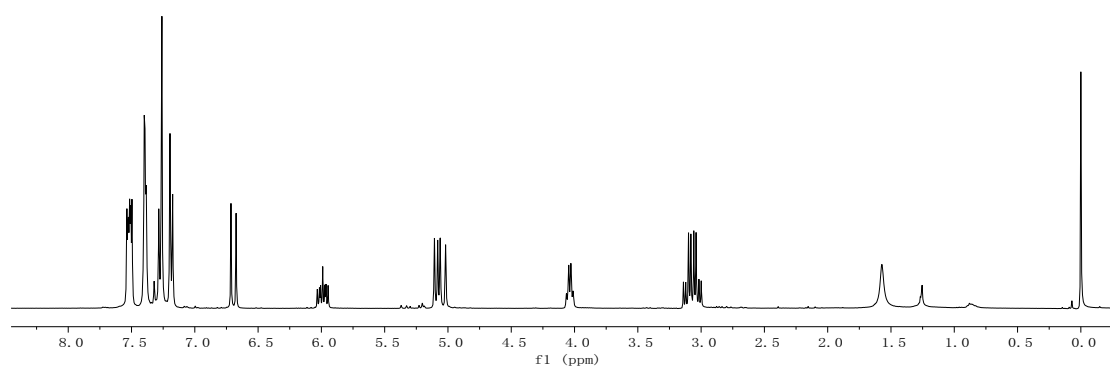
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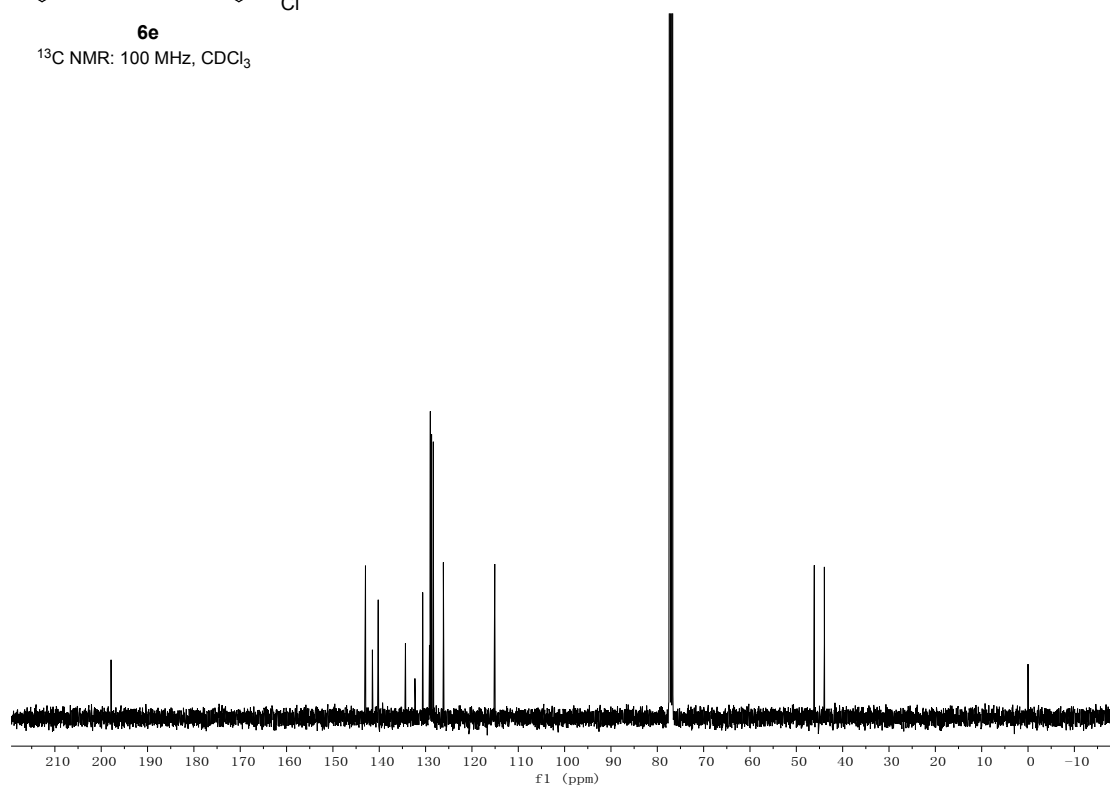
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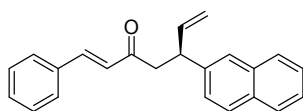
^1H NMR: 400 MHz, CDCl_3



6e

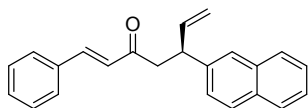
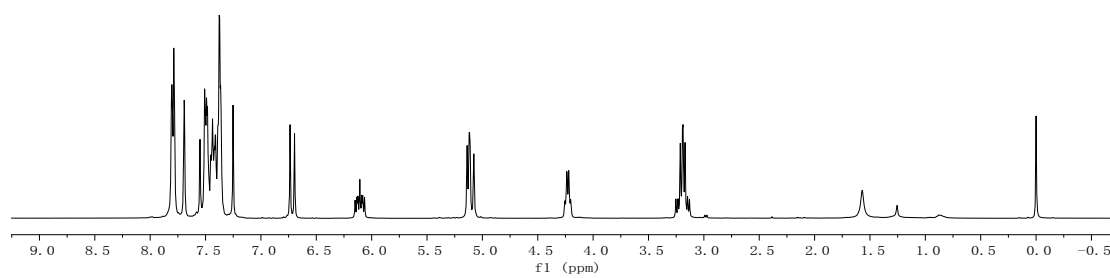
^{13}C NMR: 100 MHz, CDCl_3





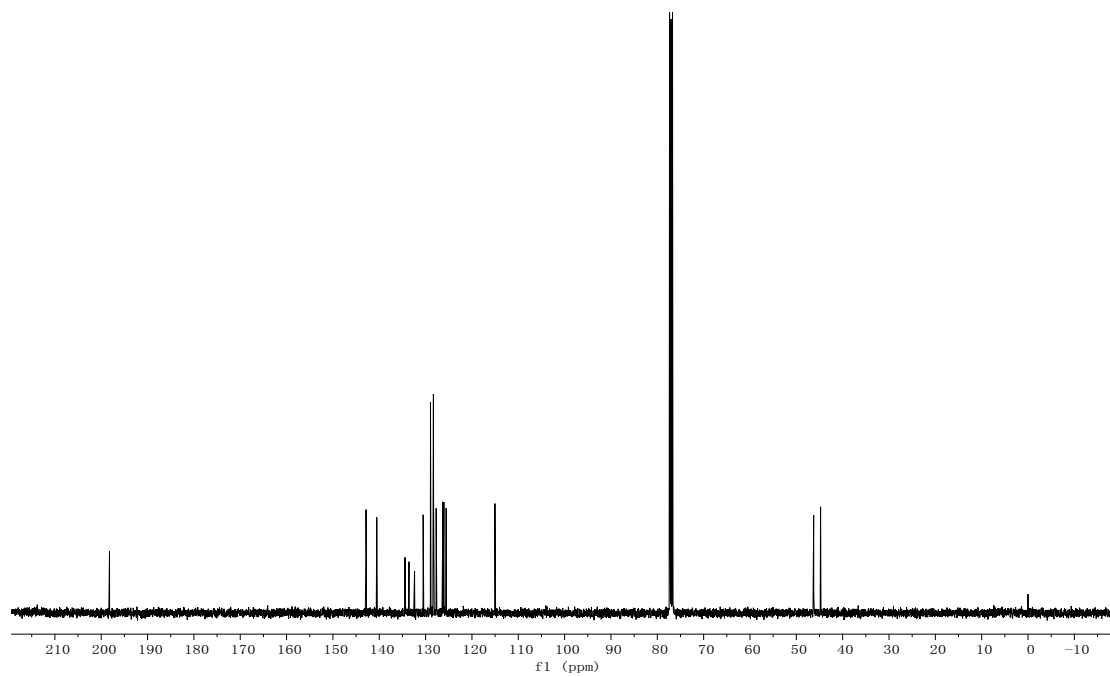
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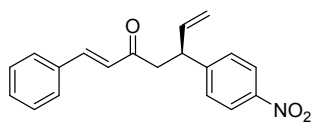
^1H NMR: 400 MHz, CDCl_3



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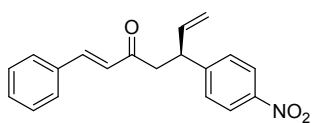
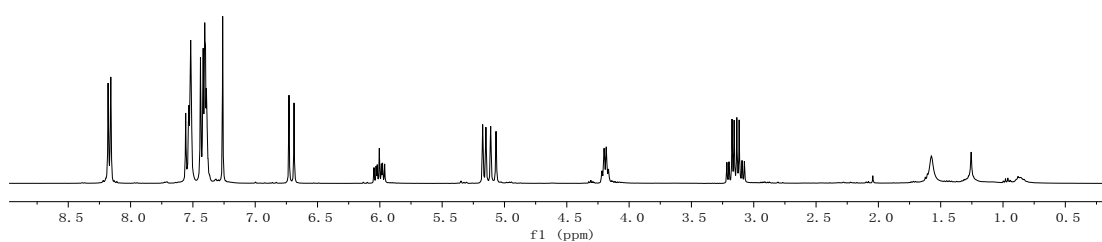
^{13}C NMR: 100 MHz, CDCl_3





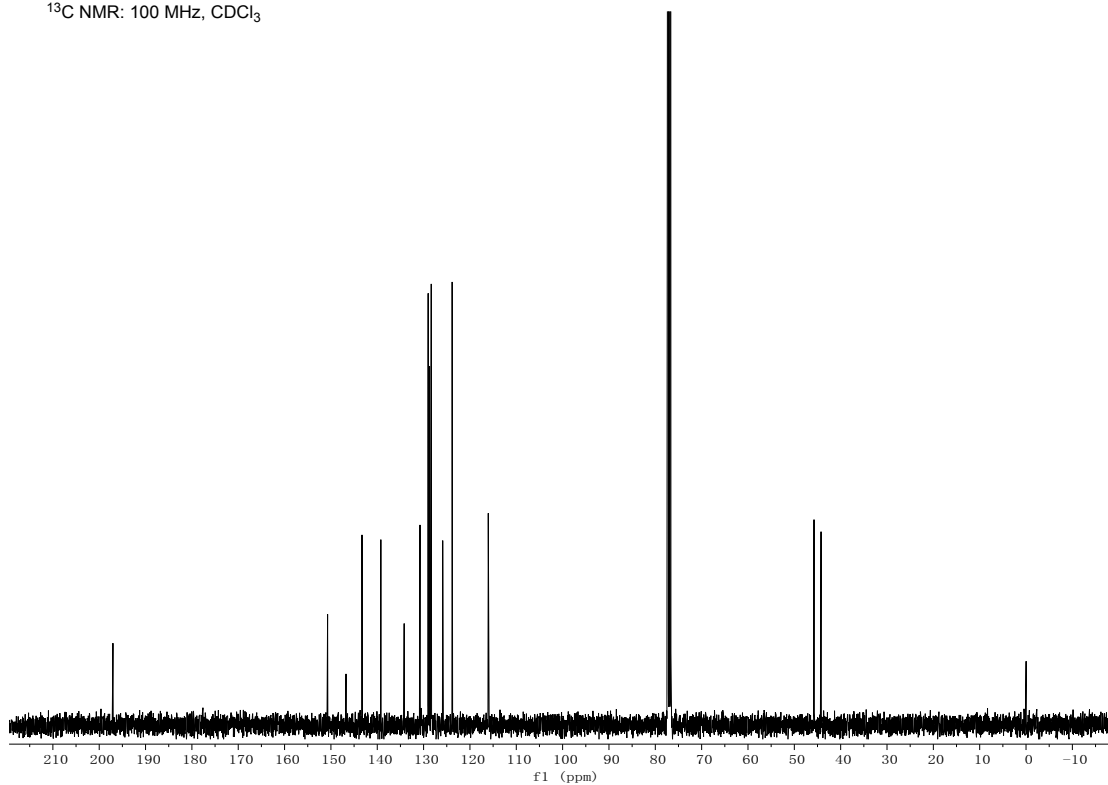
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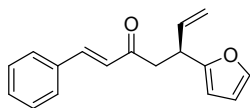
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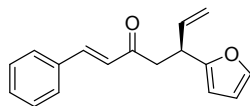
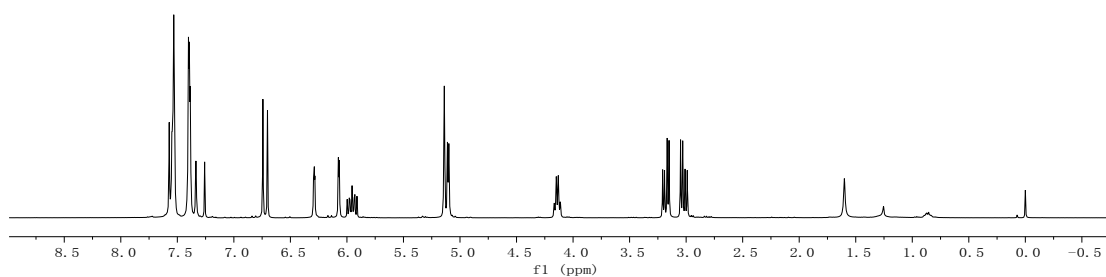
^{13}C NMR: 100 MHz, CDCl_3





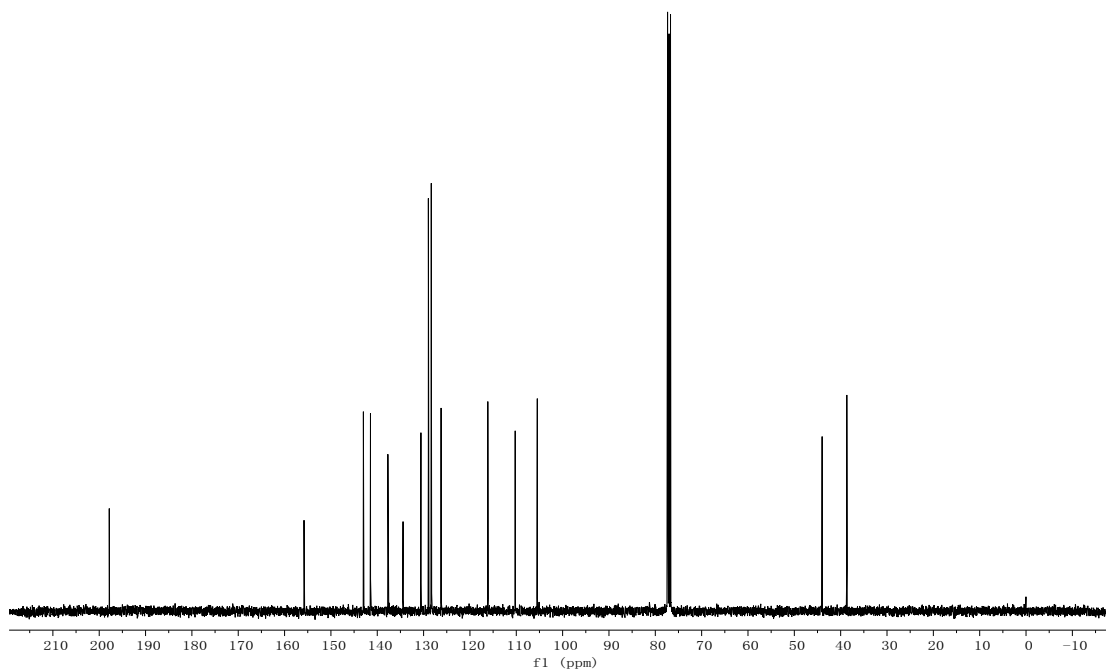
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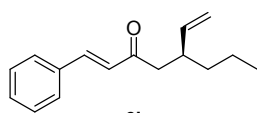
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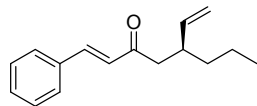
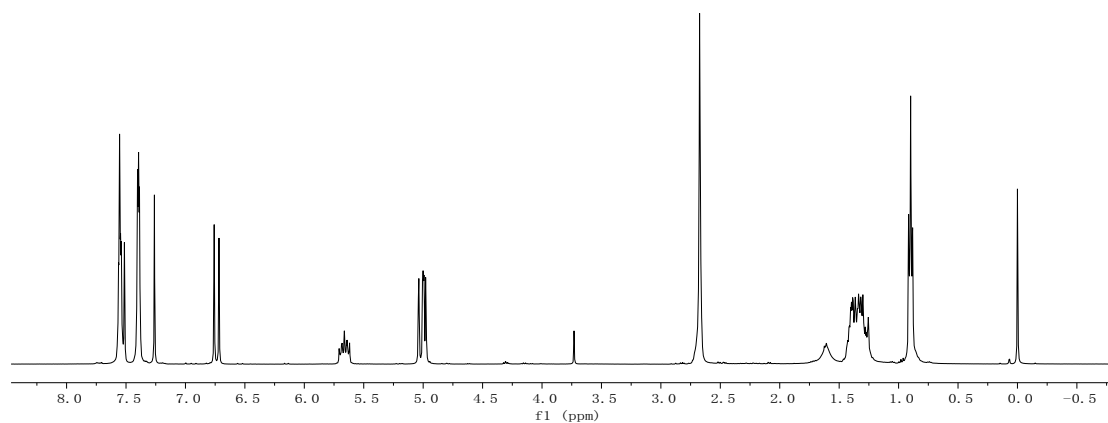
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^{13}C NMR: 100 MHz, CDCl_3

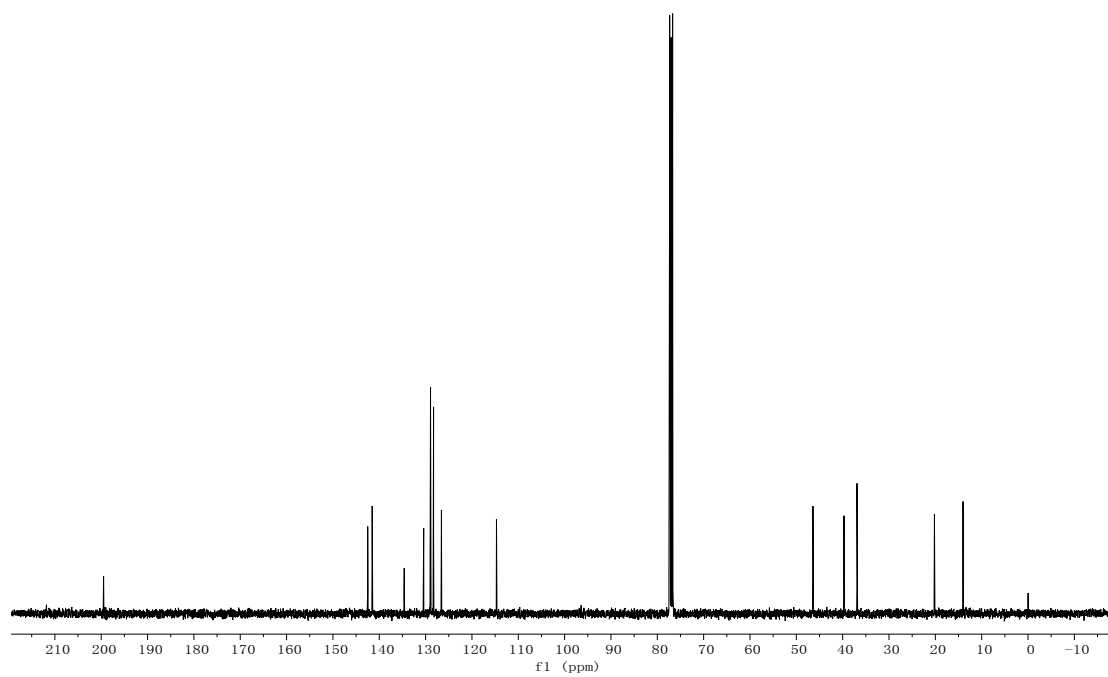


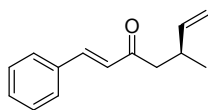


^1H NMR: 400 MHz, CDCl_3



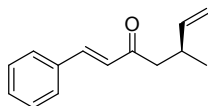
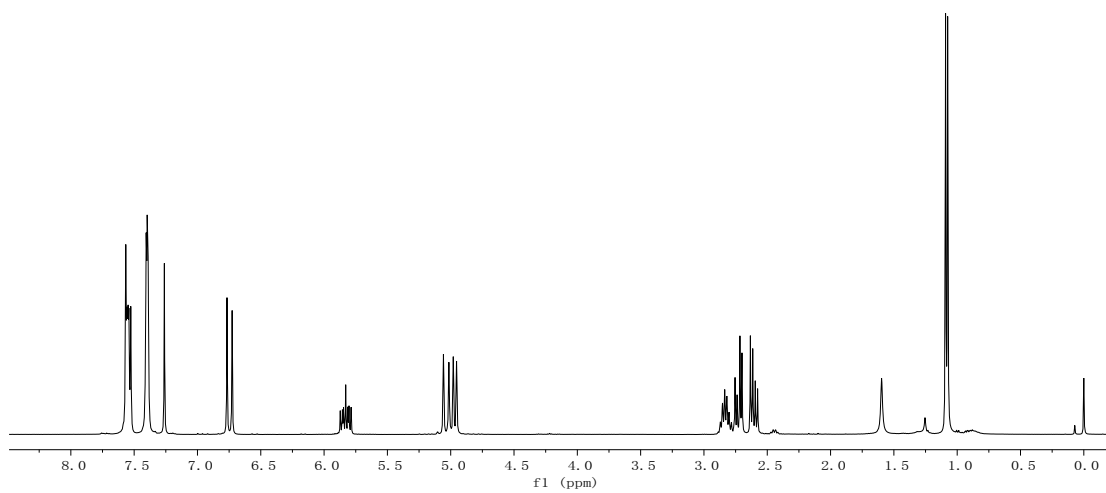
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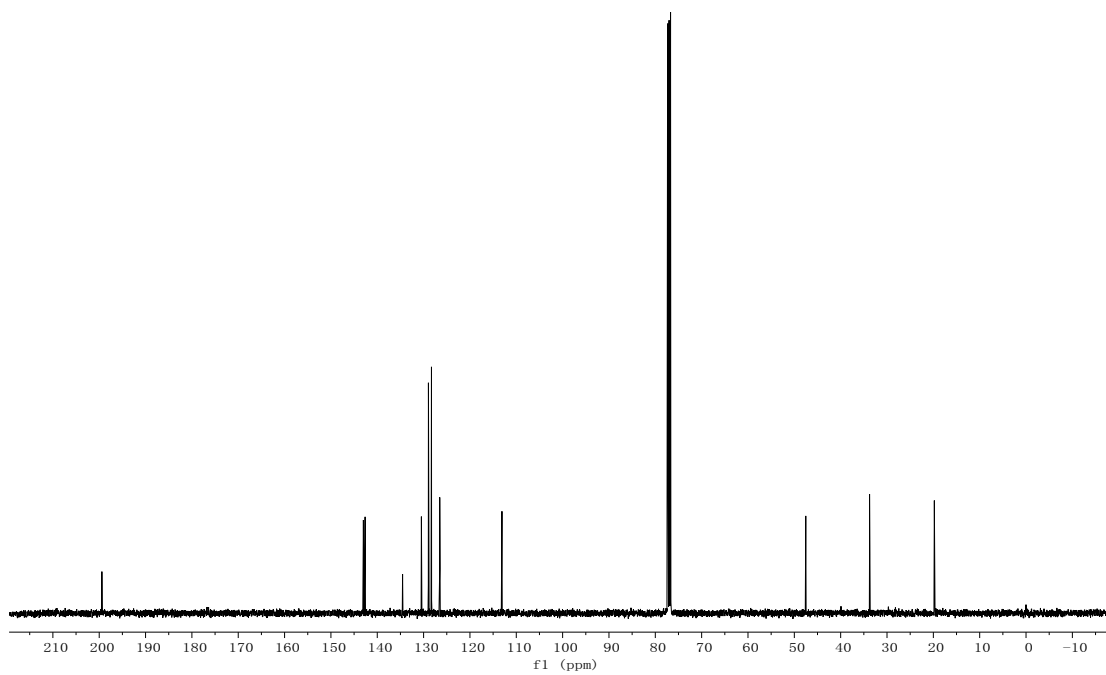
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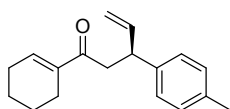
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6j

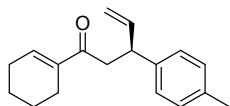
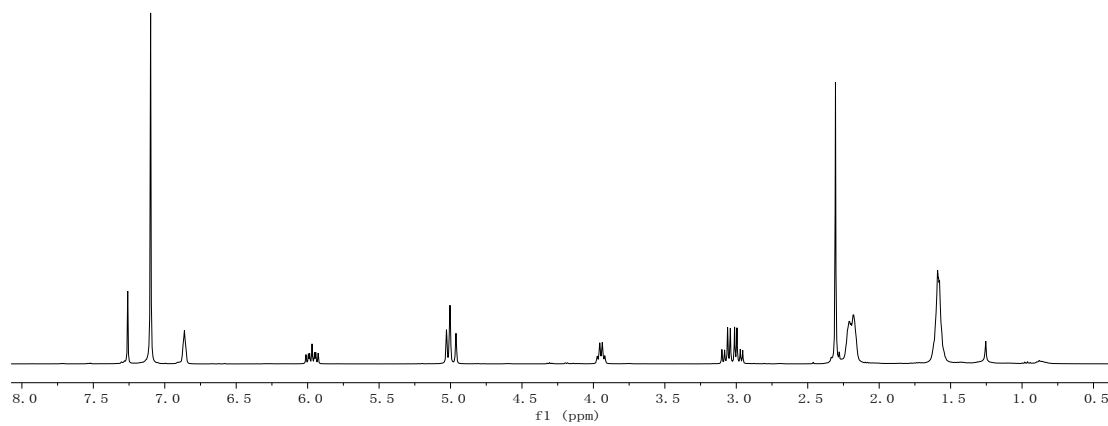
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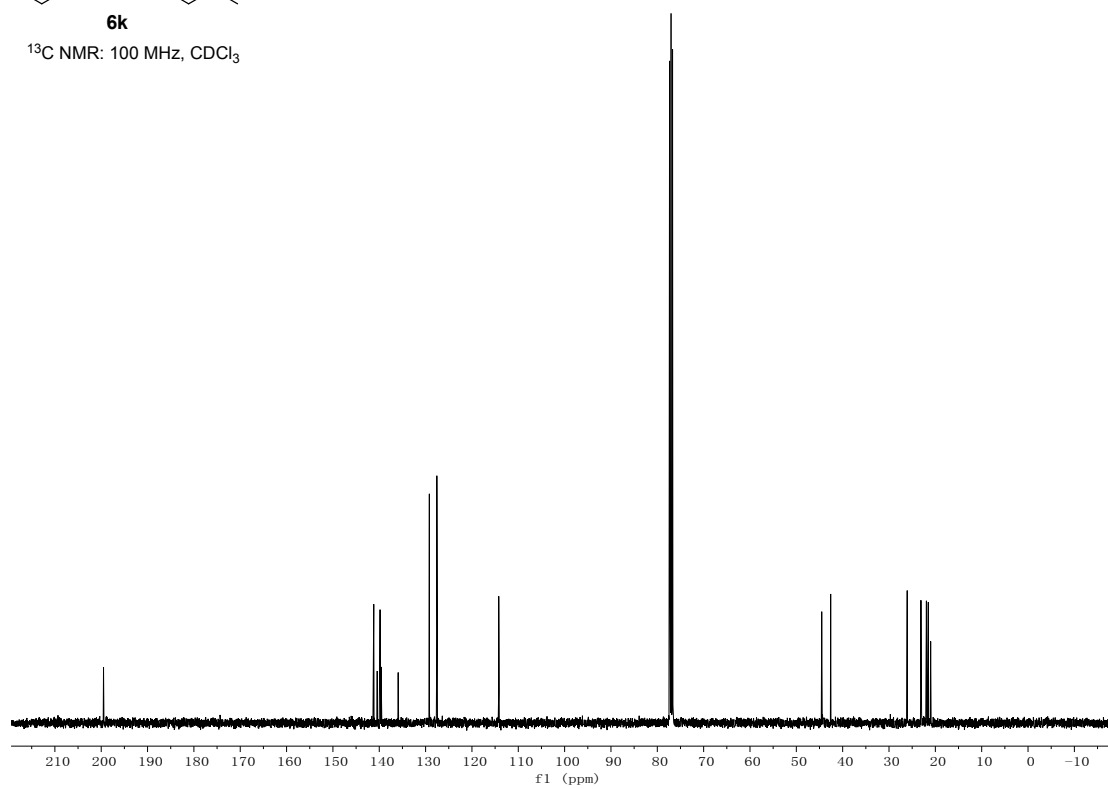
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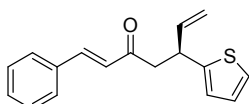
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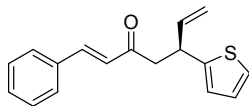
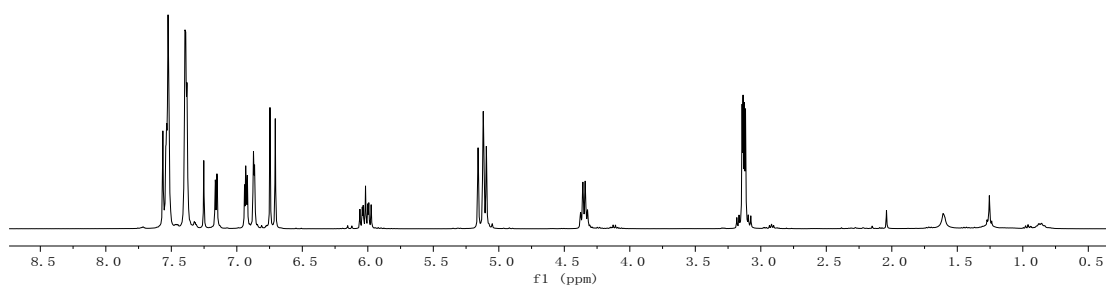
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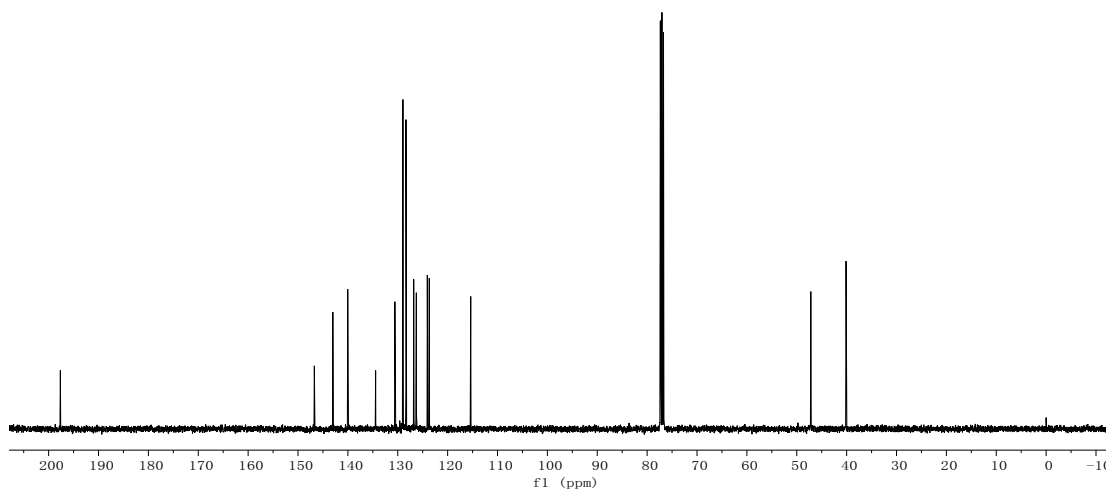
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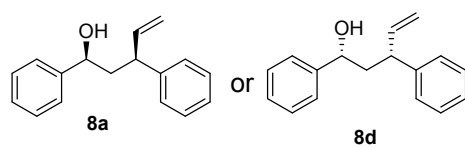
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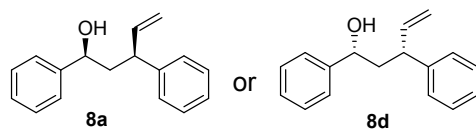
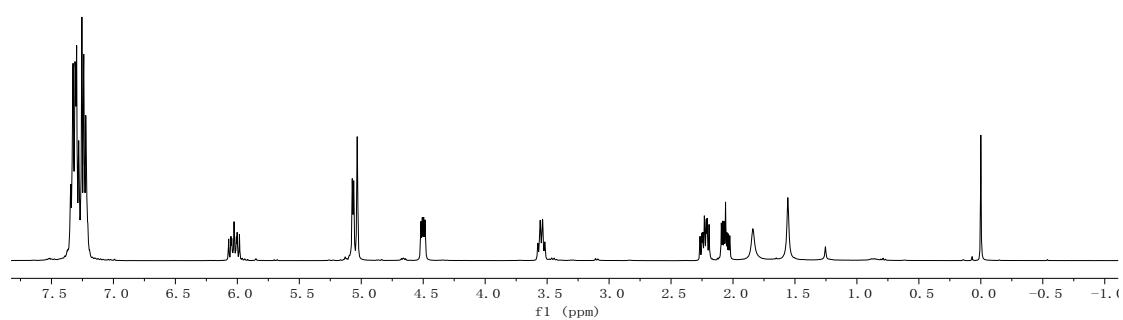
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^{13}C NMR: 100 MHz, CDCl_3

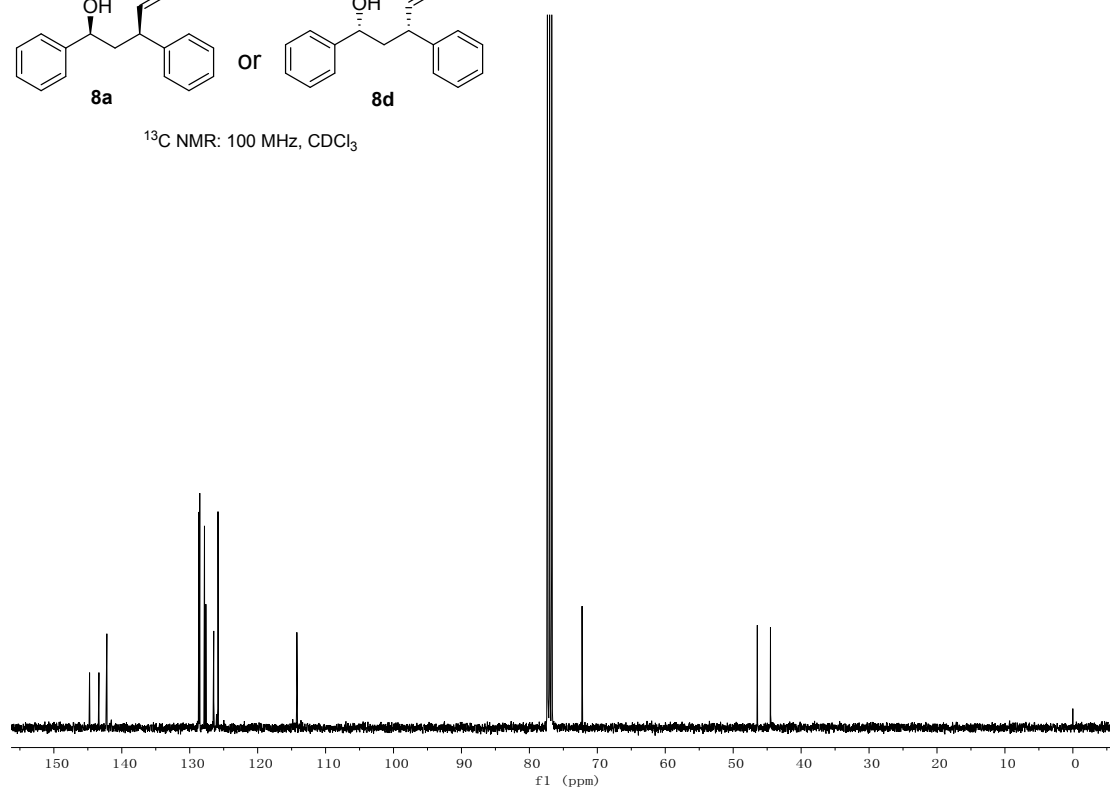


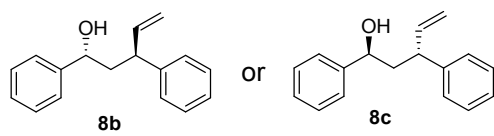


^1H NMR: 400 MHz, CDCl_3

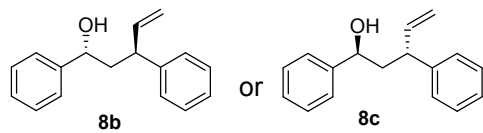
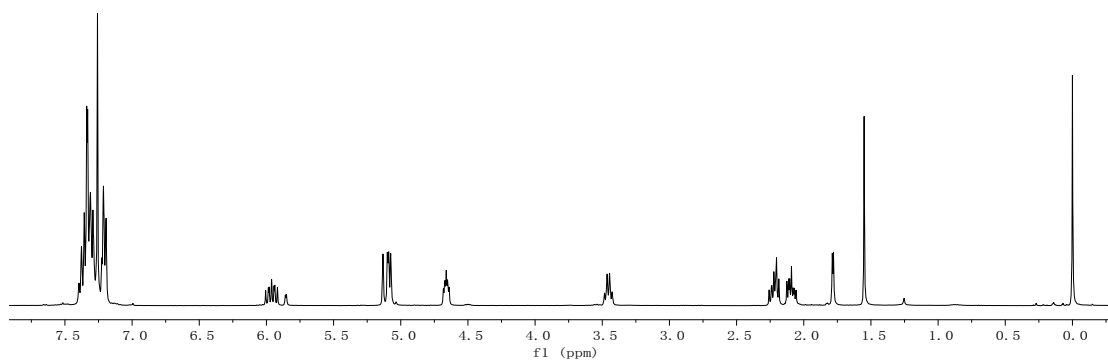


^{13}C NMR: 100 MHz, CDCl_3

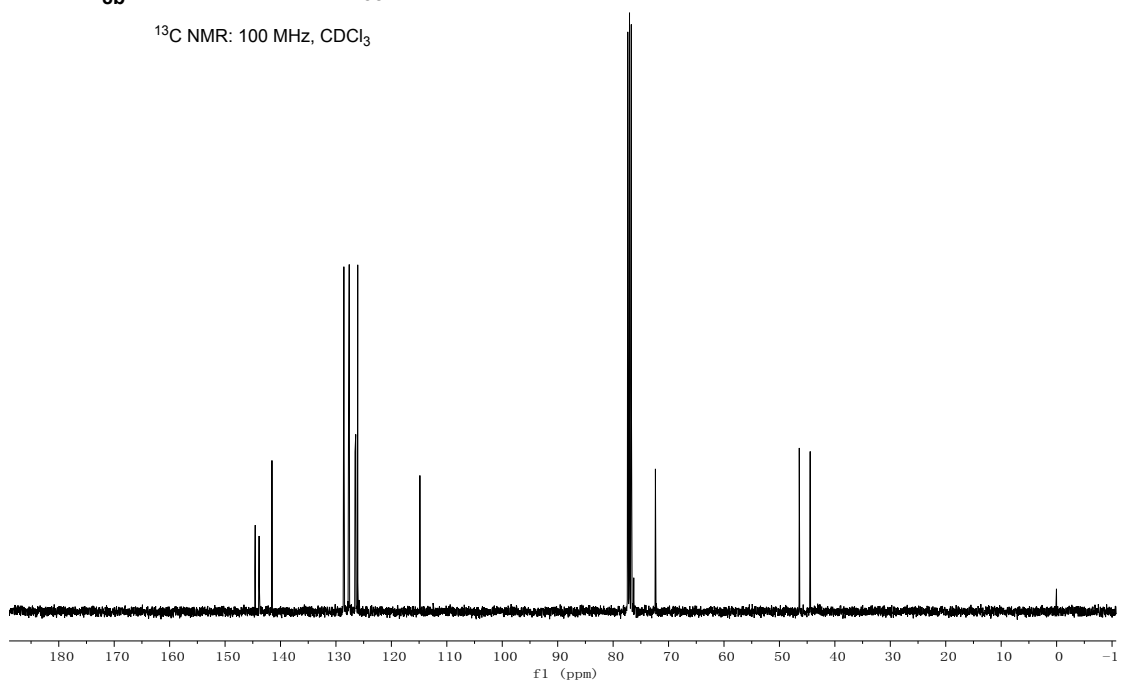


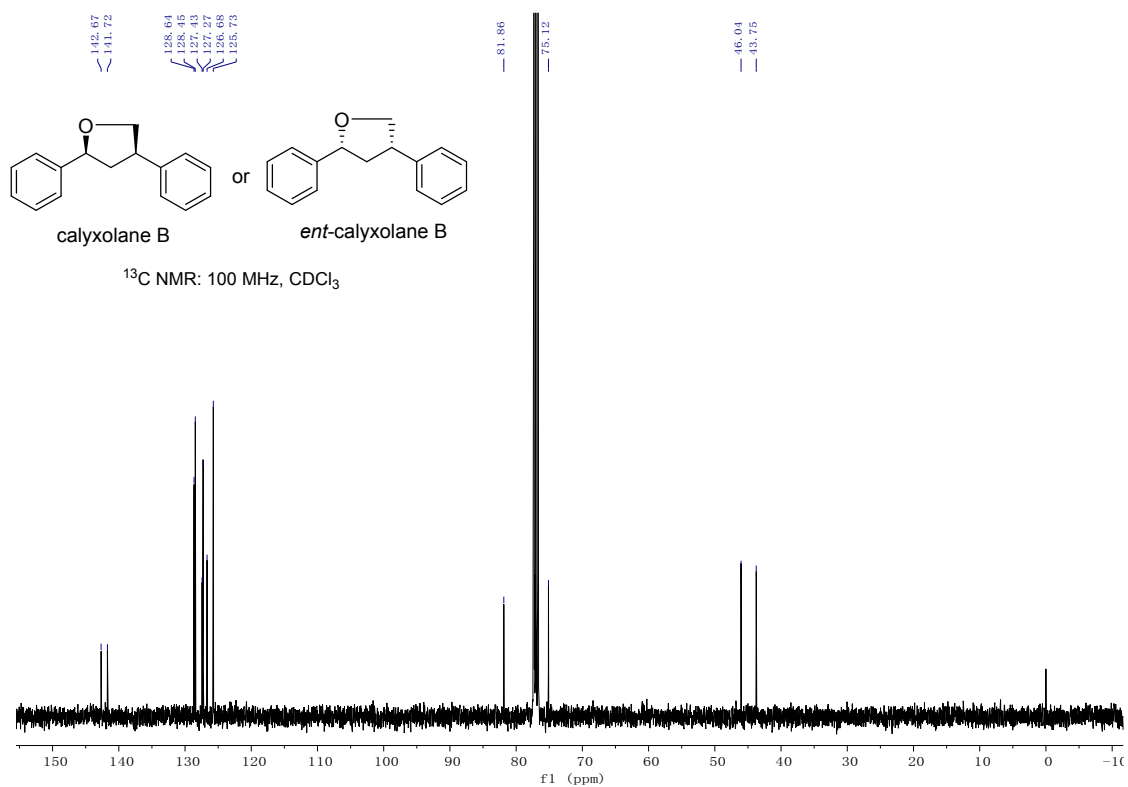
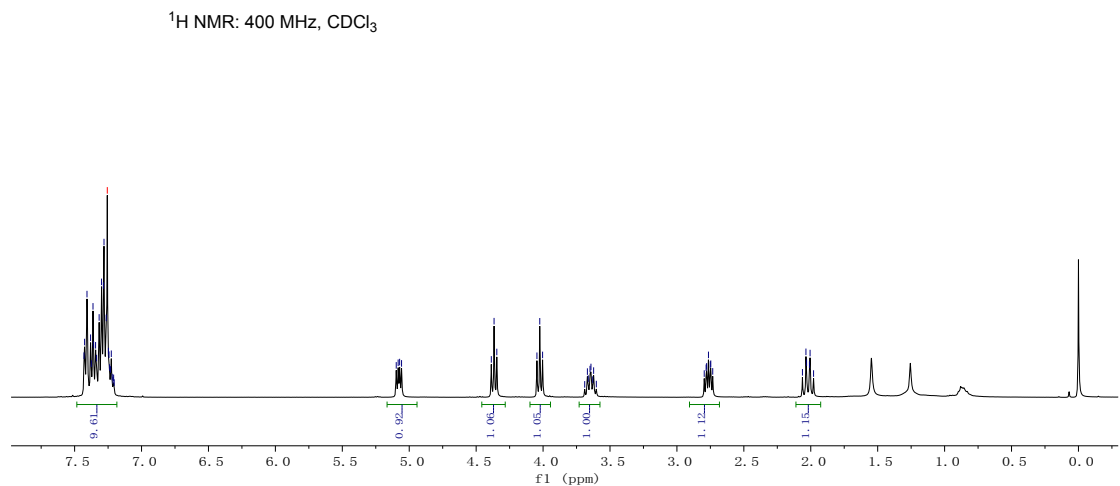
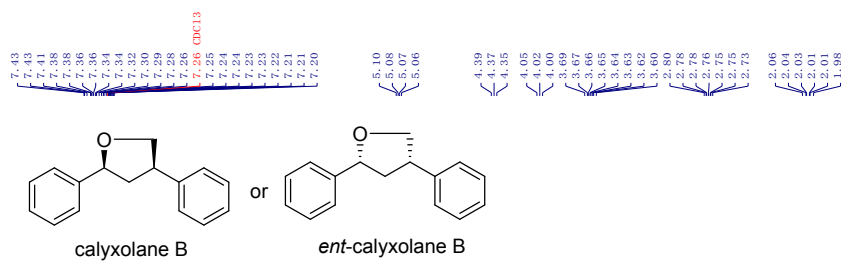


^1H NMR: 400 MHz, CDCl_3



^{13}C NMR: 100 MHz, CDCl_3





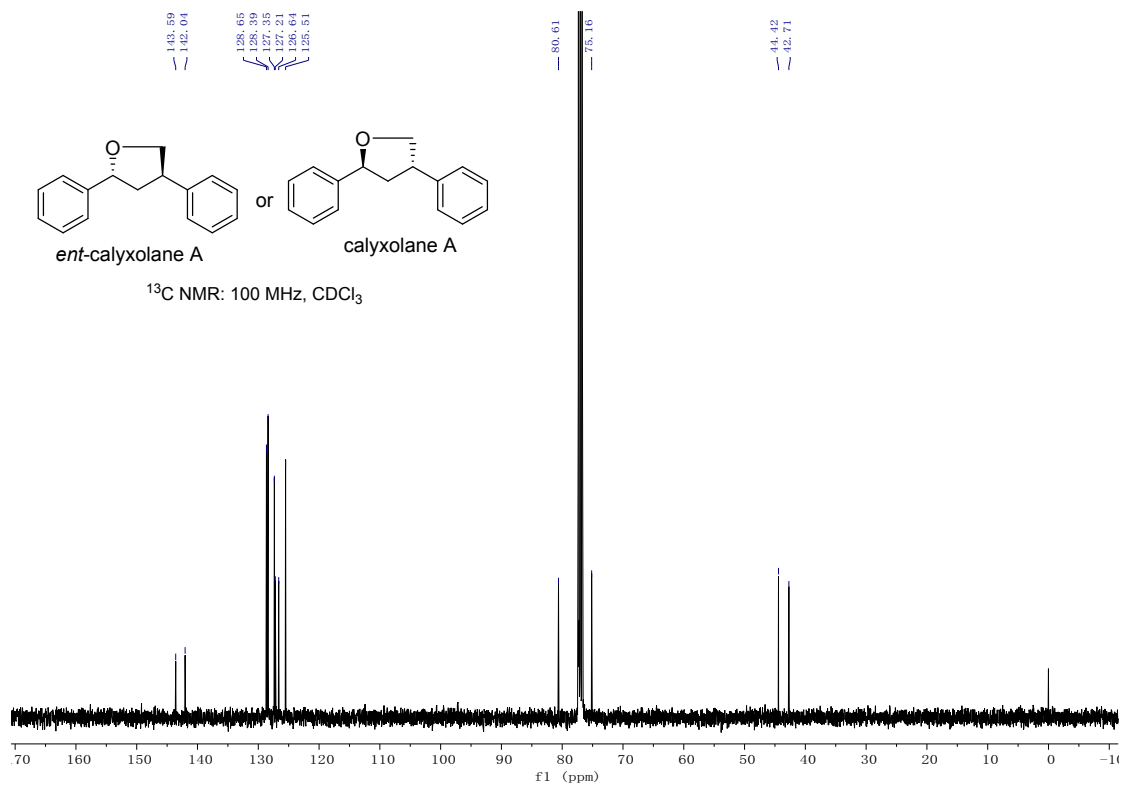
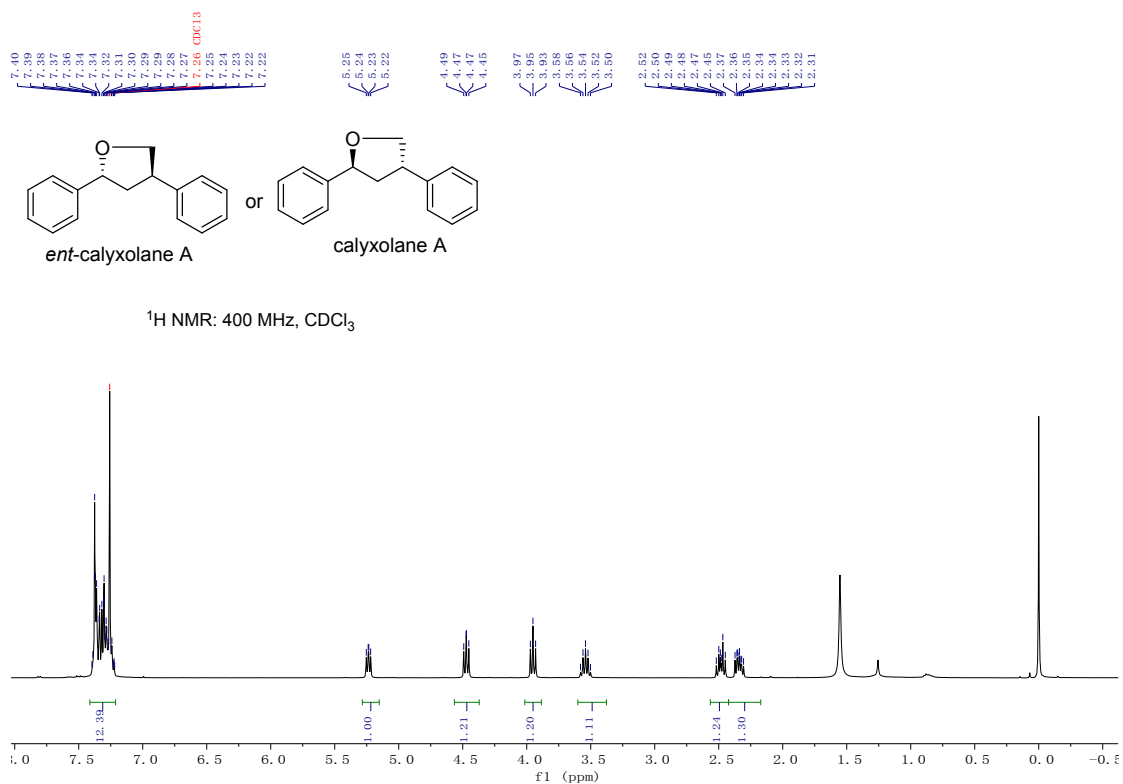
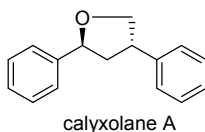
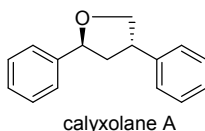
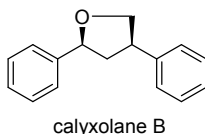


Table S5. Comparison of the ^1H NMR data of natural and synthetic calyxolane A

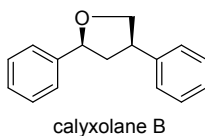
Natural δ ^1H [ppm, mult, J (Hz)] 300 MHz	Synthetic δ ^1H [ppm, mult, J (Hz)] 400 MHz	Err (natural–synthetic) $\Delta\delta$ (ppm)
7.38, m, 2H	7.38, m, 2H	—
7.37, m, 4H	7.37, m, 4H	—
7.32, m, 2H	7.32, m, 2H	—
7.26, m, 2H	7.26, m, 2H	—
5.24, dd, 1H (5.7, 7.8)	5.24, dd, 1H (5.8, 7.8)	—
4.47, t, 1H (8.0)	4.47, dd, 1H (7.3, 8.5)	—
3.95, t, 1H (8.1)	3.95, t, 1H (8.2)	—
3.54, m, 1H (7.8)	3.54, m, 1H	—
2.48, ddd, 1H (7.8, 7.8, 12.6)	2.48, dt, 1H (7.7, 12.6)	—
2.34, ddd, 1H (5.7, 8.4, 12.6)	2.34, ddd, 1H (5.8, 8.3, 12.6)	—

Table S6. Comparison of the ^{13}C NMR data of natural and synthetic calyxolane A

Natural δ ^{13}C (ppm) 75 MHz	Synthetic δ ^{13}C (ppm) 100 MHz	Err (natural – synthetic) $\Delta\delta$ (ppm)
143.6	143.6	—
142.0	142.0	—
128.6	128.7	-0.1
128.4	128.4	—
127.3	127.4	-0.1
127.2	127.2	—
126.6	126.6	—
125.5	125.5	—
80.6	80.6	—
75.1	75.2	-0.1
44.4	44.4	—
42.7	42.7	—

Table S7. Comparison of the ^1H NMR data of natural and synthetic calyxolane B

Natural $\delta\ ^1\text{H}$ [ppm, mult, J (Hz)] 300 MHz	Synthetic $\delta\ ^1\text{H}$ [ppm, mult, J (Hz)] 400 MHz	Err (natural–synthetic) $\Delta\delta$ (ppm)
7.26 – 7.38, m, 10H	7.20 - 7.42, m, 10H	—
5.08, dd, 1H (5.7, 10.2)	5.08, dd, 1H (5.7, 10.2)	—
4.37, t, 1H (8.4)	4.37, t, 1H (8.2)	—
4.03, t, 1H (8.4)	4.02, t, 1H (8.5)	0.01
3.65, m, 1H (8.1)	3.65, m, 1H	—
2.77, m, 1H (6.3)	2.76, ddd, 1H (5.7, 7.3, 12.7)	0.01
2.02, q, 1H (10.5)	2.02, dt, 1H (10.4, 12.4)	—

Table S8. Comparison of the ^{13}C NMR data of natural and synthetic calyxolane B

Natural $\delta\ ^{13}\text{C}$ (ppm) 75 MHz	Synthetic $\delta\ ^{13}\text{C}$ (ppm) 100 MHz	Err (natural–synthetic) $\Delta\delta$ (ppm)
142.6	142.7	-0.1
141.7	141.7	—
128.6	128.6	—
128.4	128.4	—
127.4	127.4	—
127.2	127.3	-0.1
126.6	126.7	-0.1
125.7	125.7	—
81.8	81.9	-0.1
75.1	75.1	-0.1
46.0	46.0	—
43.7	43.7	—