Supporting Information

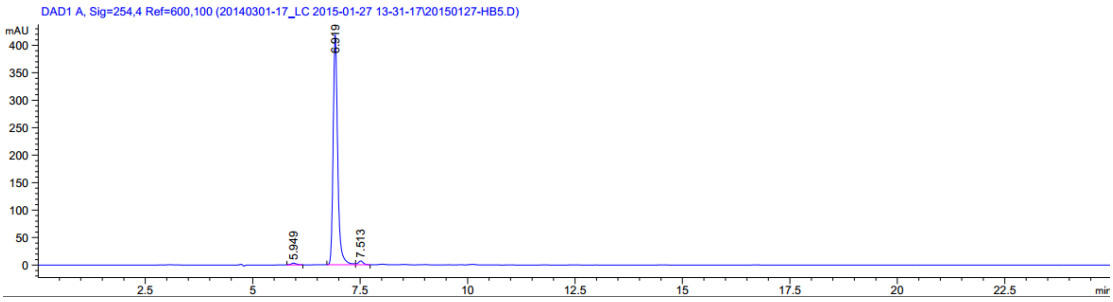
Synthesis, Biological Evaluation and Mechanisms Study of a Class of Benzylideneindanone Derivatives as Novel Anticancer Agents

Jinhui Hu, Jun Yan, Jie Chen, Yanqing Pang, Ling Huang *, Xingshu Li *

Institute of Drug Synthesis and Pharmaceutical Process, School of Pharmaceutical Sciences, Sun Yat-sen University, Guangzhou 510006, China

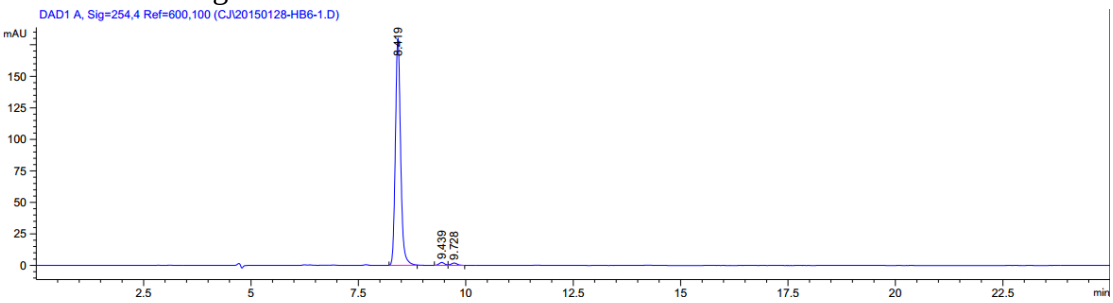
HPLC chromatograms of target compounds

HPLC chromatograms of **5a**



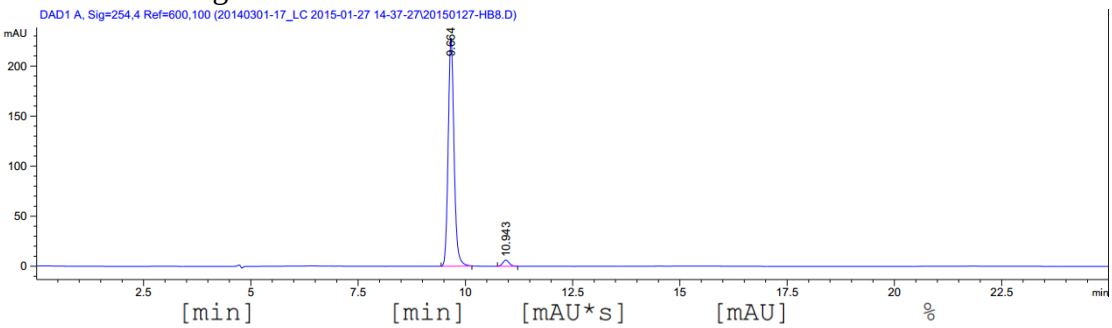
	[min]		[min]	[mAU*s]	[mAU]	%
1	5.949	BB	0.1308	28.18645	3.13816	0.8898
2	6.919	BV	0.1123	3083.09839	416.69141	97.3269
3	7.513	VB	0.1211	56.48975	6.92816	1.7833

HPLC chromatograms of **5b**



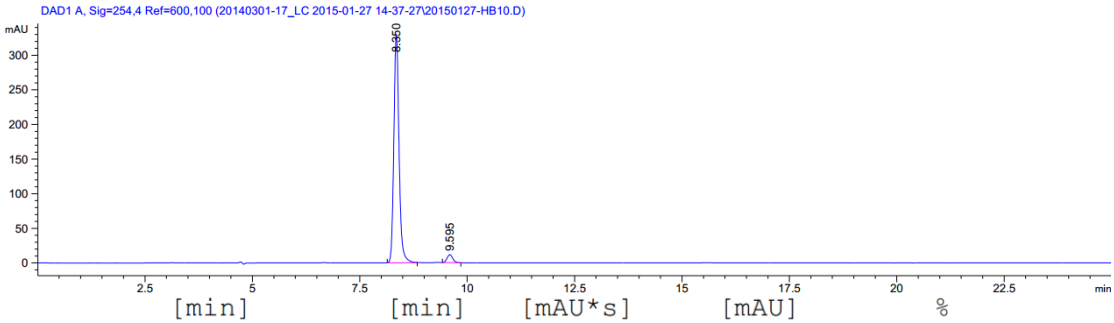
	[min]		[min]	[mAU*s]	[mAU]	%
1	8.419	BB	0.1313	1530.47546	179.85263	97.5303
2	9.439	BV	0.1387	20.55617	2.29023	1.3100
3	9.728	VB	0.1478	18.19886	1.86628	1.1597

HPLC chromatograms of **5c**



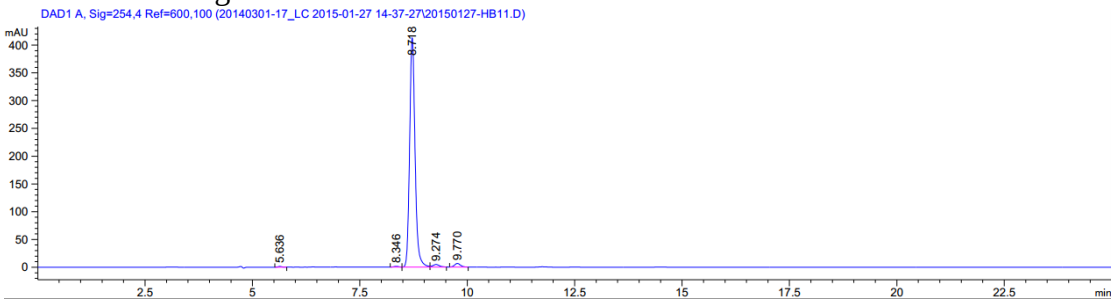
	[min]		[min]	[mAU*s]	[mAU]	%
1	9.664	BB	0.1473	2167.92749	227.31937	97.1078
2	10.943	BB	0.1622	64.56911	6.16702	2.8922

HPLC chromatograms of **5d**



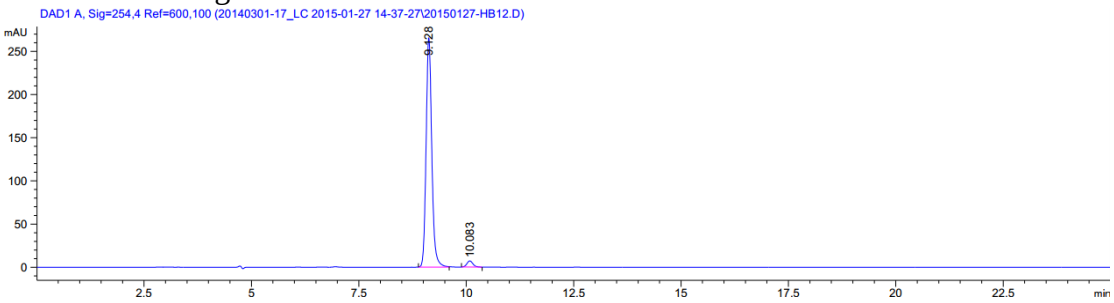
	[min]		[min]	[mAU*s]	[mAU]	%
1	8.350	BB	0.1300	2766.88965	329.36151	96.2952
2	9.595	BB	0.1431	106.45258	11.59441	3.7048

HPLC chromatograms of **5e**



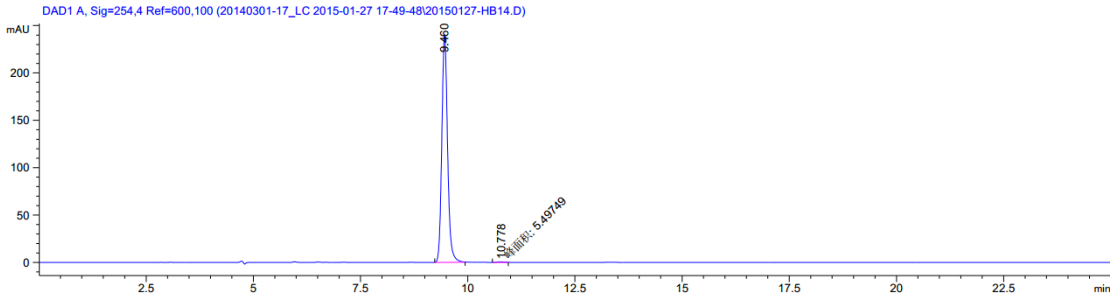
	[min]		[min]	[mAU*s]	[mAU]	%
1	5.636	BB	0.0947	8.52647	1.36819	0.2266
2	8.346	BV	0.1163	10.80013	1.42653	0.2871
3	8.718	VV	0.1346	3627.74585	412.60800	96.4291
4	9.274	VB	0.1646	51.71420	4.69196	1.3746
5	9.770	BB	0.1494	63.29773	6.50932	1.6825

HPLC chromatograms of **5f**



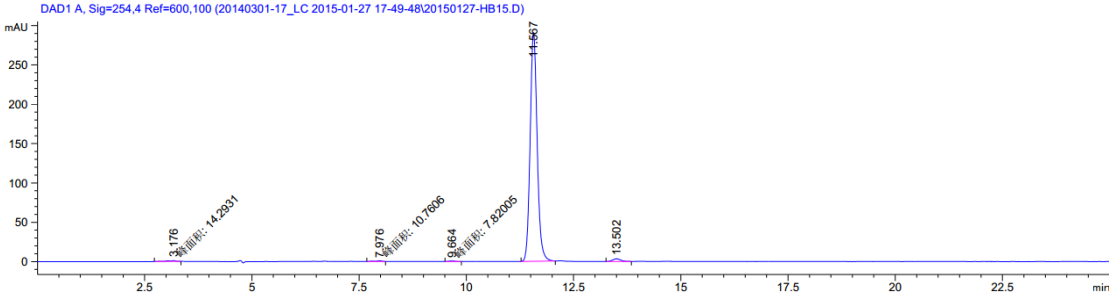
#	[min]		[min]	[mAU*s]	[mAU]	%
1	9.128	BB	0.1413	2444.09473	265.66727	97.2215
2	10.083	BB	0.1499	69.85068	7.15722	2.7785

HPLC chromatograms of **5g**



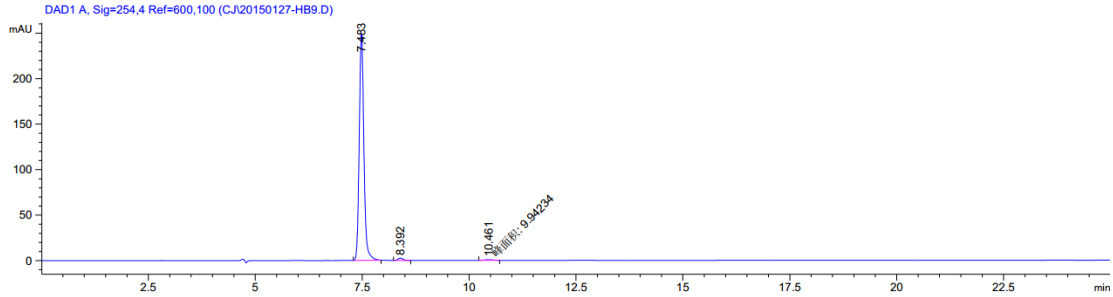
	[min]		[min]	[mAU*s]	[mAU]	%
1	9.460	BB	0.1432	2245.84058	240.02560	99.7558
2	10.778	MM	0.1651	5.49749	5.55101e-1	0.2442

HPLC chromatograms of **5h**



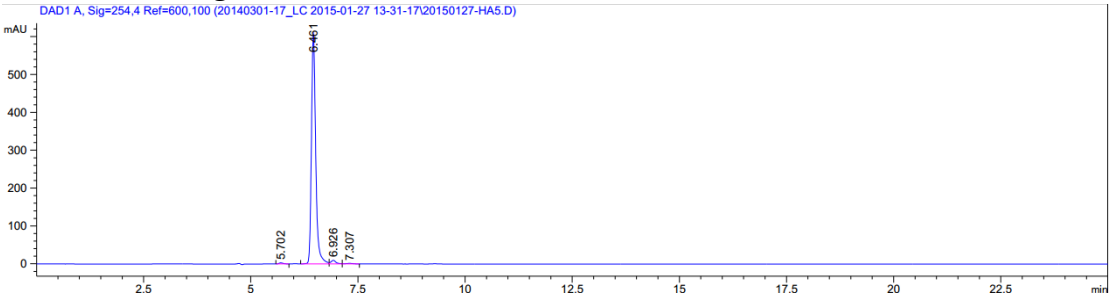
	[min]		[min]	[mAU*s]	[mAU]	%
1	3.176	MM	0.2115	14.29315	1.12651	0.4233
2	7.976	MM	0.1955	10.76062	9.17482e-1	0.3187
3	9.664	MM	0.1681	7.82005	7.75224e-1	0.2316
4	11.567	BB	0.1746	3299.86987	290.29559	97.7284
5	13.502	BB	0.1987	43.82802	3.43786	1.2980

HPLC chromatograms of **5i**



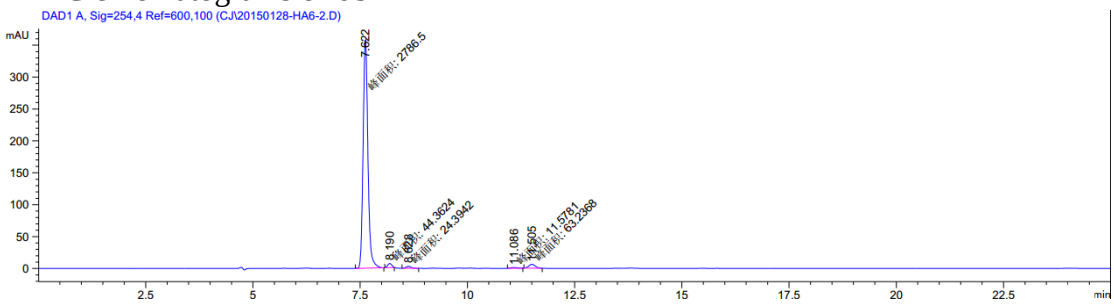
	[min]		[min]	[mAU*s]	[mAU]	%
1	7.483	BB	0.1164	1886.52441	248.94904	98.3869
2	8.392	BB	0.1313	20.98818	2.46522	1.0946
3	10.461	MM	0.2648	9.94234	6.25746e-1	0.5185

HPLC chromatograms of **6a**



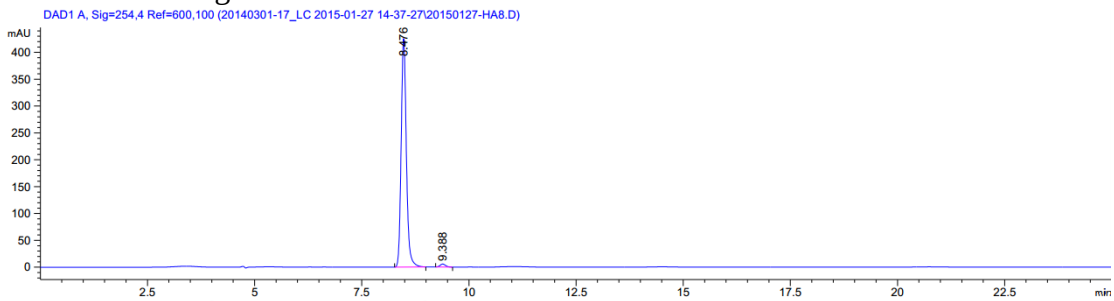
	[min]		[min]	[mAU*s]	[mAU]	%
1	5.702	BB	0.1082	20.75567	2.87731	0.4784
2	6.461	VV	0.1052	4218.76172	606.12622	97.2378
3	6.926	VB	0.1234	79.72931	9.55048	1.8377
4	7.307	BB	0.1888	19.35796	1.45903	0.4462

HPLC chromatograms of **6b**



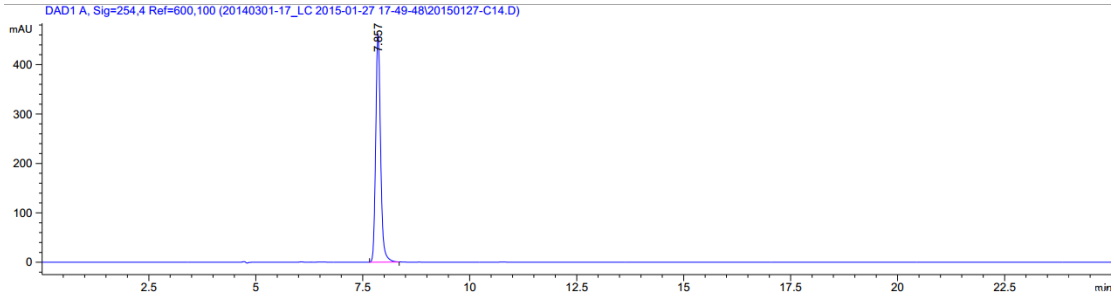
	[min]		[min]	[mAU*s]	[mAU]	%
1	7.622	MM	0.1297	2786.49927	358.09259	95.1001
2	8.190	MM	0.1141	44.36235	6.47758	1.5140
3	8.628	MM	0.1360	24.39417	2.99031	0.8325
4	11.086	MM	0.1629	11.57808	1.18474	0.3951
5	11.505	MM	0.1742	63.23684	6.05195	2.1582

HPLC chromatograms of **6c**



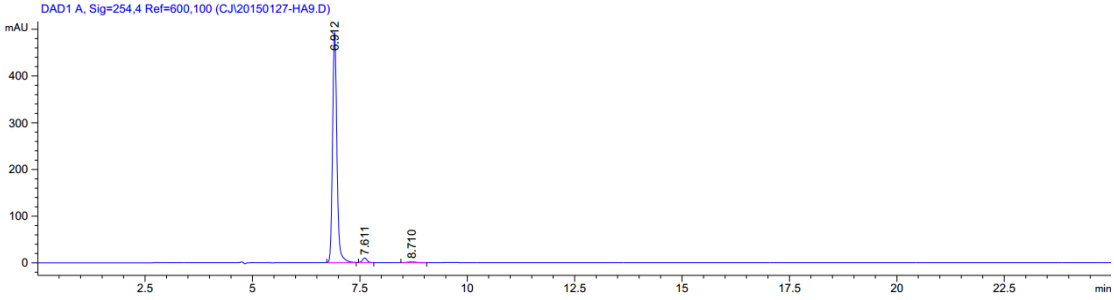
	[min]		[min]	[mAU*s]	[mAU]	%
1	8.476	BB	0.1284	3591.13208	425.67303	98.6347
2	9.388	BB	0.1369	49.70747	5.63316	1.3653

HPLC chromatograms of **6d**



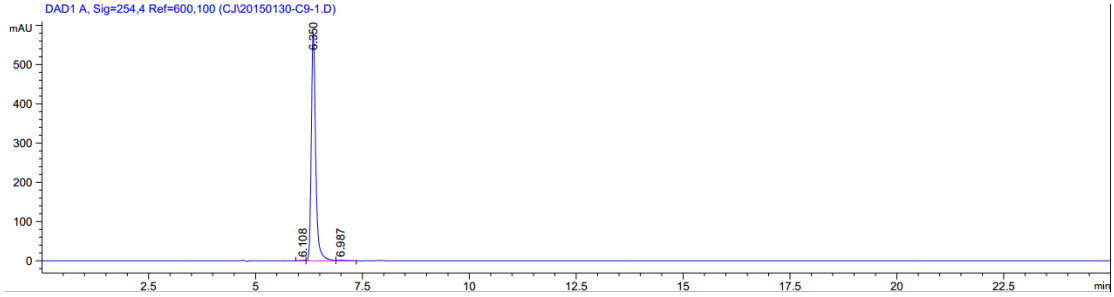
#	[min]		[min]	[mAU*s]	[mAU]	%
1	7.857	BB	0.1211	3676.74585	460.75665	100.0000

HPLC chromatograms of **6e**



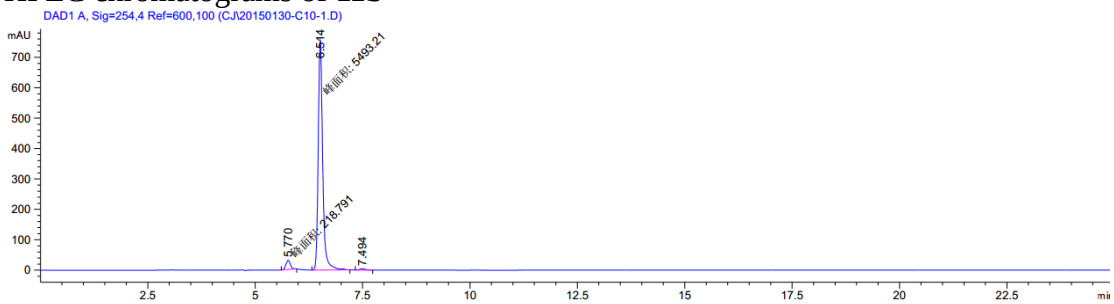
	[min]		[min]	[mAU*s]	[mAU]	%
1	6.912	BB	0.1087	3491.04443	492.52240	97.1783
2	7.611	BB	0.1186	77.88567	10.03156	2.1681
3	8.710	BB	0.2125	23.48086	1.66545	0.6536

HPLC chromatograms of **11a**



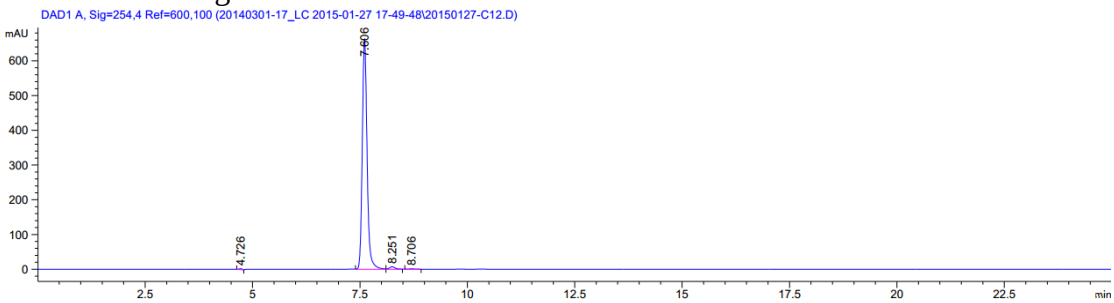
	[min]		[min]	[mAU*s]	[mAU]	%
1	6.108	BV	0.1220	9.58950	1.24376	0.2299
2	6.350	VB	0.1071	4140.26904	581.48535	99.2709
3	6.987	BB	0.1920	20.81682	1.55672	0.4991

HPLC chromatograms of **11b**



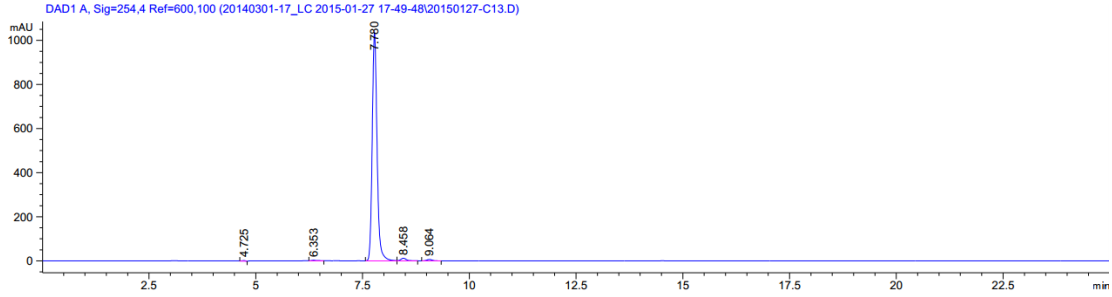
	[min]		[min]	[mAU*s]	[mAU]	%
1	5.770	MM	0.1207	218.79074	30.20711	3.8040
2	6.514	MM	0.1211	5493.20752	755.96948	95.5065
3	7.494	BB	0.1465	39.65899	4.11224	0.6895

HPLC chromatograms of **12a**



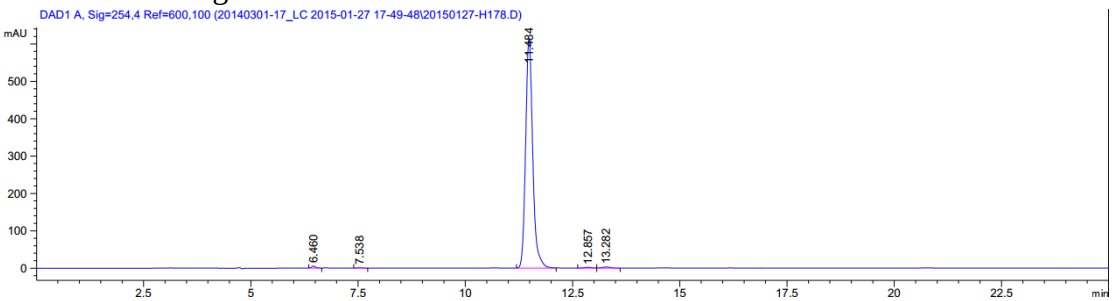
	[min]		[min]	[mAU*s]	[mAU]	%
1	4.726	BV	0.0871	14.23811	2.54985	0.2715
2	7.606	VV	0.1185	5153.48779	664.05670	98.2827
3	8.251	VB	0.1364	64.90562	7.11895	1.2378
4	8.706	BB	0.1470	10.90375	1.10605	0.2079

HPLC chromatograms of **12b**



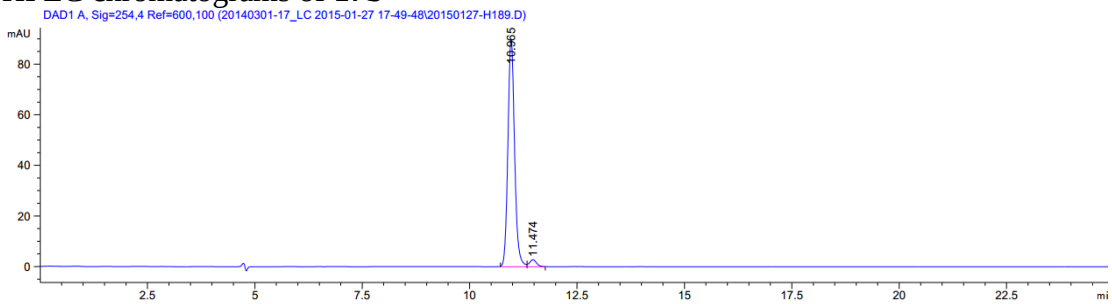
	[min]		[min]	[mAU*s]	[mAU]	%
1	4.725	BV	0.0880	14.53700	2.57028	0.1740
2	6.353	VV	0.1345	25.89314	2.73330	0.3100
3	7.780	BV	0.1220	8149.89795	1033.83801	97.5576
4	8.458	VB	0.1382	109.37187	11.79230	1.3092
5	9.064	BB	0.1350	54.23836	6.14055	0.6493

HPLC chromatograms of **17a**



	[min]		[min]	[mAU*s]	[mAU]	%
1	6.460	BB	0.0968	34.22178	5.33618	0.4766
2	7.538	BB	0.1124	8.20953	1.13493	0.1143
3	11.484	BB	0.1767	7078.66699	613.24799	98.5740
4	12.857	BV	0.1861	23.53583	1.98843	0.3277
5	13.282	VB	0.1938	36.43209	2.91480	0.5073

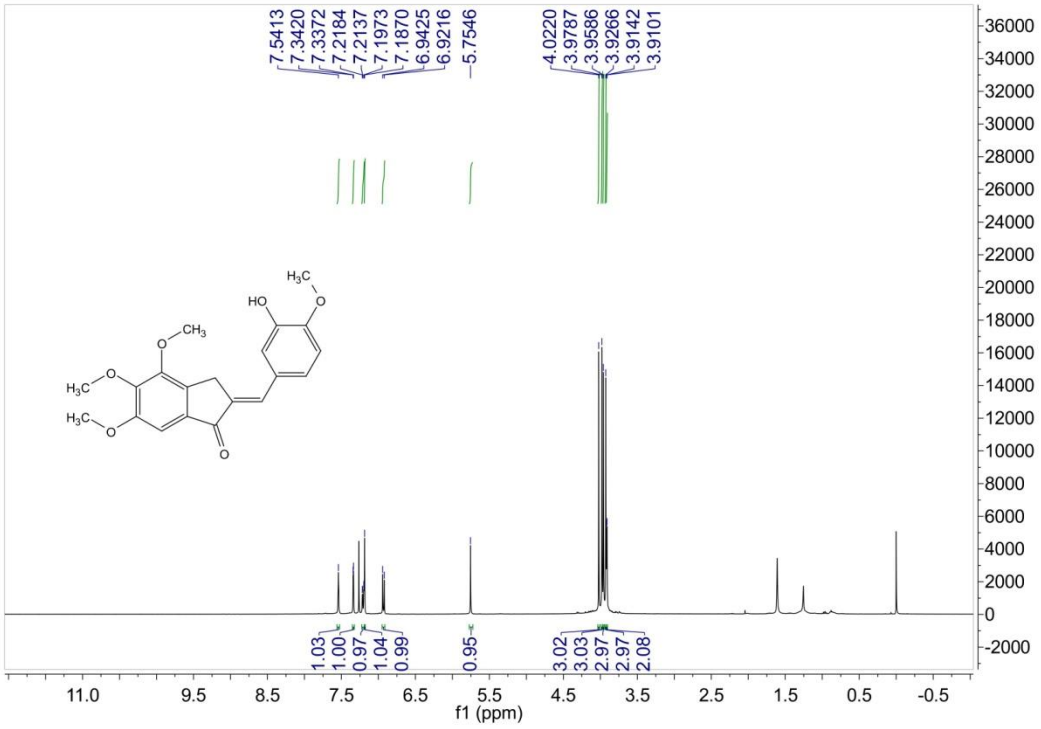
HPLC chromatograms of **17b**

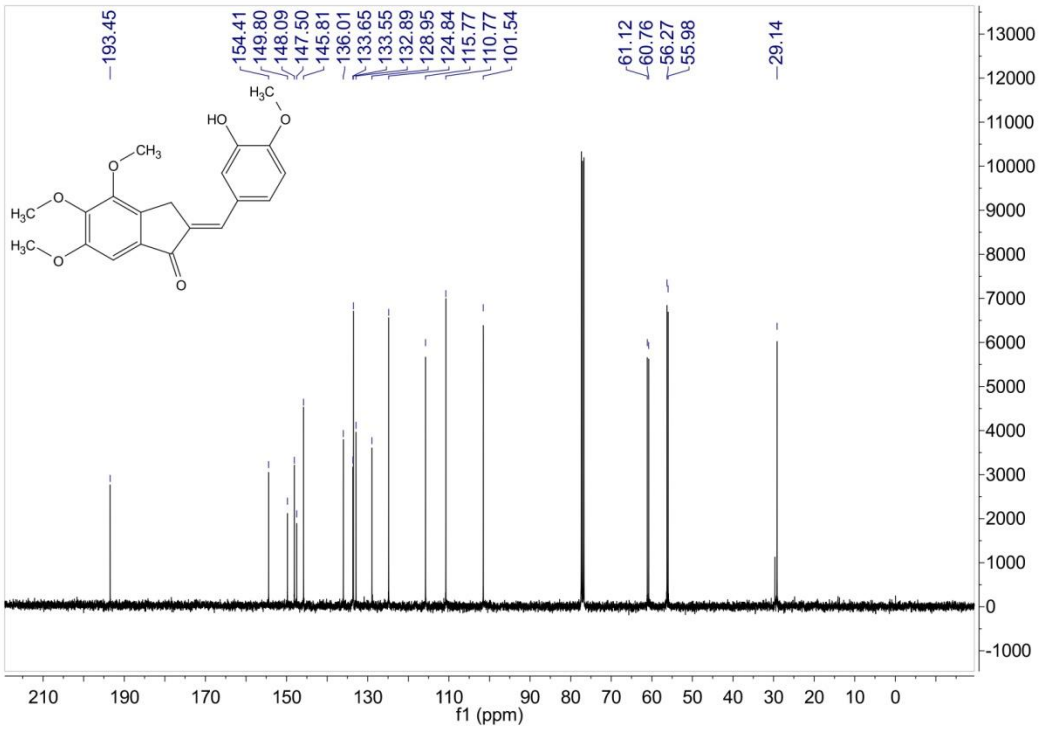


	[min]		[min]	[mAU*s]	[mAU]	%
1	10.965	BB	0.1655	968.28186	89.99854	96.8336
2	11.474	BB	0.1761	31.66253	2.75532	3.1664

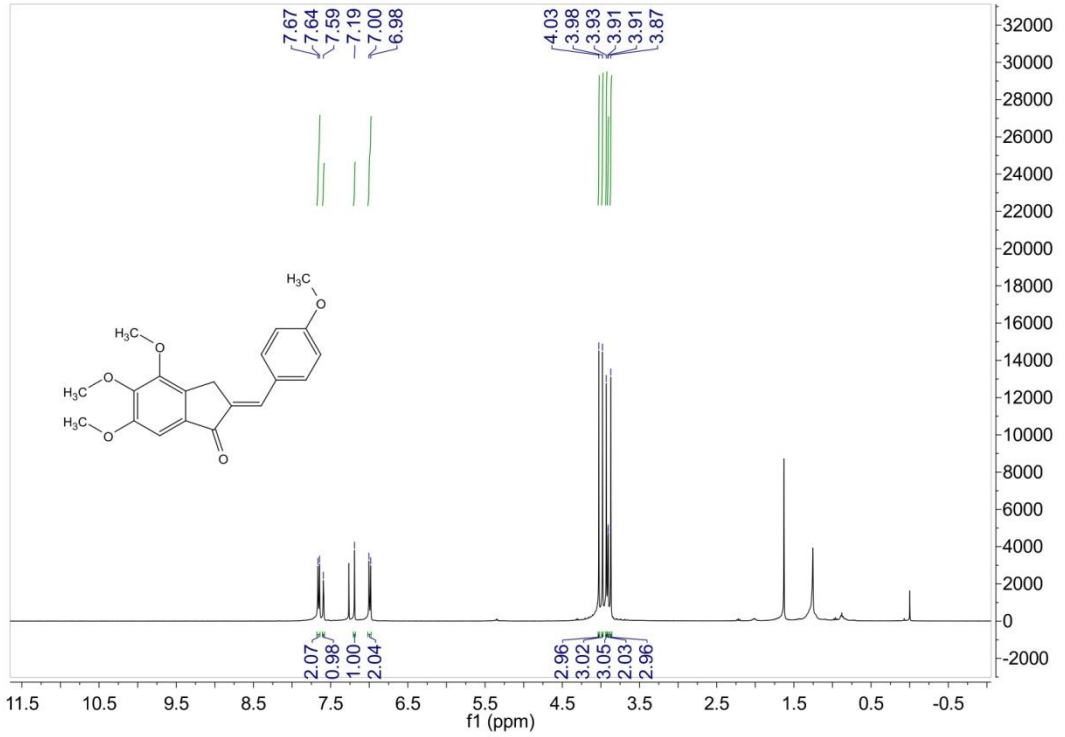
NMR spectra of typical compounds

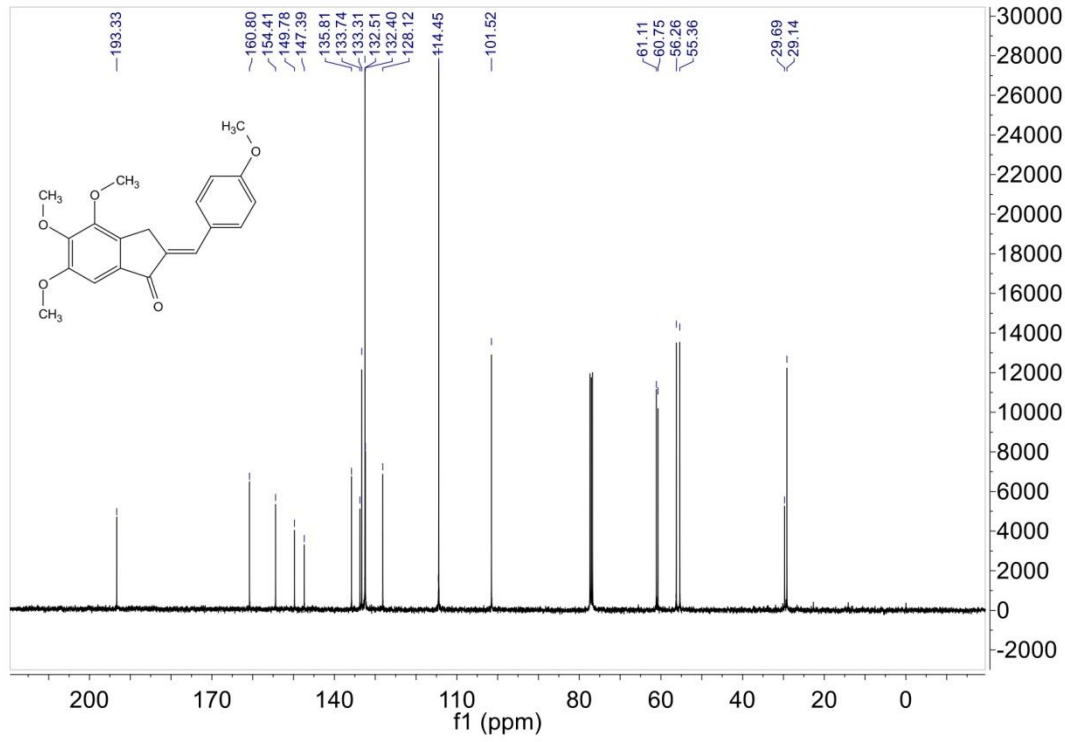
5a



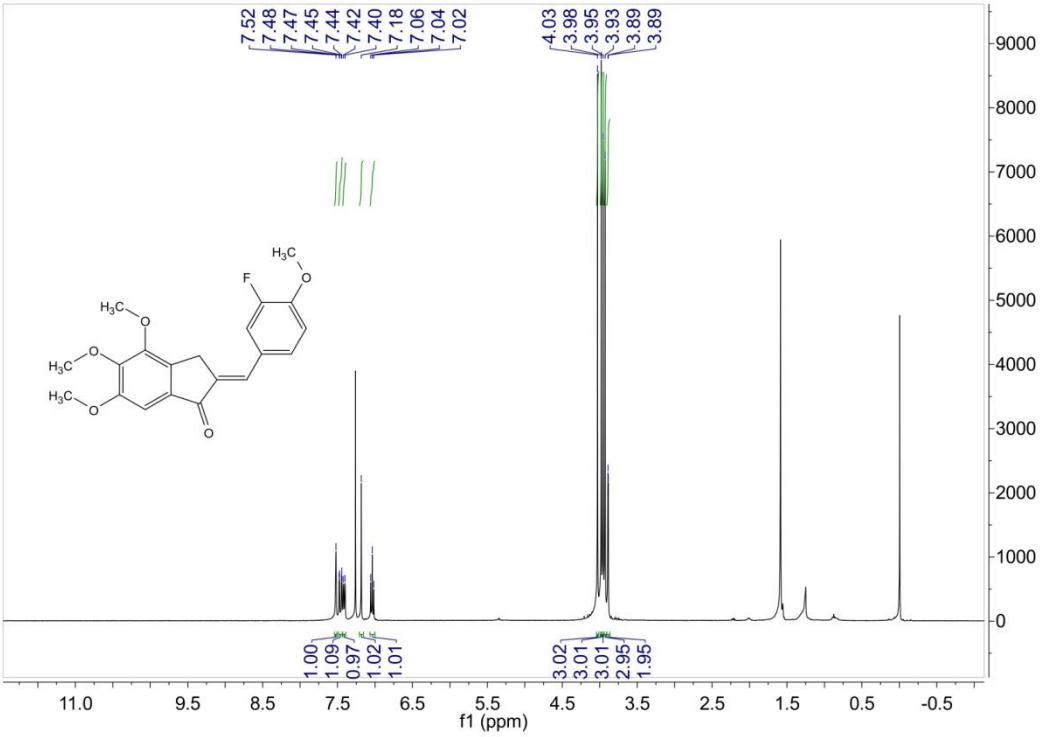


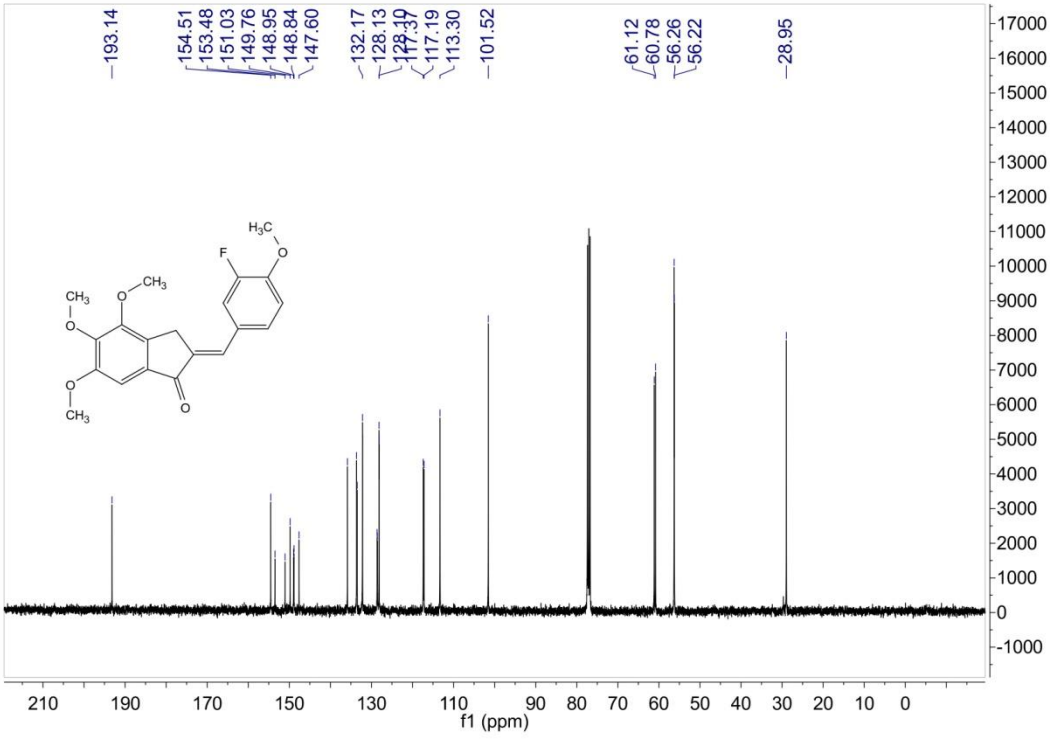
5c


7.67
7.64
7.59
7.19
7.00
6.98
4.03
3.98
3.93
3.91
3.91
3.87
2.07
0.98
1.00
2.04
2.96
3.02
3.05
2.03
2.96
f1 (ppm)

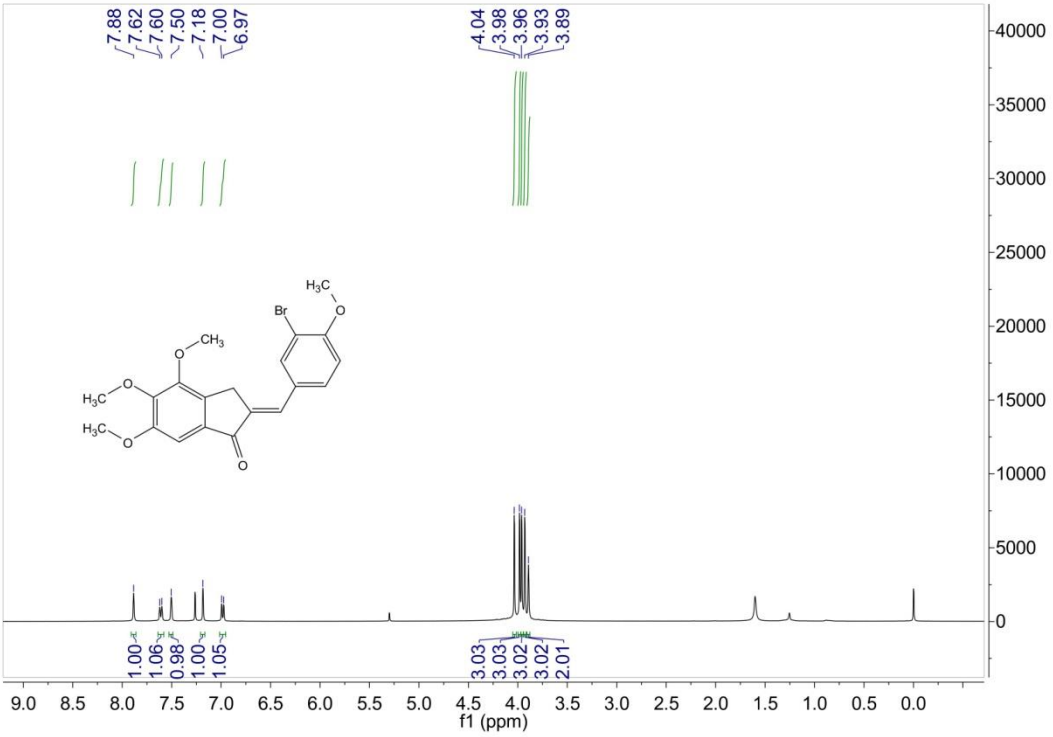

193.33
160.80
154.41
149.78
147.39
135.81
133.74
133.31
132.51
132.40
128.12
114.45
101.52
61.11
60.75
56.26
55.36
29.69
29.14
f1 (ppm)

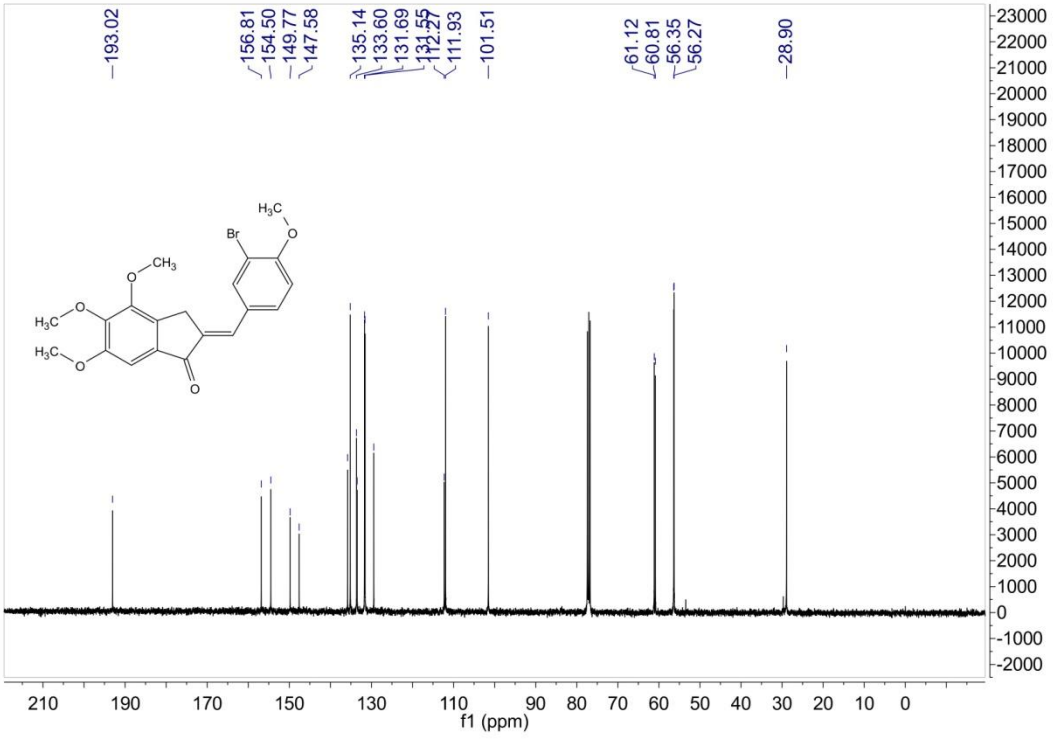
5g


7.52
7.48
7.47
7.45
7.44
7.42
7.40
7.18
7.06
7.04
7.02
4.03
3.98
3.95
3.93
3.89
3.89
1.00
1.09
0.97
1.02
1.01
3.02
3.01
3.01
2.95
1.95
f1 (ppm)

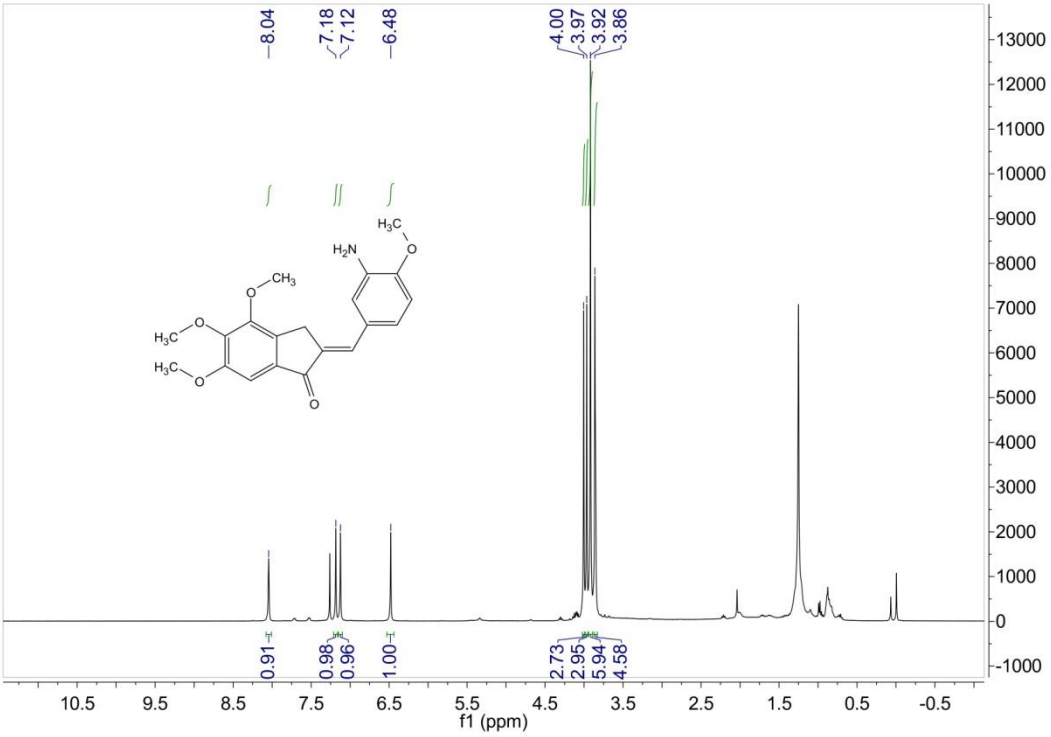

193.14
154.51
153.48
151.03
149.76
148.95
148.84
147.60
132.17
128.13
117.19
113.30
101.52
61.12
60.78
56.26
56.22
28.95
f1 (ppm)

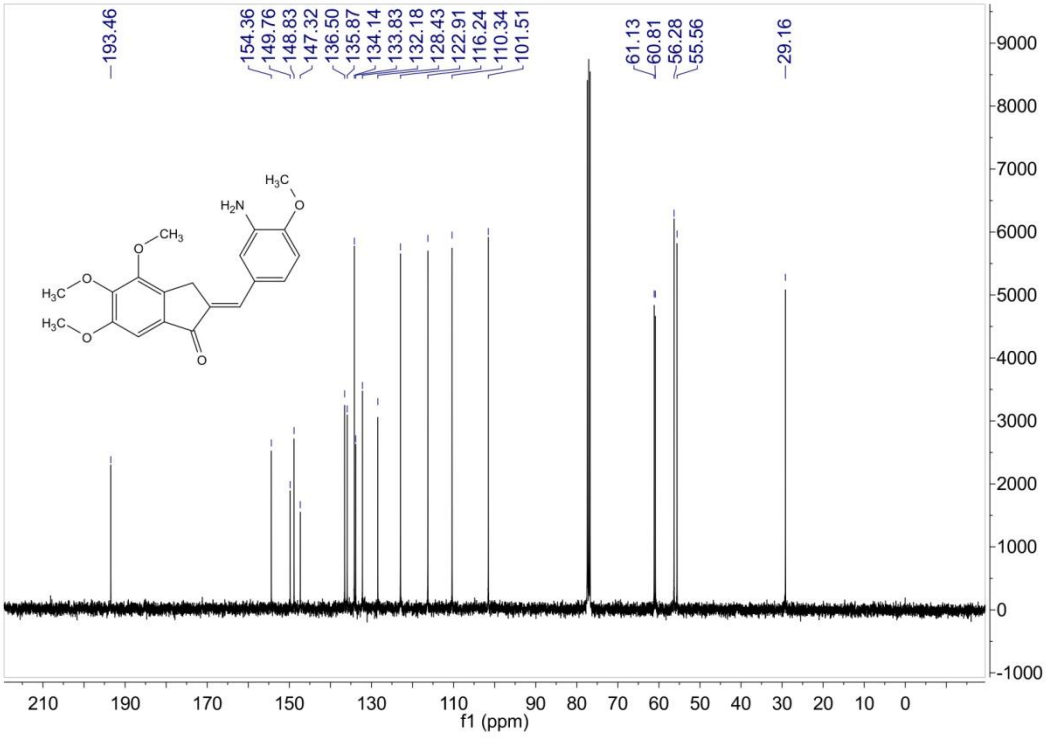
5h


7.88
7.62
7.60
7.50
7.18
7.00
6.97
4.04
3.98
3.96
3.93
3.89
1.00
1.06
0.98
1.00
1.05
3.03
3.03
3.02
3.02
2.01
f1 (ppm)


193.02
156.81
154.50
149.77
147.58
135.14
133.60
131.69
131.55
112.27
111.93
101.51
61.12
60.81
56.35
56.27
28.90
f1 (ppm)

5i


8.04
7.18
7.12
6.48
4.00
3.97
3.92
3.86
0.91
0.98
0.96
1.00
2.73
2.95
5.94
4.58
f1 (ppm)


193.46
154.36
149.76
148.83
147.32
136.50
135.87
134.14
133.83
132.18
128.43
122.91
116.24
110.34
101.51
61.13
60.81
56.28
55.56
29.16
f1 (ppm)