Synthesis and biological evaluation of novel neoflavonoid derivatives as potential antidiabetic agents

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[c] *Key Laboratory for Biotech-Drugs Ministry of Health, Jinan 250062, Shandong, China*

[d] *Key Laboratory for Rare & Uncommon Diseases of Shandong Province, Jinan 250062, Shandong, China*

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E-Mail: xiaojing6@gmail.com (X. Wang)
[1] These authors contributed equally.

Supporting Information

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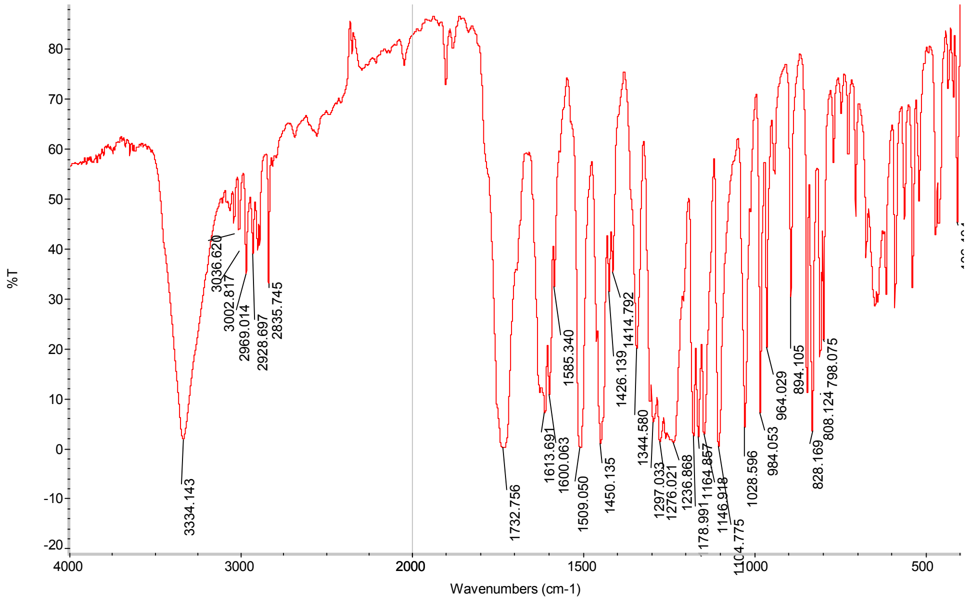
IR(KBr) of compounds 4a-8n

4a



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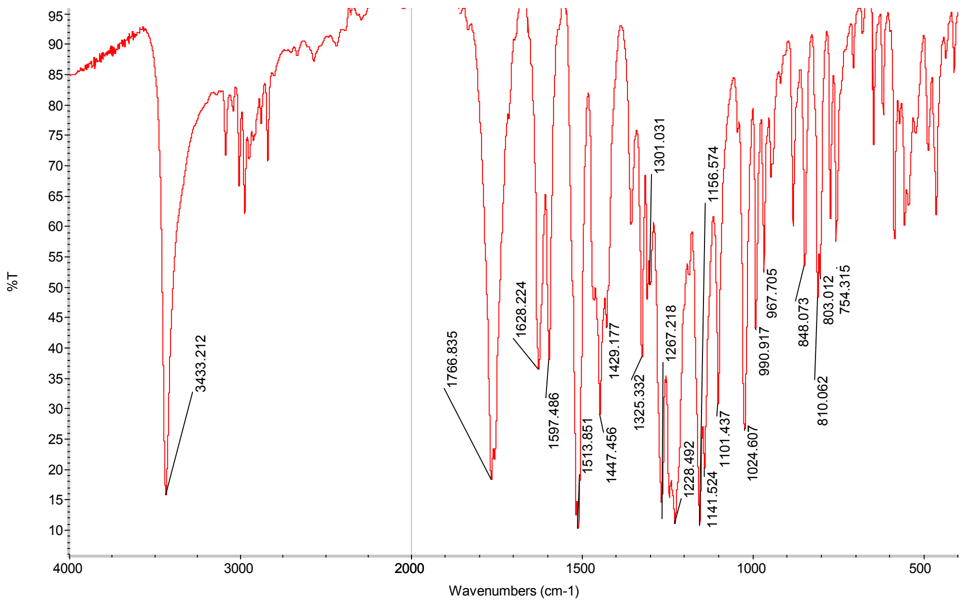

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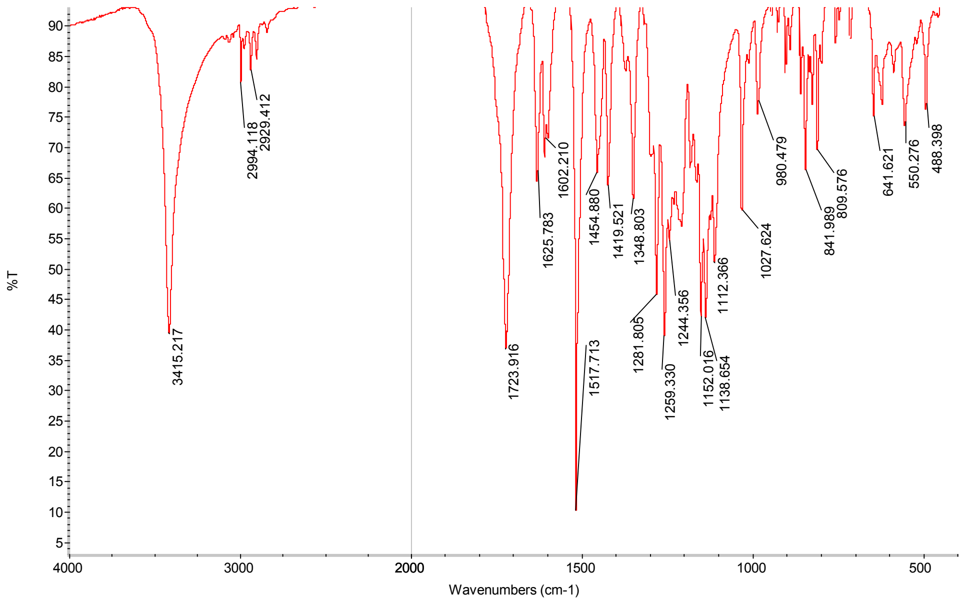
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1348.803
1281.805
1259.330
1244.356
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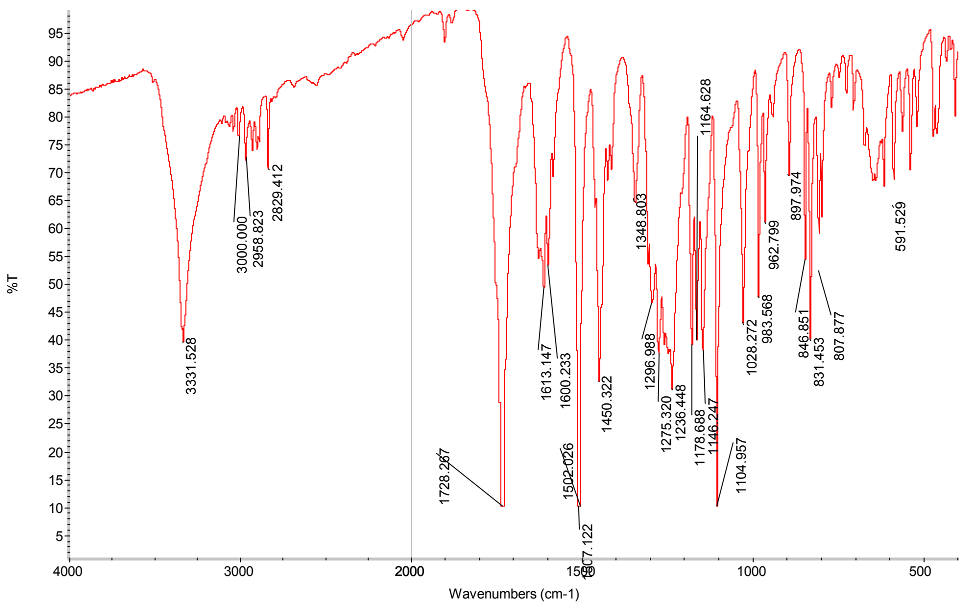
550.276
488.398

4d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1450.322
1348.803
1296.988
1275.320
1236.448
1178.688
1164.628
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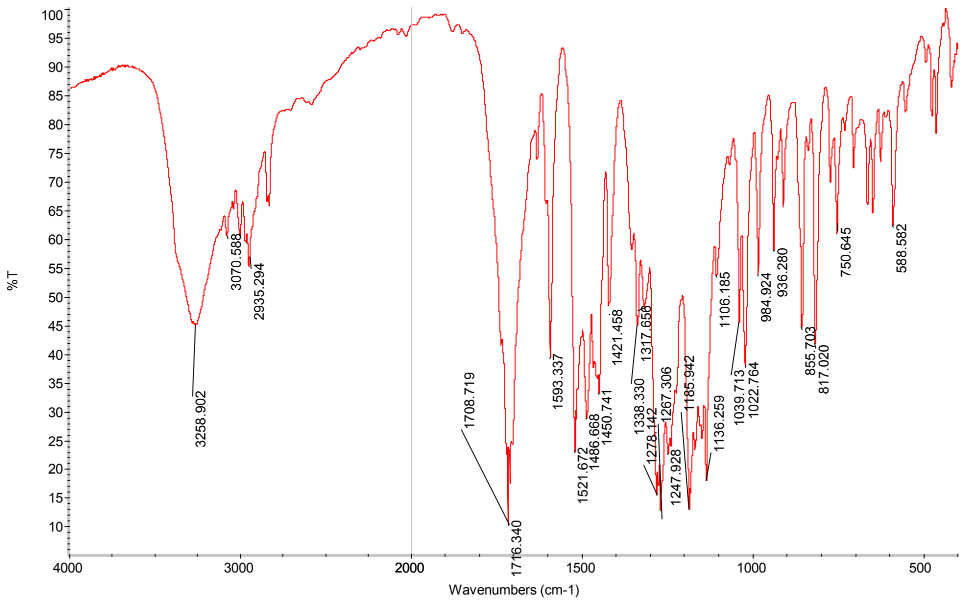
4e



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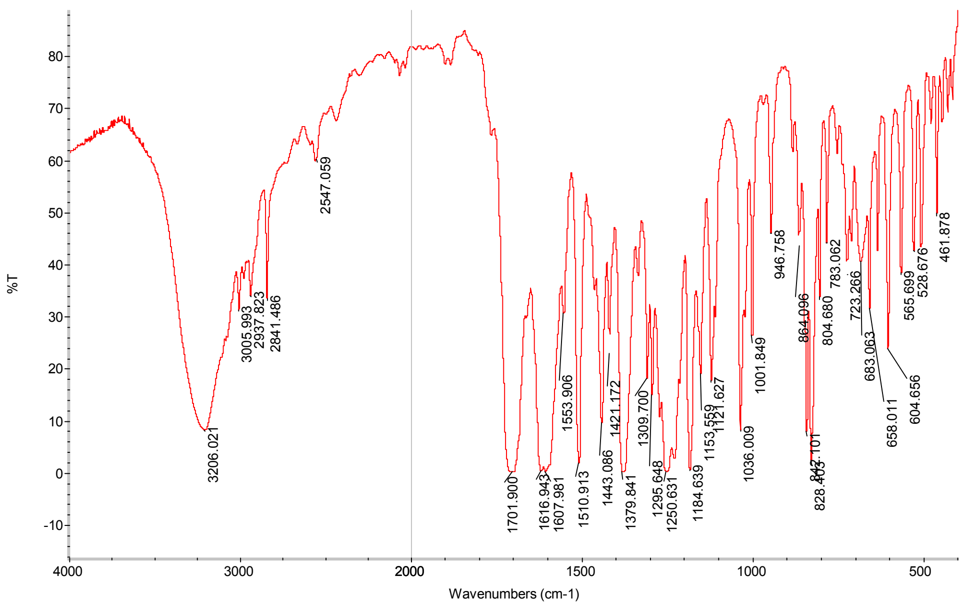

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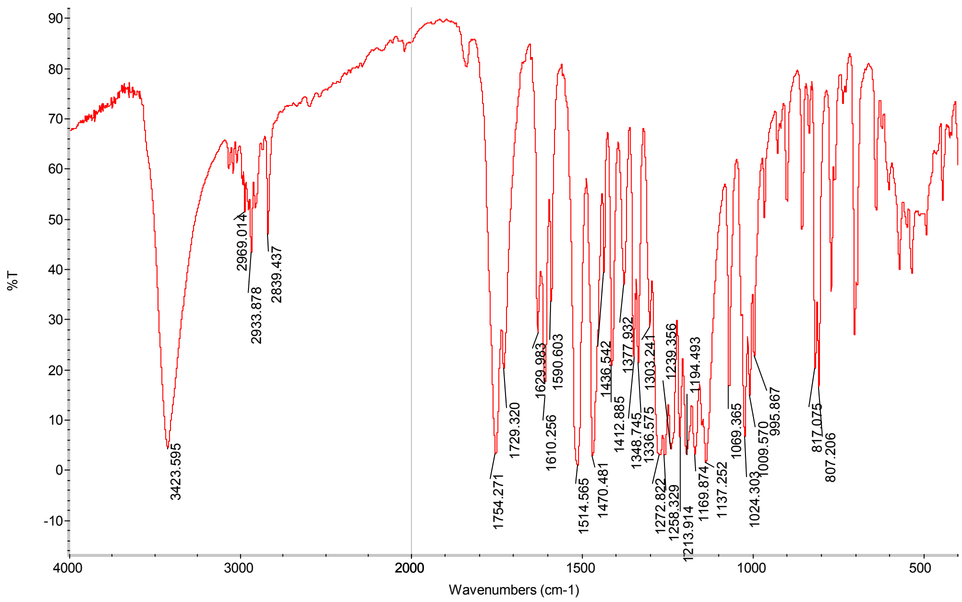
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1436.542
1412.885
1377.932
1348.745
1336.575
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1272.822
1258.329
1239.356
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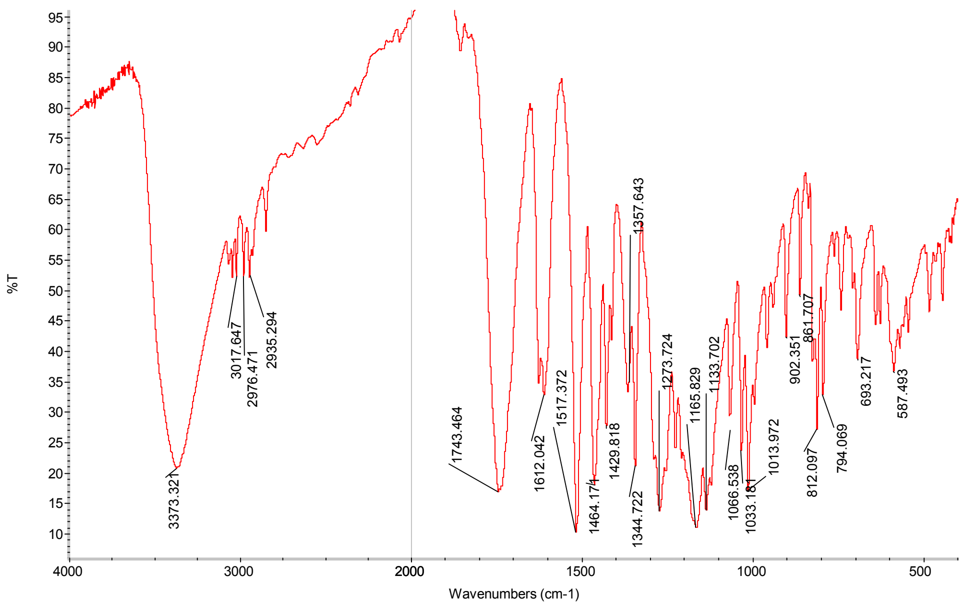
4h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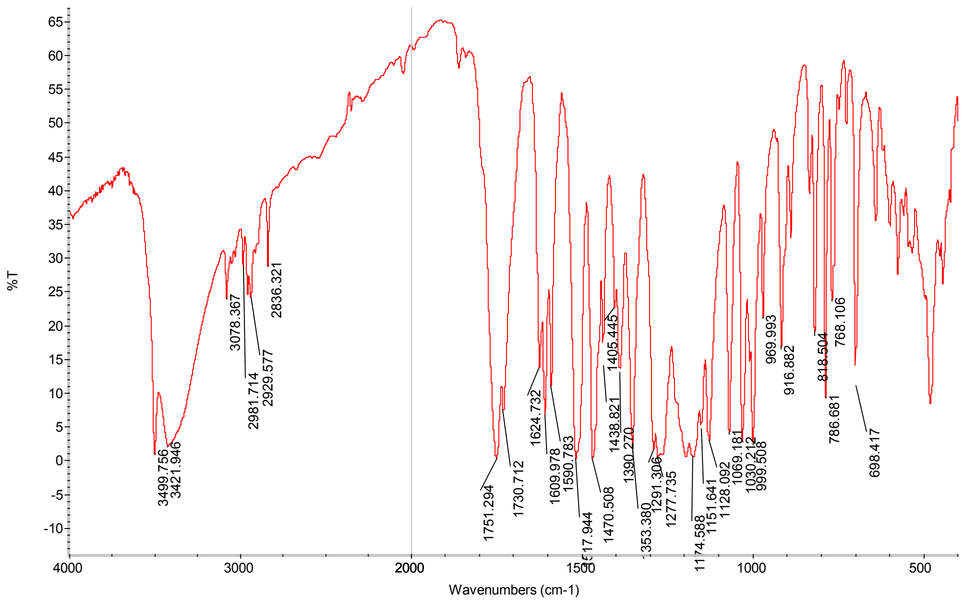
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1517.944
1470.508
1438.821
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1277.735
1174.588
1151.641
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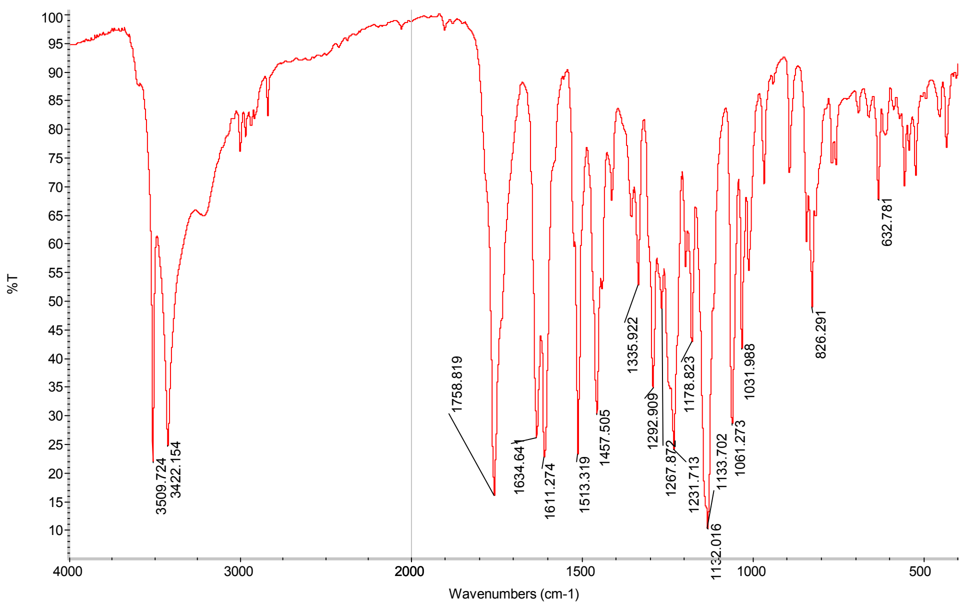
4j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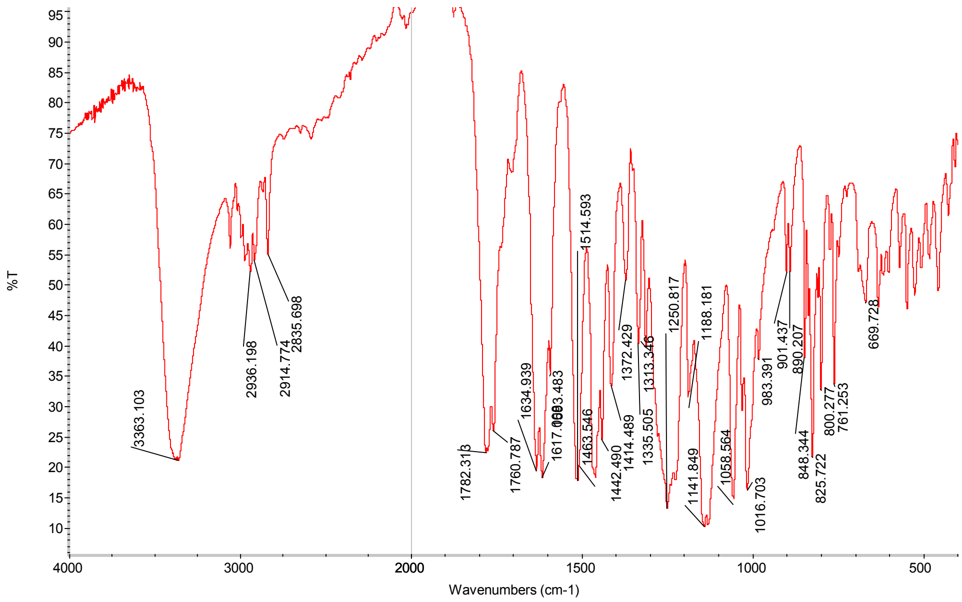
4k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1514.593
1463.546
1442.490
1414.489
1372.429
1335.505
1313.346
1250.817
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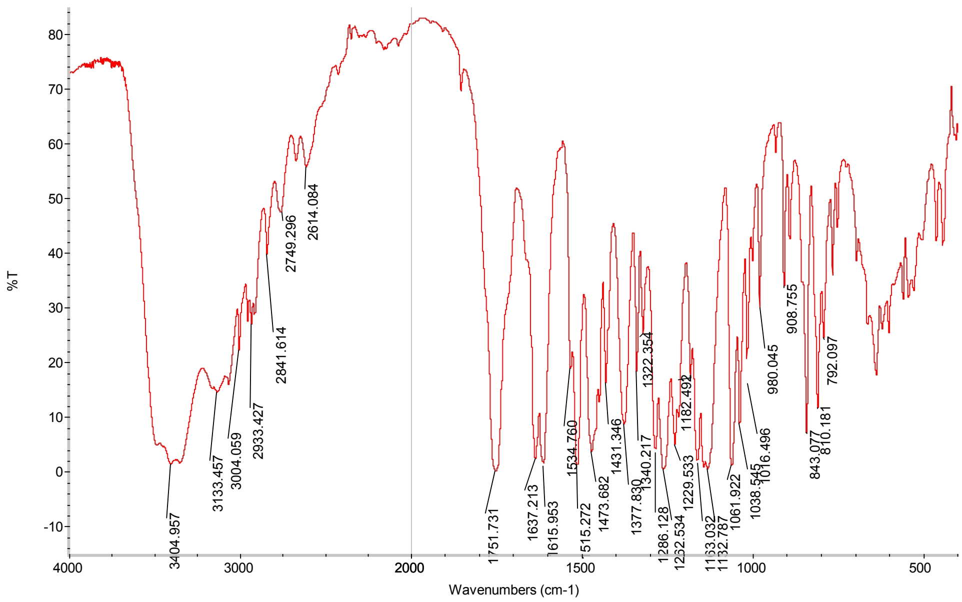
4l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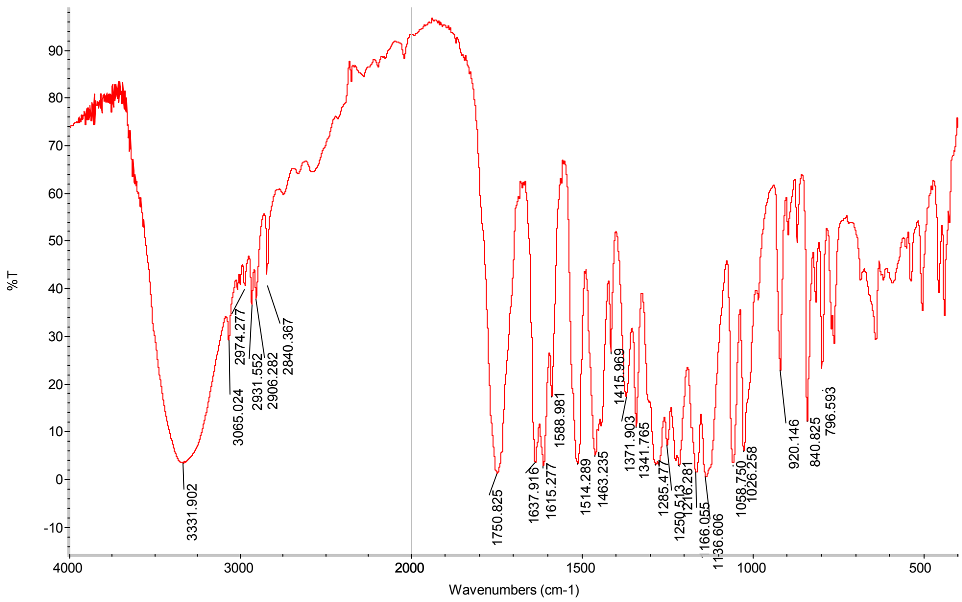
4m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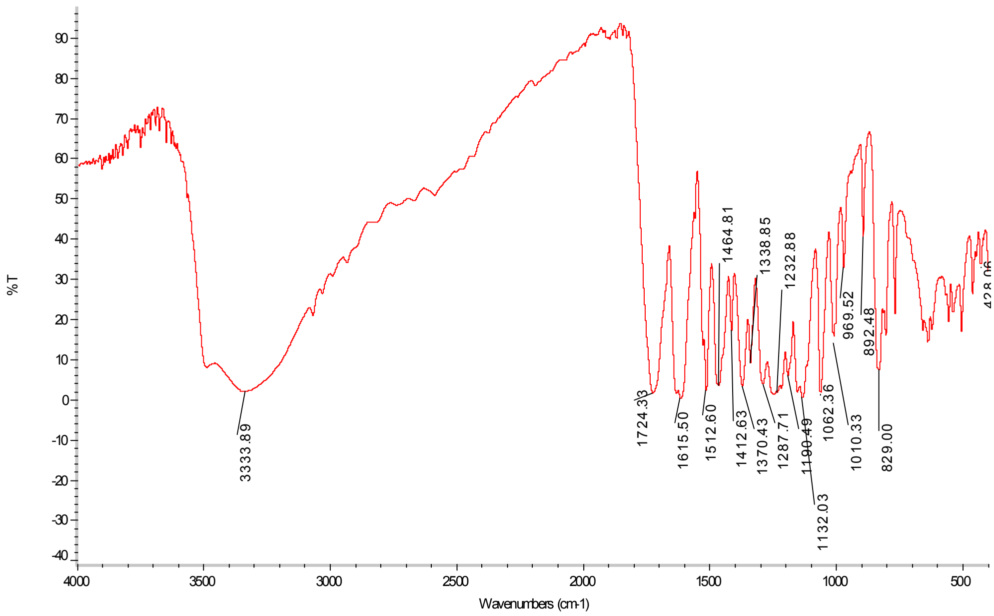
4n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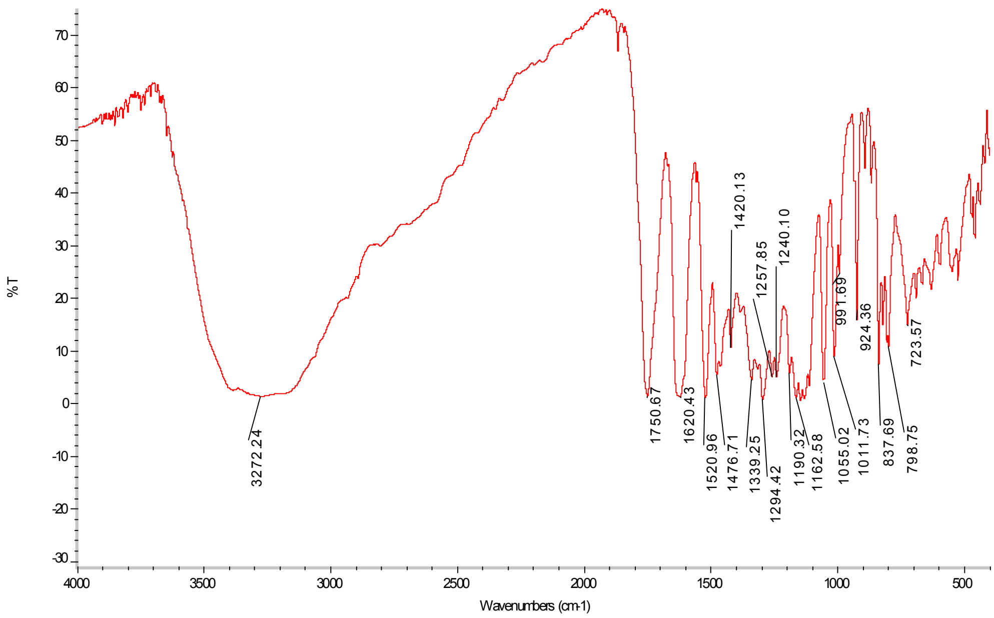
892.48
829.00

4o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50
40
30
20
10
0
-10
-20
-30
4000
3500
3000
2500
2000
1500
1000
500
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1750.67
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1520.96
1476.71
1420.13
1339.25
1294.42
1257.85
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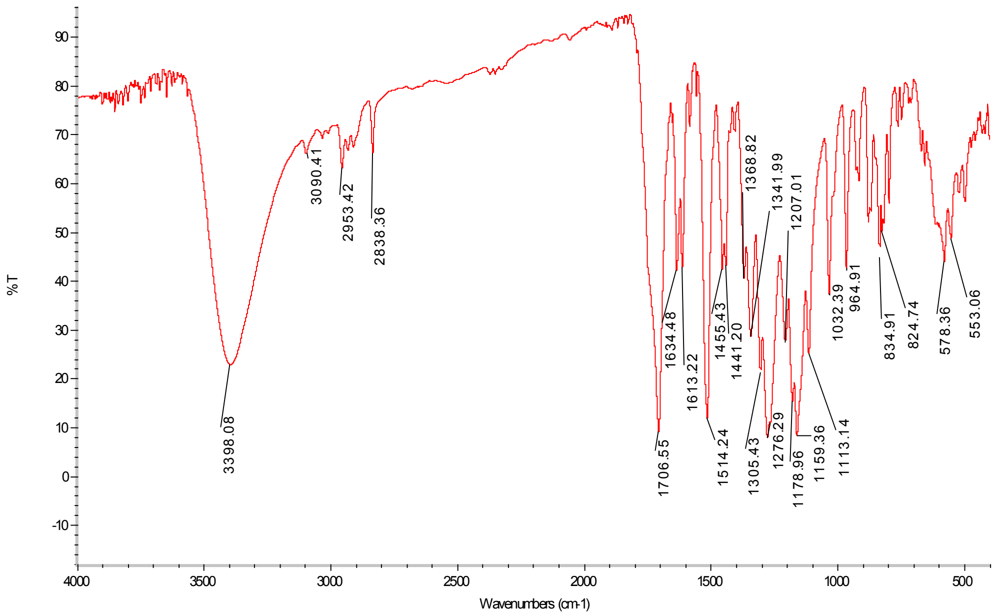
4p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60
50
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20
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0
-10
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3500
3000
2500
2000
1500
1000
500
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2953.42
2838.36
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1514.24
1455.43
1441.20
1368.82
1341.99
1305.43
1276.29
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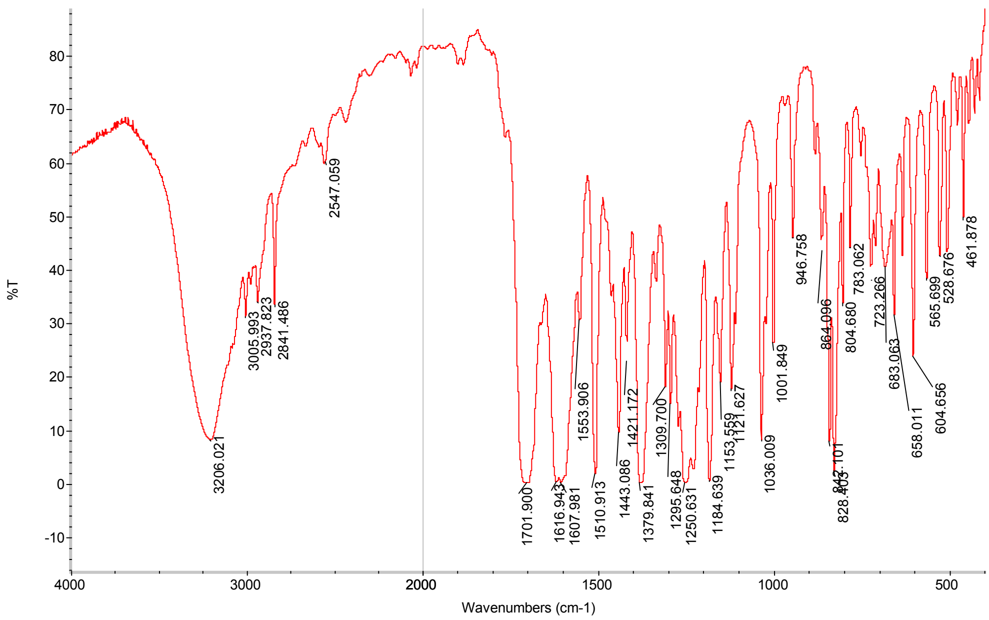
553.06

8a



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1295.648
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1001.849
946.758
864.096
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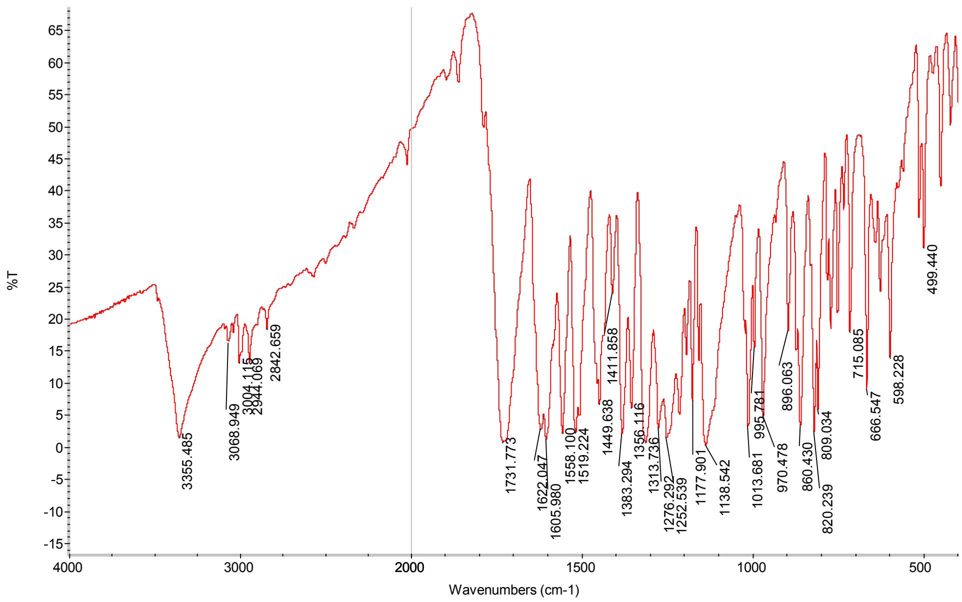
8b



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1519.224
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1276.292
1252.539
1177.901
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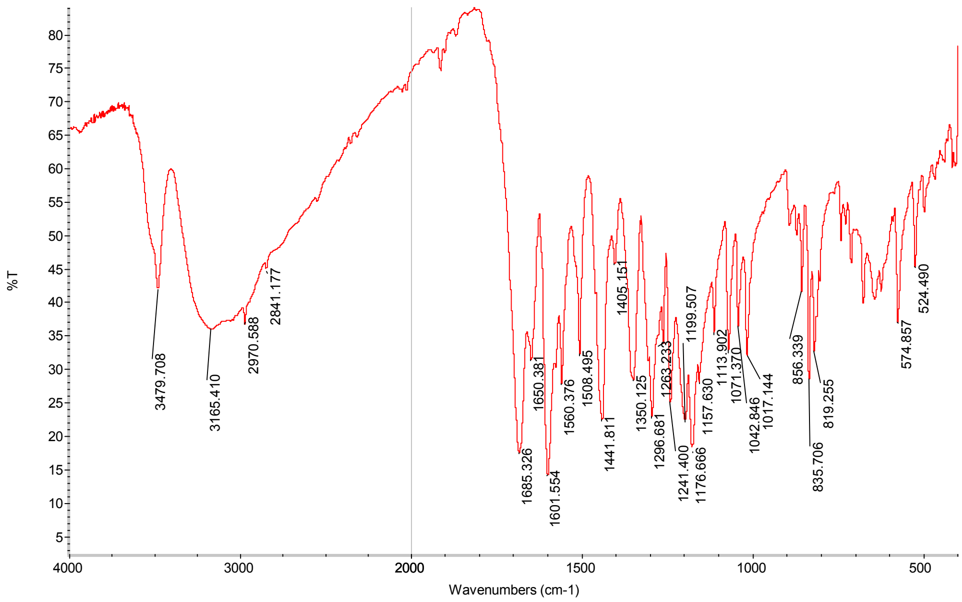
8c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1441.811
1405.151
1350.125
1296.681
1263.233
1241.400
1199.507
1176.666
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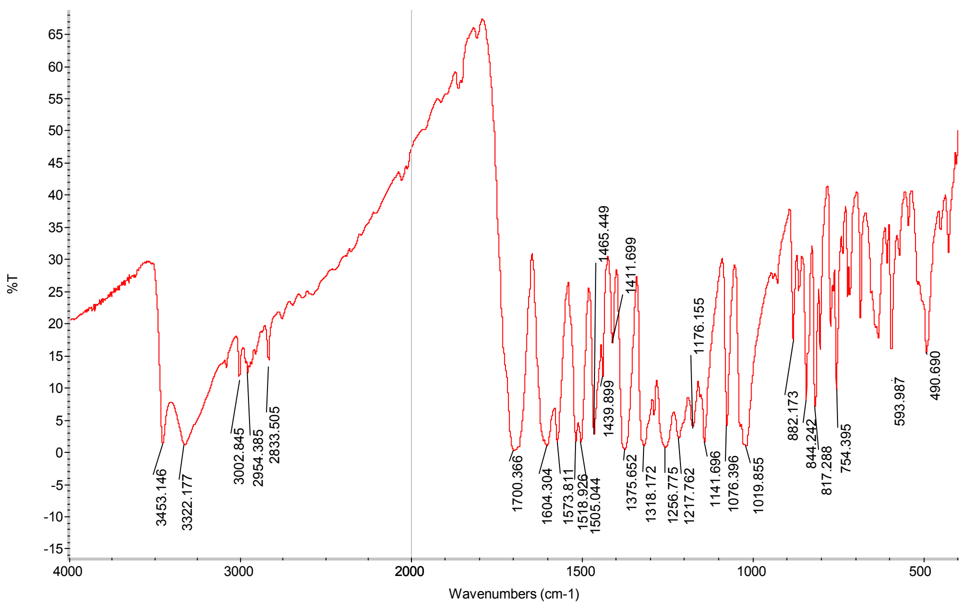
8d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1411.699
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1318.172
1256.775
1217.762
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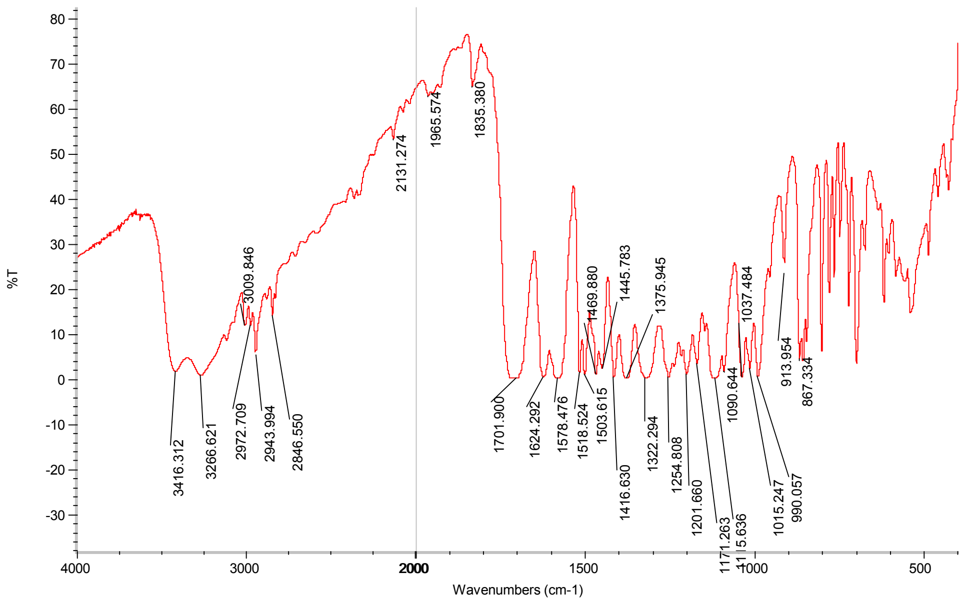
490.690

8e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1578.476
1518.524
1503.615
1469.880
1445.783
1416.630
1375.945
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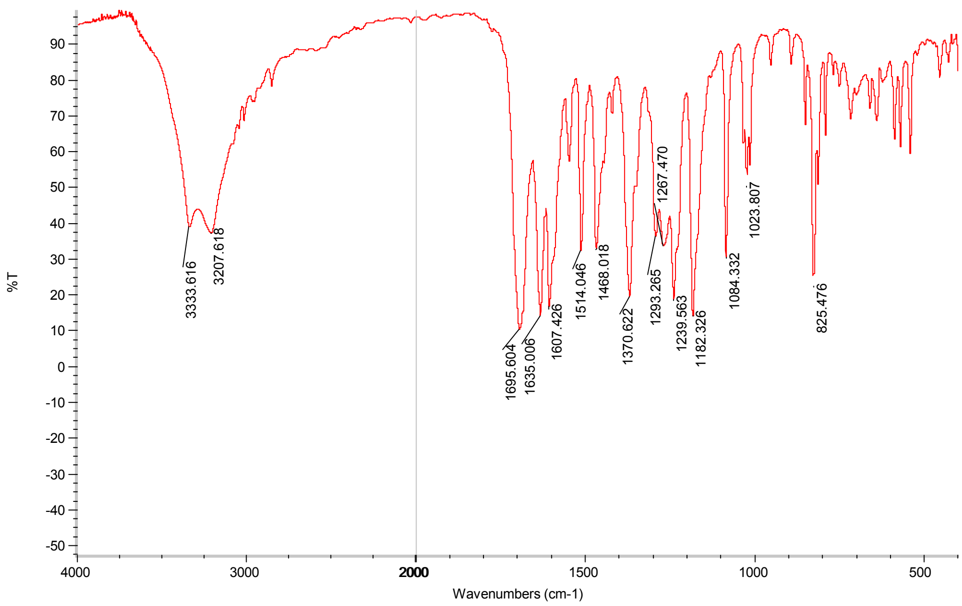
8f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Wavenumbers (cm-1)
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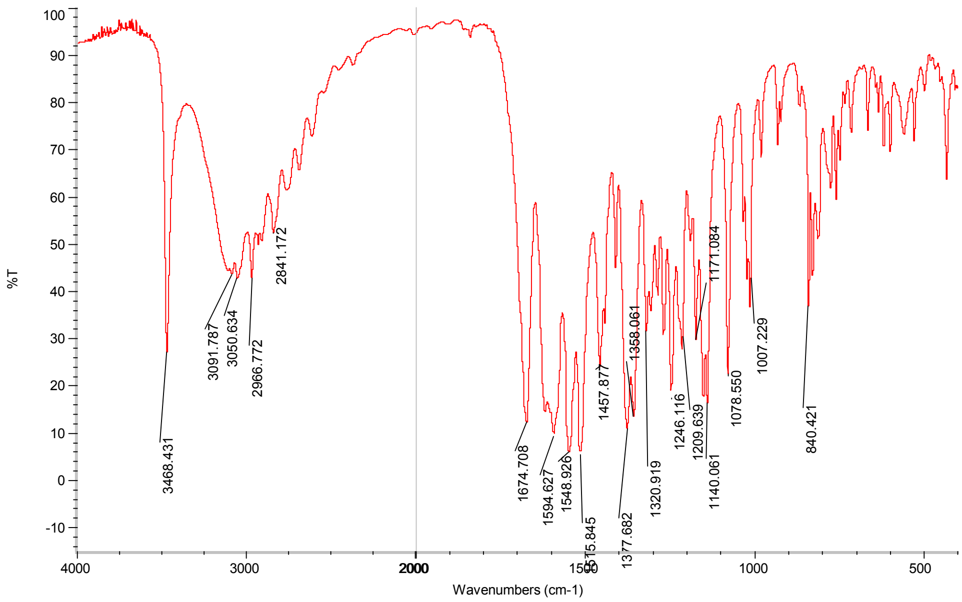
825.476

8g



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1457.877
1377.682
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1246.116
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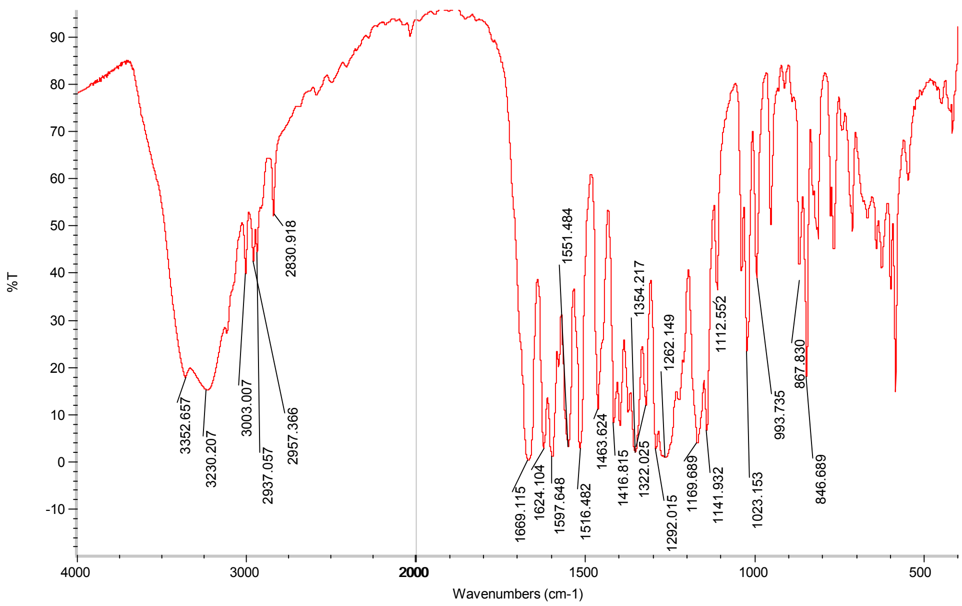
840.421

8h



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1463.624
1416.815
1354.217
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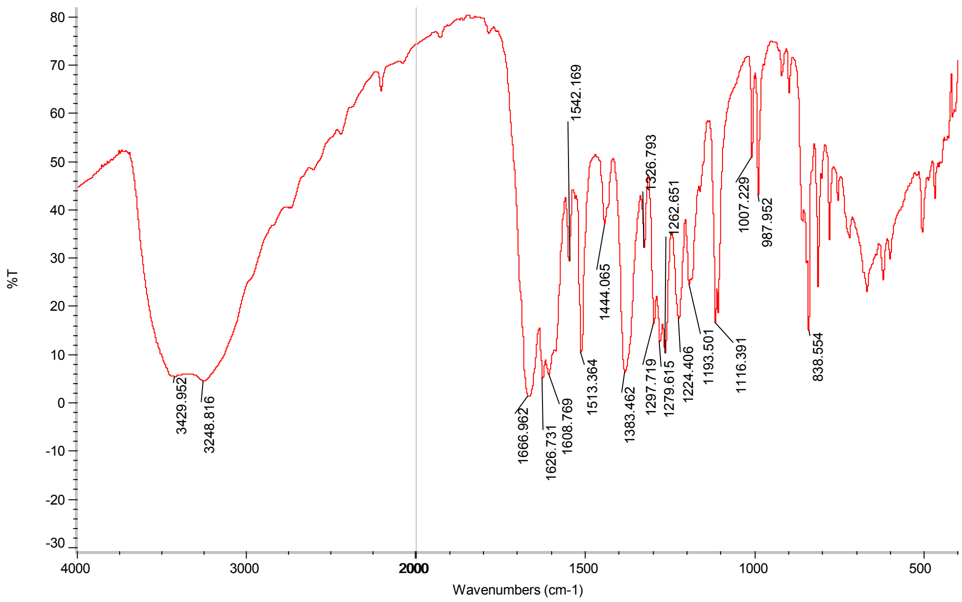
8i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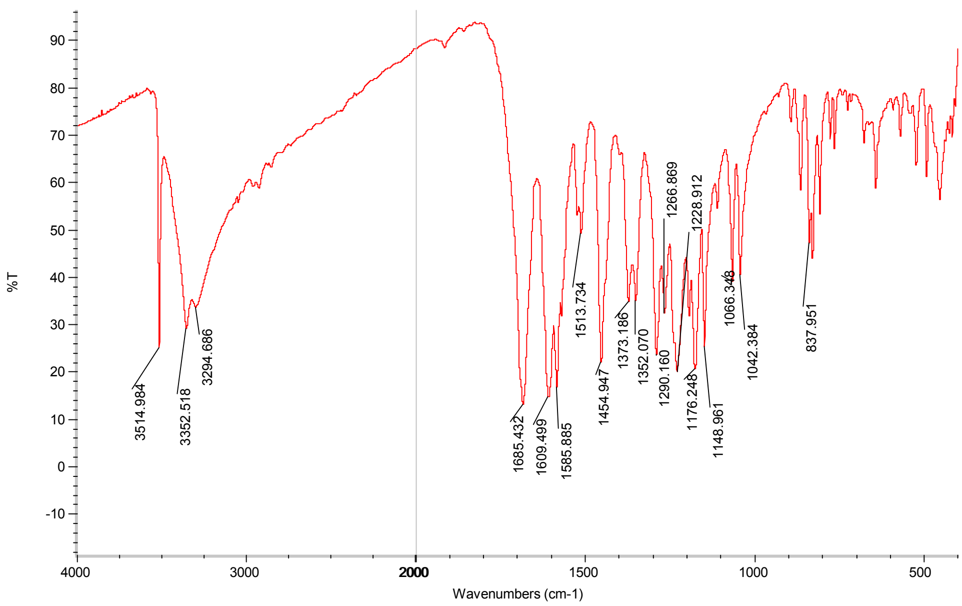
8j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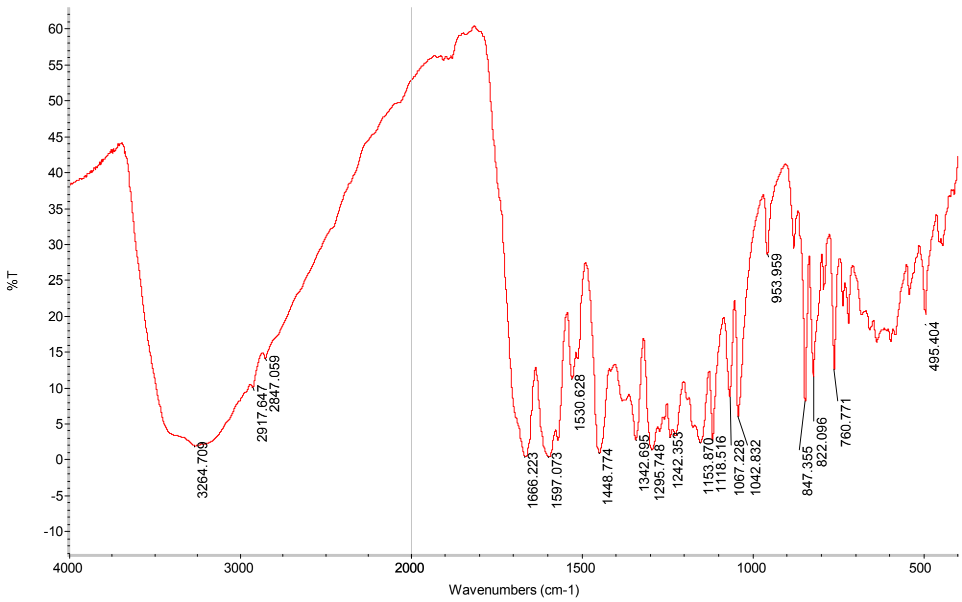
8k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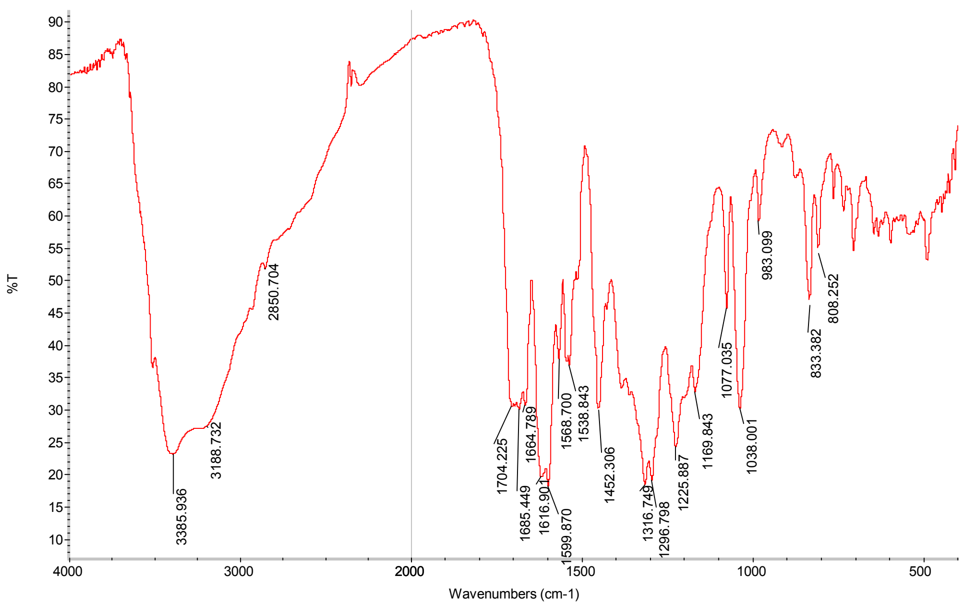
8l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1538.843
1452.306
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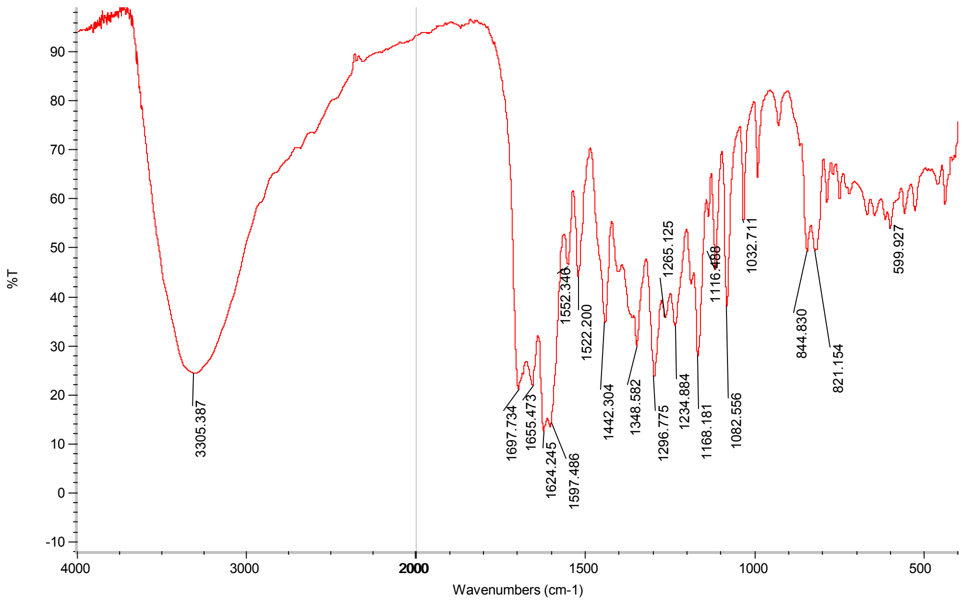
1296.798
1225.887
1169.843
1077.035
1038.001
983.099
833.382
808.252

8m



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Wavenumbers (cm-1)
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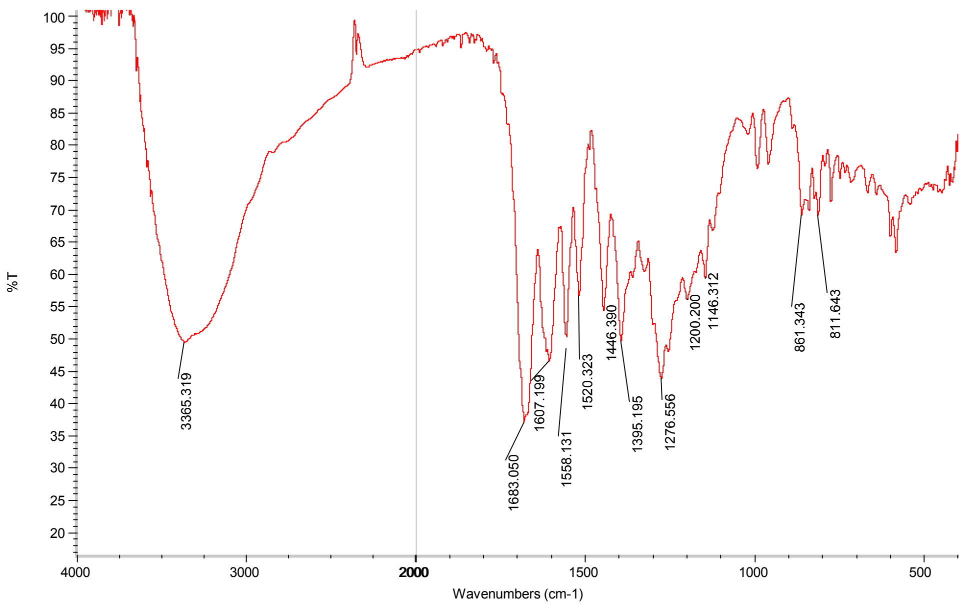
1168.181
1116.408
1082.556
1032.711
844.830
821.154
599.927

8n



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Wavenumbers (cm-1)
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1146.312
861.343
811.643

HPLC spectra of compounds 4a-8n

Specify methods used: Instrument:Agilent 1100;

Column:Agilent SB-C18, 30 x 2.1 mm,3.5 um;

Detector:DAD detector, 254 nm;

Flow rate: 1 ml / min

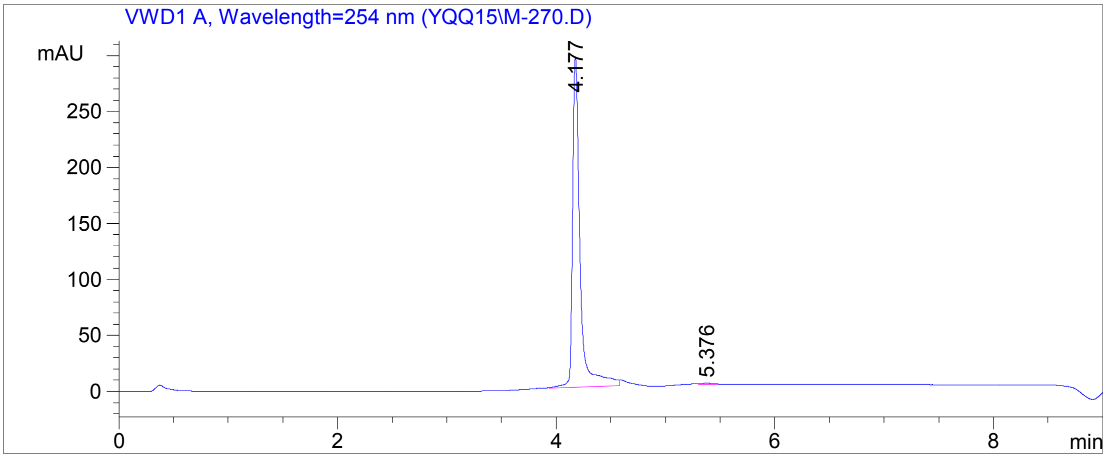
Mobile phase: methanol: water (0.1% glacial acetic acid); gradient elution

Injection volume: 5 ul

Temperature: 25 ° C

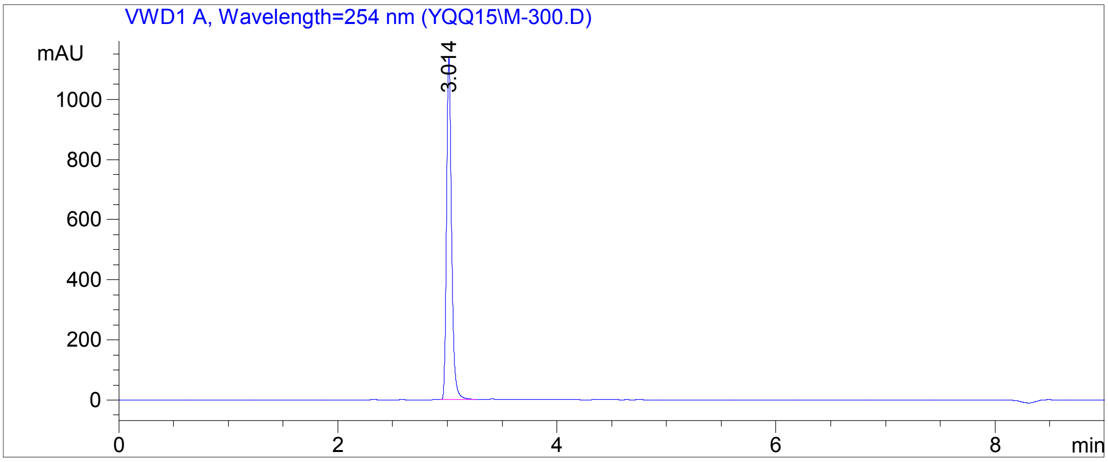
Spectra without purity table means that the purity is close to 100%.

4a

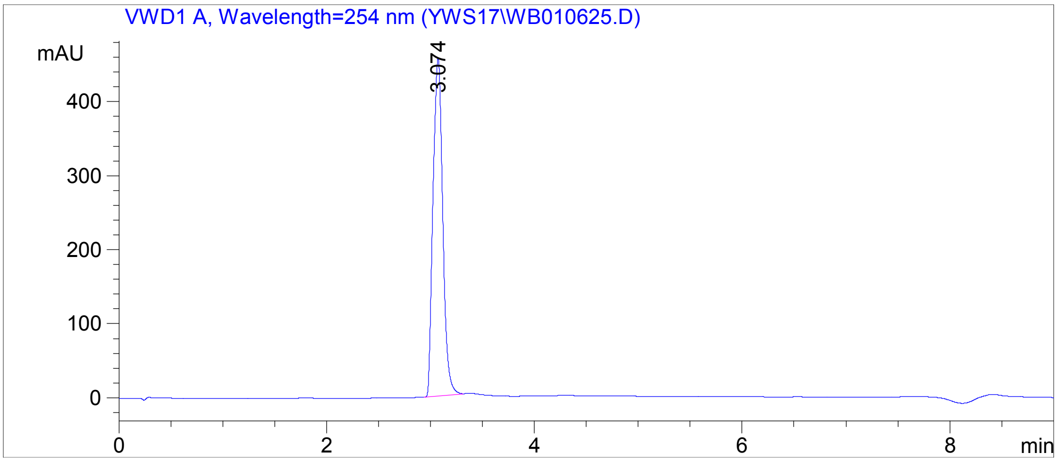


This means that the purity is close to 100%.

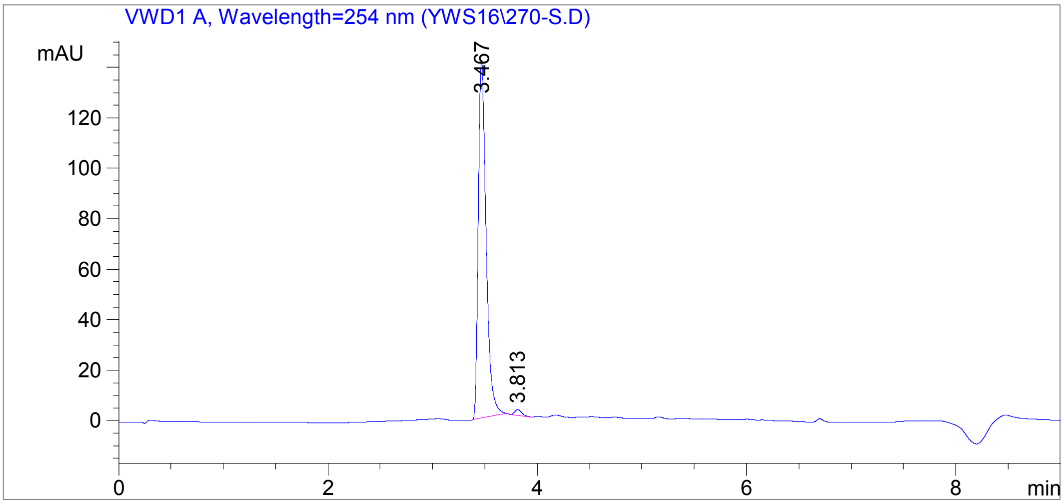
4b



4c

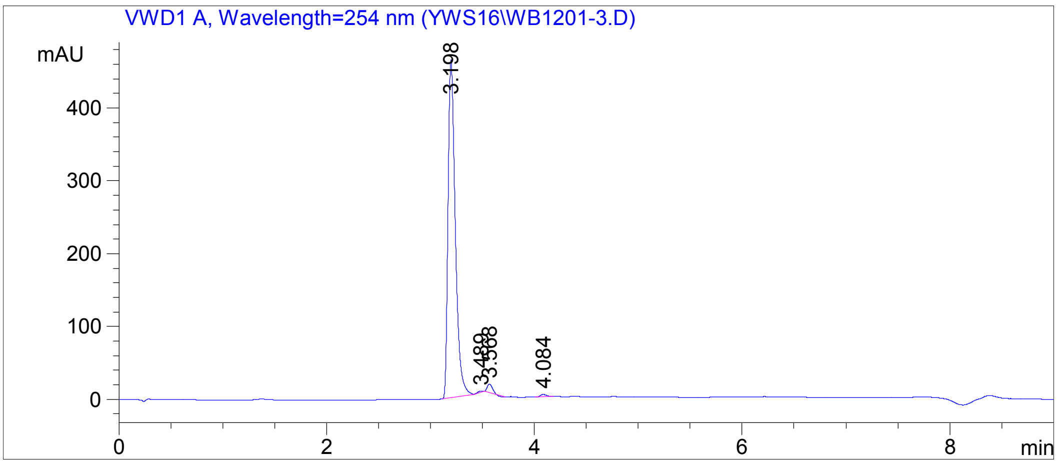


4d



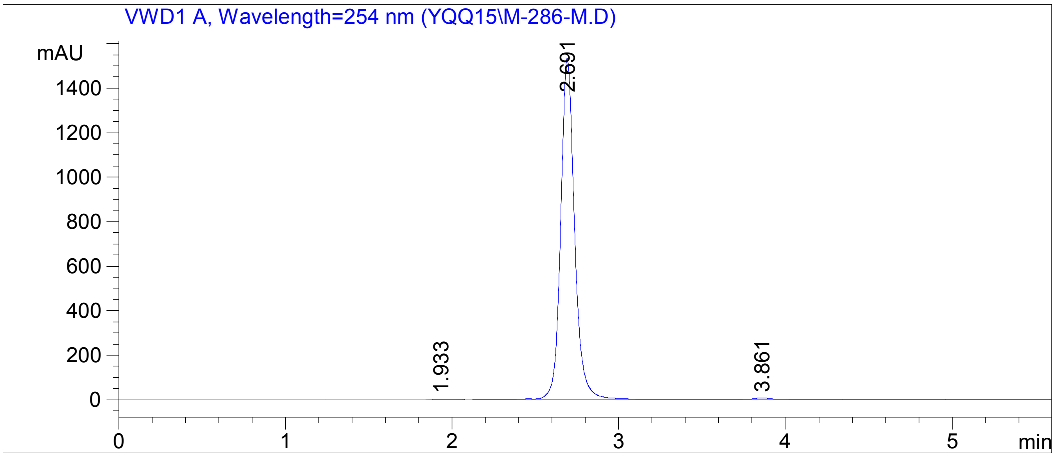
#	Meas. Ret. Time	Main Peak Heigh	Main Peak Area	Main Peak Area %
1	3.467	141.791	732.287	98.647
2	3.813	2.263	10.043	1.352

4e



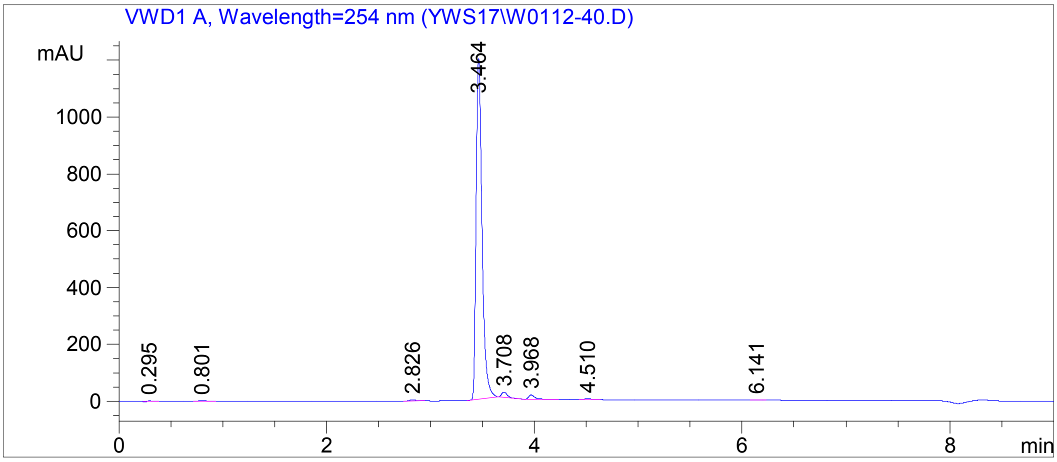
#	Meas. Ret. Time	Main Peak Heigh	Main Peak Area	Main Peak Area %
1	3.198	464.090	2246.243	97.457
2	3.489	1.799	5.456	0.236
3	3.568	12.042	40.789	1.769
4	4.084	3.167	12.358	0.536

4f



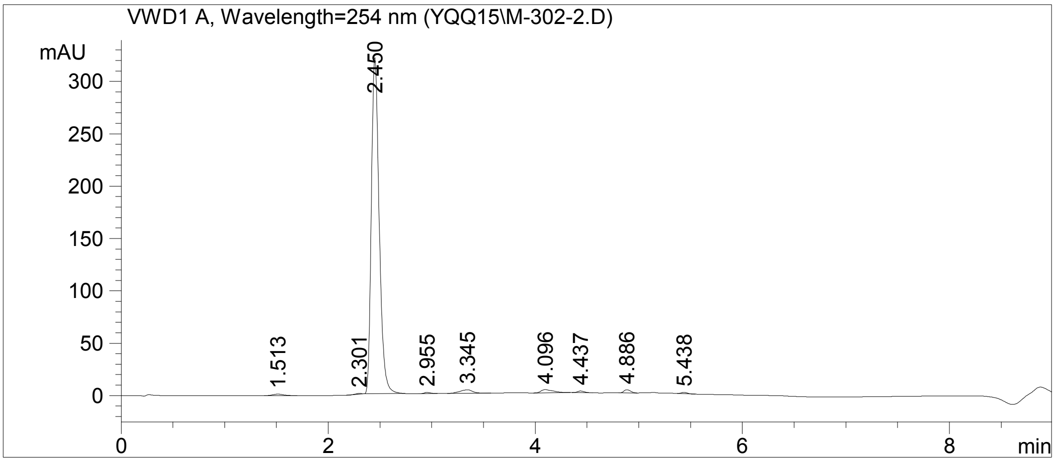
#	Meas. Ret. Time	Main Peak Heigh	Main Peak Area	Main Peak Area %
1	1.933	1.660	7.876	0.088
2	2.691	1534.656	8880.228	99.419
3	3.861	7.018	43.950	0.492

4g



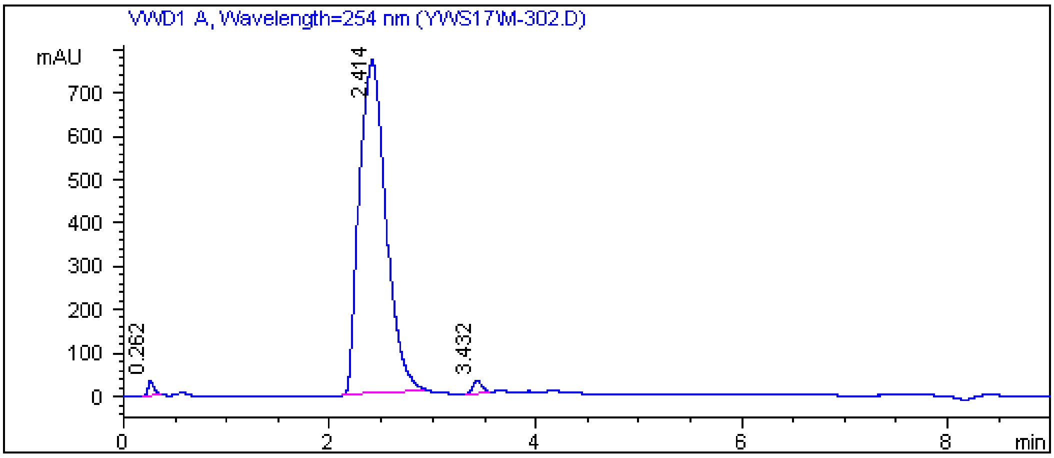
#	Meas. Ret. Time	Main Peak Heigh	Main Peak Area	Main Peak Area %
1	0.295	1.491	1.160	0.023
2	0.801	2.101	10.154	0.206
3	2.826	4.213	17.405	0.353
4	3.464	1199.614	4734.924	96.282
5	3.708	18.724	68.369	1.390
6	3.968	14.836	65.314	1.328
7	4.510	3.189	15.779	0.320
8	6.141	1.314	4.620	0.094

4h



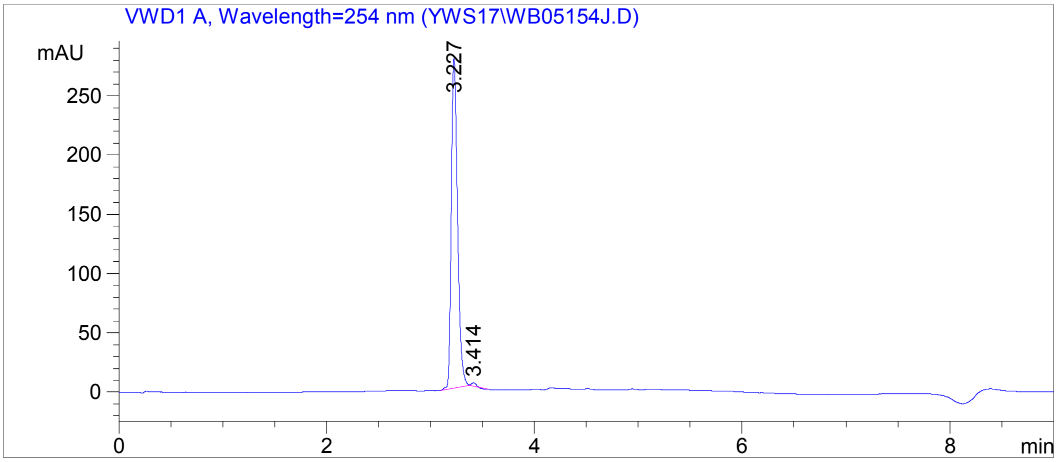
#	Meas. Ret. Time	Main Peak Heigh	Main Peak Area	Main Peak Area %
1	1.513	1.481	11.082	0.619
2	2.301	0.728	2.826	0.157
3	2.450	321.301	1689.159	94.404
4	2.955	1.157	5.148	0.287
5	3.345	3.365	29.293	1.637
6	4.096	3.104	25.509	1.425
7	4.437	1.601	7.032	0.393
8	4.886	3.069	13.798	0.771
9	5.438	1.336	5.432	0.303

4i



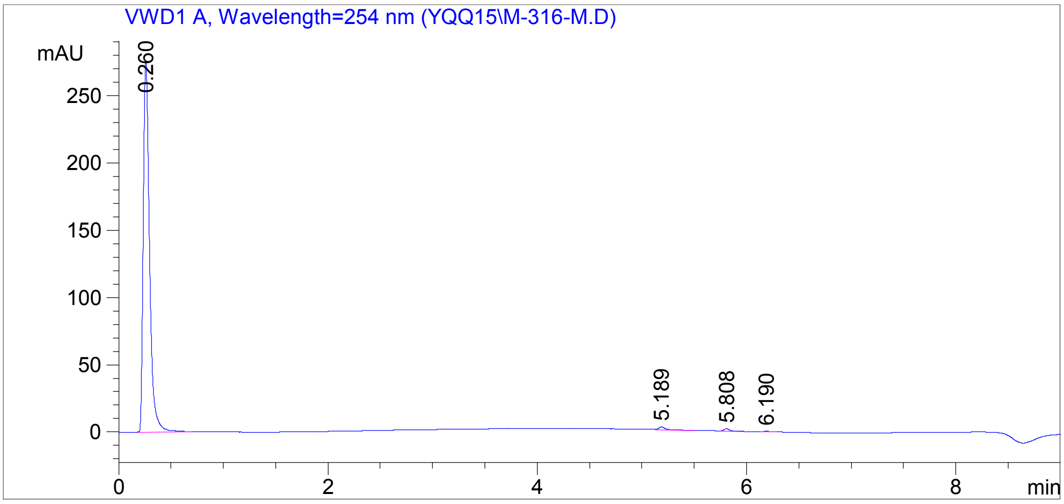
#	Meas. Ret. Time	Main Peak Heigh	Main Peak Area	Main Peak Area %
1	0.262	33.969	156.412	1.104
2	2.414	765.840	13819.979	97.605
3	3.432	27.611	182.690	1.290

4j



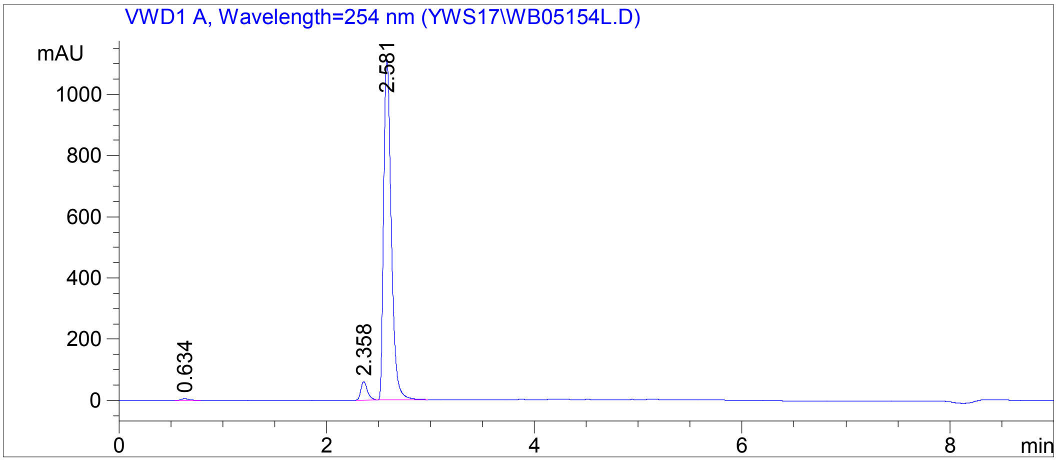
#	Meas. Ret. Time	Main Peak Heigh	Main Peak Area	Main Peak Area %
1	3.227	278.253	1156.969	99.544
2	3.414	2.633	5.297	0.455

4k



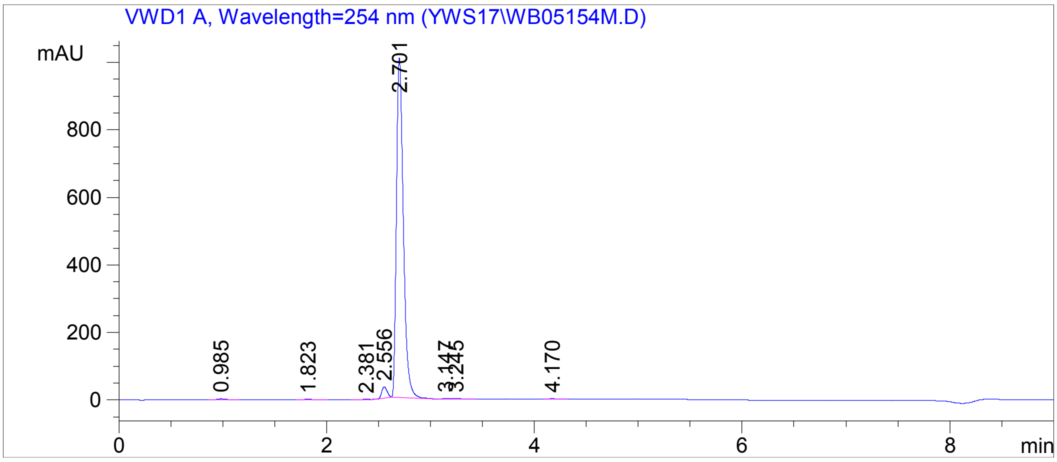
#	Meas. Ret. Time	Main Peak Heigh	Main Peak Area	Main Peak Area %
1	0.260	276.218	1145.243	98.563
2	5.189	2.071	8.785	0.756
3	5.808	1.723	6.377	0.548
4	6.190	0.426	1.525	0.131

4l



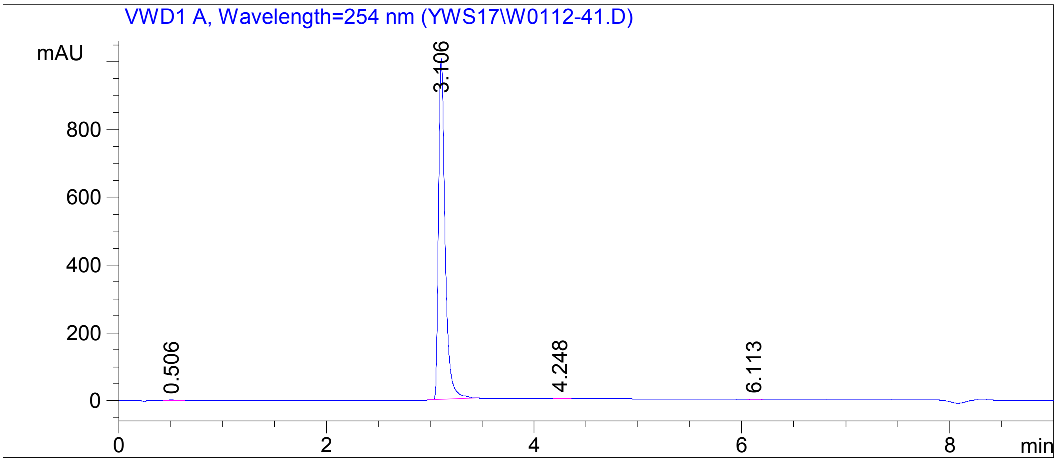
#	Meas. Ret. Time	Main Peak Heigh	Main Peak Area	Main Peak Area %
1	0.634	5.482	28.580	0.480
2	2.358	60.194	258.971	4.349
3	2.581	1116.142	5666.079	95.170

4m



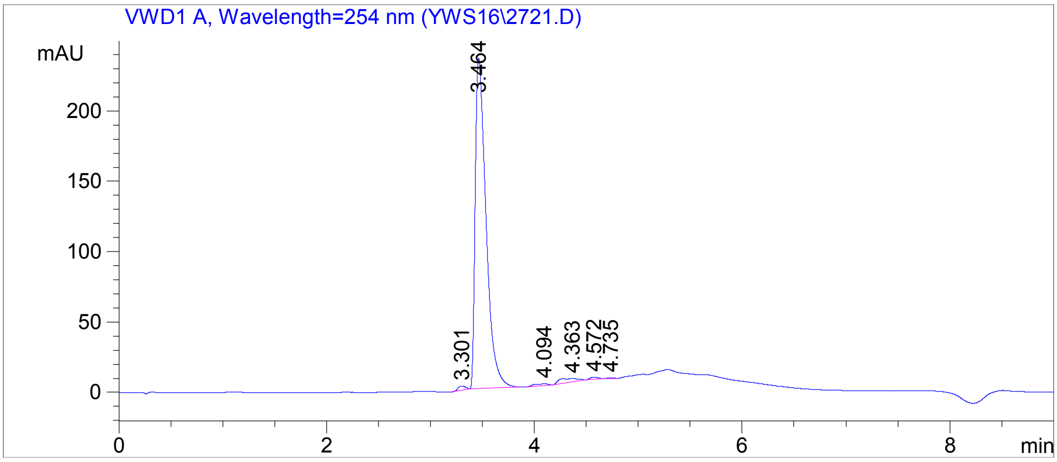
#	Meas. Ret. Time	Main Peak Heigh	Main Peak Area	Main Peak Area %
1	0.985	3.725	23.665	0.490
2	1.823	2.222	14.663	0.303
3	2.381	1.181	3.812	0.078
4	2.556	33.072	113.869	2.358
5	2.701	1004.659	4655.777	96.418
6	3.147	1.751	5.118	0.106
7	3.245	1.820	5.227	0.108
8	4.170	1.382	6.615	0.137

4n



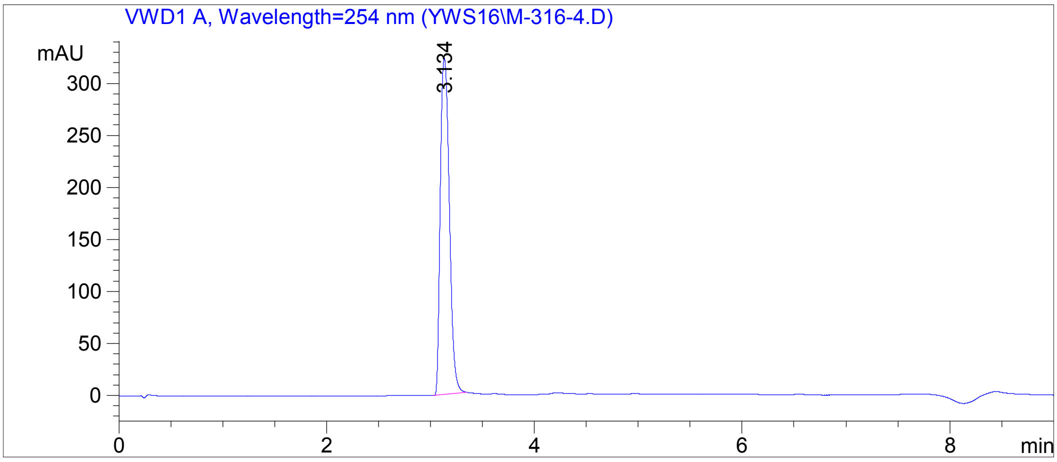
#	Meas. Ret. Time	Main Peak Heigh	Main Peak Area	Main Peak Area %
1	0.506	1.996	9.523	0.213
2	3.106	1006.852	4440.542	99.569
3	4.248	1.135	4.863	0.109
4	6.113	1.338	4.830	0.108

4o

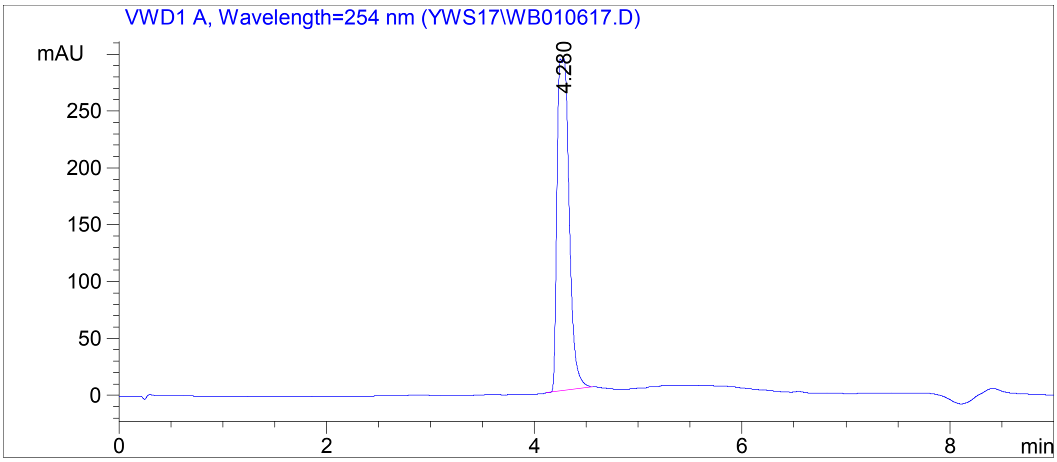


#	Meas. Ret. Time	Main Peak Heigh	Main Peak Area	Main Peak Area %
1	3.301	2.937	14.289	0.807
2	3.464	234.961	1698.379	95.913
3	4.094	1.288	11.179	0.631
4	4.363	2.452	35.783	2.020
5	4.572	1.561	8.546	0.482
6	4.735	0.606	2.568	0.145

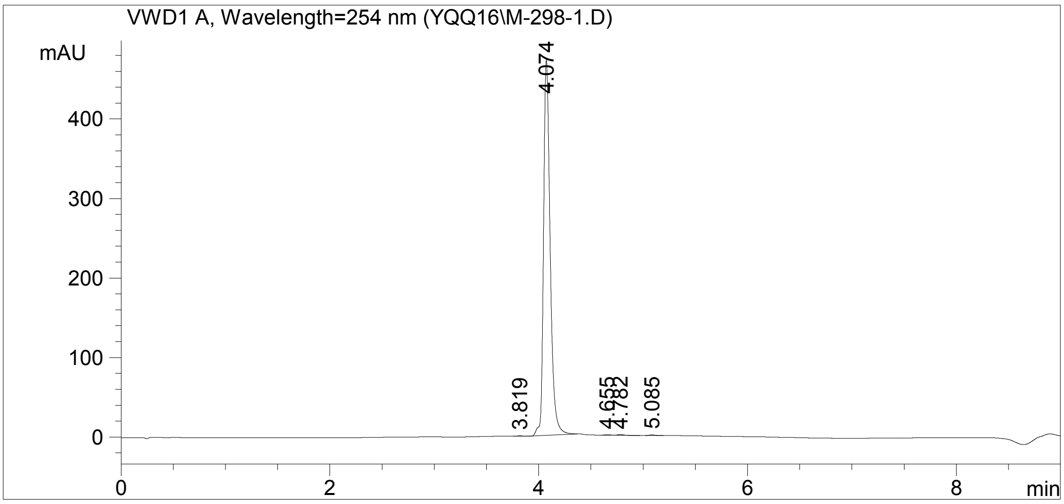
4p



8a

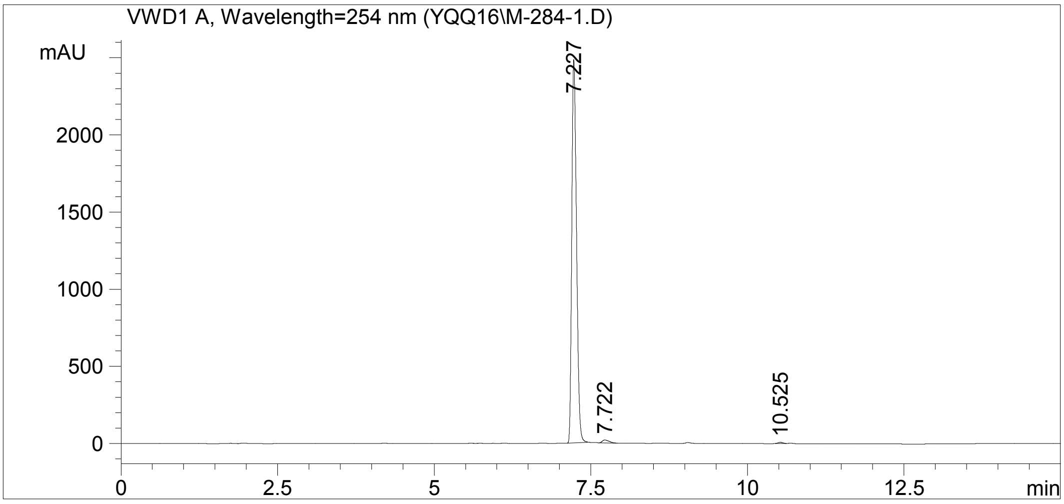


8b



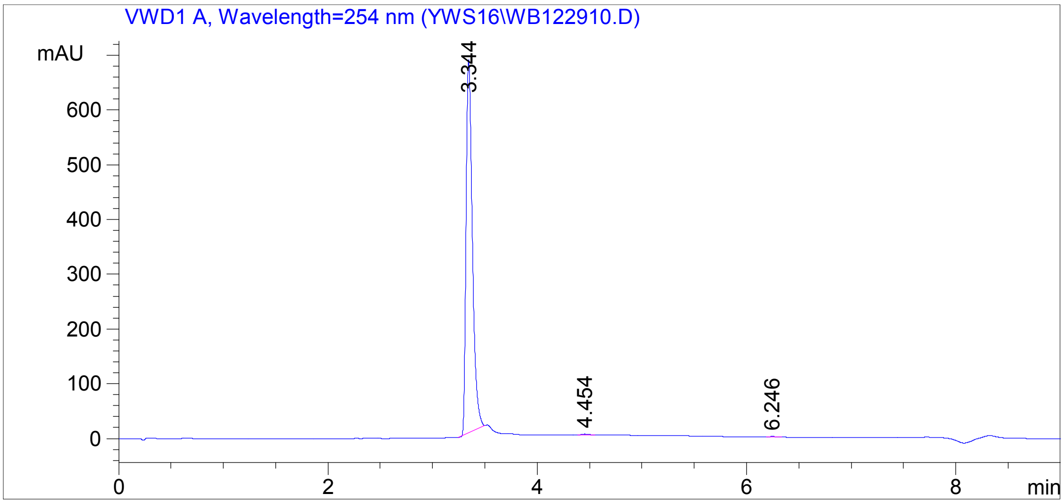
#	Meas. Ret. Time	Main Peak Heigh	Main Peak Area	Main Peak Area %
1	3.819	0.499	1.838	0.087
2	4.074	472.236	2084.687	99.495
3	4.655	0.540	1.930	0.092
4	4.782	0.882	3.557	0.169
5	5.085	0.818	3.253	0.155

8c

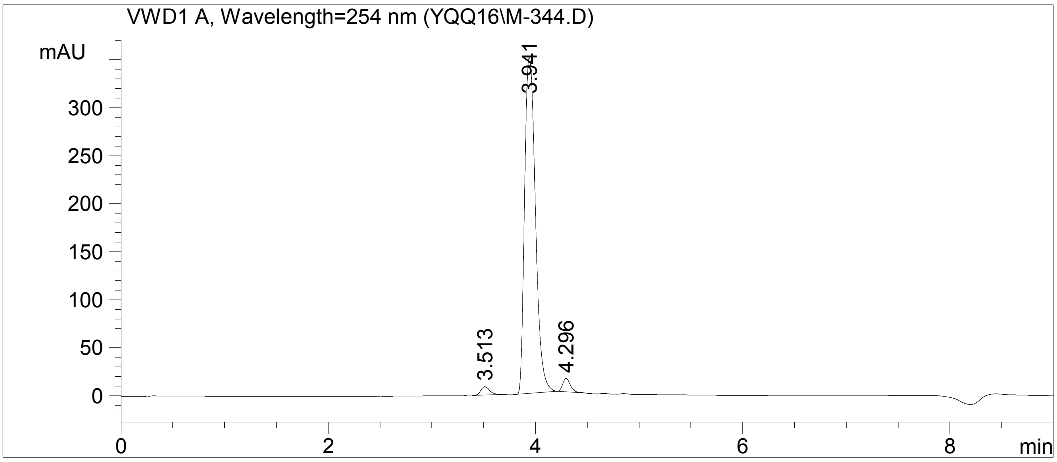


#	Meas. Ret. Time	Main Peak Heigh	Main Peak Area	Main Peak Area %
1	7.227	2485.287	13036.486	98.631
2	7.722	18.726	137.708	1.041
3	10.525	7.840	43.215	0.327

8d

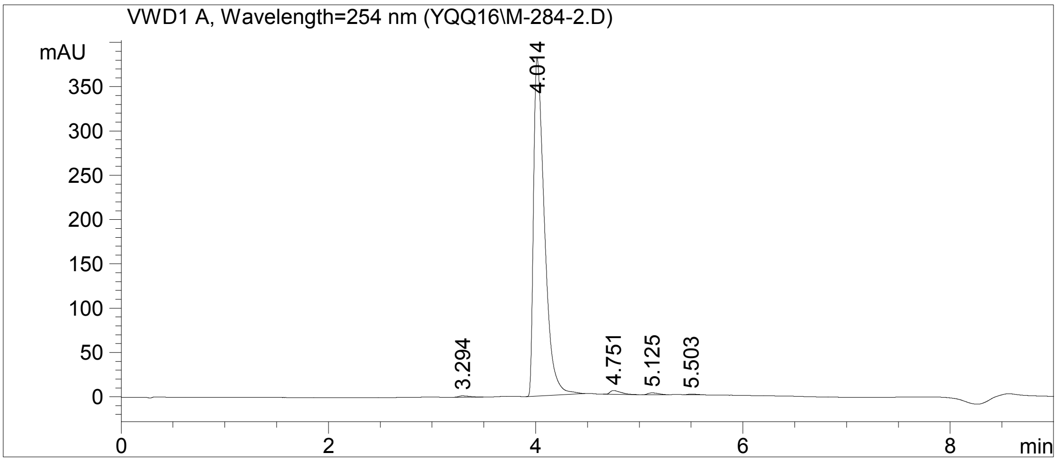


8e



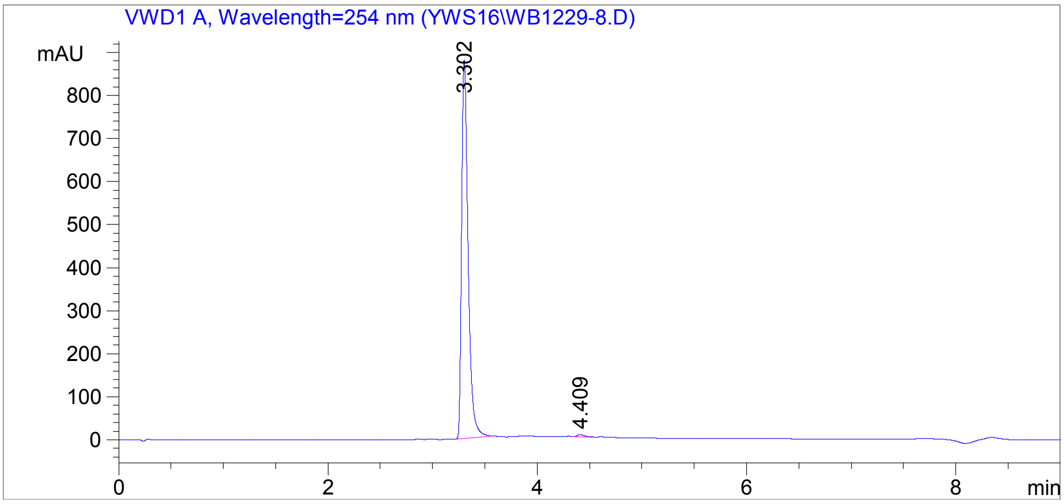
#	Meas. Ret. Time	Main Peak Heigh	Main Peak Area	Main Peak Area %
1	3.513	8.703	51.003	1.915
2	3.941	349.673	2542.413	95.462
3	4.296	14.008	69.857	2.623

8f

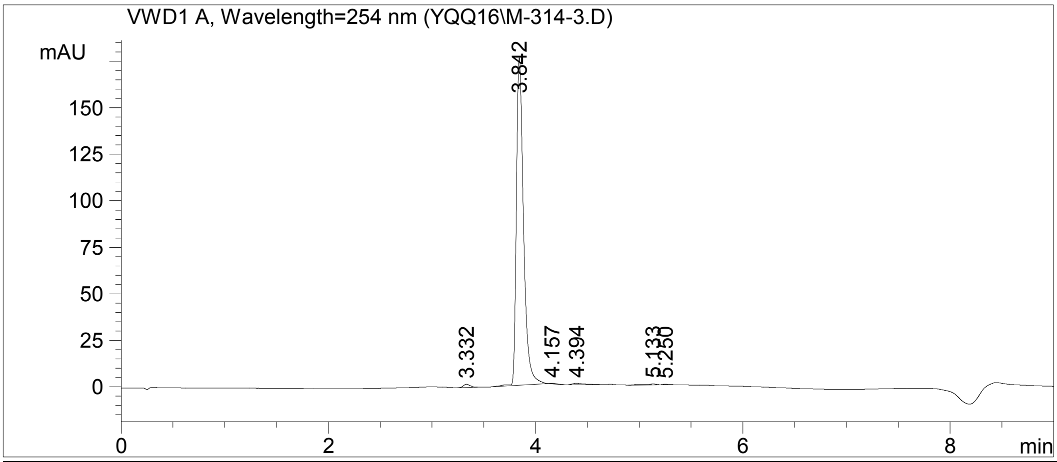


#	Meas. Ret. Time	Main Peak Heigh	Main Peak Area	Main Peak Area %
1	3.294	1.540	11.228	0.392
2	4.014	382.008	2795.469	97.814
3	4.751	4.389	31.548	1.103
4	5.125	2.046	14.979	0.524
5	5.503	0.856	4.693	0.164

8g

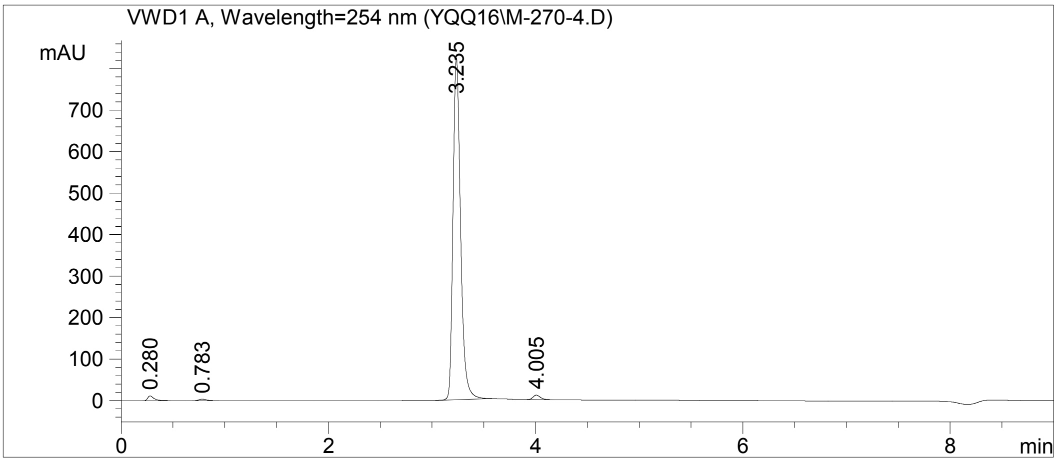


8h



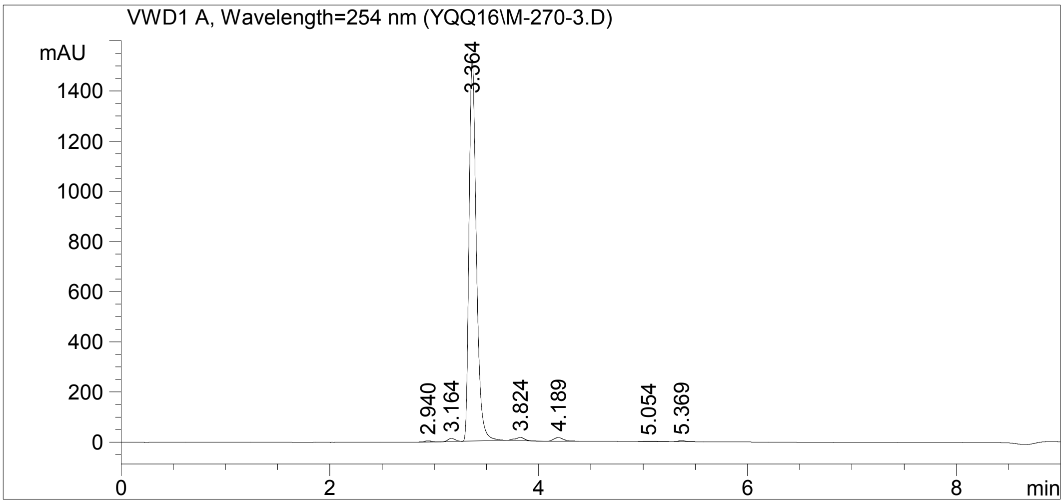
#	Meas. Ret. Time	Main Peak Heigh	Main Peak Area	Main Peak Area %
1	3.332	1.667	7.381	0.851
2	3.842	176.033	846.854	97.719
3	4.157	0.362	1.461	0.168
4	4.394	0.788	6.169	0.711
5	5.133	0.481	3.684	0.425
6	5.250	0.279	1.071	0.123

8i



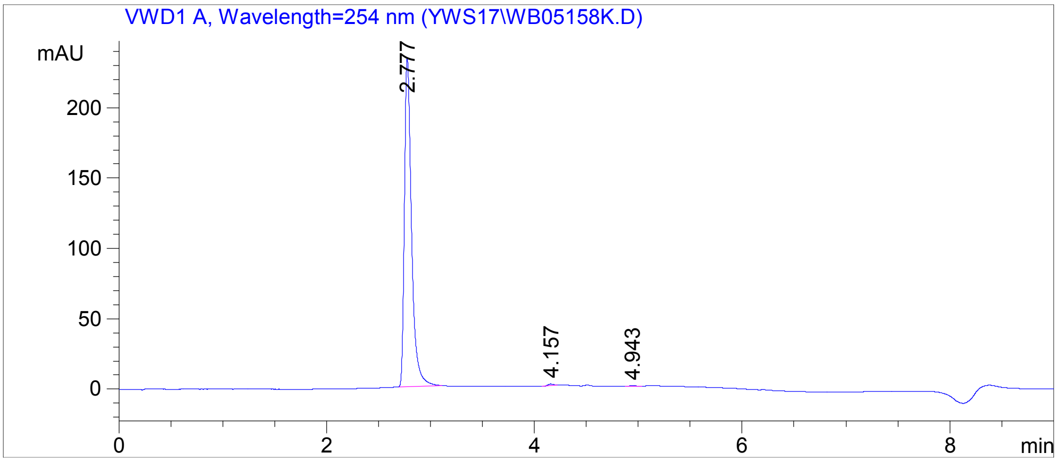
#	Meas. Ret. Time	Main Peak Heigh	Main Peak Area	Main Peak Area %
1	0.280	11.688	50.440	1.170
2	0.783	3.748	20.324	0.471
3	3.235	823.973	4186.617	97.133
4	4.005	10.821	52.784	1.224

8j



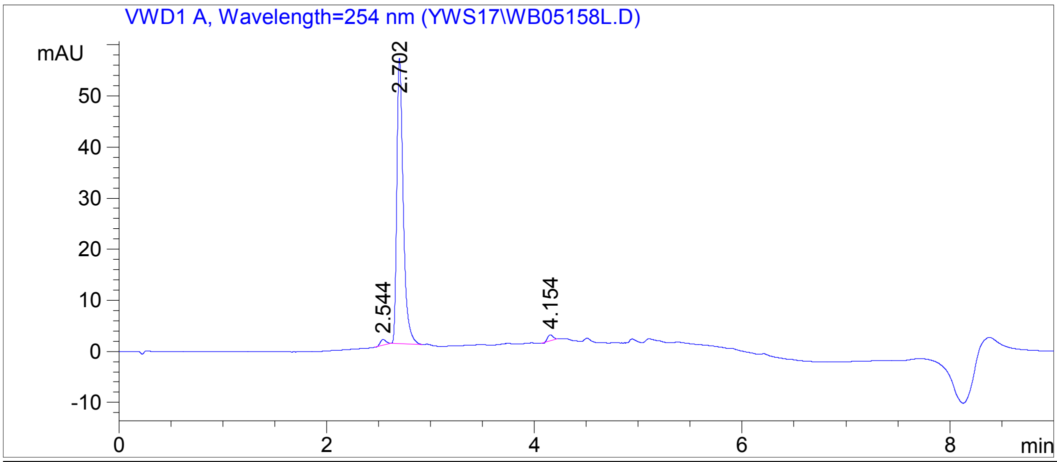
#	Meas. Ret. Time	Main Peak Heigh	Main Peak Area	Main Peak Area %
1	2.940	4.972	23.764	0.307
2	3.164	13.072	66.116	0.855
3	3.364	1520.333	7429.652	96.116
4	3.824	13.174	83.438	1.079
5	4.189	14.707	93.487	1.209
6	5.054	1.839	13.262	0.171
7	5.369	4.655	20.112	0.260

8k



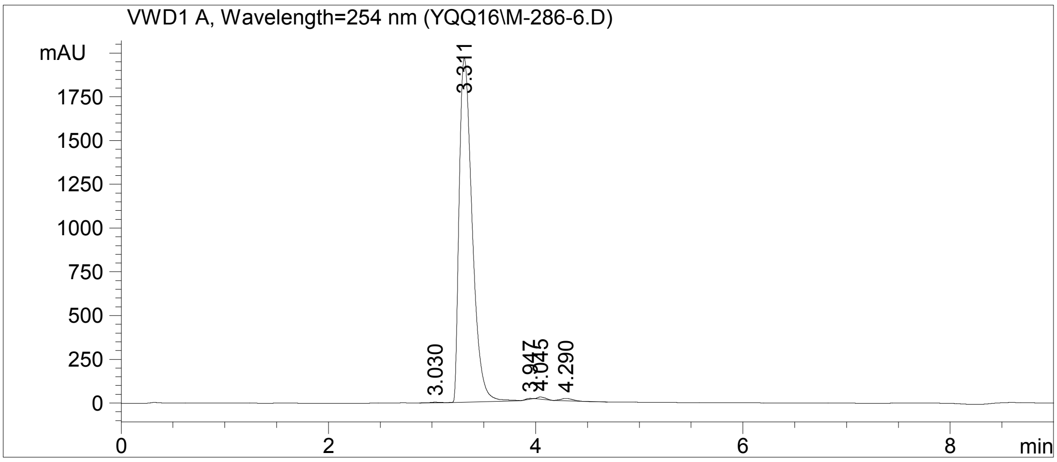
#	Meas. Ret. Time	Main Peak Heigh	Main Peak Area	Main Peak Area %
1	2.777	233.587	1112.374	99.330
2	4.157	1.222	4.429	0.395
3	4.943	0.764	3.074	0.274

8l



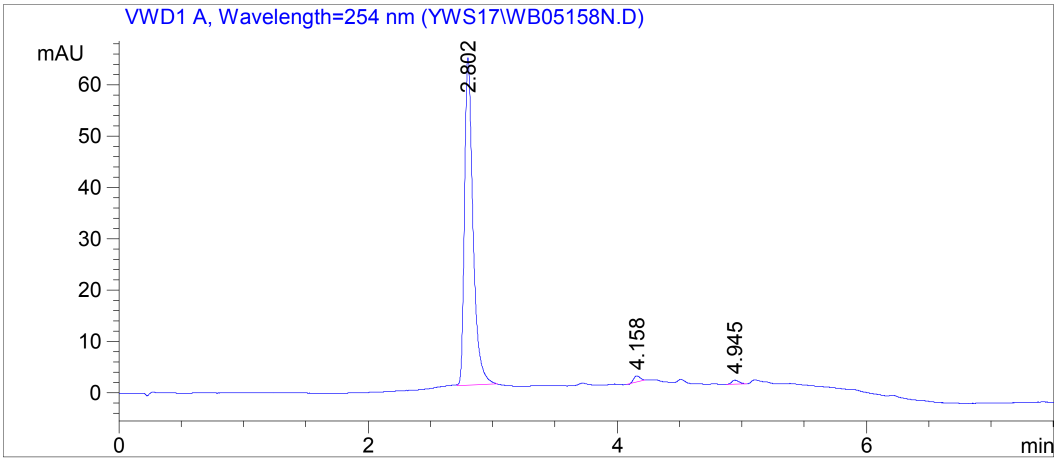
#	Meas. Ret. Time	Main Peak Heigh	Main Peak Area	Main Peak Area %
1	2.544	1.126	4.277	1.723
2	2.702	55.846	239.564	96.522
3	4.154	1.198	4.353	1.753

8m



#	Meas. Ret. Time	Main Peak Heigh	Main Peak Area	Main Peak Area %
1	3.030	3.231	22.030	0.127
2	3.311	1967.617	17106.301	98.780
3	3.947	5.054	21.349	0.123
4	4.045	12.753	70.976	0.409
5	4.290	13.339	96.883	0.559

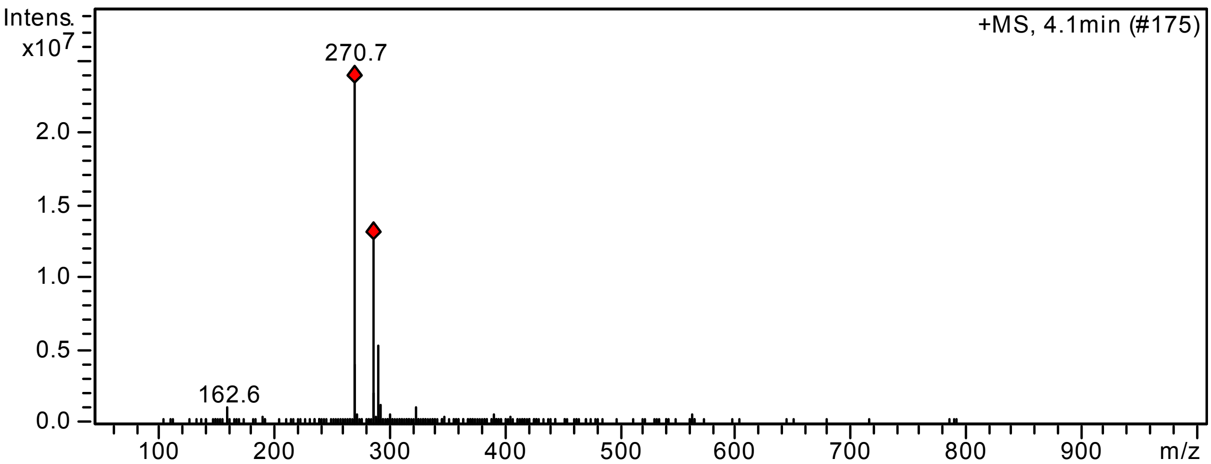
8n

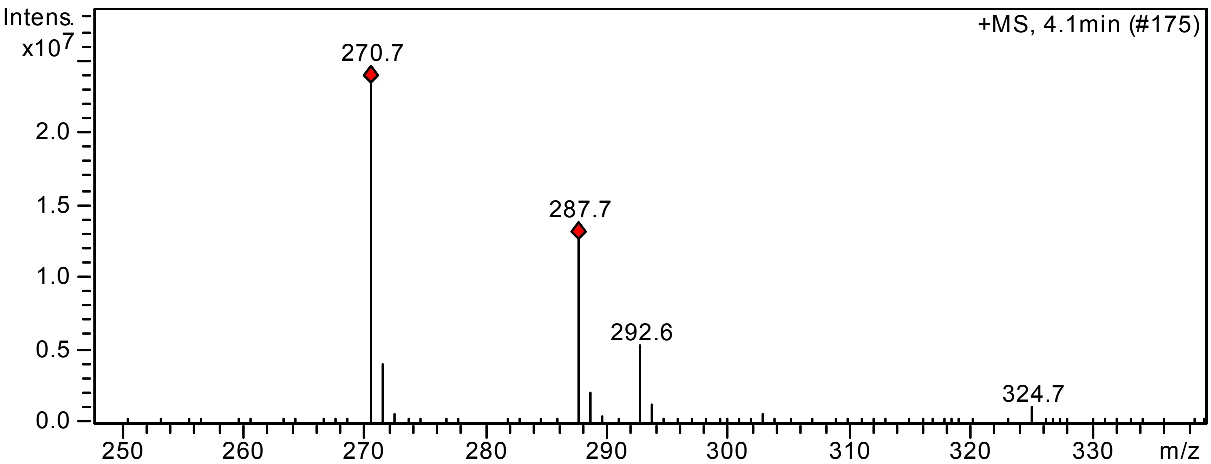


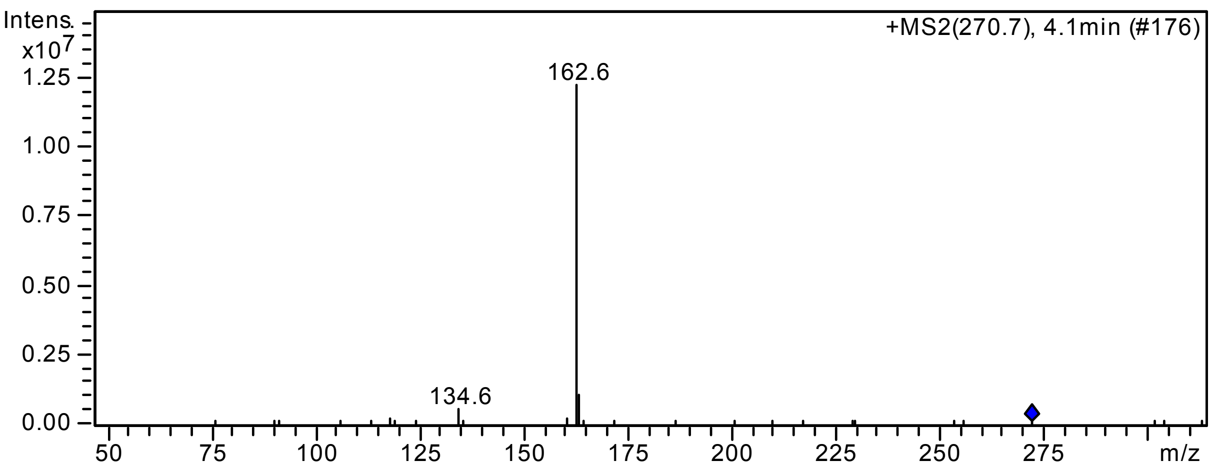
#	Meas. Ret. Time	Main Peak Heigh	Main Peak Area	Main Peak Area %
1	2.802	63.695	302.276	97.631
2	4.158	1.180	4.310	1.391
3	4.945	0.763	3.025	0.977

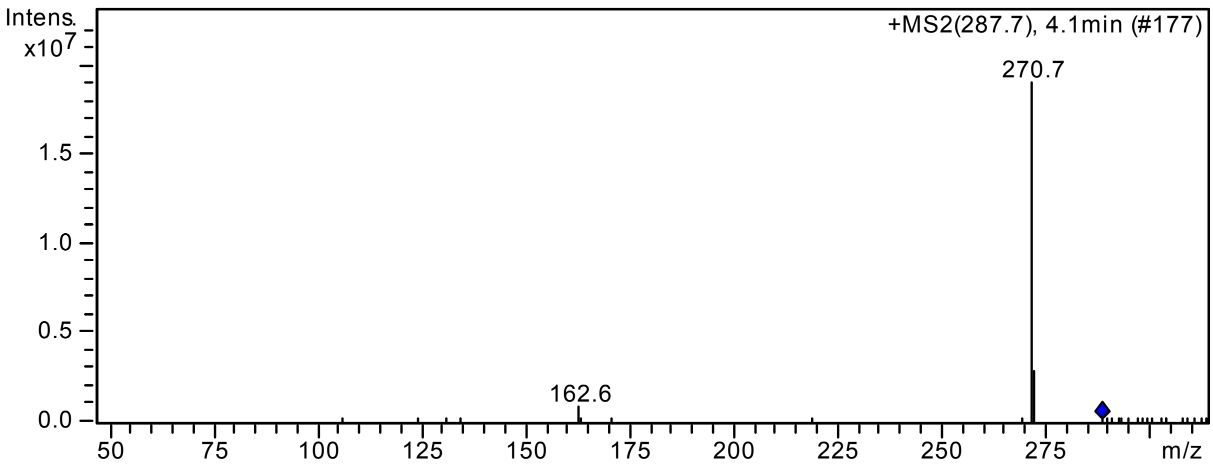
Mass spectrum of compounds 4a-8n

4a





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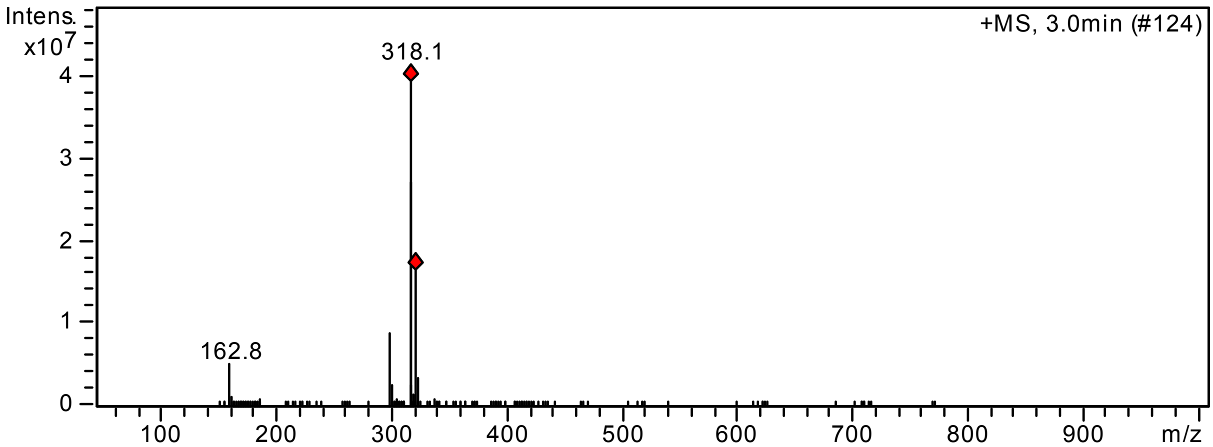
270.7
162.6
m/z

4b


Intens.
x10^7
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318.1
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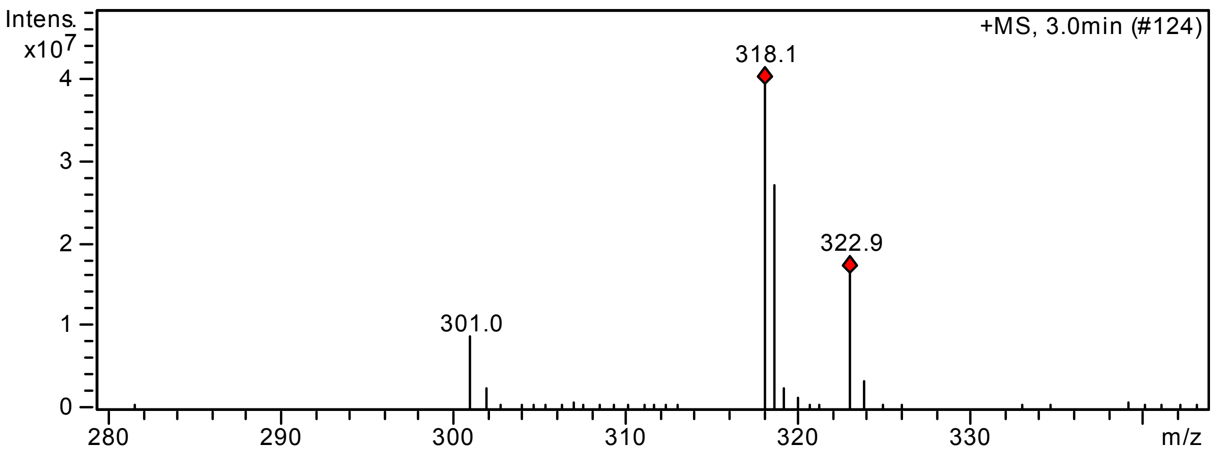
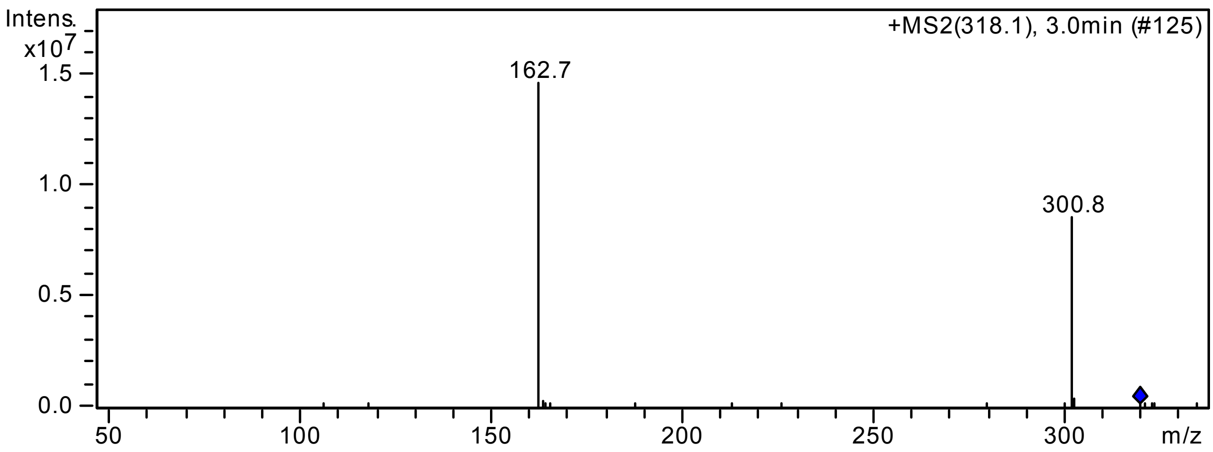
m/z


Intens.
x10^7
+MS, 3.0min (#124)
318.1
322.9
301.0
m/z


Intens.
x10^7
1.5
1.0
0.5
0.0
+MS2(318.1), 3.0min (#125)
162.7
300.8
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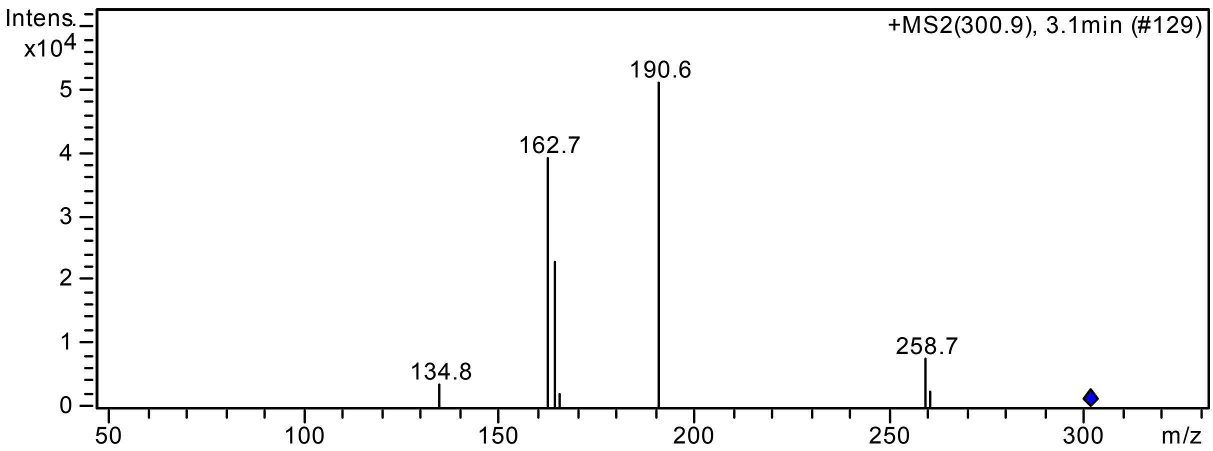
100
150
200
250
300
m/z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x10^4
5
4
3
2
1
0
+MS2(300.9), 3.1min (#129)
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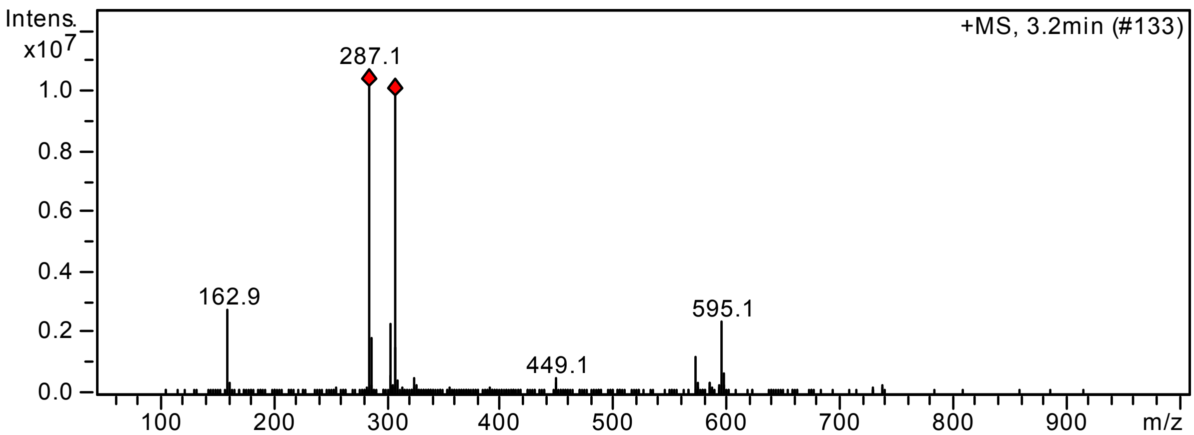
162.7
134.8
258.7
50
100
150
200
250
300
m/z

4c


Intens.
x10^7
1.0
0.8
0.6
0.4
0.2
0.0
+MS, 3.2min (#133)
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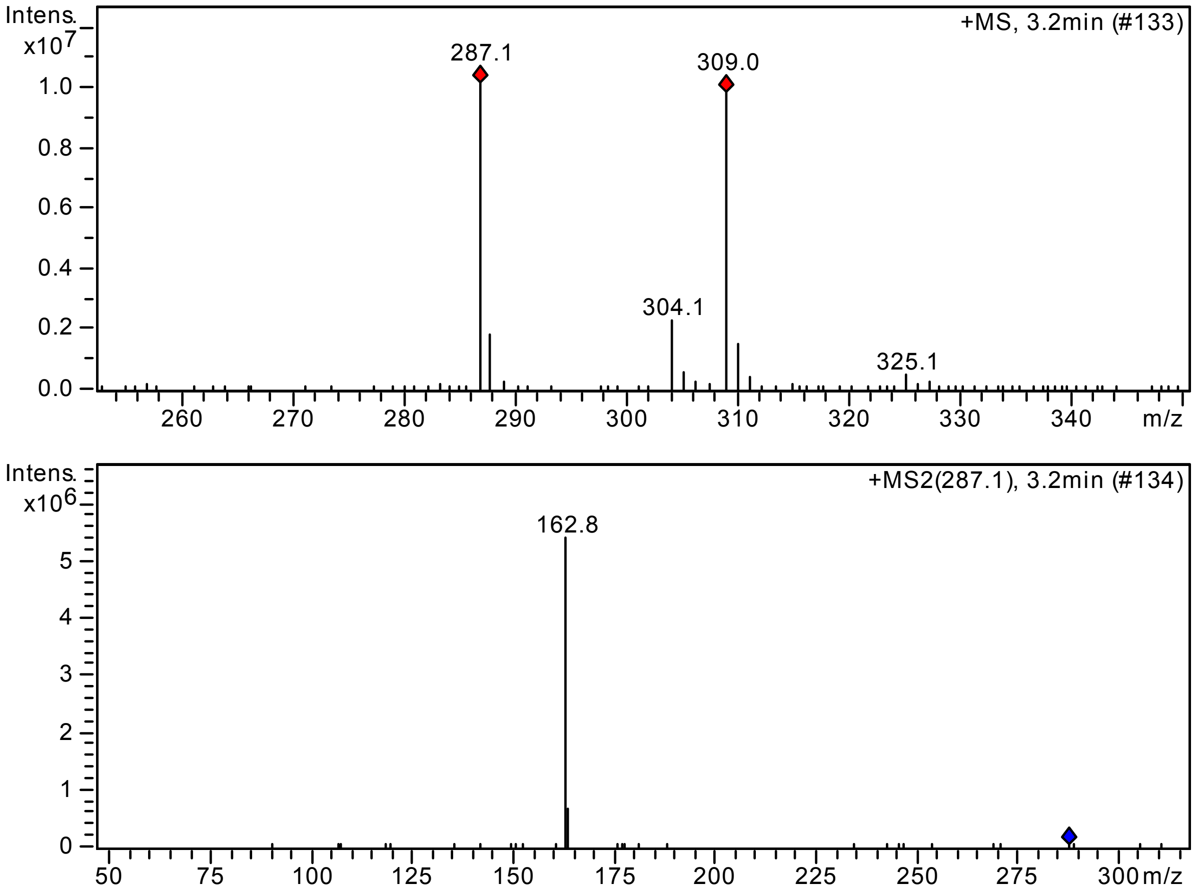
162.9
449.1
595.1
100
200
300
400
500
600
700
800
900
m/z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+MS, 3.2min (#133)
287.1
309.0
304.1
325.1
1.0
0.8
0.6
0.4
0.2
0.0
260
270
280
290
300
310
320
330
340
m/z
Intens.
x10^6
+MS2(287.1), 3.2min (#134)
162.8
5
4
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1
0
50
75
100
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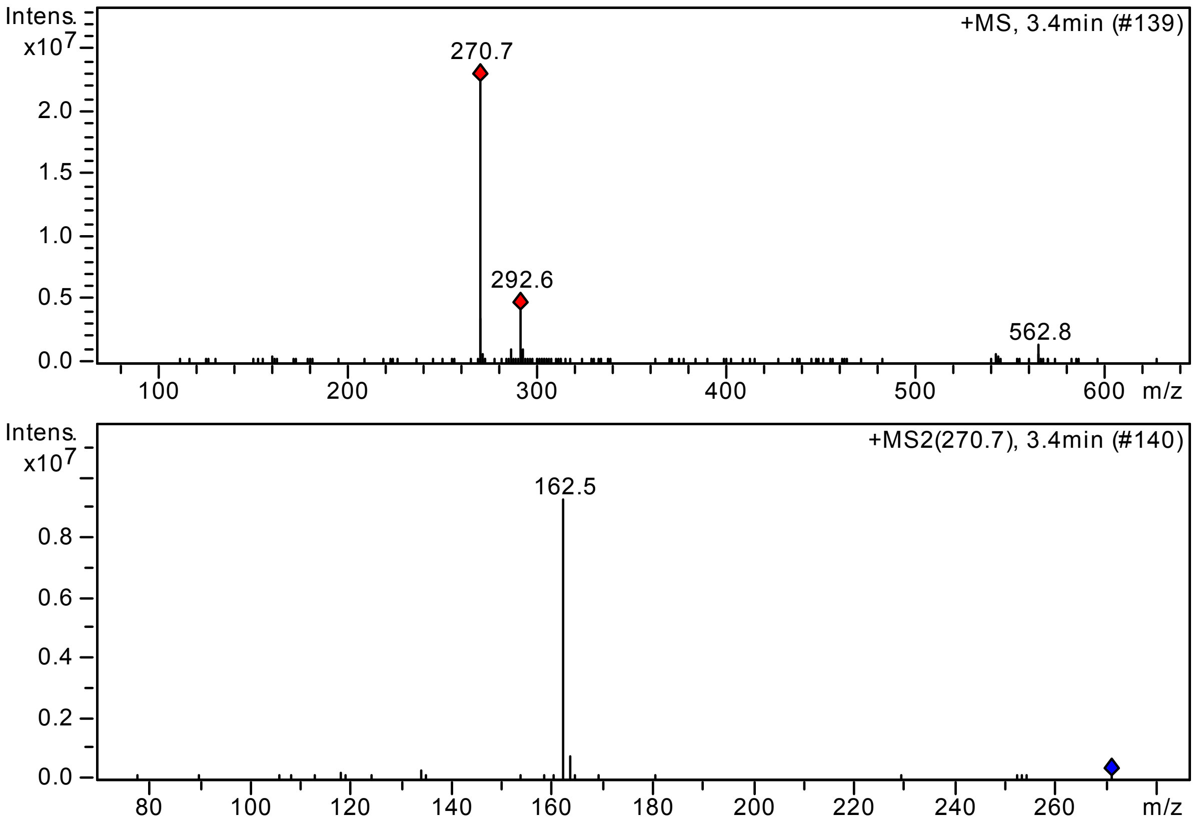
150
175
200
225
250
275
300
m/z

4d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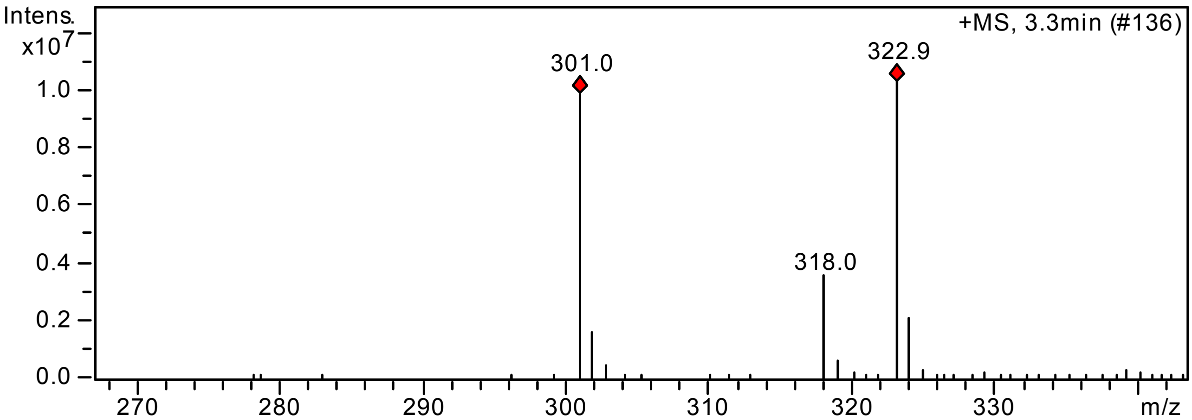
292.6
562.8
2.0
1.5
1.0
0.5
0.0
100
200
300
400
500
600
m/z
Intens.
x10^7
+MS2(270.7), 3.4min (#140)
162.5
0.8
0.6
0.4
0.2
0.0
80
100
120
140
160
180
200
220
240
260
m/z

4e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+MS, 3.3min (#136)
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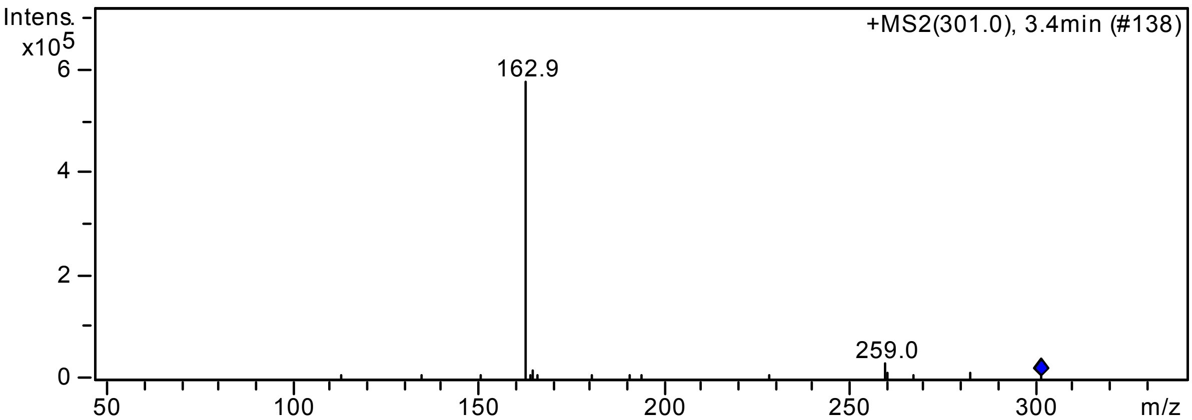
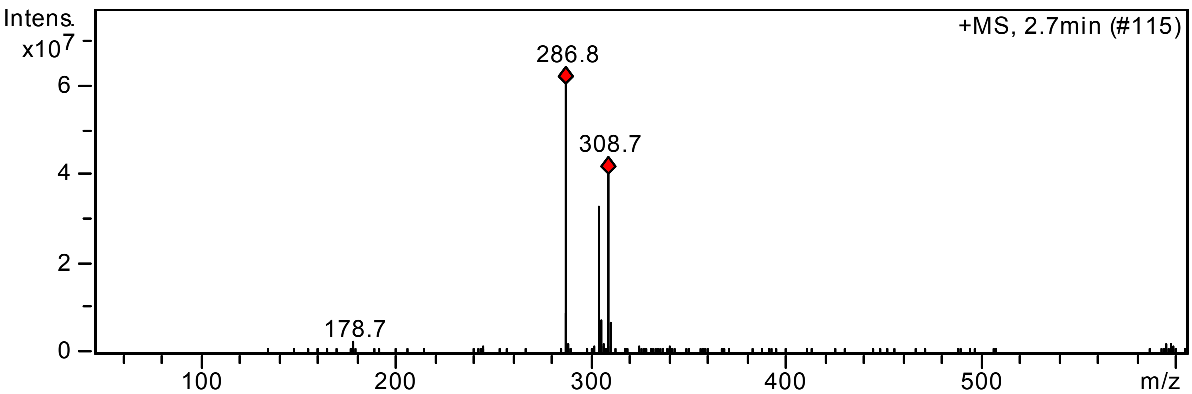
322.9
318.0
m/z


Intens.
x10^5
+MS2(301.0), 3.4min (#138)
162.9
259.0
m/z

4f


Intens.
x10^7
+MS, 2.7min (#115)
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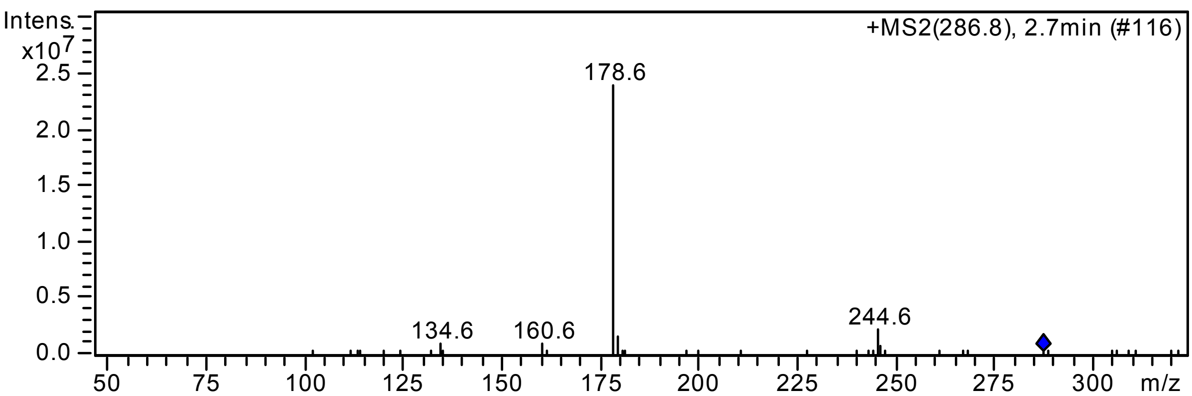
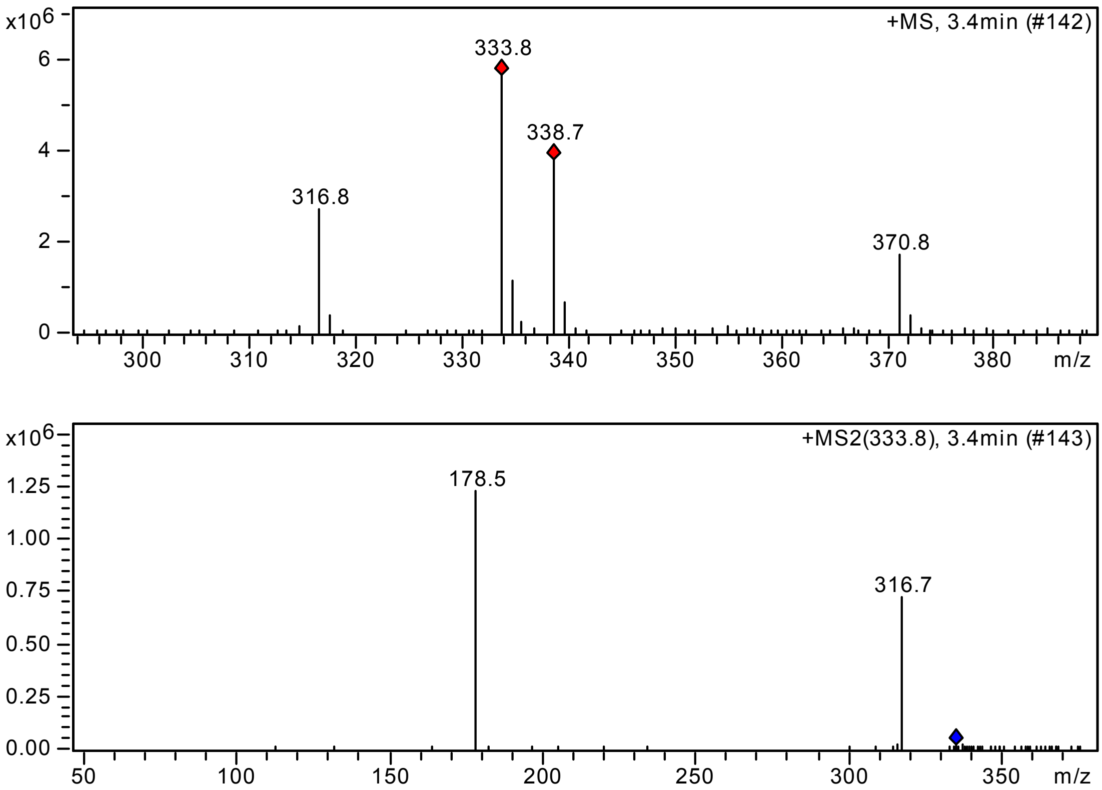
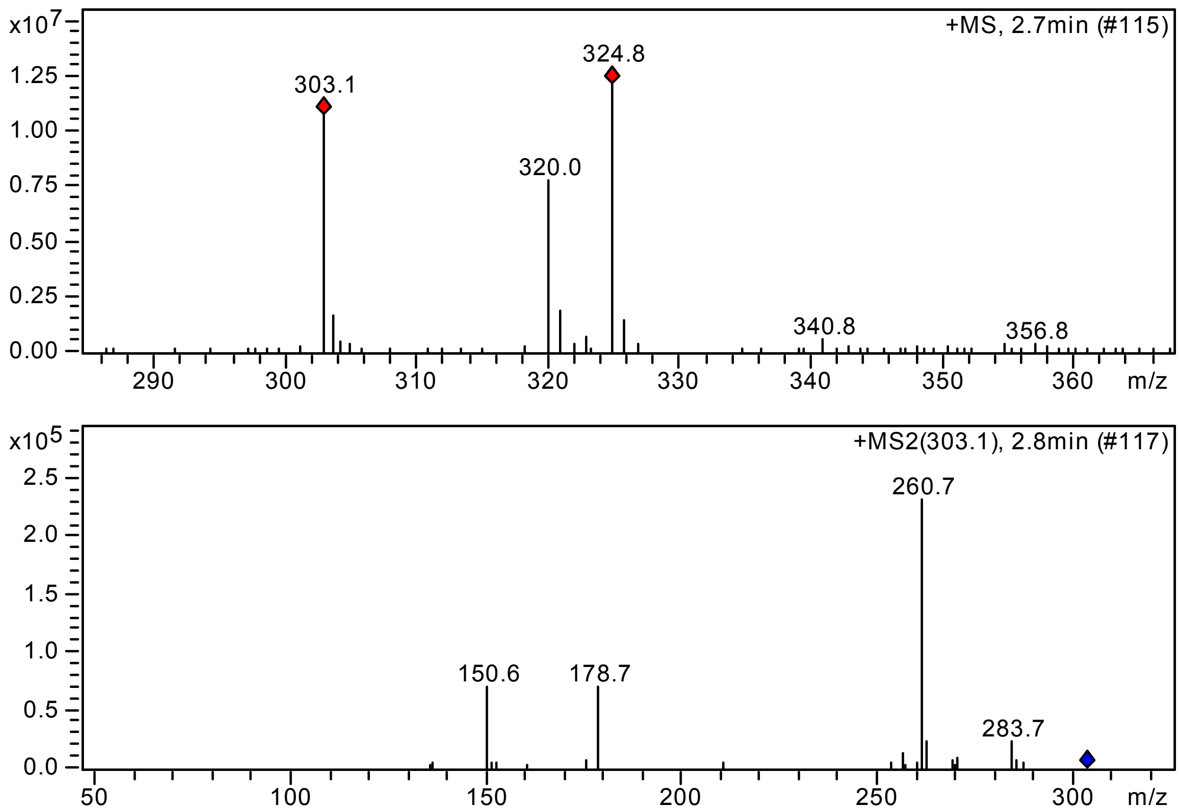
308.7
178.7
m/z


Intens.
x10^7
+MS2(286.8), 2.7min (#116)
178.6
134.6
160.6
244.6
m/z

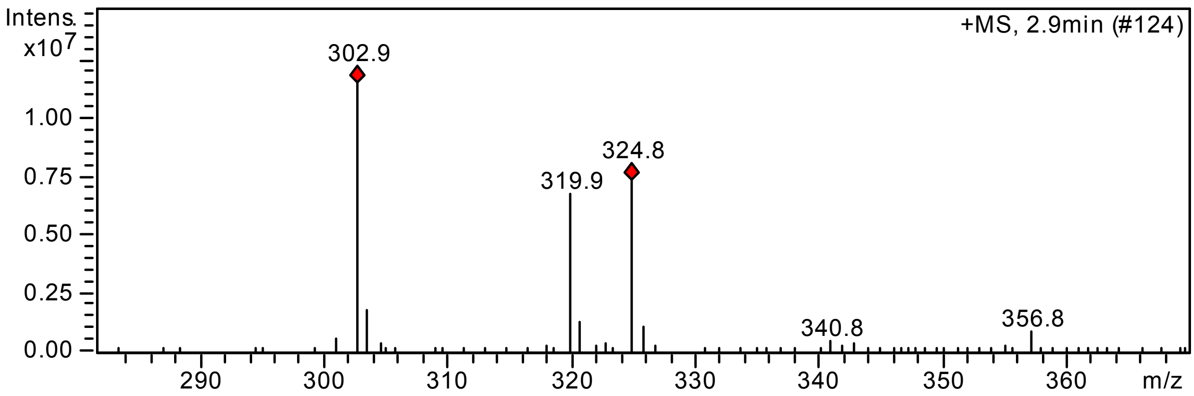
4g

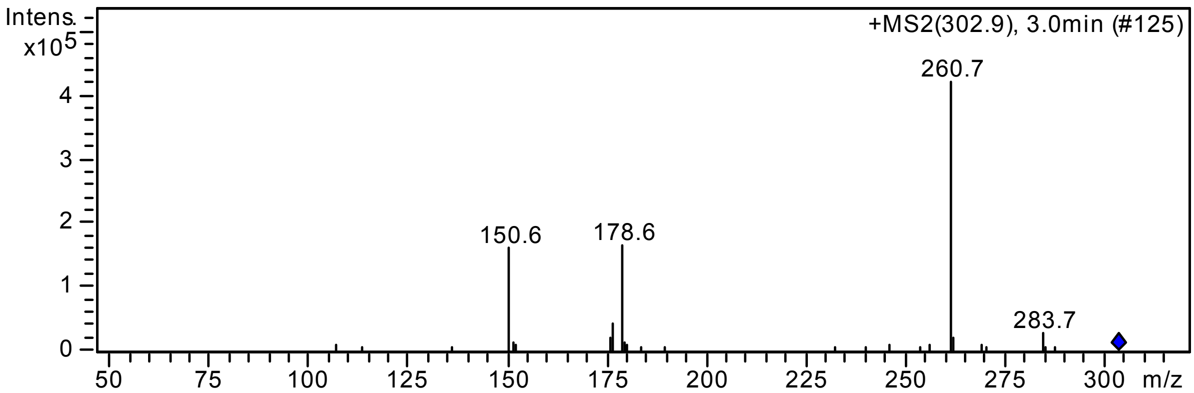

x10^6
+MS, 3.4min (#142)
333.8
338.7
316.8
370.8
m/z
+MS2(333.8), 3.4min (#143)
178.5
316.7
m/z

4h

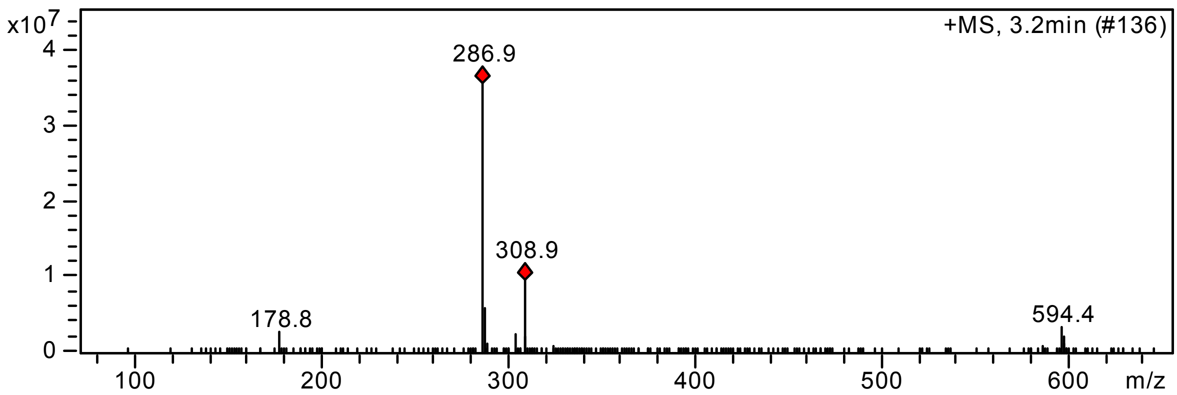

x10^7
+MS, 2.7min (#115)
303.1
324.8
320.0
340.8
356.8
m/z
x10^5
+MS2(303.1), 2.8min (#117)
260.7
150.6
178.7
283.7
m/z

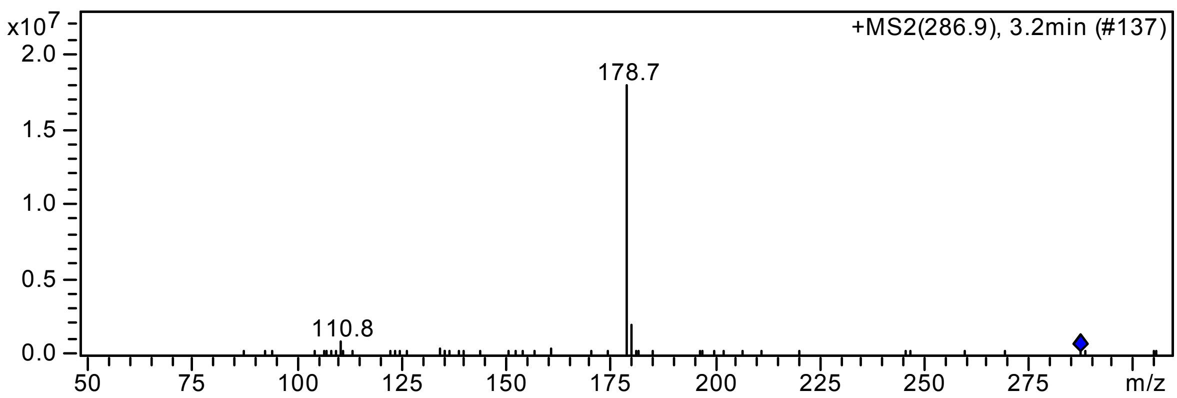
4i


Intens.
x10^7
+MS, 2.9min (#124)
302.9
324.8
319.9
340.8
356.8
m/z

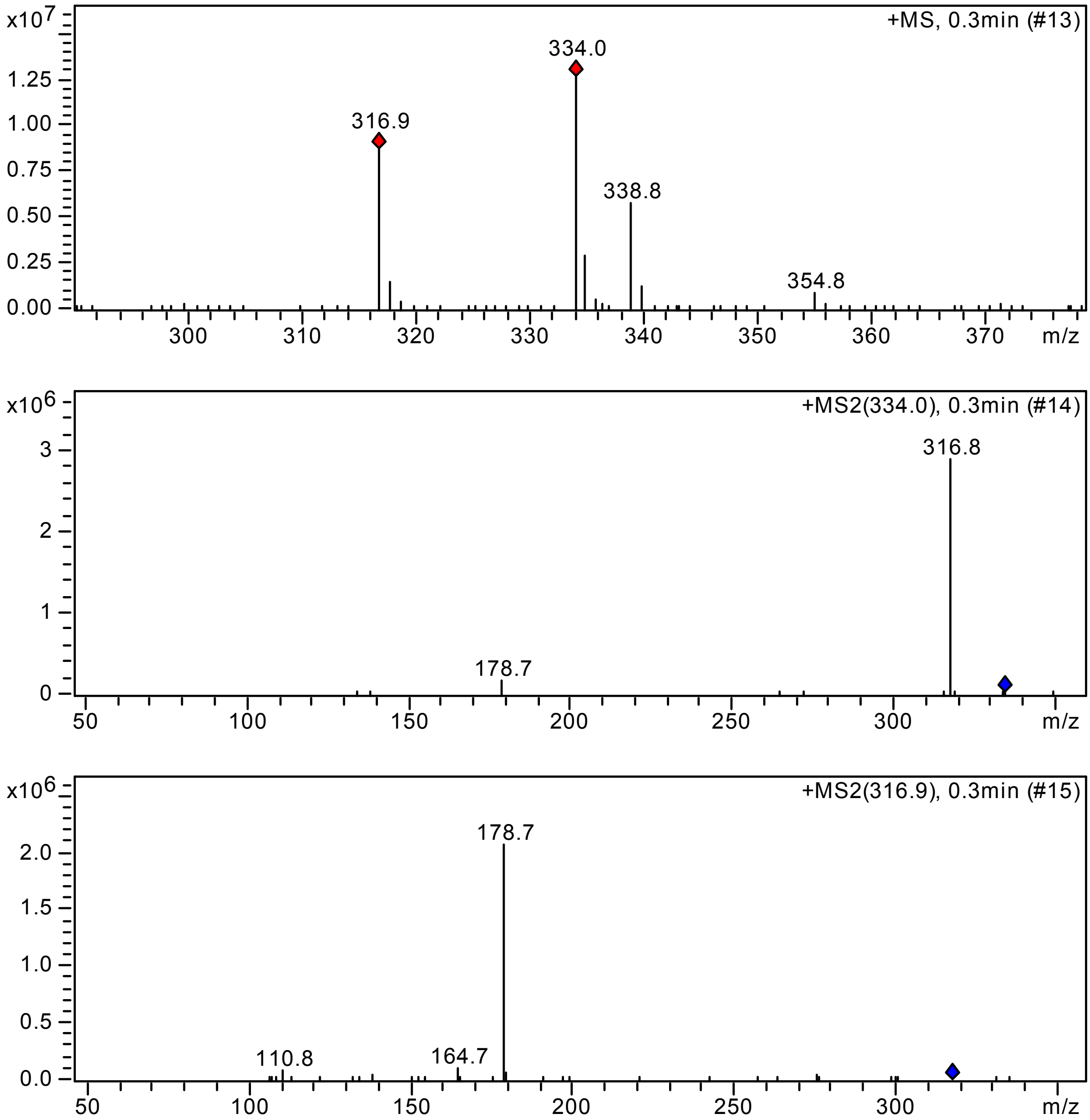

Intens.
x10^5
+MS2(302.9), 3.0min (#125)
260.7
150.6
178.6
283.7
m/z

4j


x10^7
+MS, 3.2min (#136)
286.9
308.9
178.8
594.4
m/z

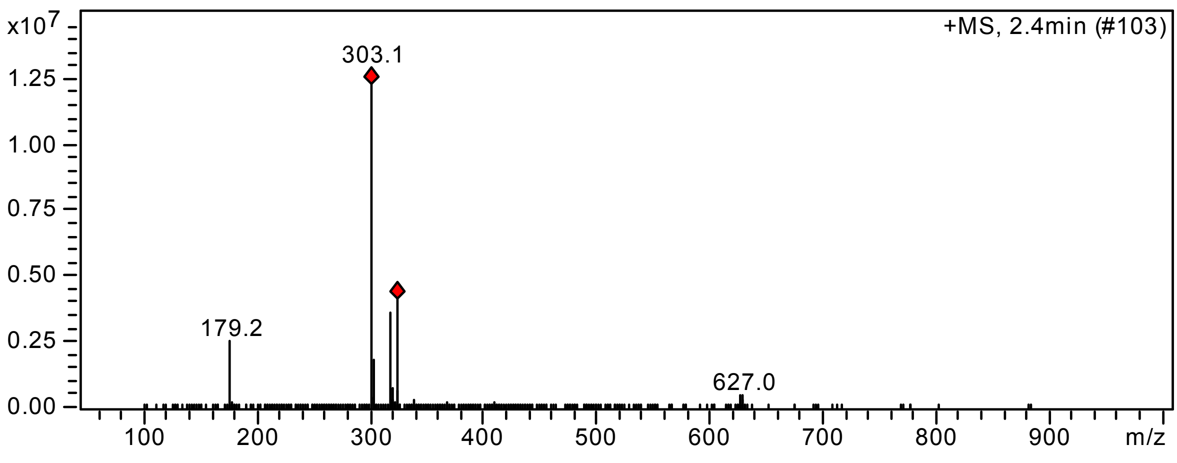

x10^7
+MS2(286.9), 3.2min (#137)
178.7
110.8
m/z

4k

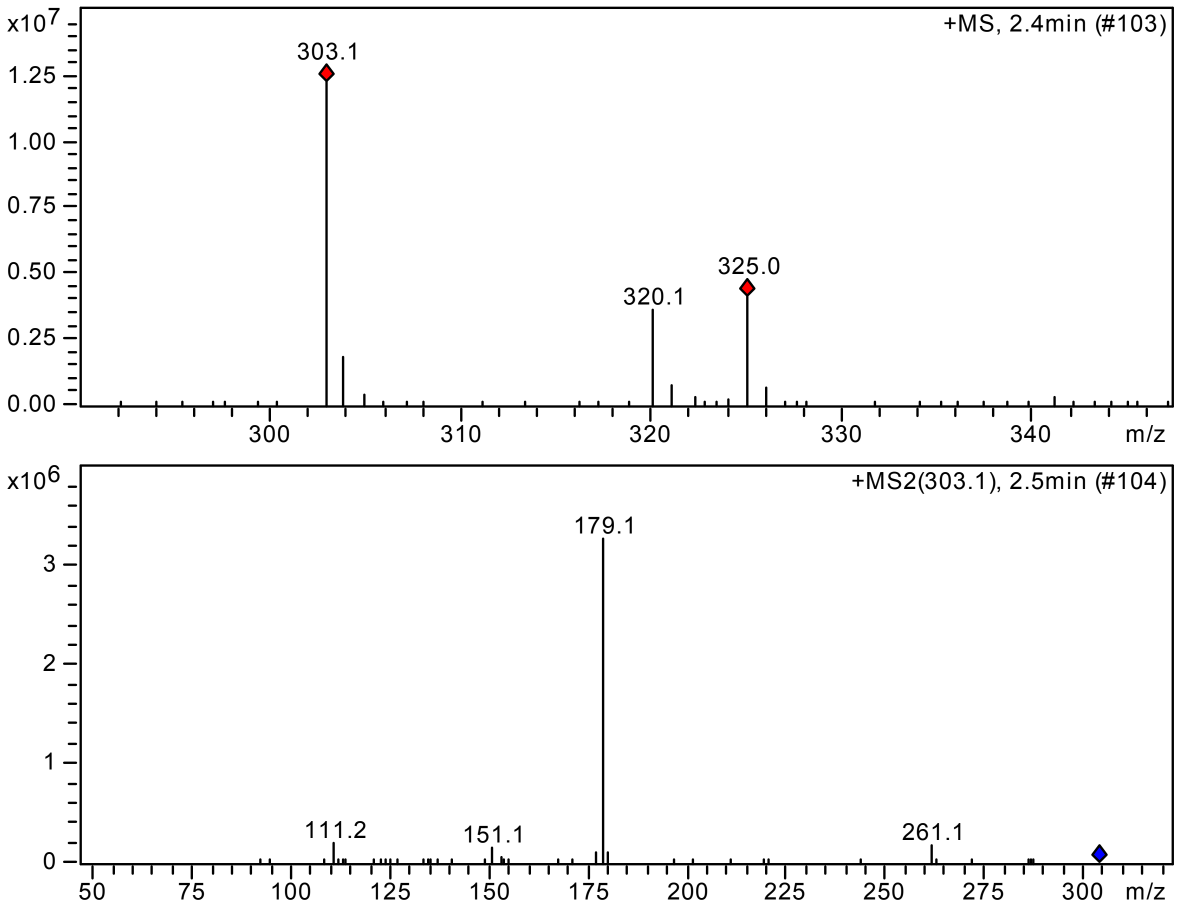


x10^7
+MS, 0.3min (#13)
334.0
316.9
338.8
354.8
m/z
x10^6
+MS2(334.0), 0.3min (#14)
316.8
178.7
m/z
x10^6
+MS2(316.9), 0.3min (#15)
178.7
110.8
164.7
m/z

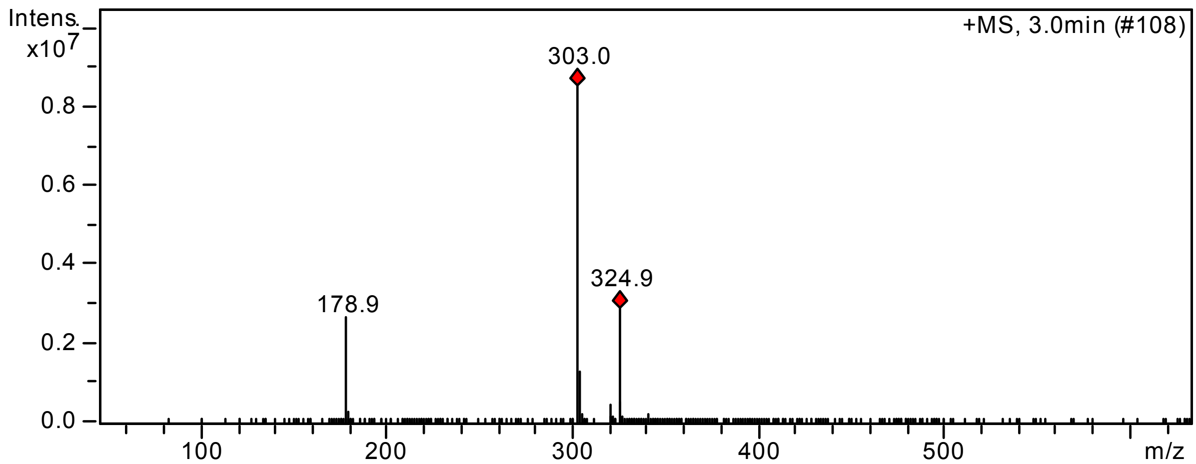
4l

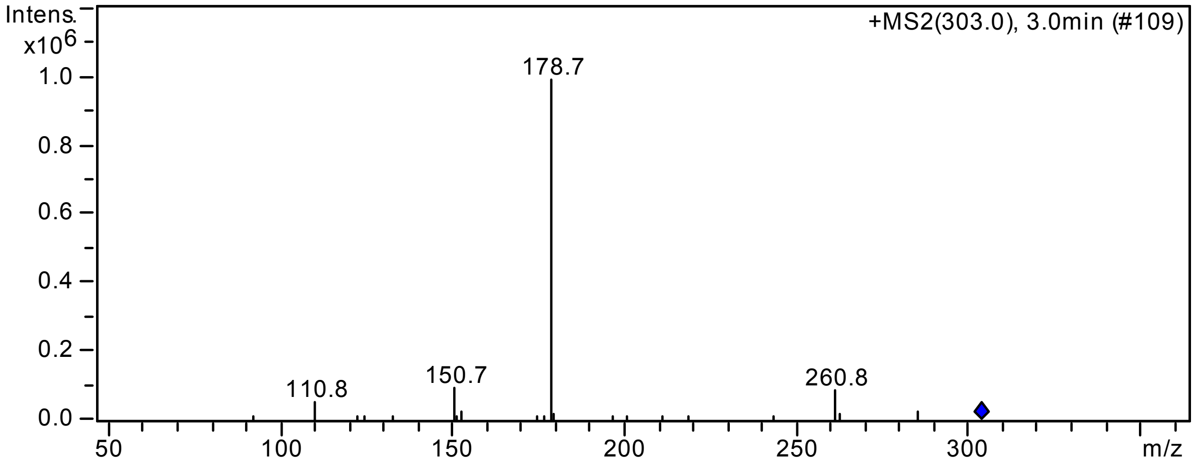


x10^7
+MS, 2.4min (#103)
303.1
179.2
627.0
m/z

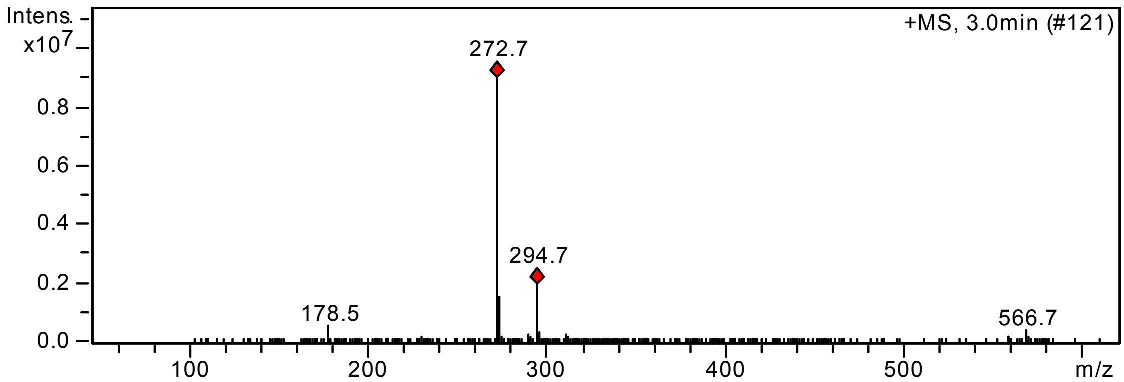

+MS, 2.4min (#103)
x10^7
303.1
320.1
325.0
m/z
+MS2(303.1), 2.5min (#104)
x10^6
179.1
111.2
151.1
261.1
m/z

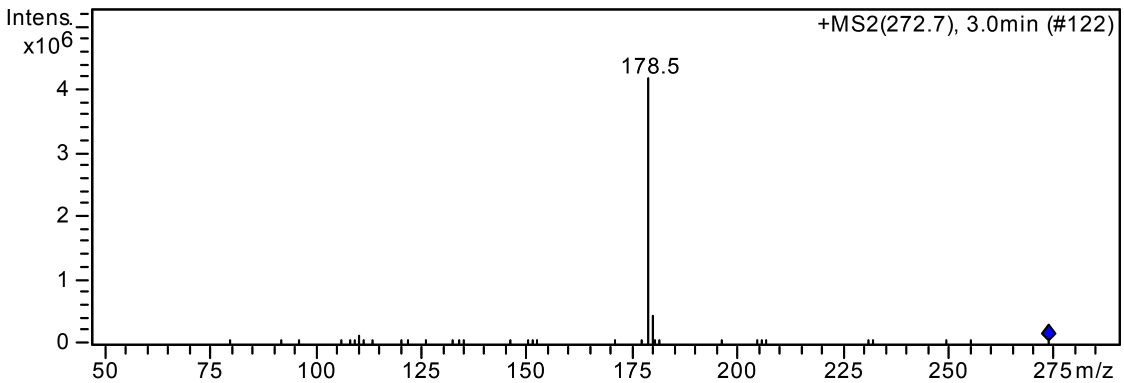
4m


Intens.
x10^7
+MS, 3.0min (#108)
303.0
324.9
178.9
m/z

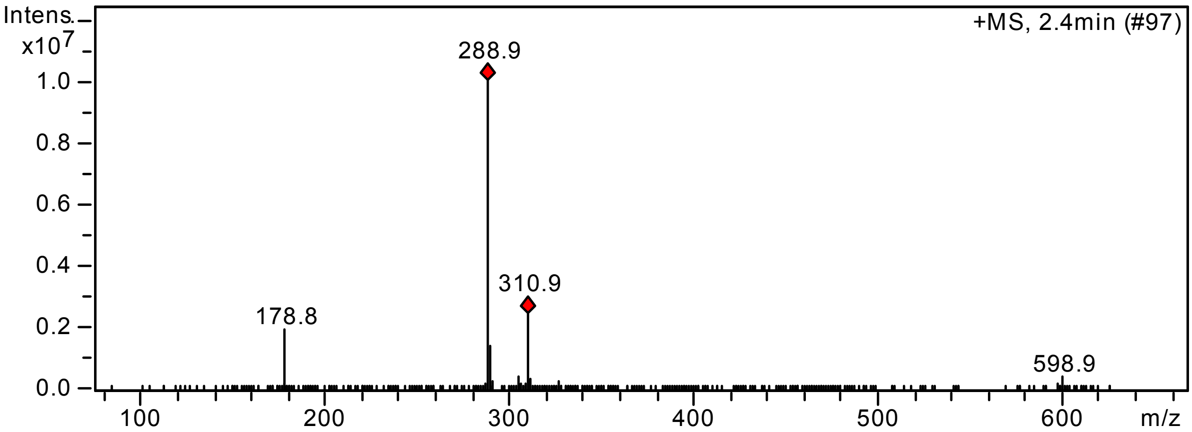

Intens.
x10^6
+MS2(303.0), 3.0min (#109)
178.7
110.8
150.7
260.8
m/z

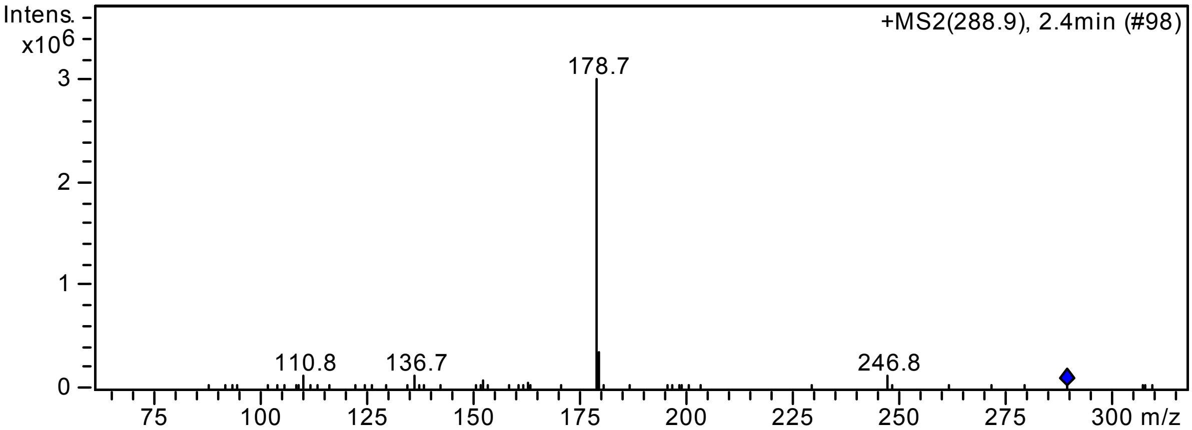
4n


Intens.
x10^7
+MS, 3.0min (#121)
272.7
294.7
178.5
566.7
m/z

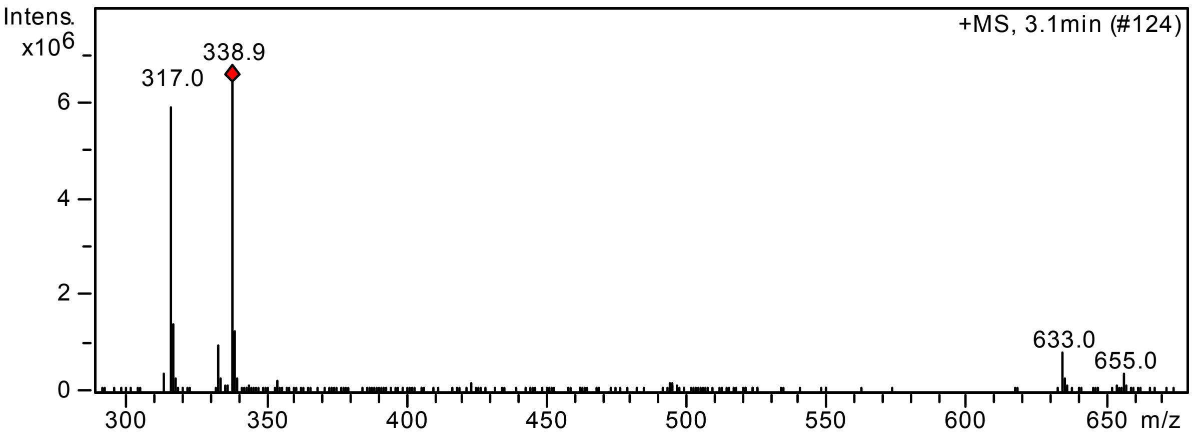

Intens.
x10^6
+MS2(272.7), 3.0min (#122)
178.5
m/z

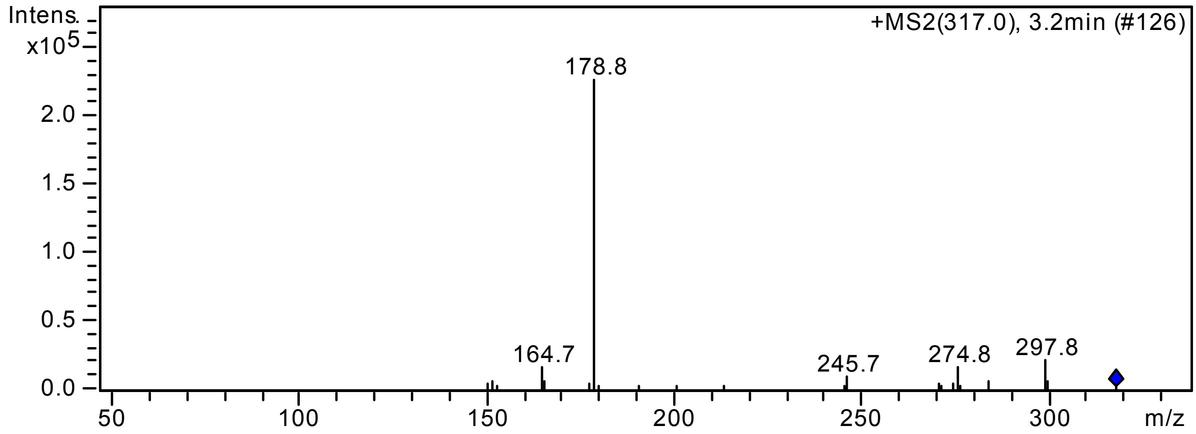
4o


Intens.
x10^7
+MS, 2.4min (#97)
288.9
310.9
178.8
598.9
m/z

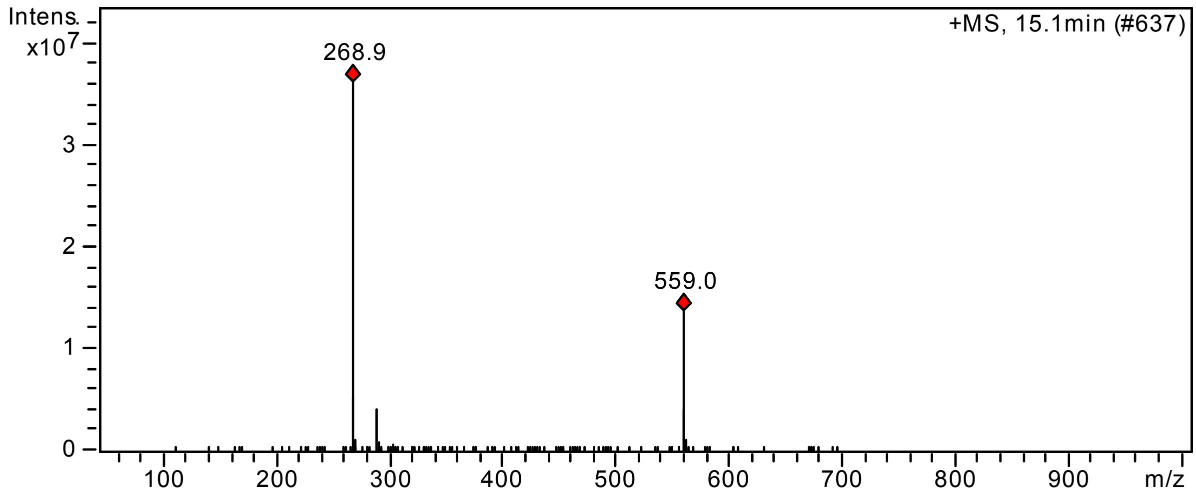

Intens.
x10^6
+MS2(288.9), 2.4min (#98)
178.7
110.8
136.7
246.8
m/z

4p

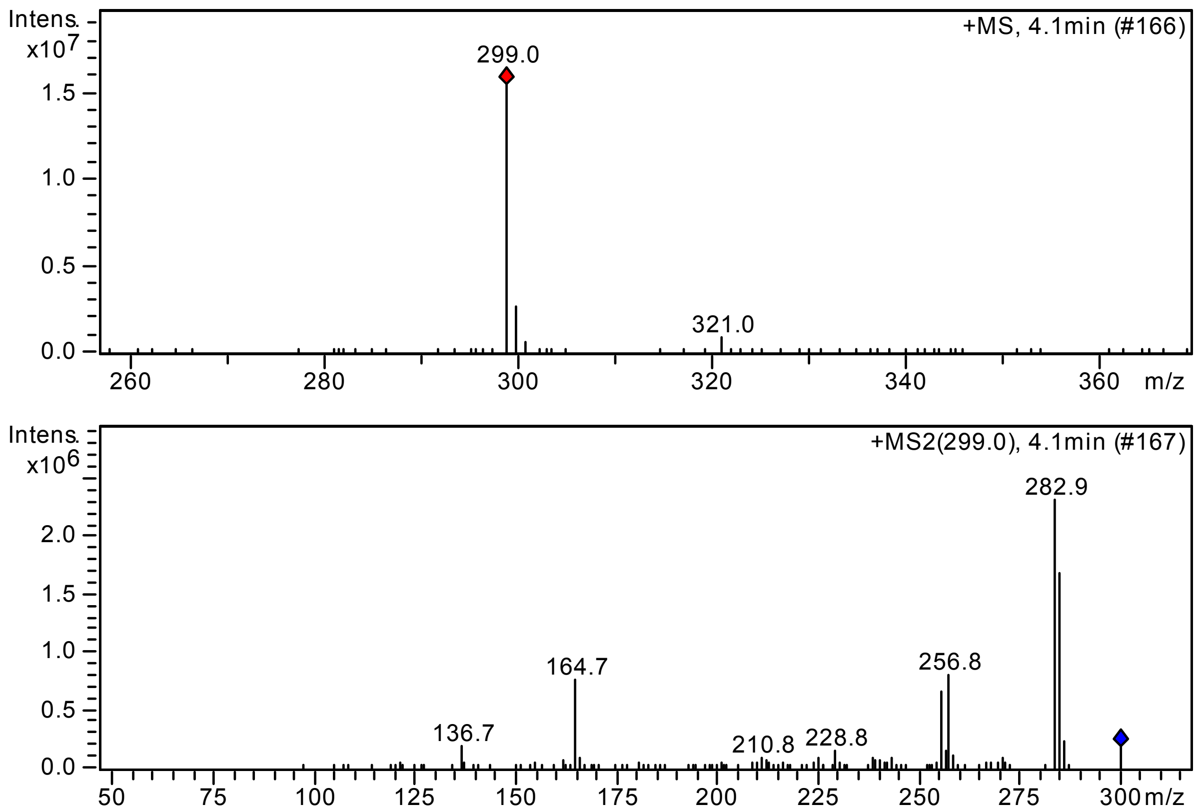

Intens.
x10^6
+MS, 3.1min (#124)
338.9
317.0
633.0
655.0
m/z


Intens.
x10^5
+MS2(317.0), 3.2min (#126)
178.8
164.7
245.7
274.8
297.8
0.0
0.5
1.0
1.5
2.0
50
100
150
200
250
300
m/z

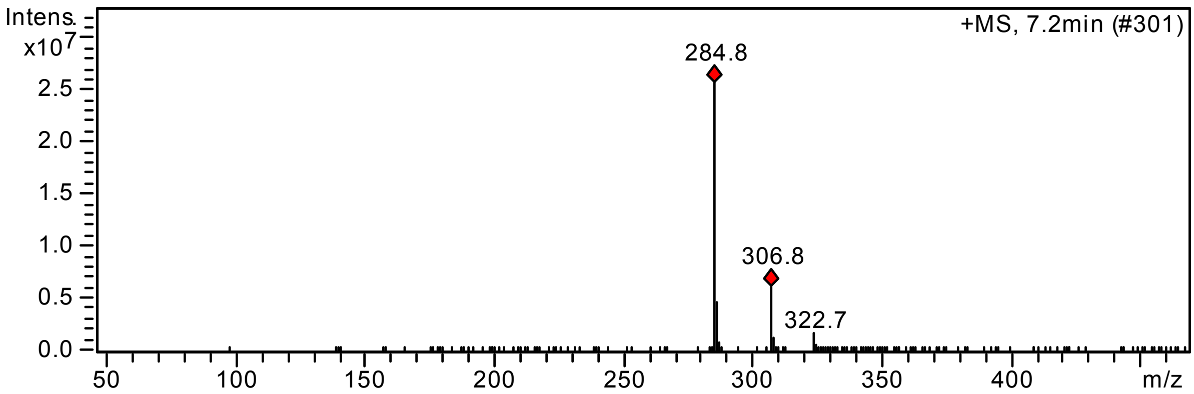
8a

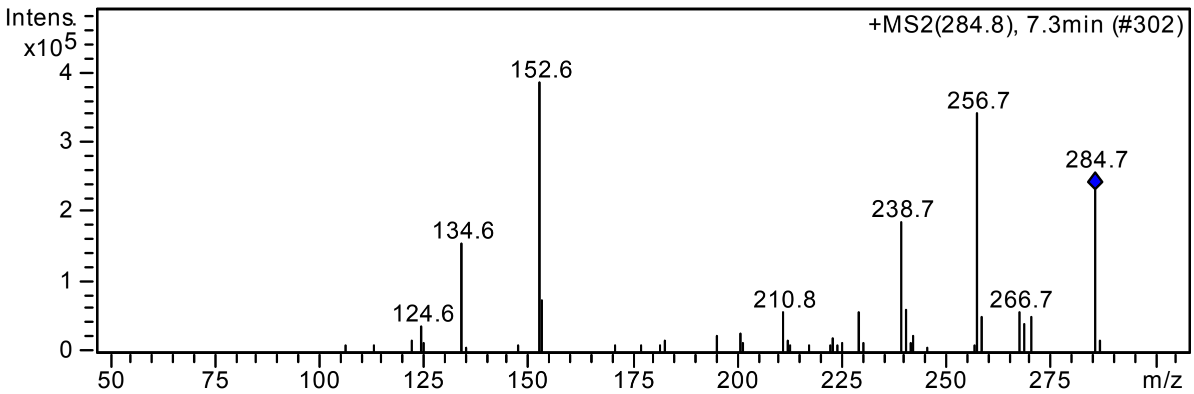

Intens.
x10^7
+MS, 15.1min (#637)
268.9
559.0
0
1
2
3
100
200
300
400
500
600
700
800
900
m/z

8b

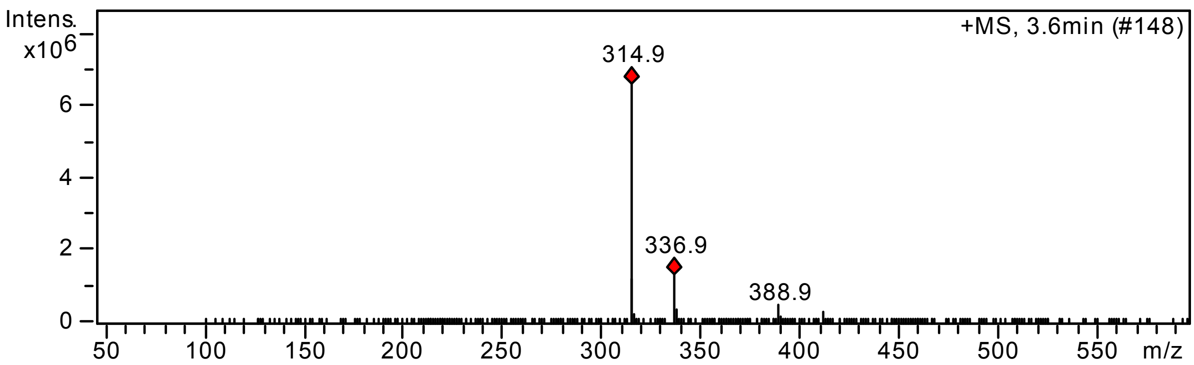

Intens.
x10^7
+MS, 4.1min (#166)
299.0
321.0
0.0
0.5
1.0
1.5
260
280
300
320
340
360
m/z
Intens.
x10^6
+MS2(299.0), 4.1min (#167)
282.9
256.8
164.7
136.7
210.8
228.8
0.0
0.5
1.0
1.5
2.0
50
75
100
125
150
175
200
225
250
275
300
m/z

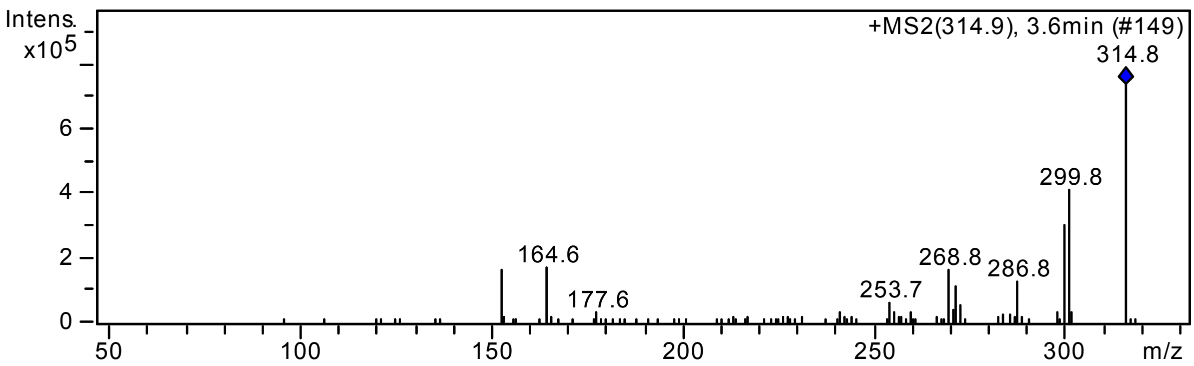
8c


Intens.
x10^7
+MS, 7.2min (#301)
284.8
306.8
322.7
m/z

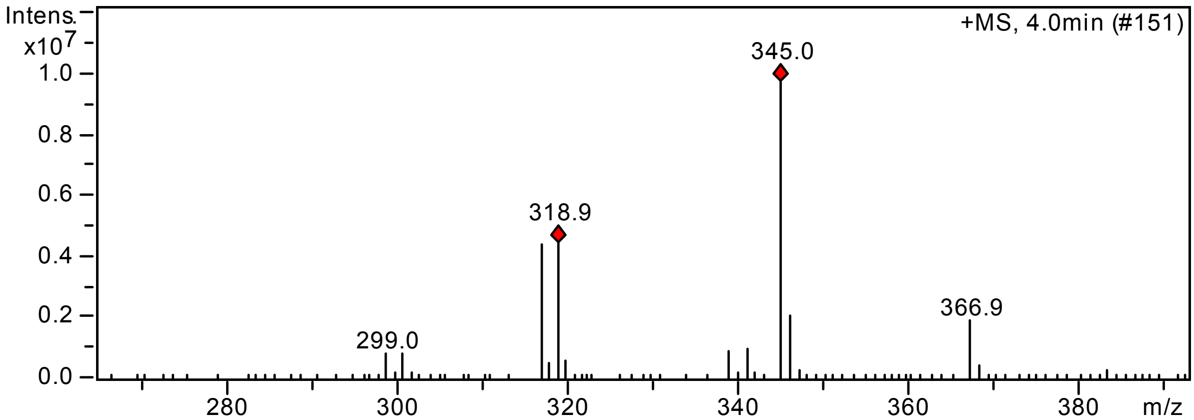

Intens.
x10^5
+MS2(284.8), 7.3min (#302)
152.6
256.7
284.7
238.7
134.6
124.6
210.8
266.7
m/z

8d

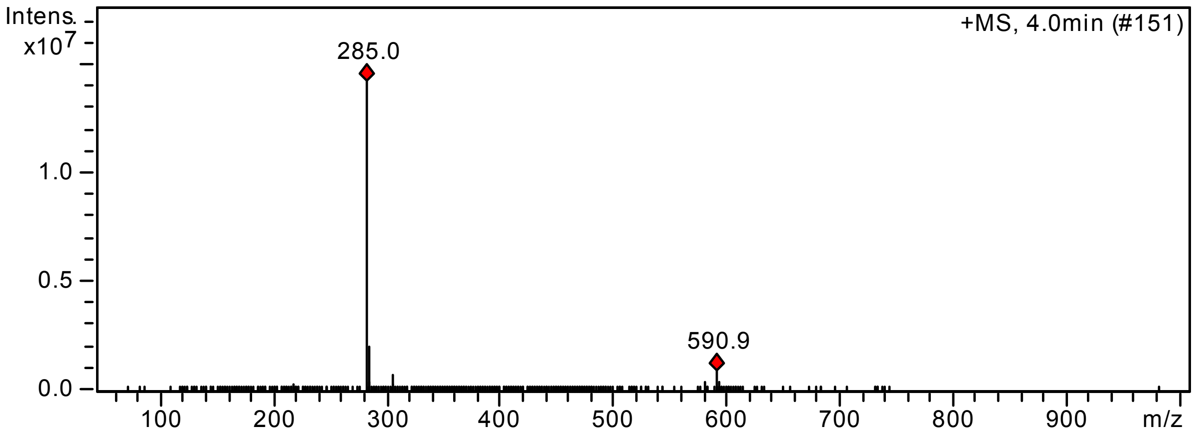

Intens.
x10^6
+MS, 3.6min (#148)
314.9
336.9
388.9
m/z

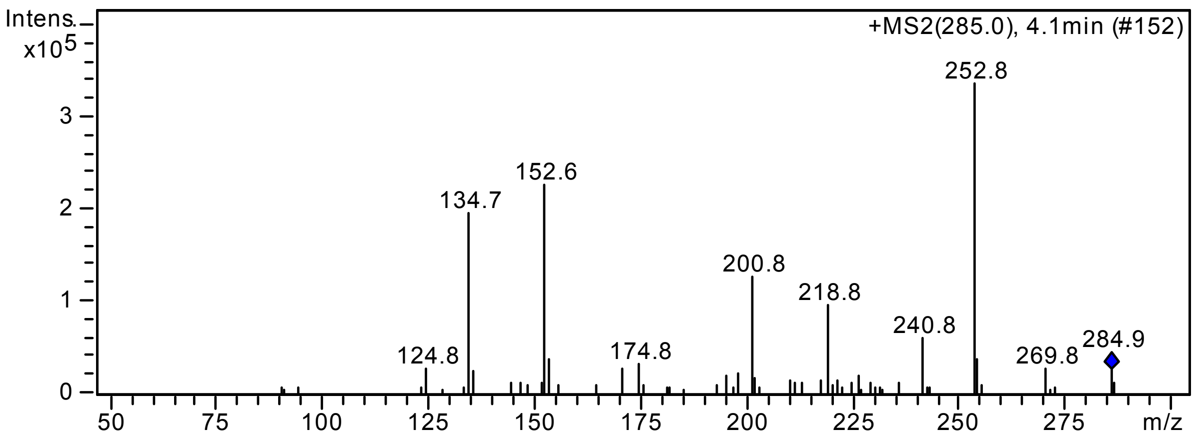

Intens.
x10^5
+MS2(314.9), 3.6min (#149)
314.8
299.8
164.6
177.6
253.7
268.8
286.8
m/z

8e

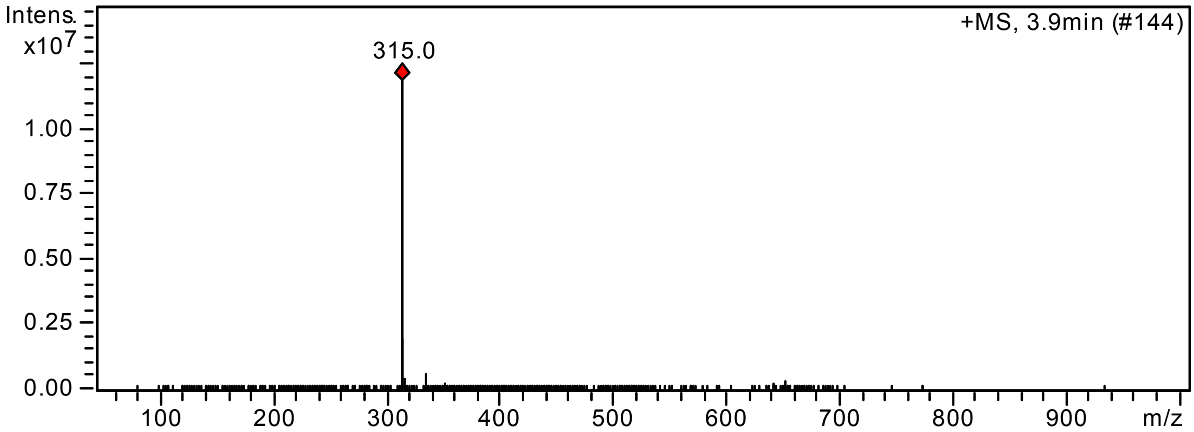

Intens.
x10^7
+MS, 4.0min (#151)
345.0
318.9
366.9
299.0
m/z

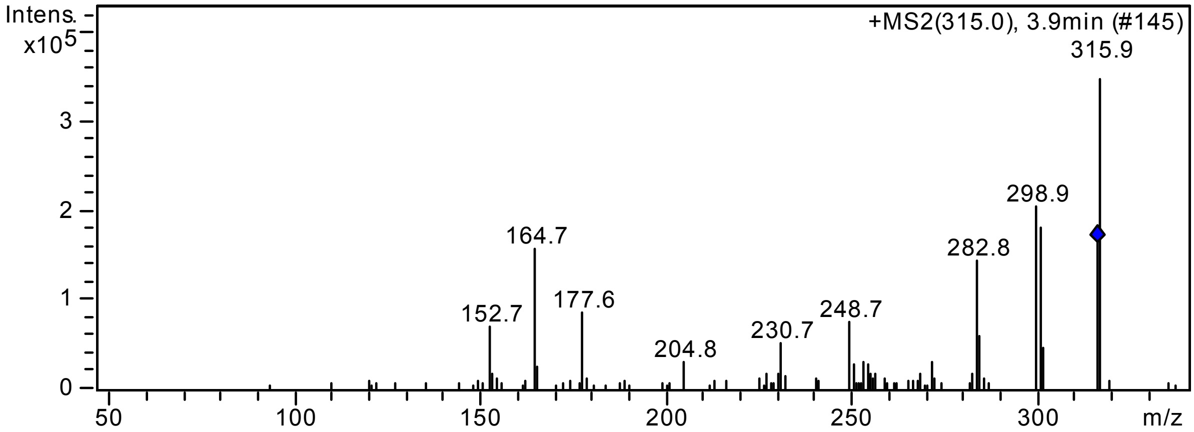
8f


Intens.
x10^7
+MS, 4.0min (#151)
285.0
590.9
m/z

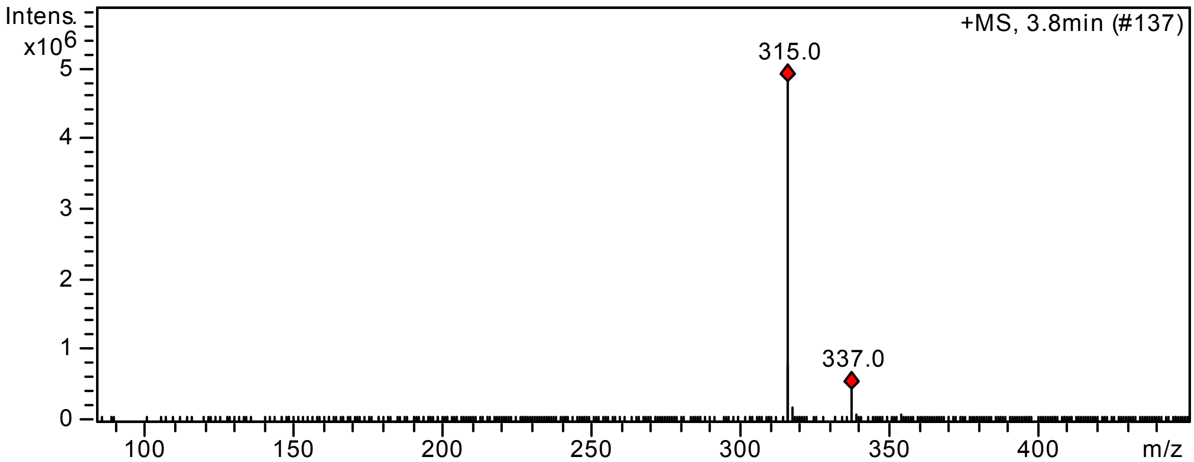

Intens.
x10^5
+MS2(285.0), 4.1min (#152)
252.8
152.6
134.7
200.8
218.8
240.8
124.8
174.8
269.8
284.9
m/z

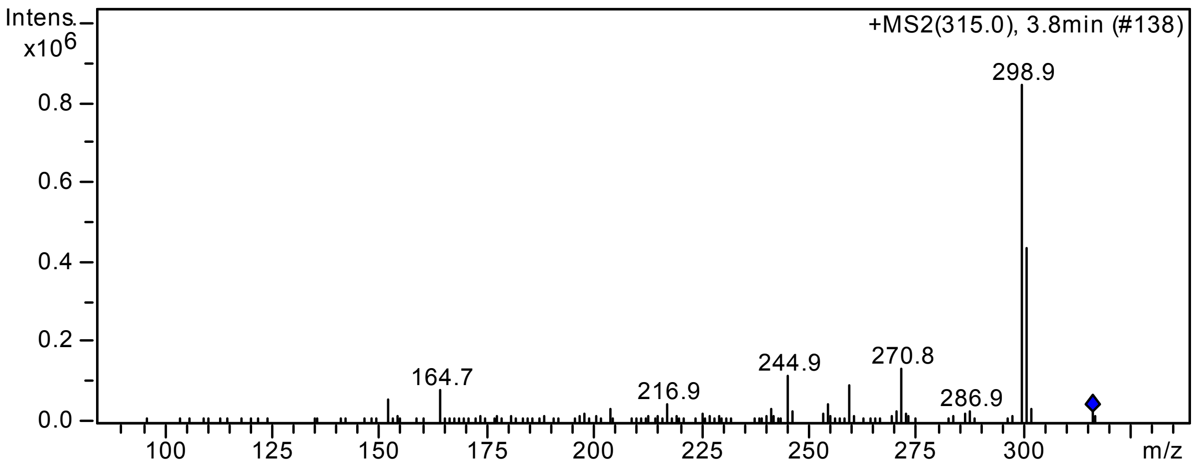
8g


Intens.
x10^7
+MS, 3.9min (#144)
315.0
1.00
0.75
0.50
0.25
0.00
100
200
300
400
500
600
700
800
900
m/z

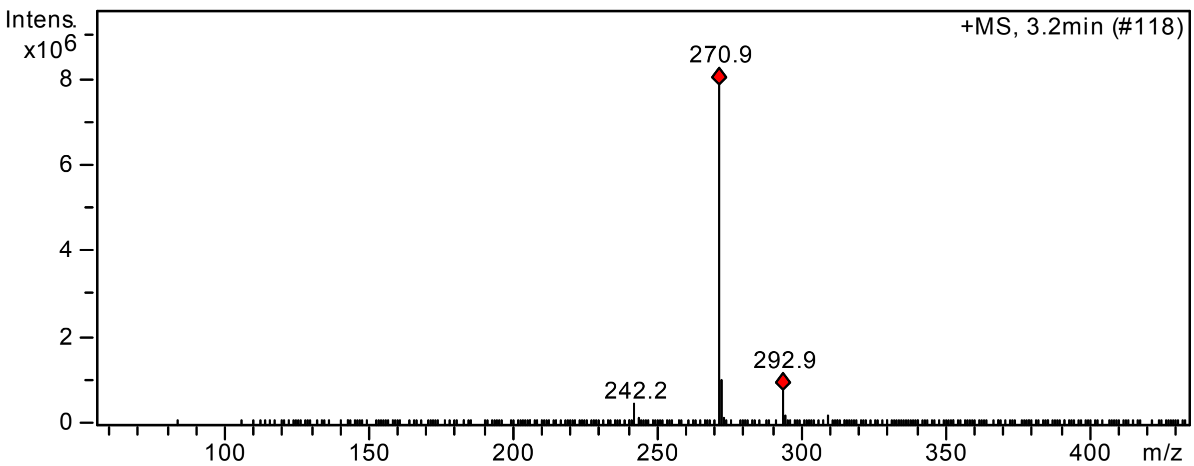

Intens.
x10^5
+MS2(315.0), 3.9min (#145)
315.9
298.9
282.8
164.7
177.6
152.7
248.7
230.7
204.8
3
2
1
0
50
100
150
200
250
300
m/z

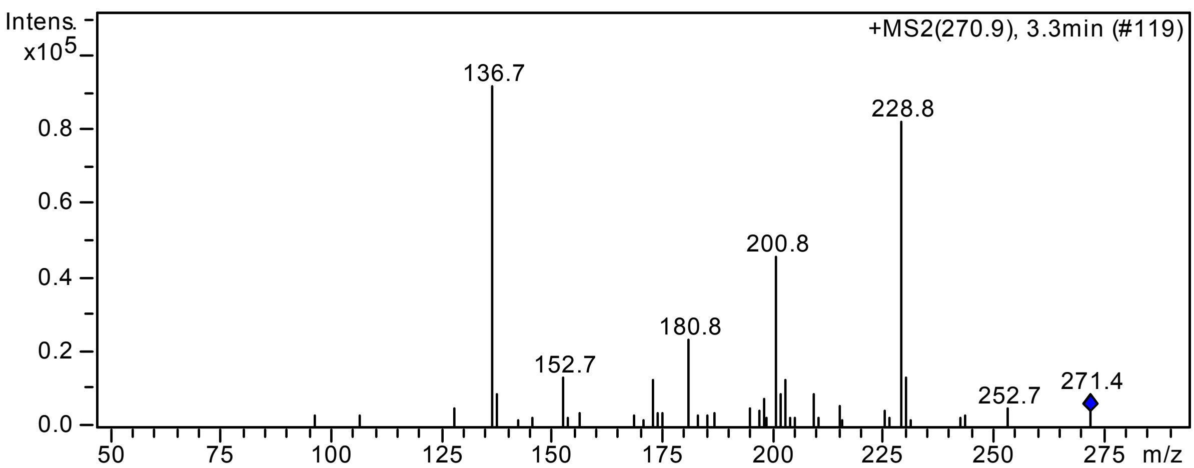
8h


Intens.
x10^6
+MS, 3.8min (#137)
315.0
337.0
5
4
3
2
1
0
100
150
200
250
300
350
400
m/z

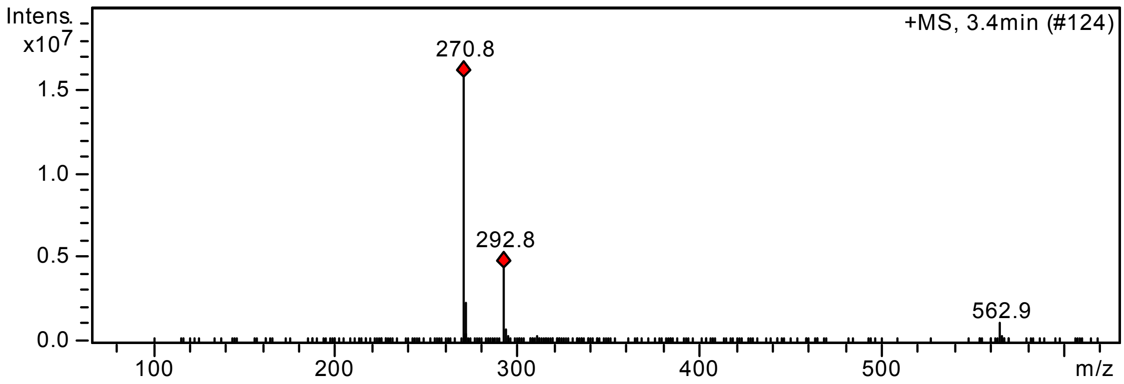

Intens.
x10^6
+MS2(315.0), 3.8min (#138)
298.9
164.7
216.9
244.9
270.8
286.9
m/z

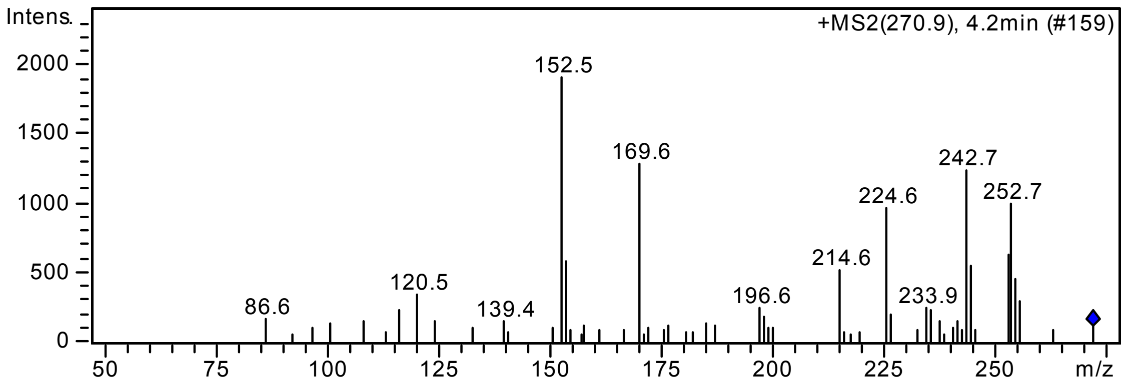
8i


Intens.
x10^6
+MS, 3.2min (#118)
270.9
242.2
292.9
m/z

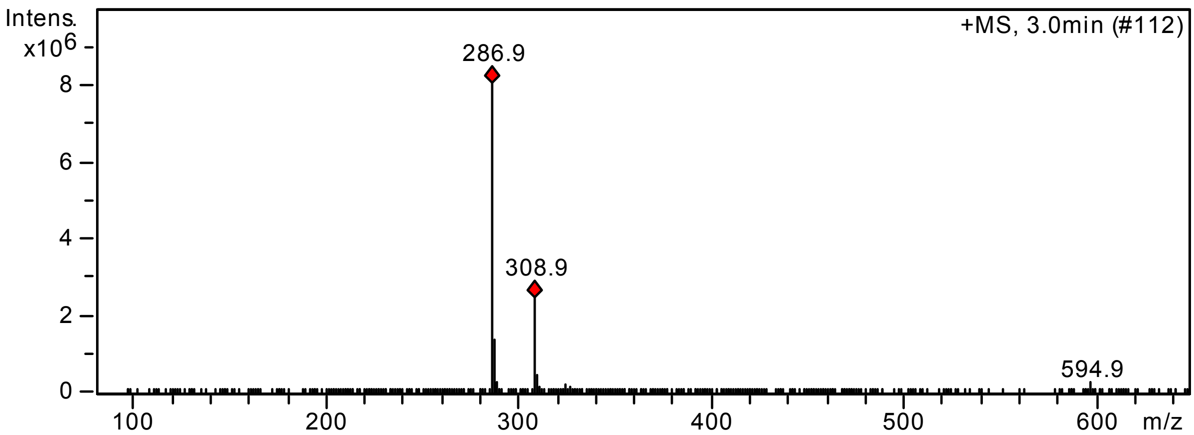

Intens.
x10^5
+MS2(270.9), 3.3min (#119)
136.7
228.8
200.8
180.8
152.7
252.7
271.4
m/z

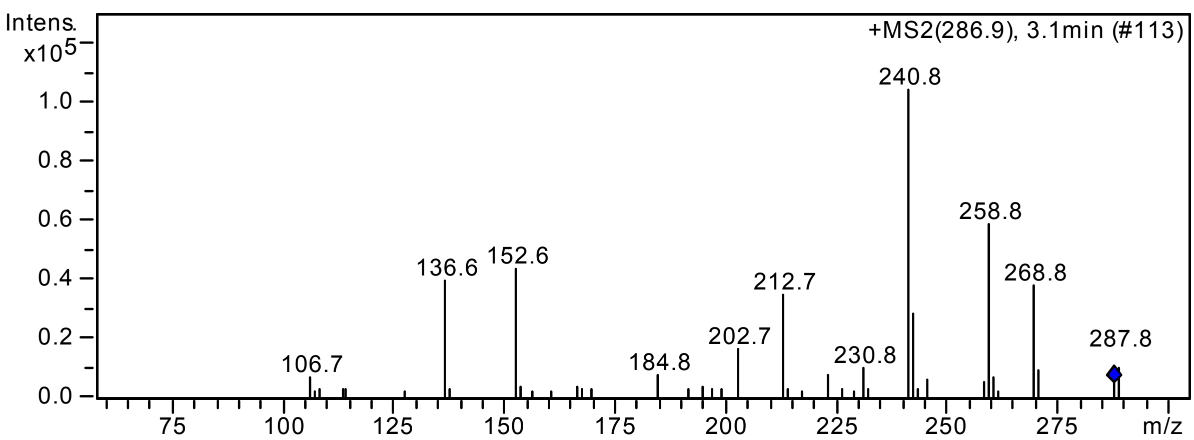
8j


Intens.
x10^7
+MS, 3.4min (#124)
270.8
292.8
562.9
m/z

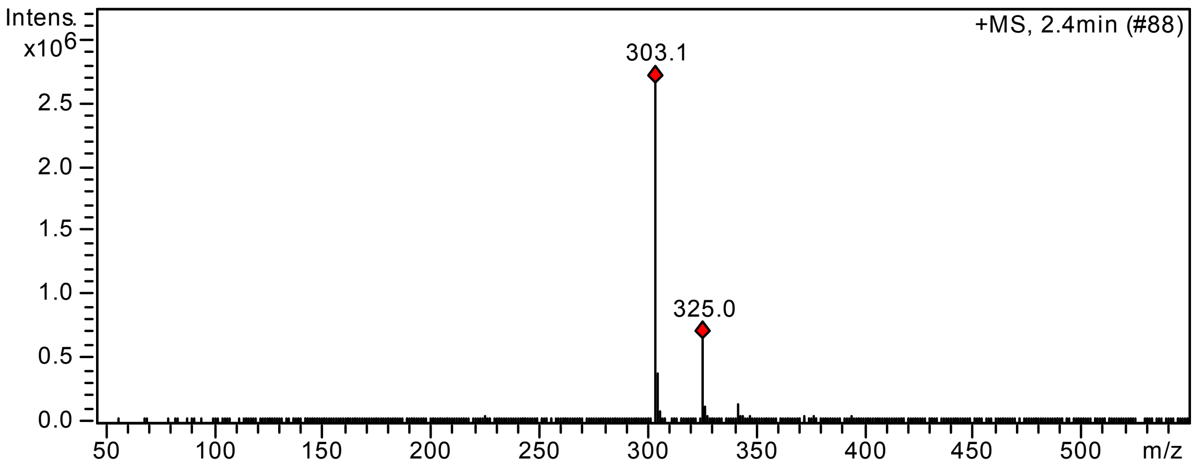

Intens.
+MS2(270.9), 4.2min (#159)
152.5
169.6
242.7
224.6
252.7
214.6
196.6
233.9
120.5
86.6
139.4
m/z

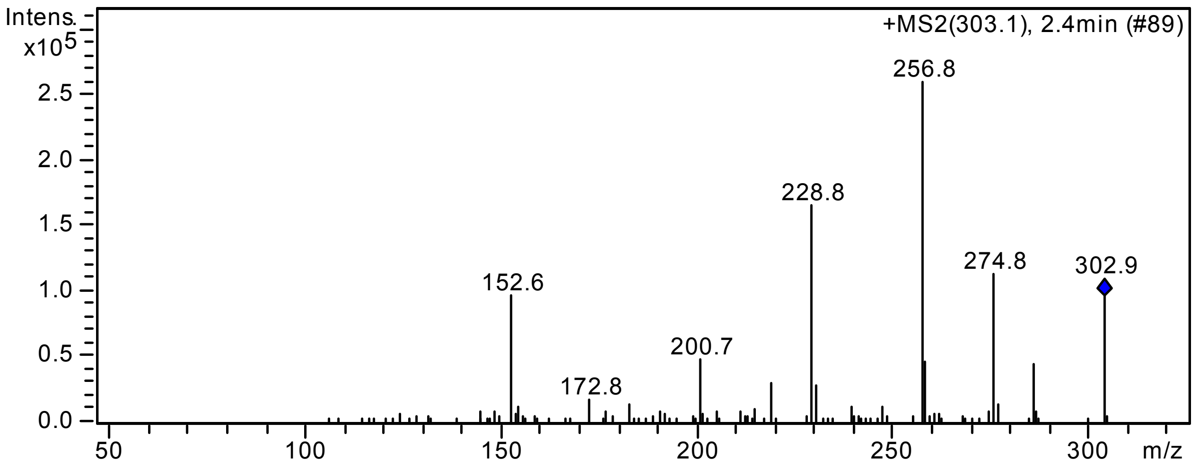
8k


Intens.
x10^6
+MS, 3.0min (#112)
286.9
308.9
594.9
m/z

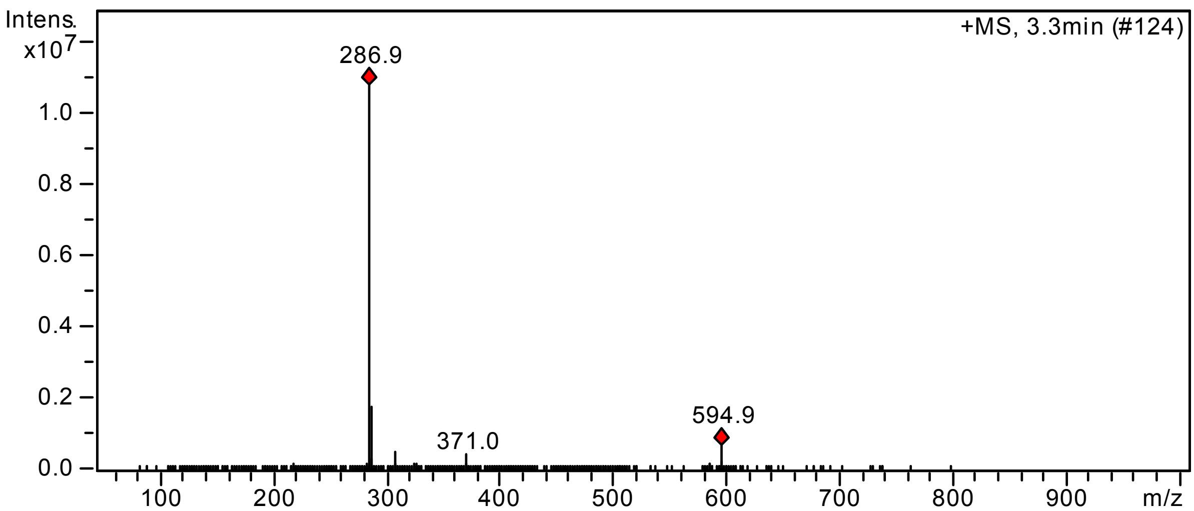

Intens.
x10^5
+MS2(286.9), 3.1min (#113)
240.8
258.8
268.8
136.6
152.6
212.7
202.7
287.8
230.8
184.8
106.7
m/z

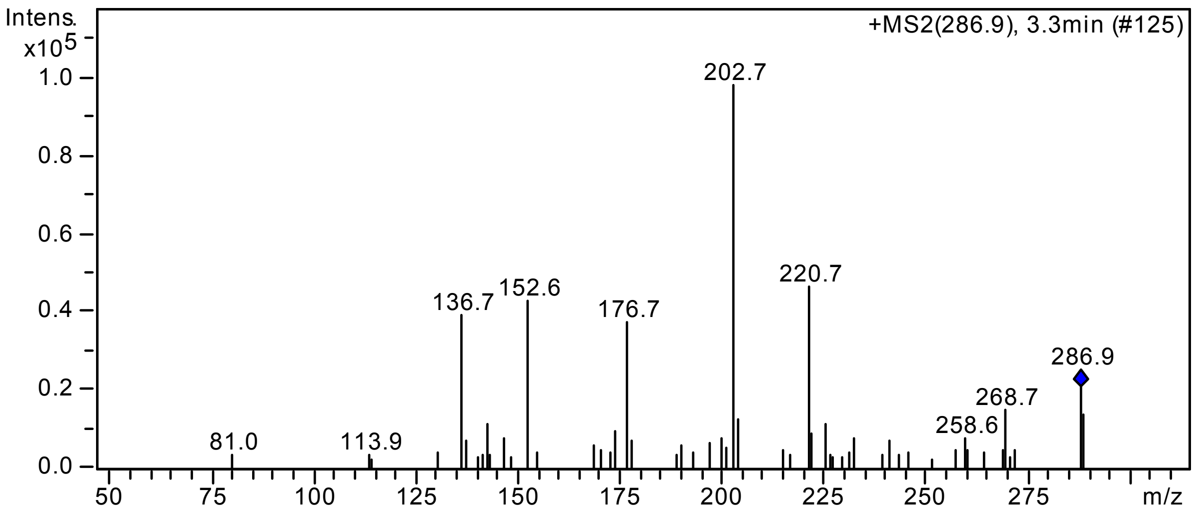
8l


Intens.
x10^6
+MS, 2.4min (#88)
303.1
325.0
m/z


Intens.
x10^5
+MS2(303.1), 2.4min (#89)
256.8
228.8
274.8
302.9
152.6
200.7
172.8
m/z

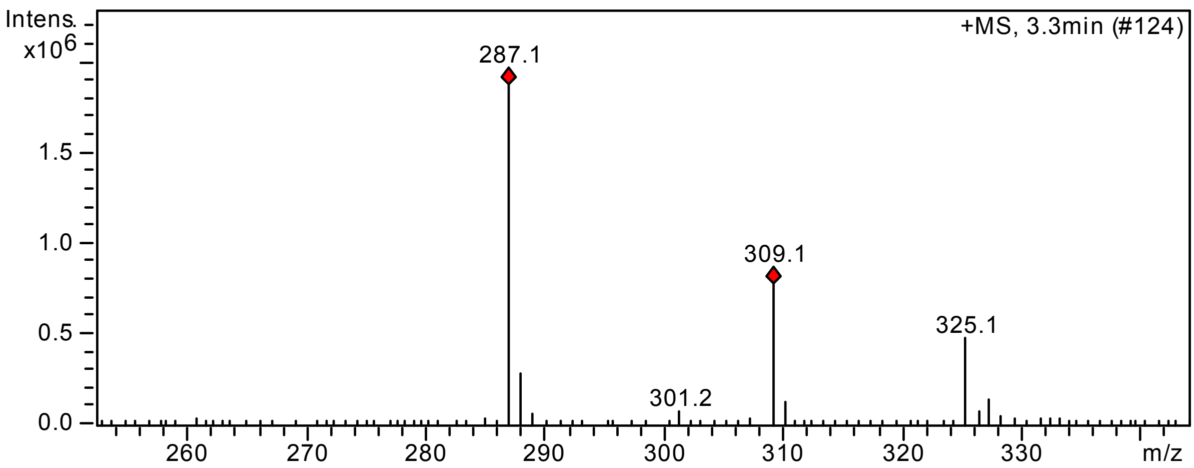
8m


Intens.
x10^7
+MS, 3.3min (#124)
286.9
594.9
371.0
m/z

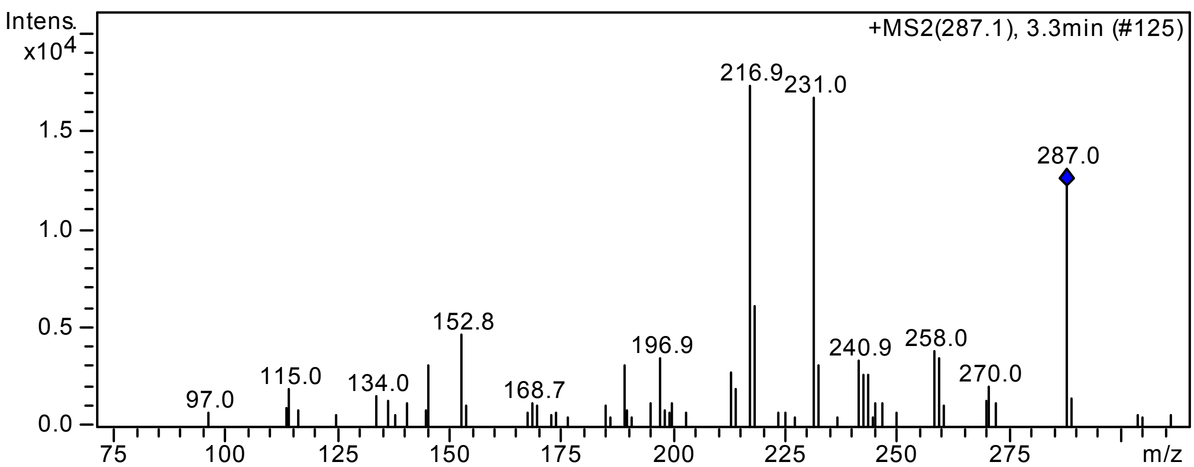


Intens.
x10^5
+MS2(286.9), 3.3min (#125)
202.7
220.7
136.7
152.6
176.7
286.9
268.7
258.6
81.0
113.9
m/z

8n

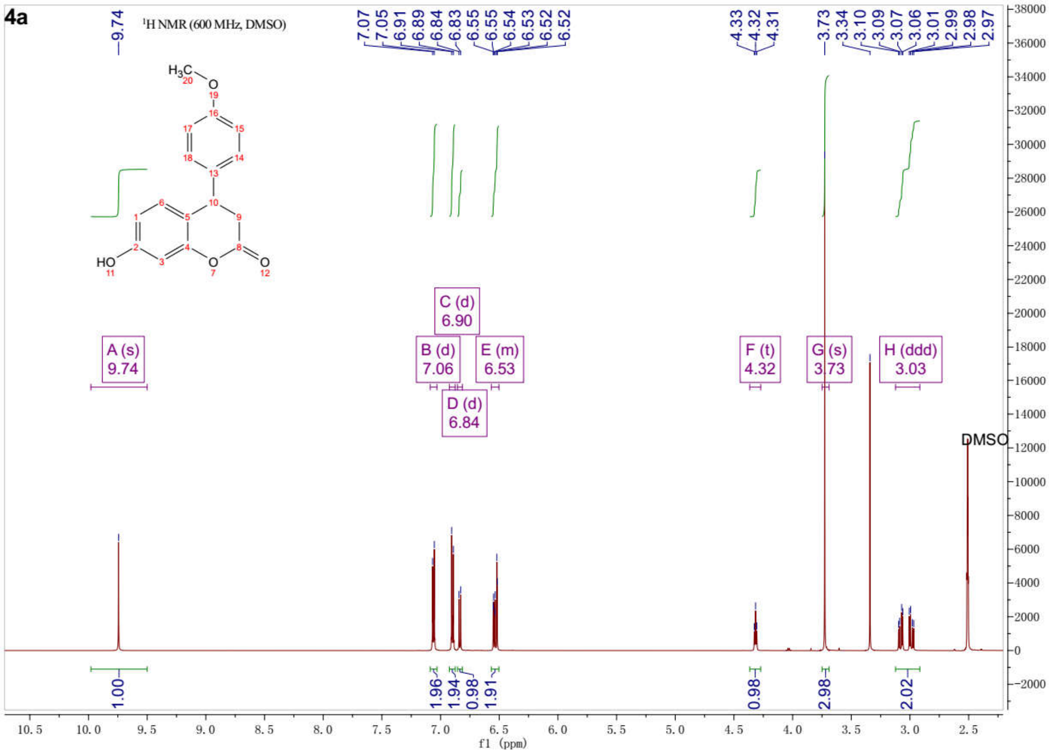


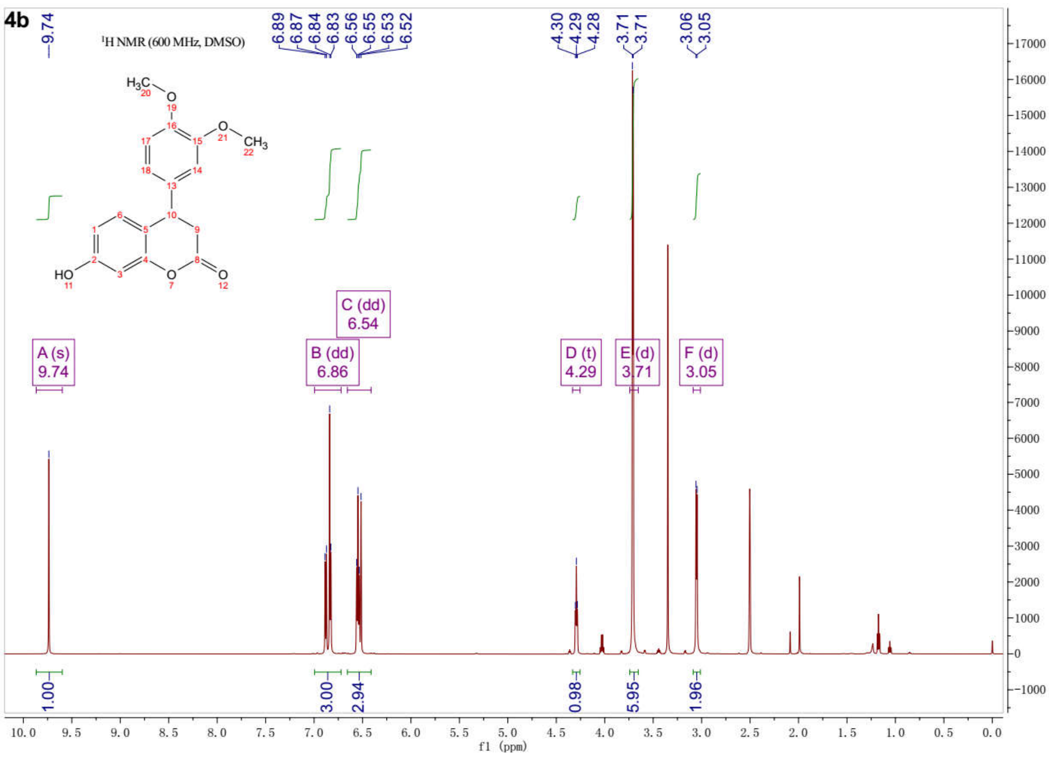
Intens.
x10^6
+MS, 3.3min (#124)
287.1
309.1
325.1
301.2
m/z

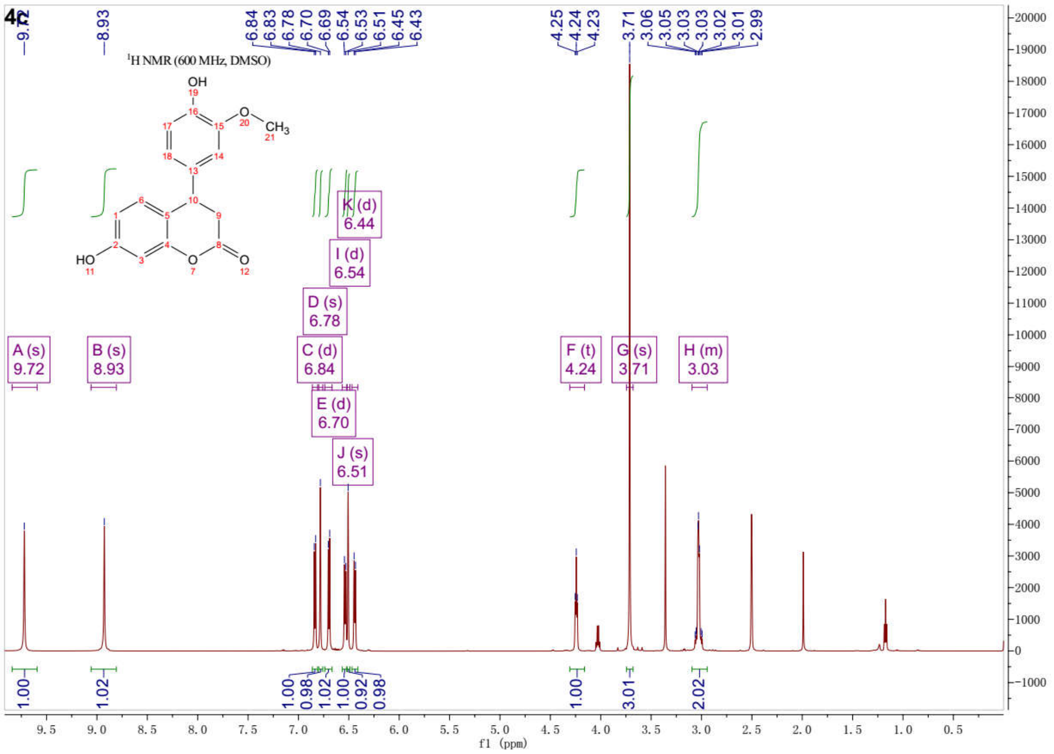


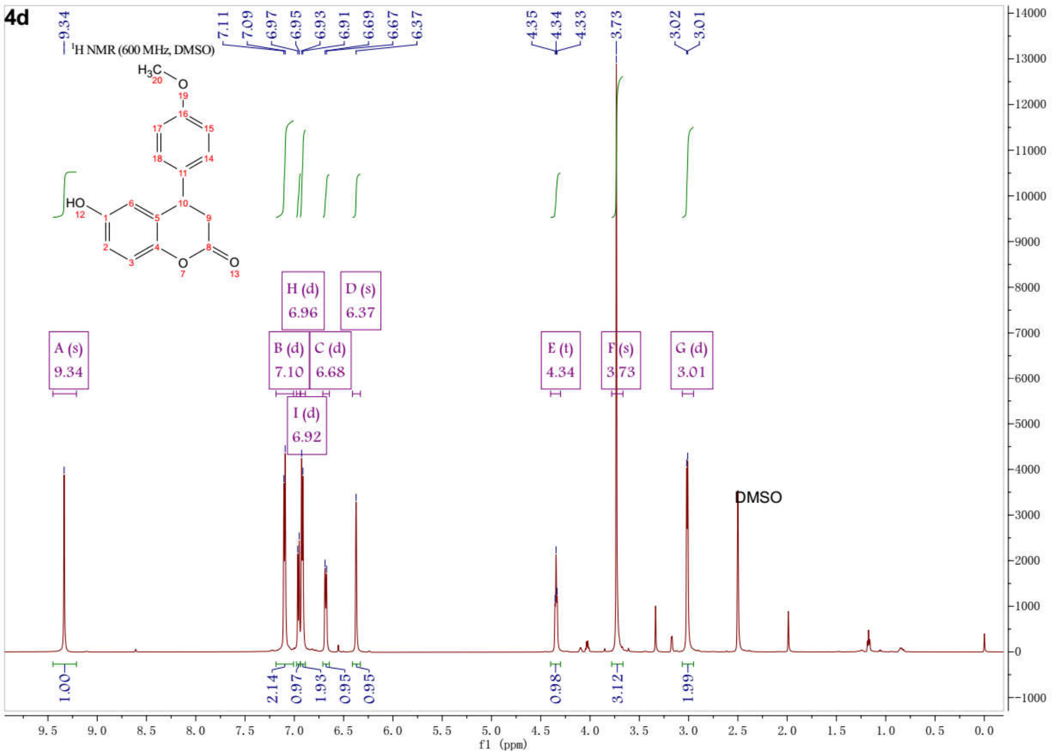
Intens.
x10^4
+MS2(287.1), 3.3min (#125)
216.9
231.0
287.0
152.8
196.9
240.9
258.0
270.0
115.0
134.0
168.7
97.0
m/z

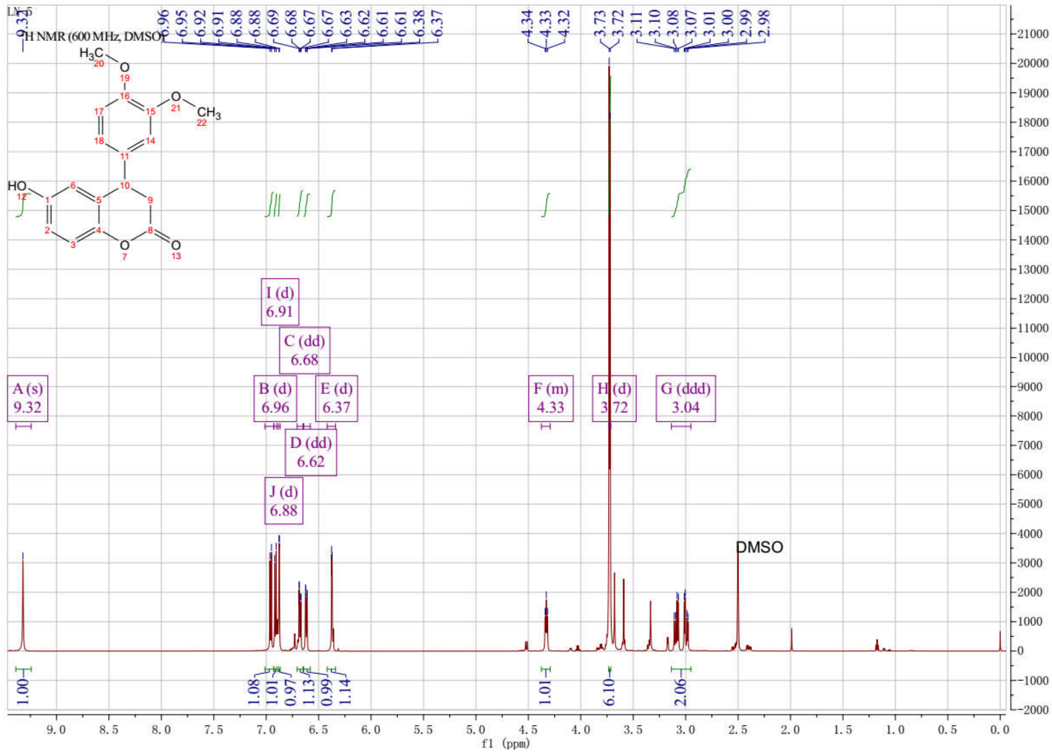
^{1}H NMR(600 MHz, DMSO-d_6) of compounds 4a-8n



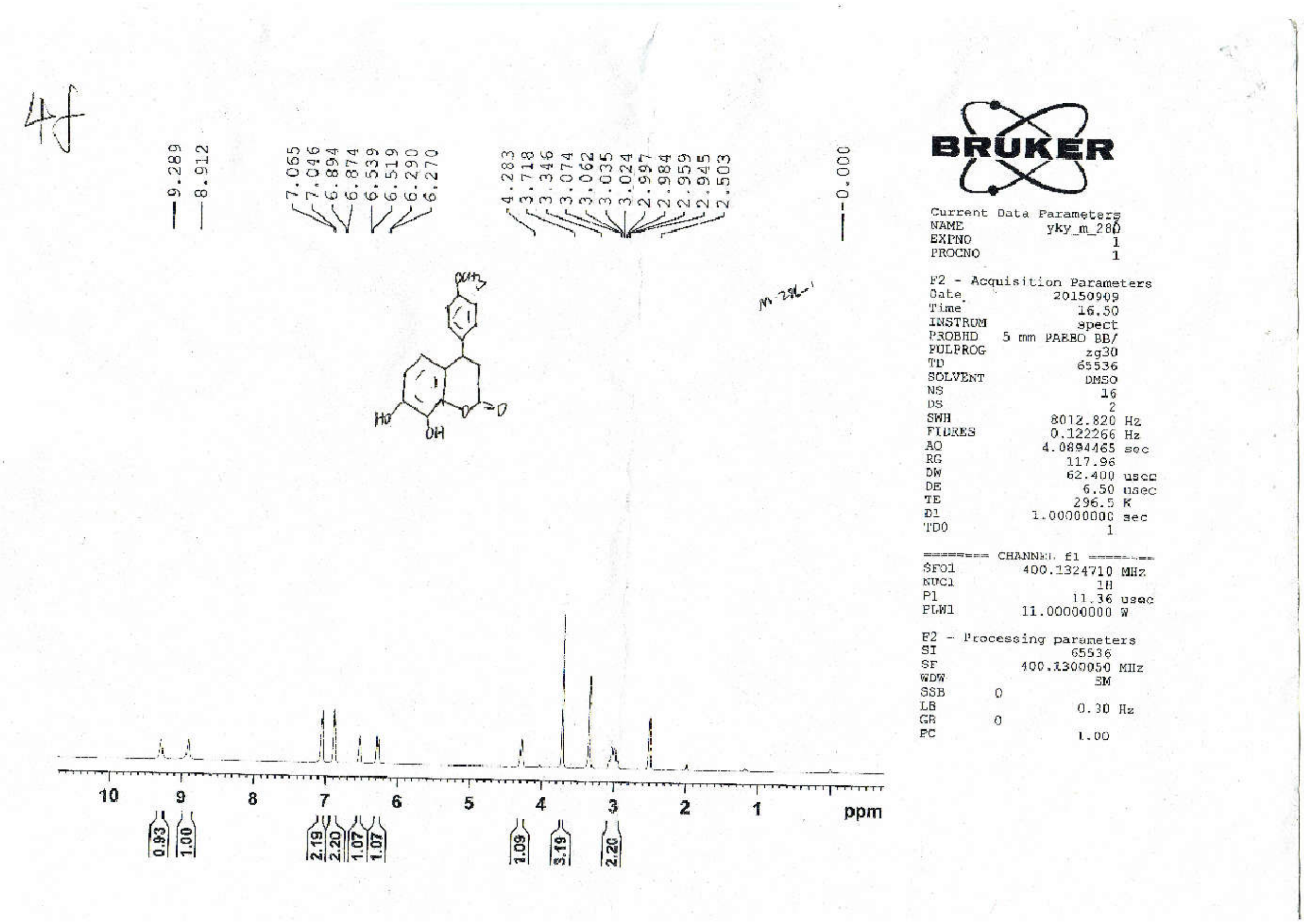


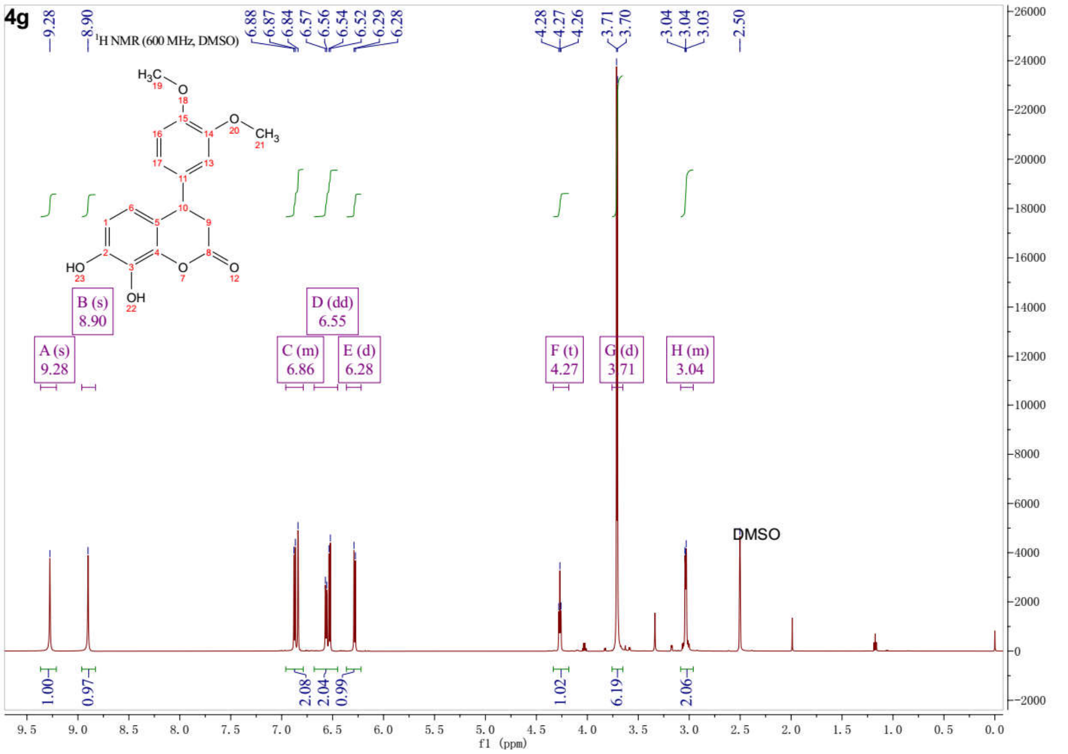

4c
¹H NMR (600 MHz, DMSO)
A (s) 9.72
B (s) 8.93
C (d) 6.84
D (s) 6.78
E (d) 6.70
I (d) 6.54
J (s) 6.51
K (d) 6.44
F (t) 4.24
G (s) 3.71
H (m) 3.03
f1 (ppm)

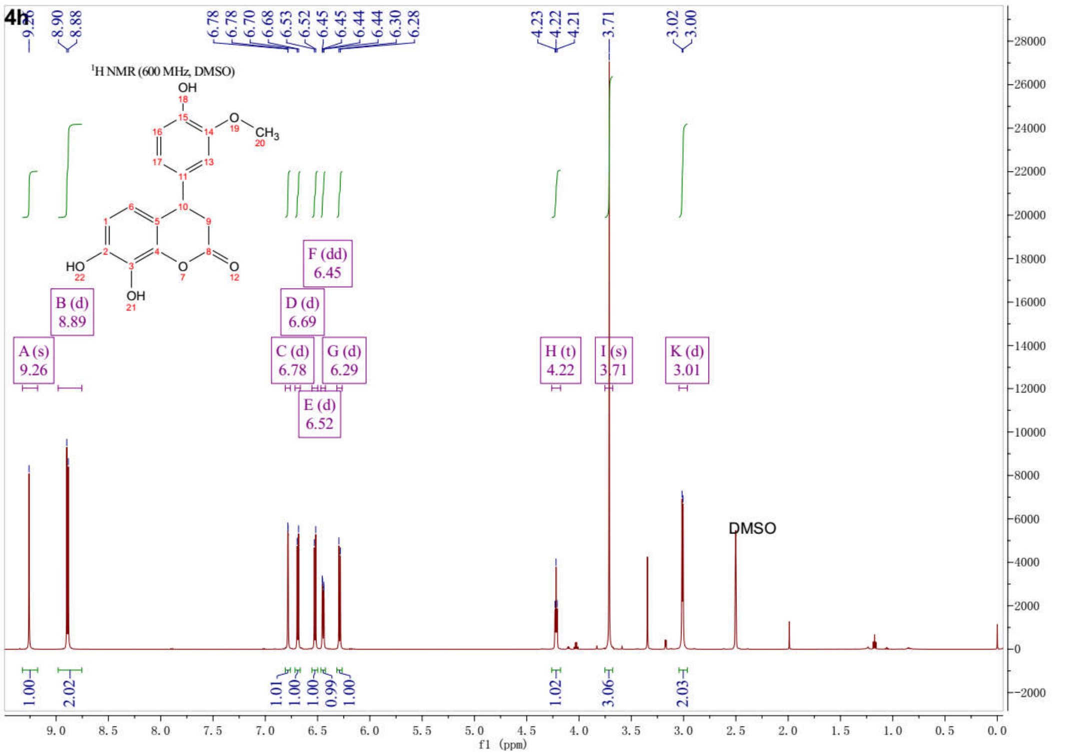

4d
¹H NMR (600 MHz, DMSO)
A (s) 9.34
B (d) 7.10
H (d) 6.96
I (d) 6.92
C (d) 6.68
D (s) 6.37
E (t) 4.34
F (s) 3.73
G (d) 3.01
DMSO
f1 (ppm)

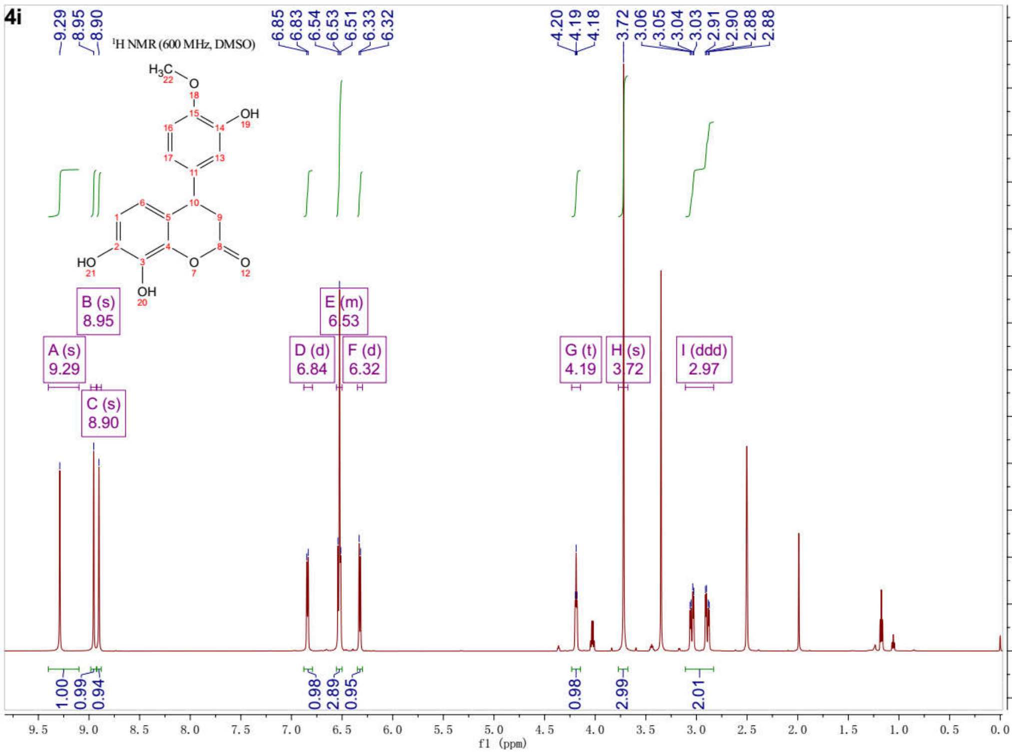


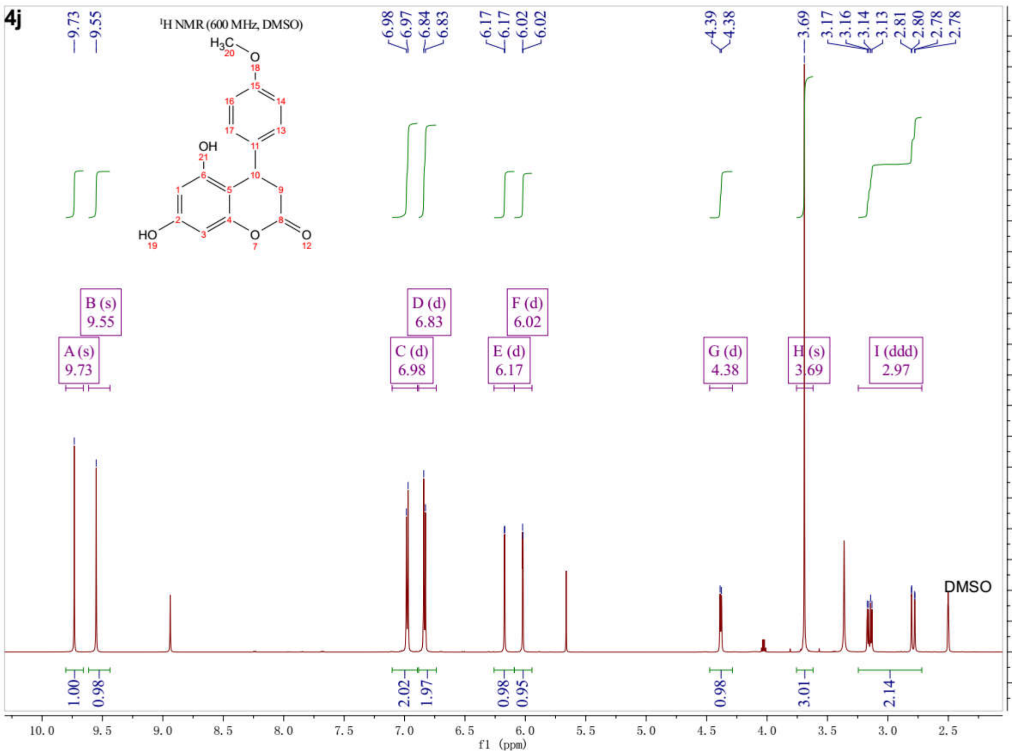
LY-5
1H NMR (600 MHz, DMSO)
A (s) 9.32
B (d) 6.96
I (d) 6.91
J (d) 6.88
C (dd) 6.68
D (dd) 6.62
E (d) 6.37
F (m) 4.33
H (d) 3.72
G (ddd) 3.04
DMSO
f1 (ppm)


4f
9.289
8.912
7.065
7.046
6.894
6.874
6.539
6.519
6.290
6.270
4.283
3.718
3.346
3.074
3.062
3.035
3.024
2.997
2.984
2.959
2.945
2.503
0.000
HO
OH
BRUKER
Current Data Parameters
NAME yky_m_280
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150909
Time 16.50
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 117.96
DW 62.400 usec
DE 6.50 usec
TE 296.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 11.36 usec
PLW1 11.00000000 W
F2 - Processing parameters
SI 65536
SF 400.1300050 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
0.93
1.00
2.19
2.20
1.07
1.07
1.09
3.19
2.20

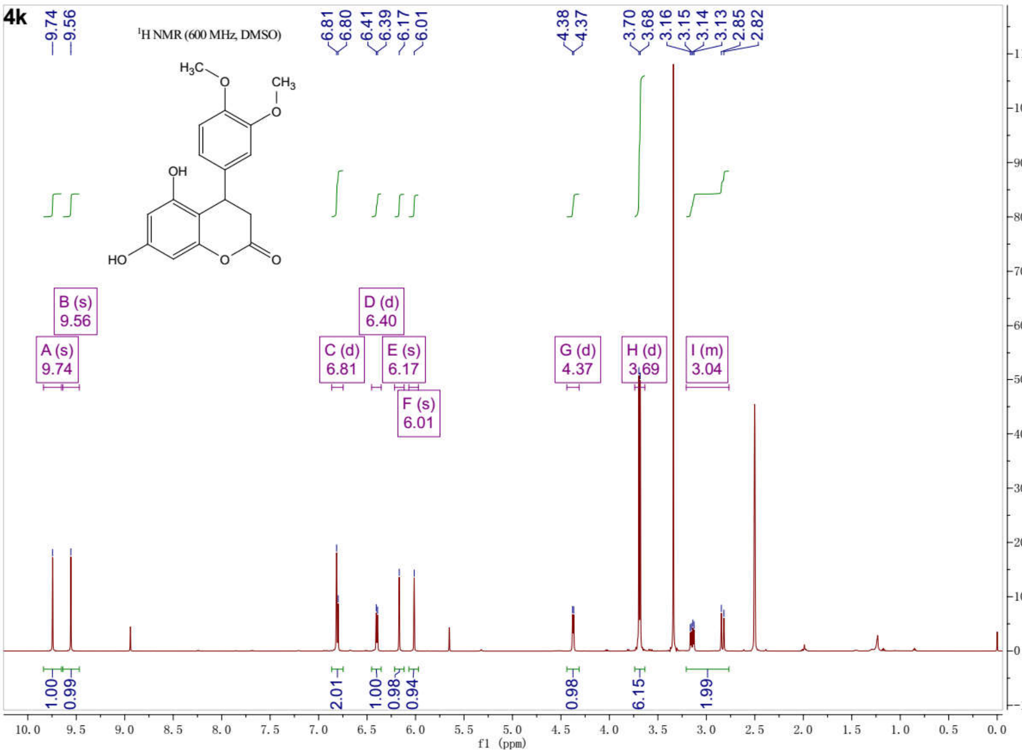

4g
¹H NMR (600 MHz, DMSO)
9.28
8.90
6.88
6.87
6.84
6.57
6.56
6.54
6.52
6.29
6.28
4.28
4.27
4.26
3.71
3.70
3.04
3.04
3.03
2.50
A (s) 9.28
B (s) 8.90
C (m) 6.86
D (dd) 6.55
E (d) 6.28
F (t) 4.27
G (d) 3.71
H (m) 3.04
DMSO
1.00
0.97
2.08
2.04
0.99
1.02
6.19
2.06
f1 (ppm)


4h
¹H NMR (600 MHz, DMSO)
9.26
8.90
8.88
6.78
6.78
6.70
6.68
6.53
6.52
6.45
6.45
6.44
6.44
6.30
6.28
4.23
4.22
4.21
3.71
3.02
3.00
A (s) 9.26
B (d) 8.89
C (d) 6.78
D (d) 6.69
E (d) 6.52
F (dd) 6.45
G (d) 6.29
H (t) 4.22
I (s) 3.71
K (d) 3.01
DMSO
1.00
2.02
1.01
1.00
1.00
0.99
1.00
1.02
3.06
2.03
f1 (ppm)


4i
¹H NMR (600 MHz, DMSO)
A (s) 9.29
B (s) 8.95
C (s) 8.90
D (d) 6.84
E (m) 6.53
F (d) 6.32
G (t) 4.19
H (s) 3.72
I (ddd) 2.97
f1 (ppm)

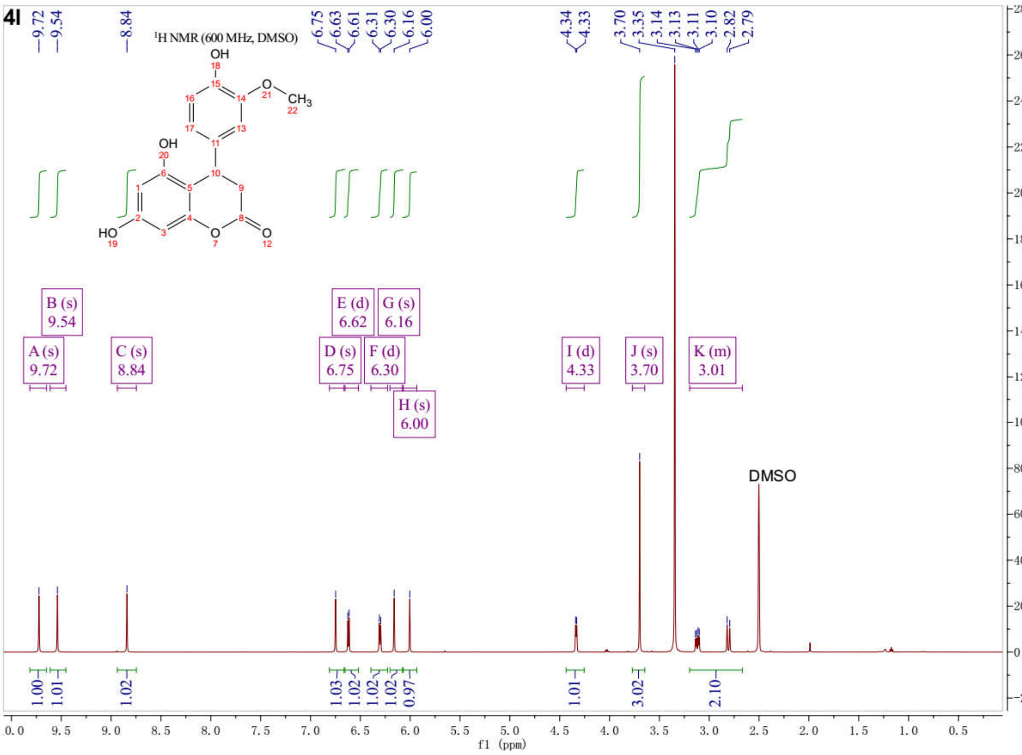

4j
¹H NMR (600 MHz, DMSO)
A (s) 9.73
B (s) 9.55
C (d) 6.98
D (d) 6.83
E (d) 6.17
F (d) 6.02
G (d) 4.38
H (s) 3.69
I (ddd) 2.97
DMSO
f1 (ppm)

4k



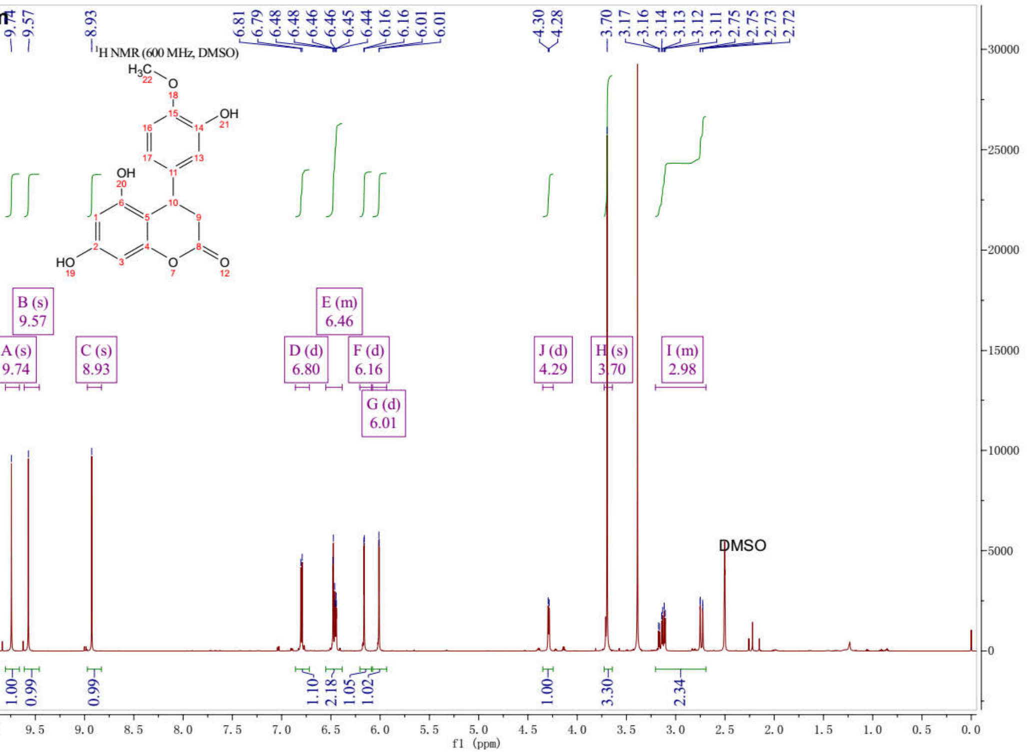
¹H NMR (600 MHz, DMSO)
A (s) 9.74
B (s) 9.56
C (d) 6.81
D (d) 6.40
E (s) 6.17
F (s) 6.01
G (d) 4.37
H (d) 3.69
I (m) 3.04
f1 (ppm)

4l

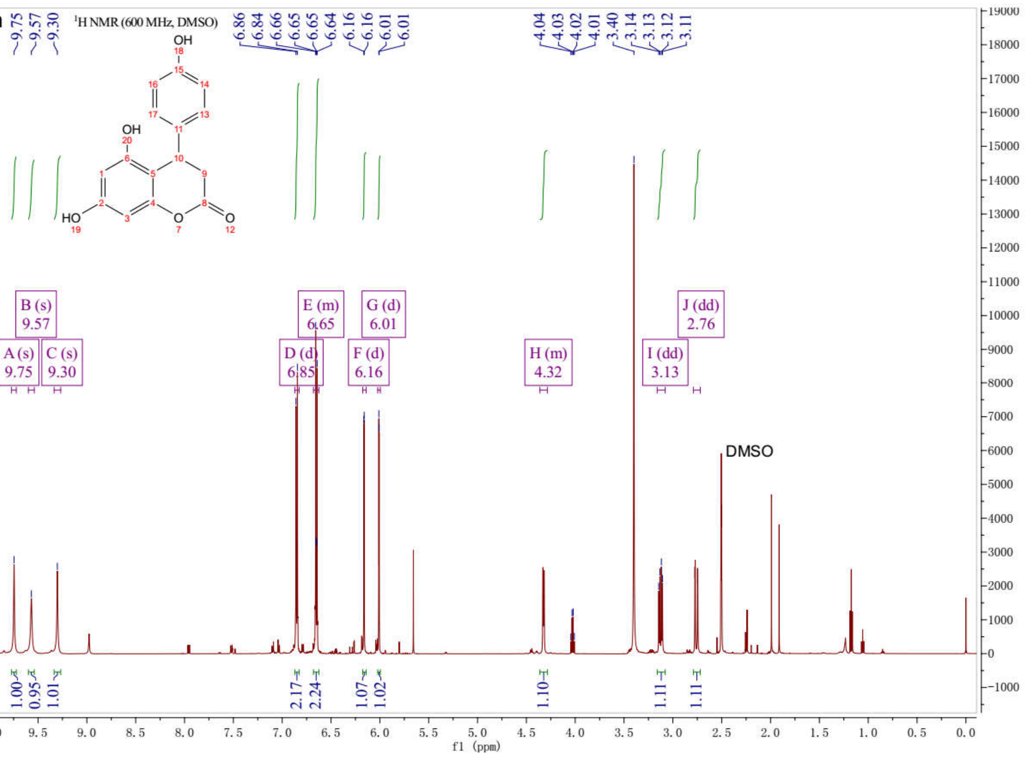


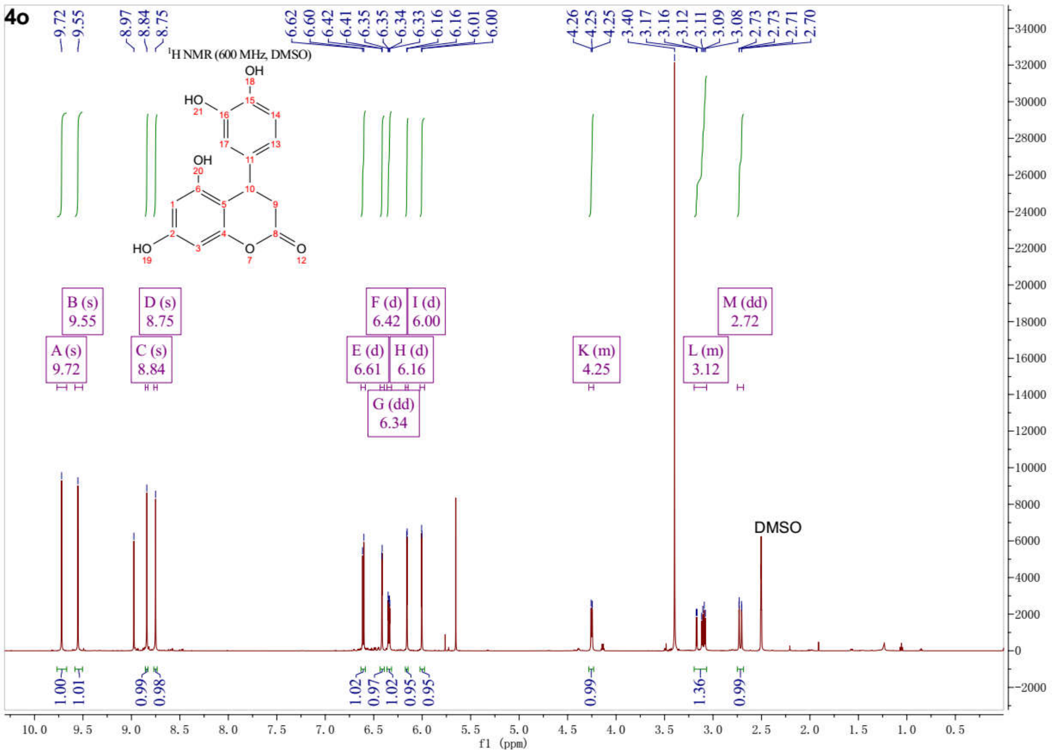
¹H NMR (600 MHz, DMSO)
A (s) 9.72
B (s) 9.54
C (s) 8.84
D (s) 6.75
E (d) 6.62
F (d) 6.30
G (s) 6.16
H (s) 6.00
I (d) 4.33
J (s) 3.70
K (m) 3.01
DMSO
f1 (ppm)

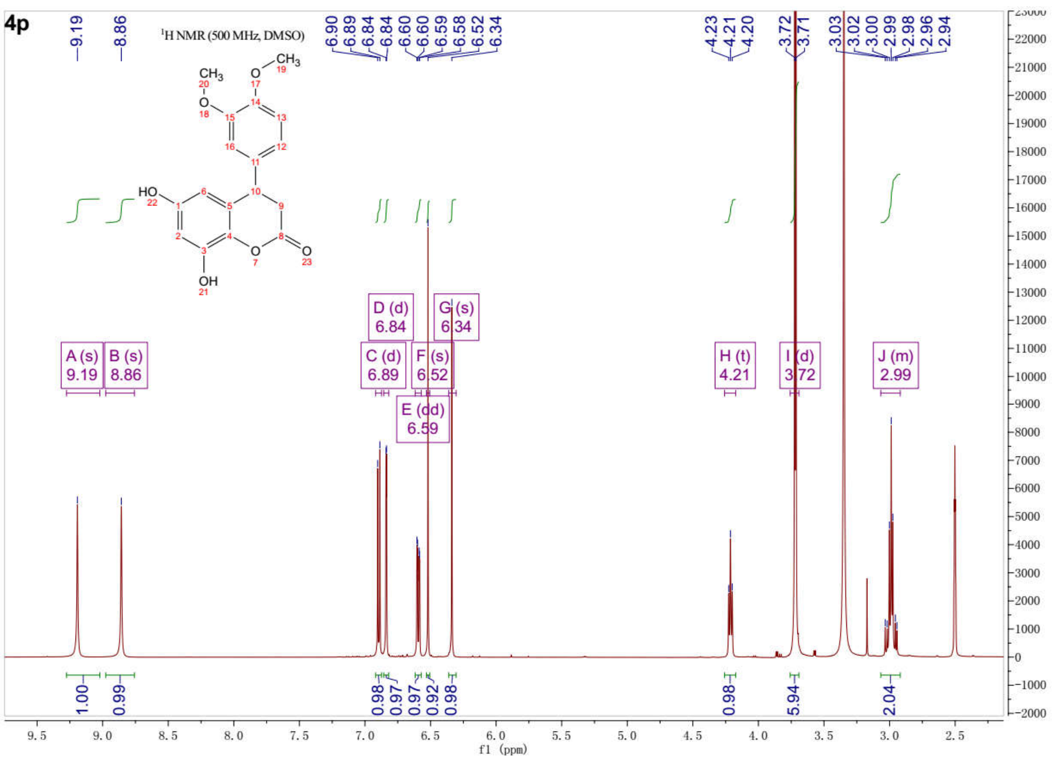
4m



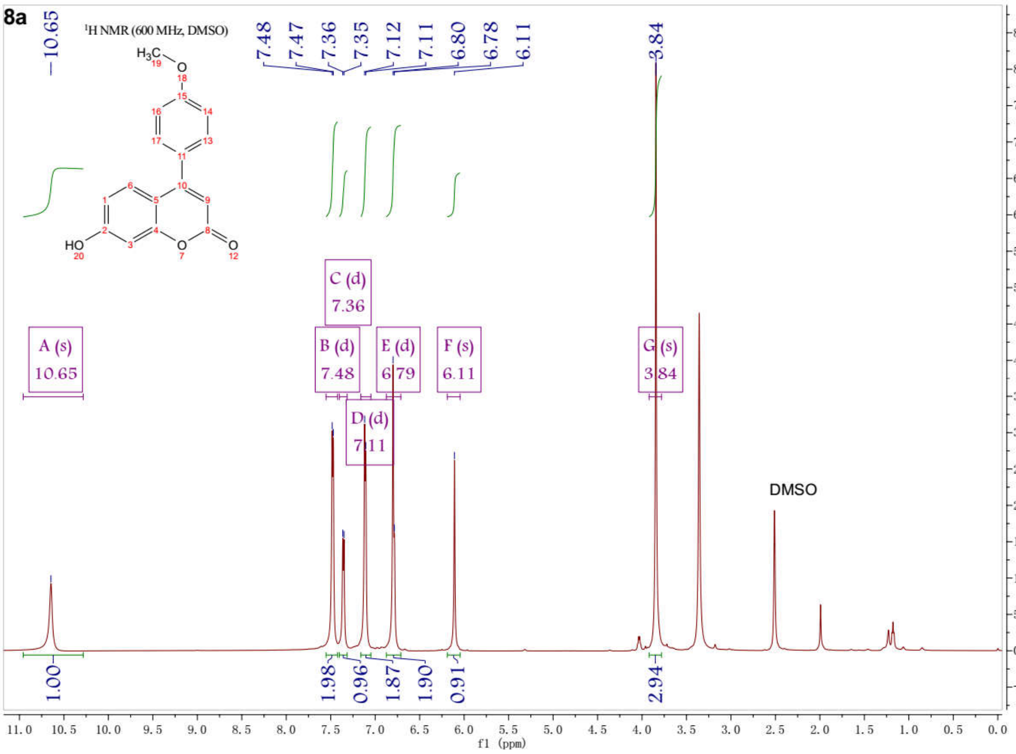
4n




4o
¹H NMR (600 MHz, DMSO)
DMSO
f1 (ppm)

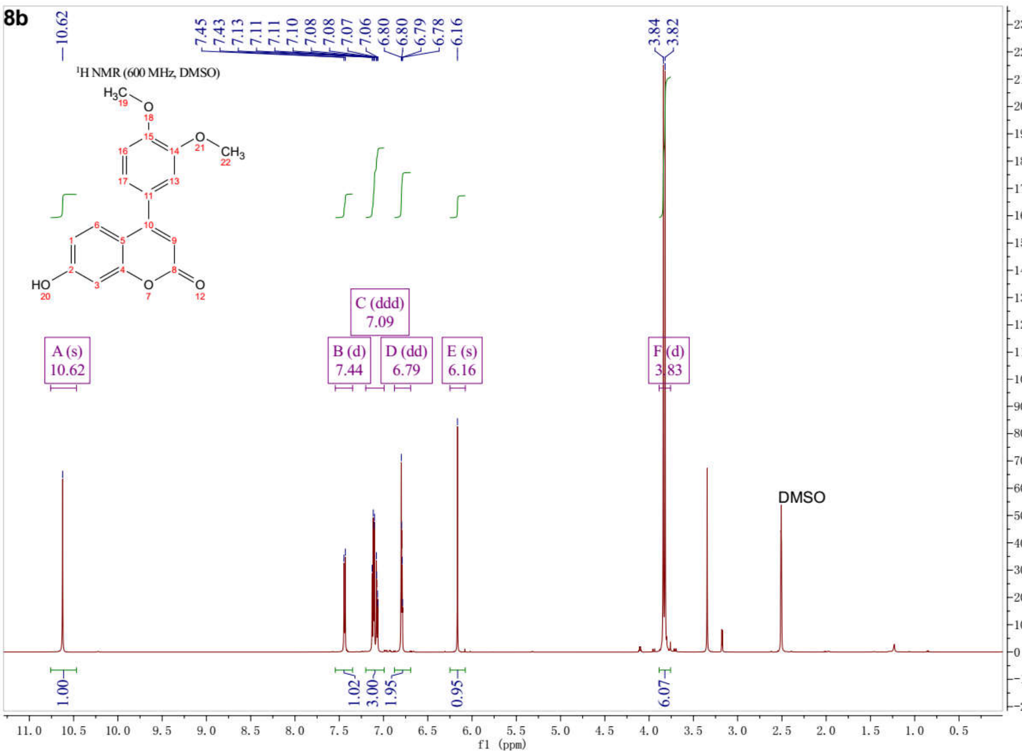

4p
¹H NMR (500 MHz, DMSO)
f1 (ppm)

8a

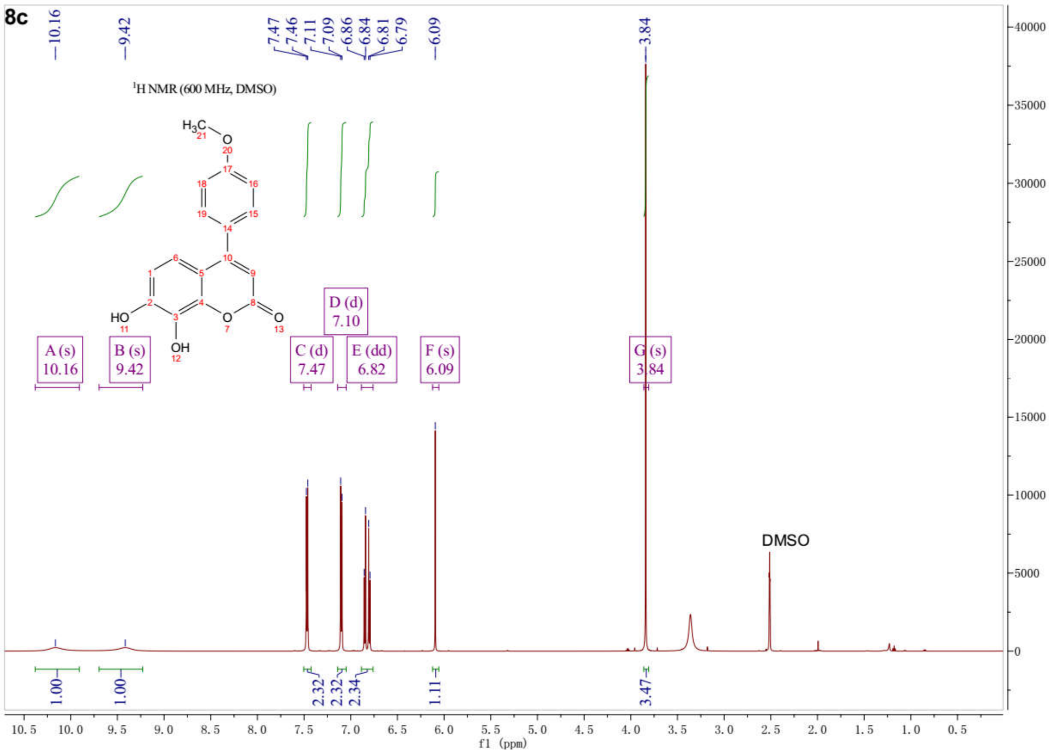


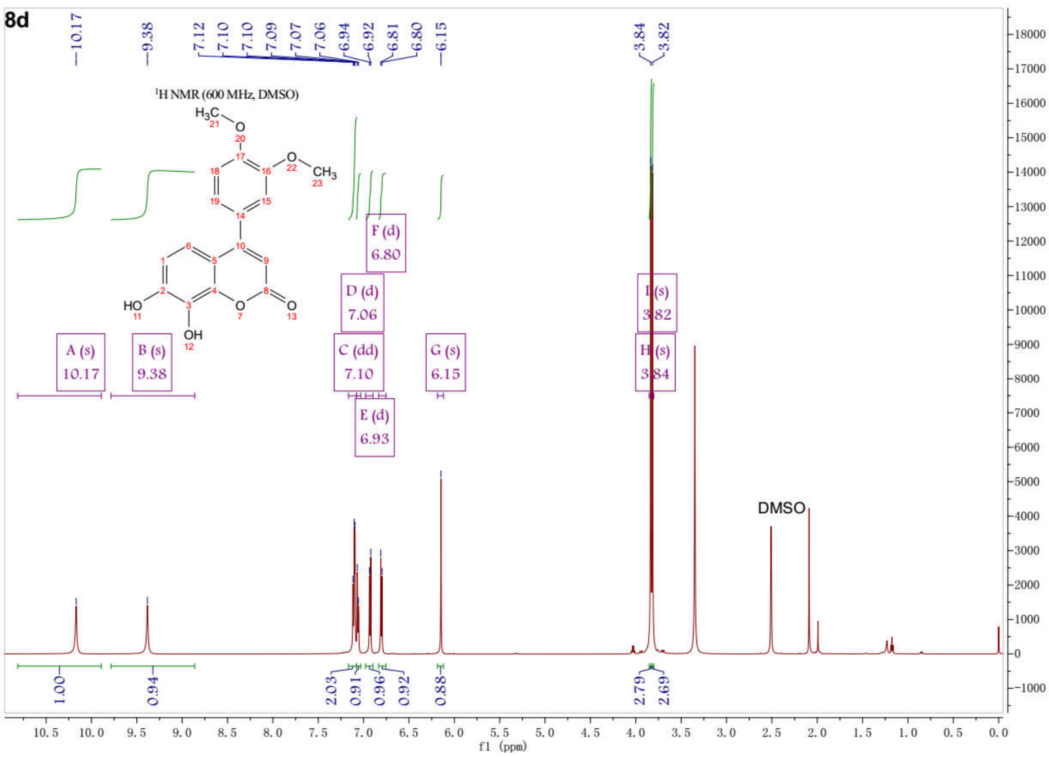
¹H NMR (600 MHz, DMSO)
10.65
7.48
7.47
7.36
7.35
7.12
7.11
6.80
6.78
6.11
3.84
A (s)
10.65
B (d)
7.48
C (d)
7.36
D (d)
7.11
E (d)
6.79
F (s)
6.11
G (s)
3.84
DMSO
1.00
1.98
0.96
1.87
1.90
0.91
2.94
f1 (ppm)

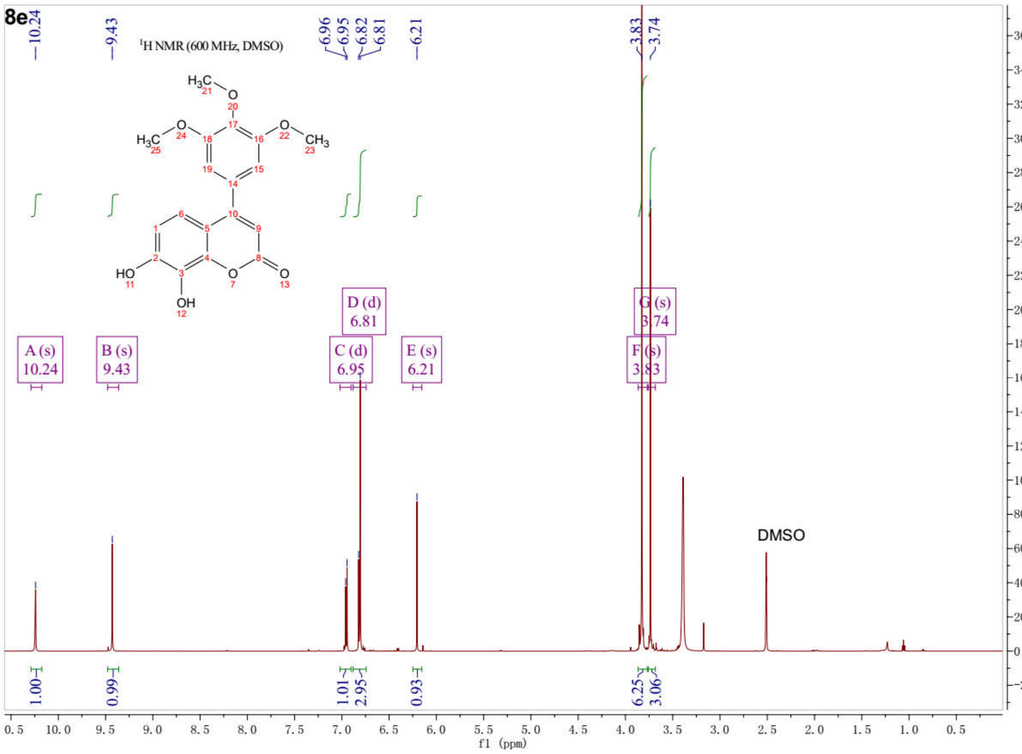
8b

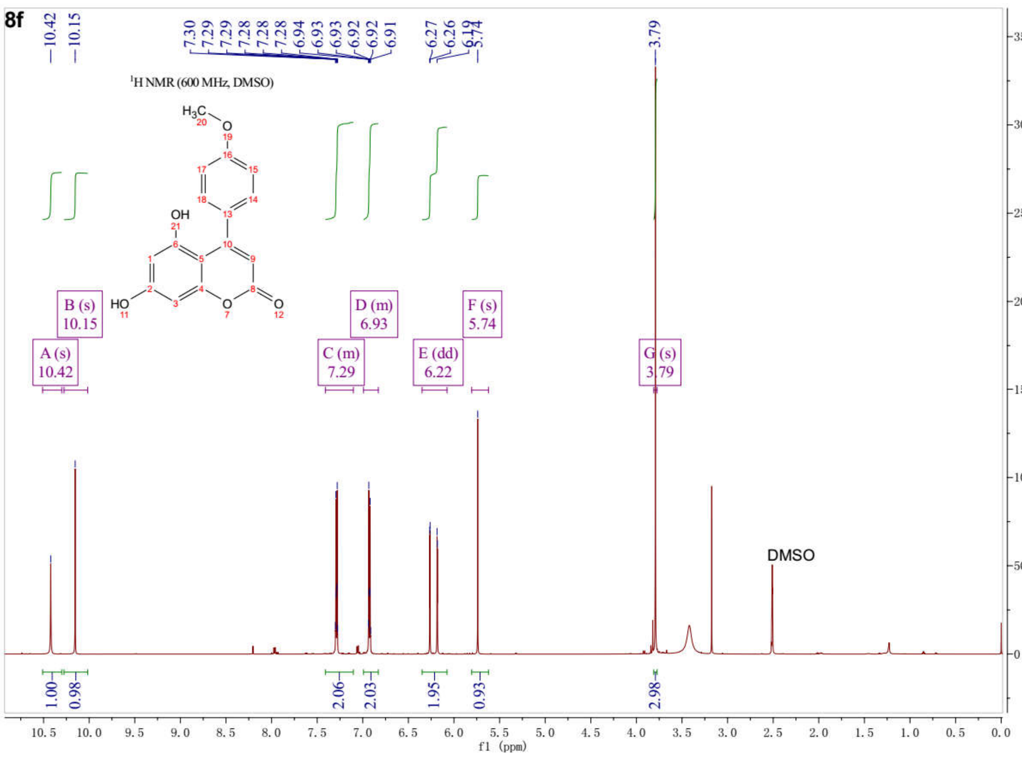


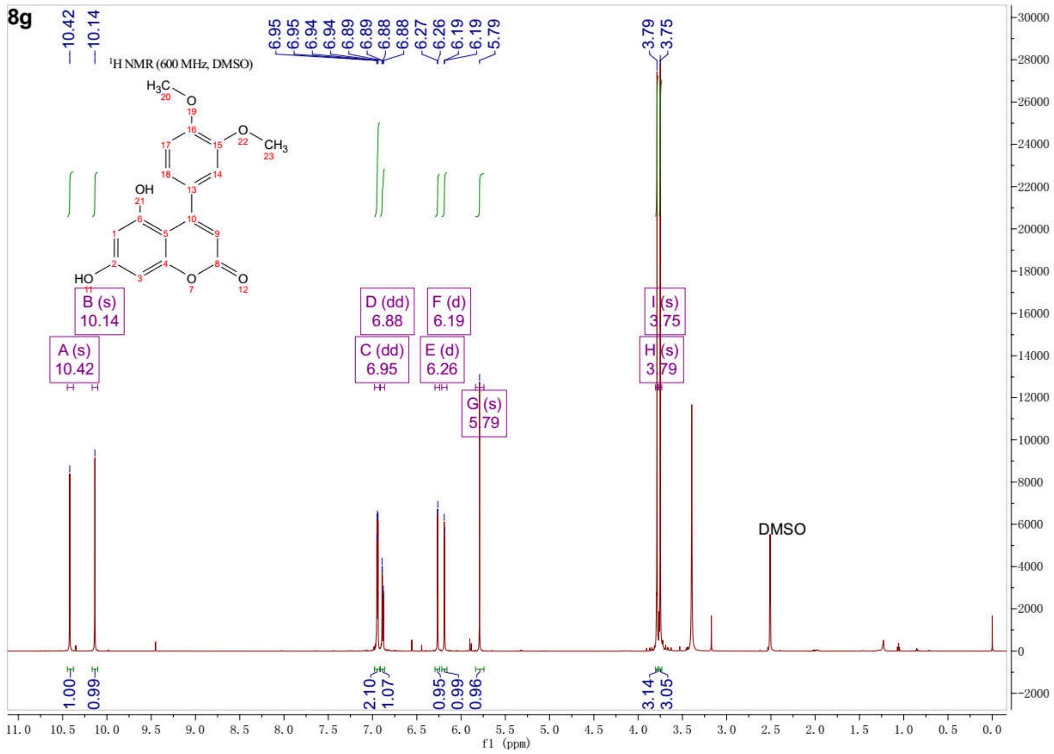
¹H NMR (600 MHz, DMSO)
10.62
7.45
7.43
7.13
7.11
7.11
7.10
7.08
7.07
7.06
6.80
6.80
6.79
6.78
6.16
3.84
3.82
A (s)
10.62
B (d)
7.44
C (ddd)
7.09
D (dd)
6.79
E (s)
6.16
F (d)
3.83
DMSO
1.00
1.02
3.00
1.95
0.95
6.07
f1 (ppm)

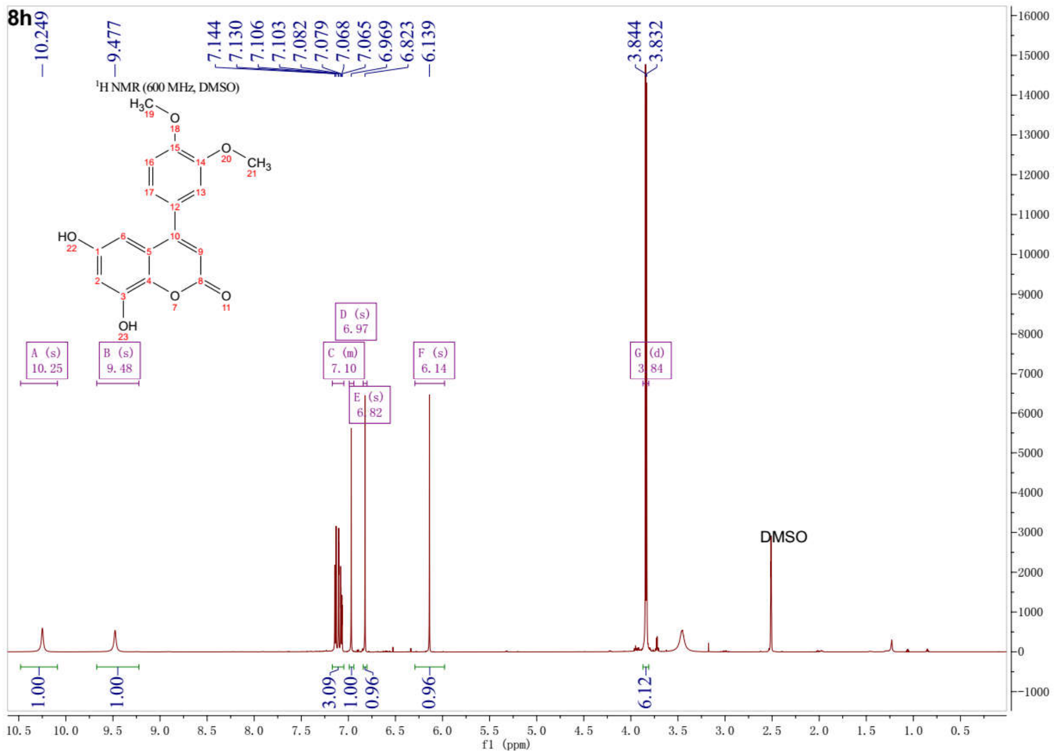

8c
¹H NMR (600 MHz, DMSO)
A (s) 10.16
B (s) 9.42
C (d) 7.47
D (d) 7.10
E (dd) 6.82
F (s) 6.09
G (s) 3.84
DMSO
f1 (ppm)

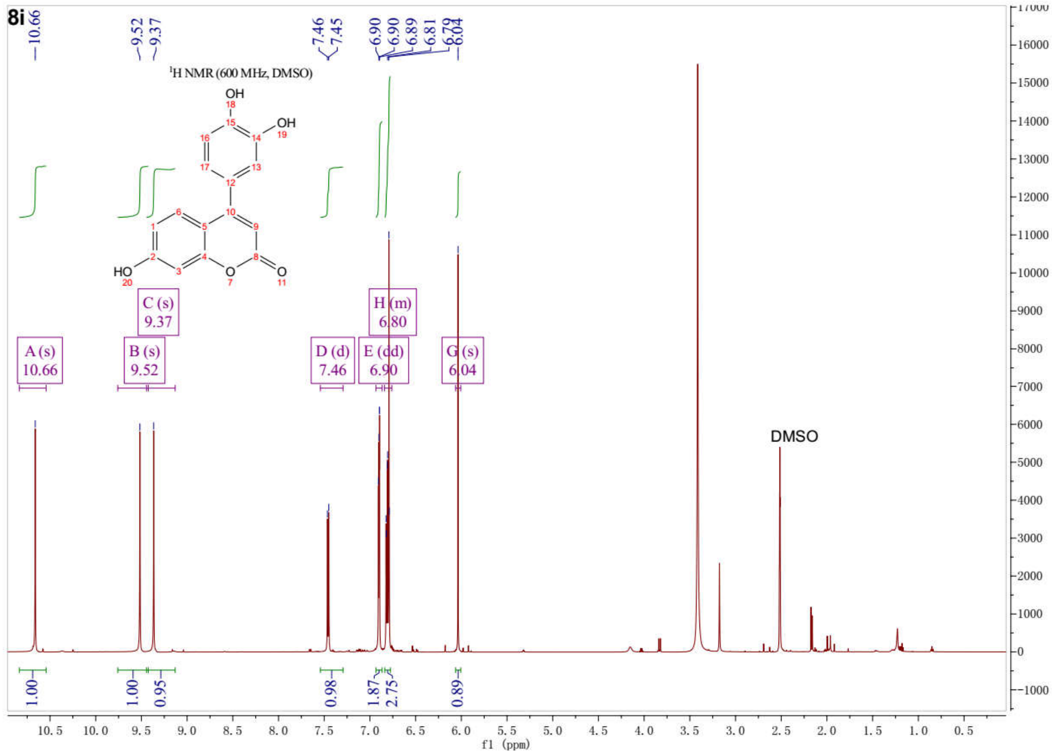

8d
¹H NMR (600 MHz, DMSO)
A (s) 10.17
B (s) 9.38
C (dd) 7.10
D (d) 7.06
E (d) 6.93
F (d) 6.80
G (s) 6.15
H (s) 3.84
I (s) 3.82
DMSO
f1 (ppm)

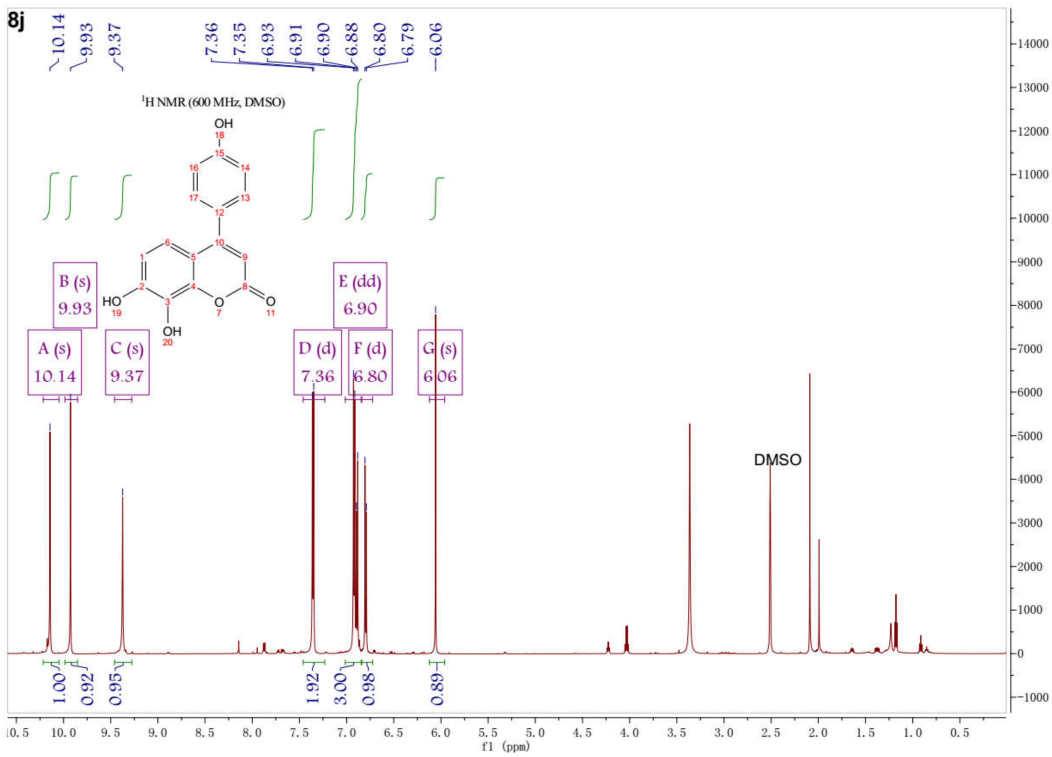

8e
1H NMR (600 MHz, DMSO)
A (s) 10.24
B (s) 9.43
C (d) 6.95
D (d) 6.81
E (s) 6.21
F (s) 3.83
G (s) 3.74
DMSO
f1 (ppm)

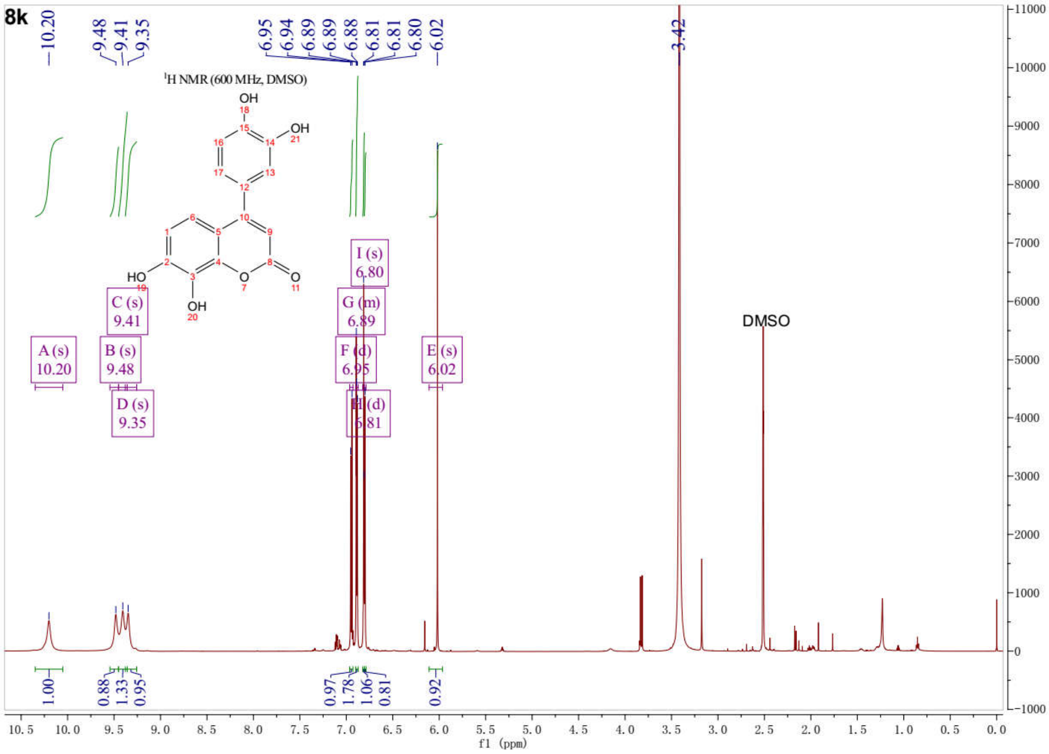

8f
1H NMR (600 MHz, DMSO)
A (s) 10.42
B (s) 10.15
C (m) 7.29
D (m) 6.93
E (dd) 6.22
F (s) 5.74
G (s) 3.79
DMSO
f1 (ppm)

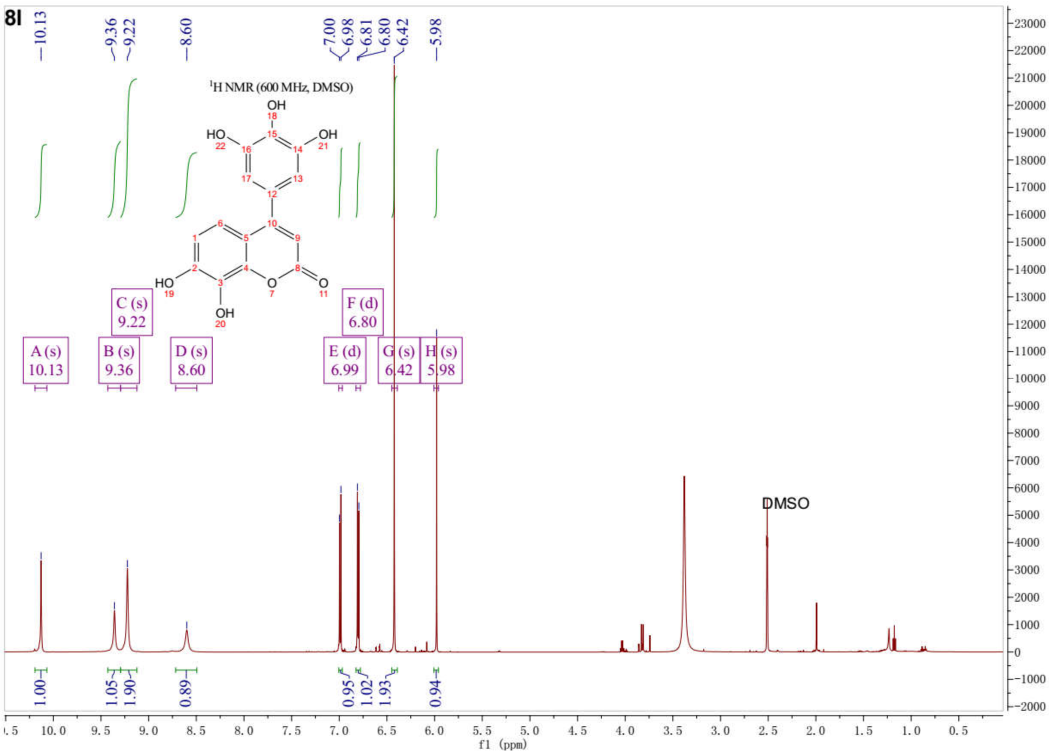

8g
1H NMR (600 MHz, DMSO)
DMSO
f1 (ppm)


8h
1H NMR (600 MHz, DMSO)
DMSO
f1 (ppm)

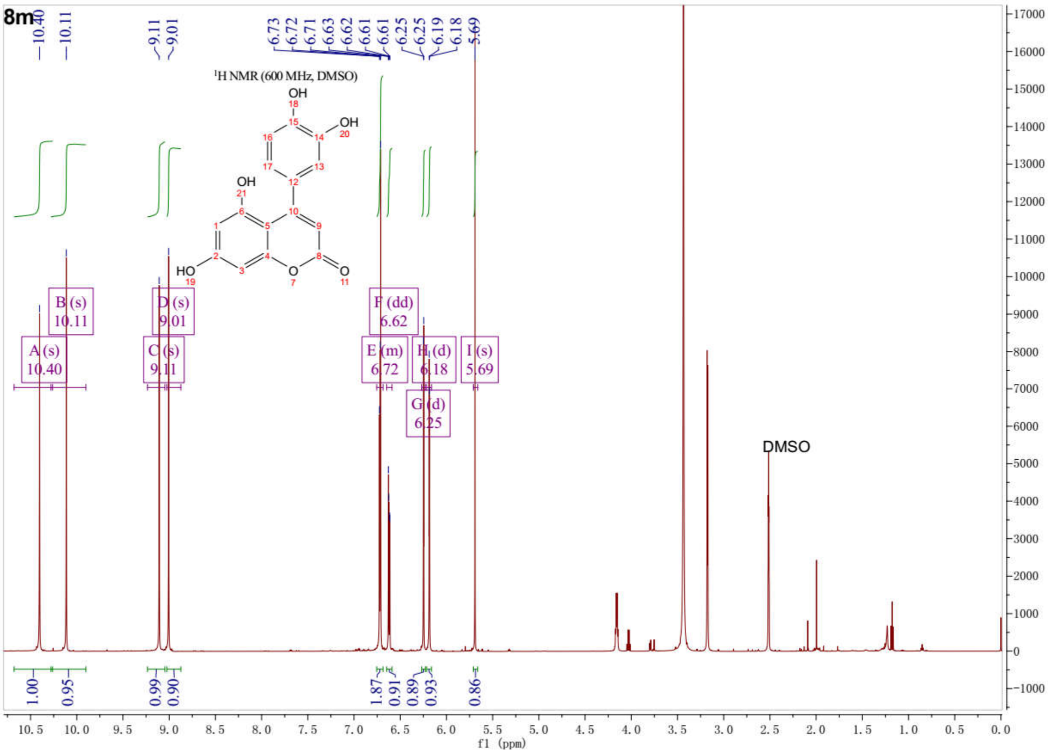

8i
1H NMR (600 MHz, DMSO)
A (s) 10.66
B (s) 9.52
C (s) 9.37
D (d) 7.46
E (dd) 6.90
H (m) 6.80
G (s) 6.04
DMSO
f1 (ppm)


8j
1H NMR (600 MHz, DMSO)
A (s) 10.14
B (s) 9.93
C (s) 9.37
D (d) 7.36
E (dd) 6.90
F (d) 6.80
G (s) 6.06
DMSO
f1 (ppm)

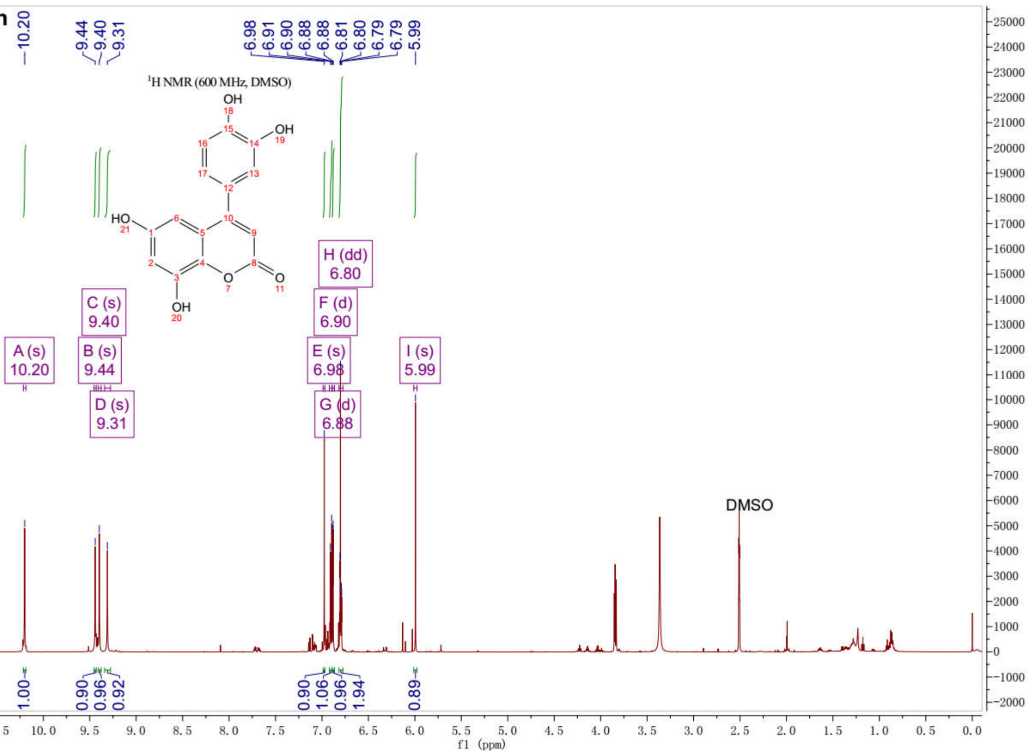

8k
¹H NMR (600 MHz, DMSO)
A (s) 10.20
B (s) 9.48
C (s) 9.41
D (s) 9.35
E (s) 6.02
F (d) 6.95
G (m) 6.89
H (d) 6.81
I (s) 6.80
DMSO
f1 (ppm)


8l
¹H NMR (600 MHz, DMSO)
A (s) 10.13
B (s) 9.36
C (s) 9.22
D (s) 8.60
E (d) 6.99
F (d) 6.80
G (s) 6.42
H (s) 5.98
DMSO
f1 (ppm)

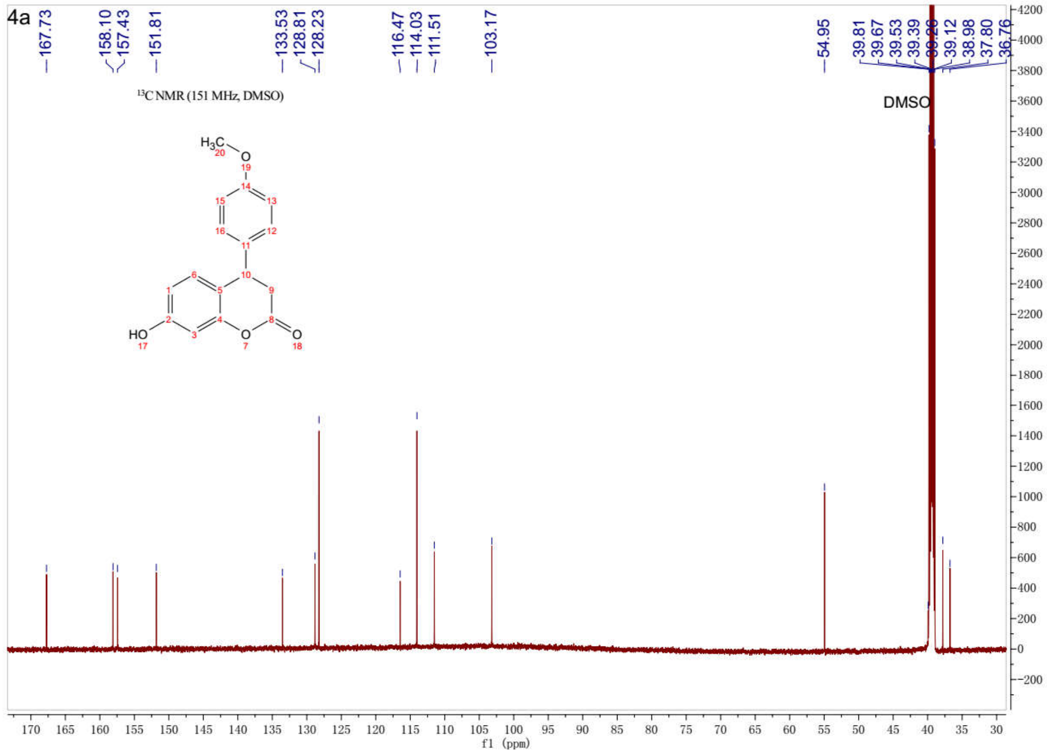
8m

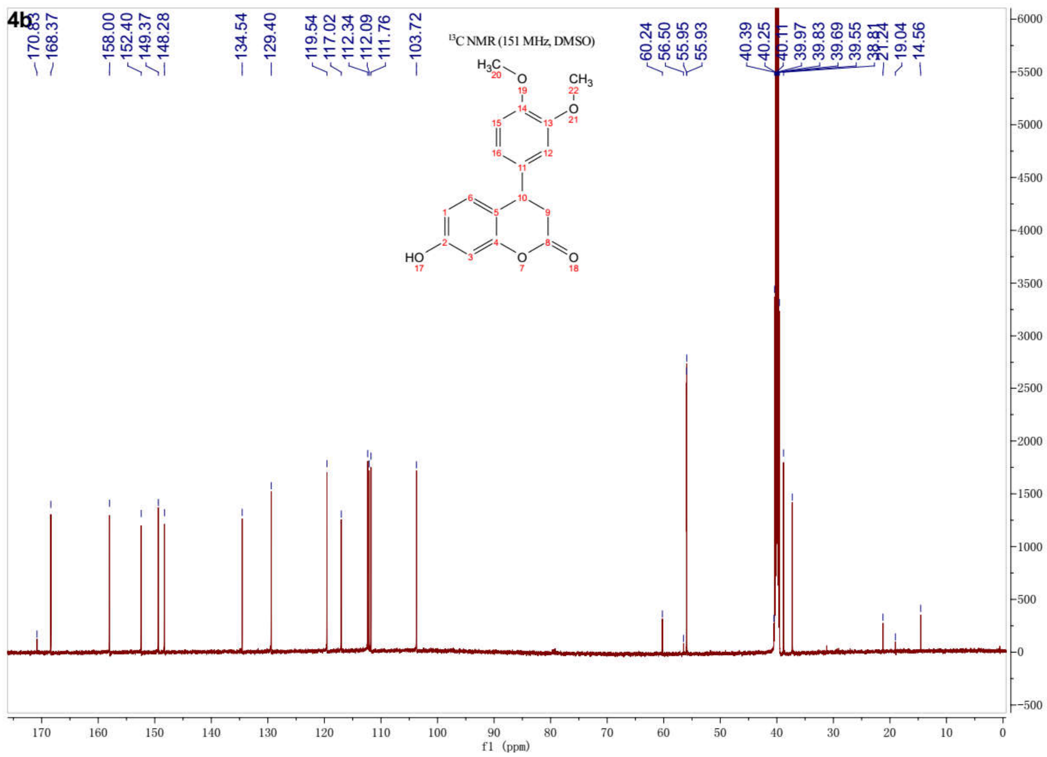


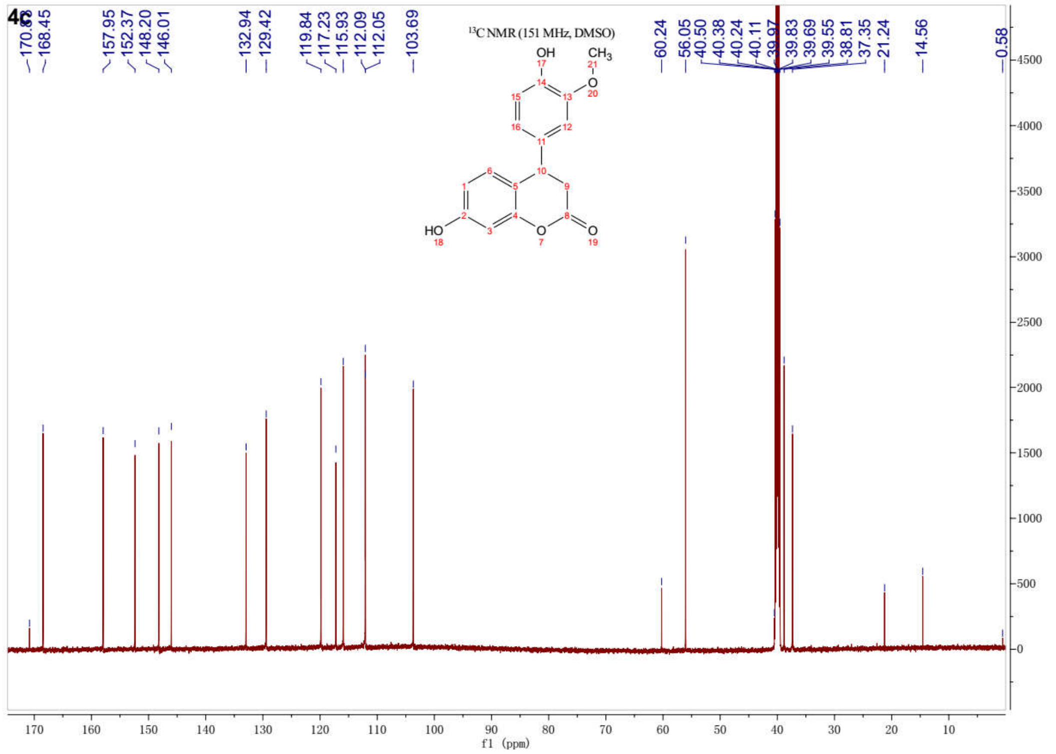
8n

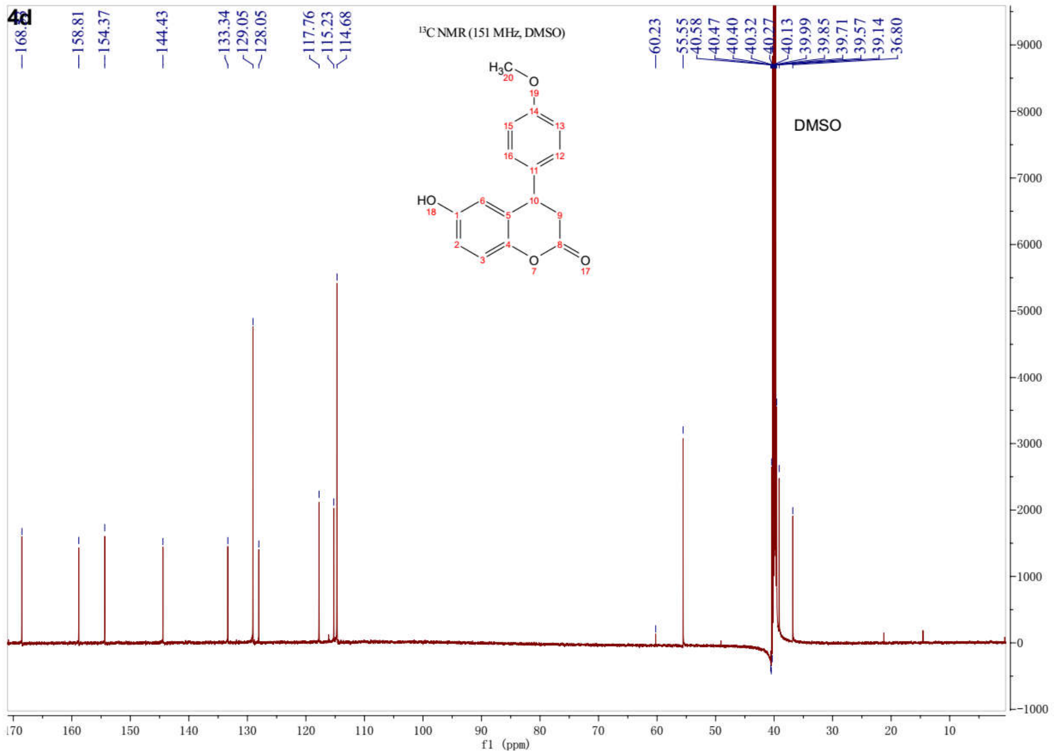


^{13}C NMR(600 MHz, DMSO-d_6) of compounds 4a-8n

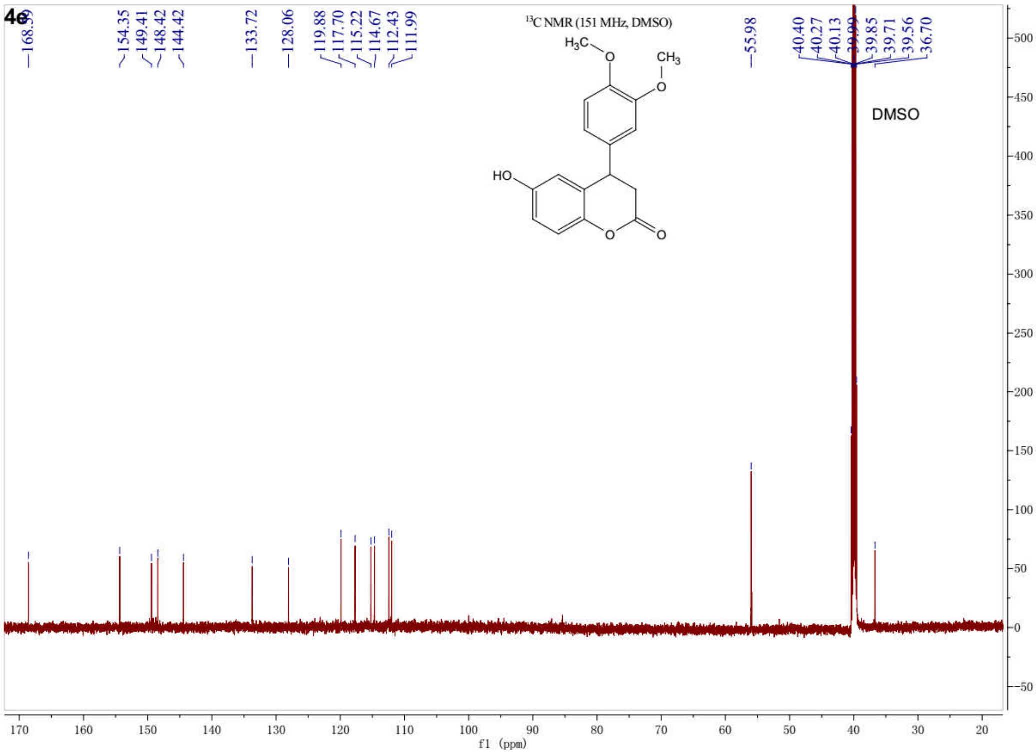





4c
13C NMR (151 MHz, DMSO)
f1 (ppm)

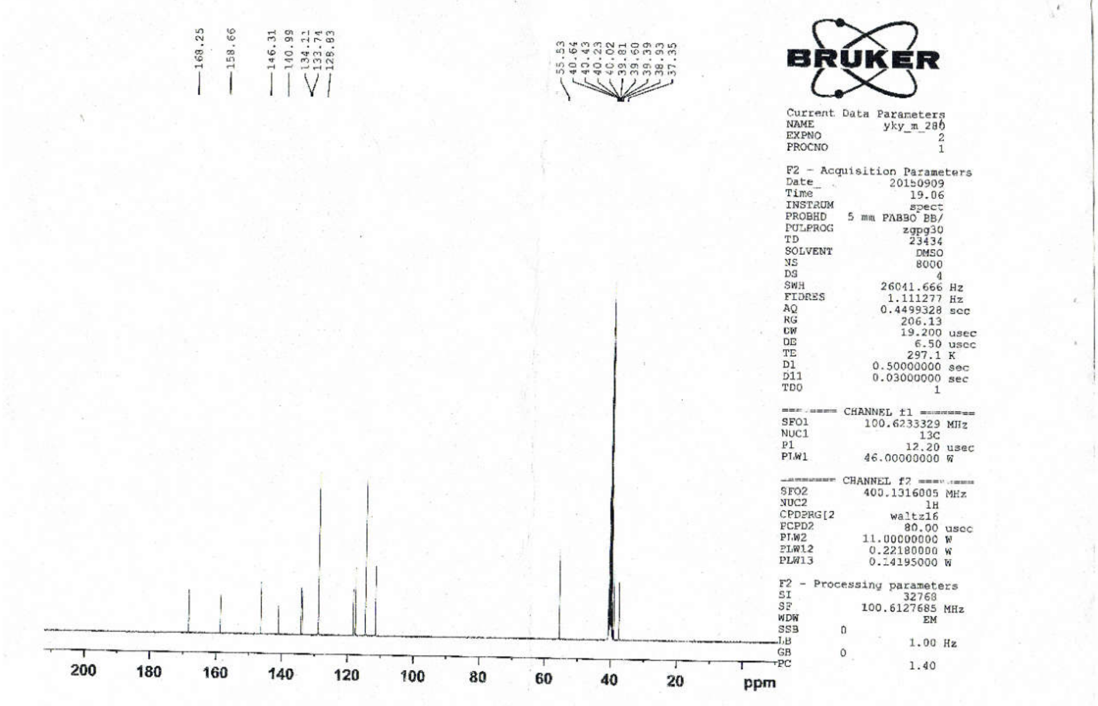

4d
13C NMR (151 MHz, DMSO)
DMSO
f1 (ppm)

4e



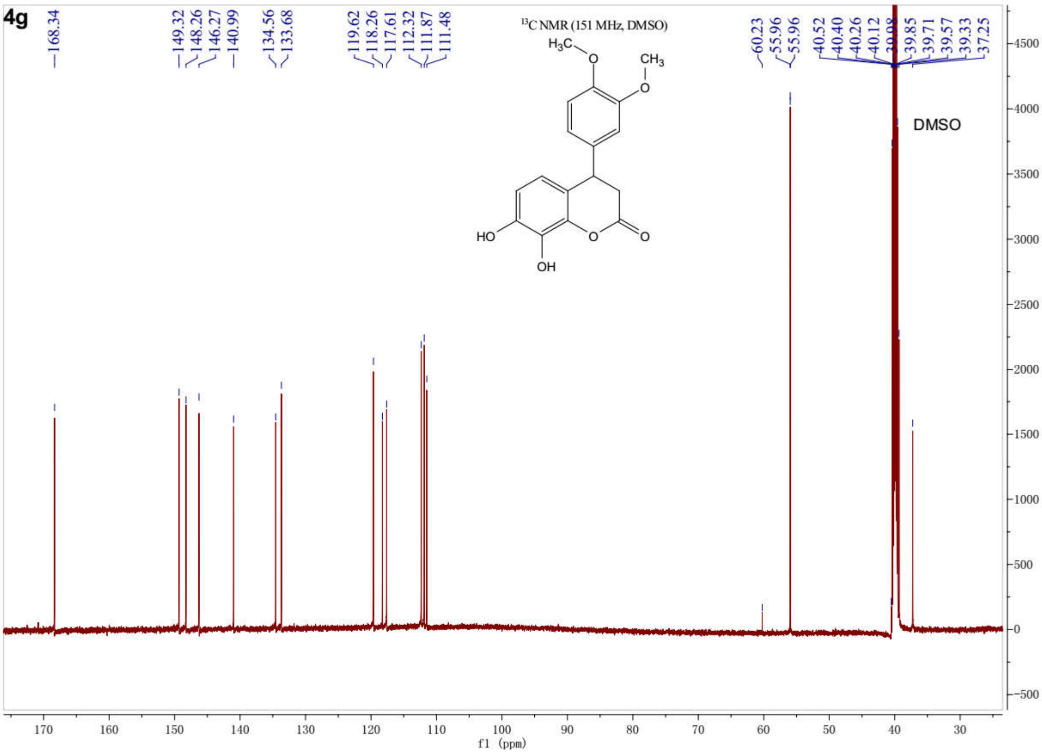
168.55
154.35
149.41
148.42
144.42
133.72
128.06
119.88
117.70
115.22
114.67
112.43
111.99
^{13}C NMR (151 MHz, DMSO)
55.98
40.40
40.27
40.13
39.99
39.85
39.71
39.56
36.70
DMSO
f1 (ppm)

4f

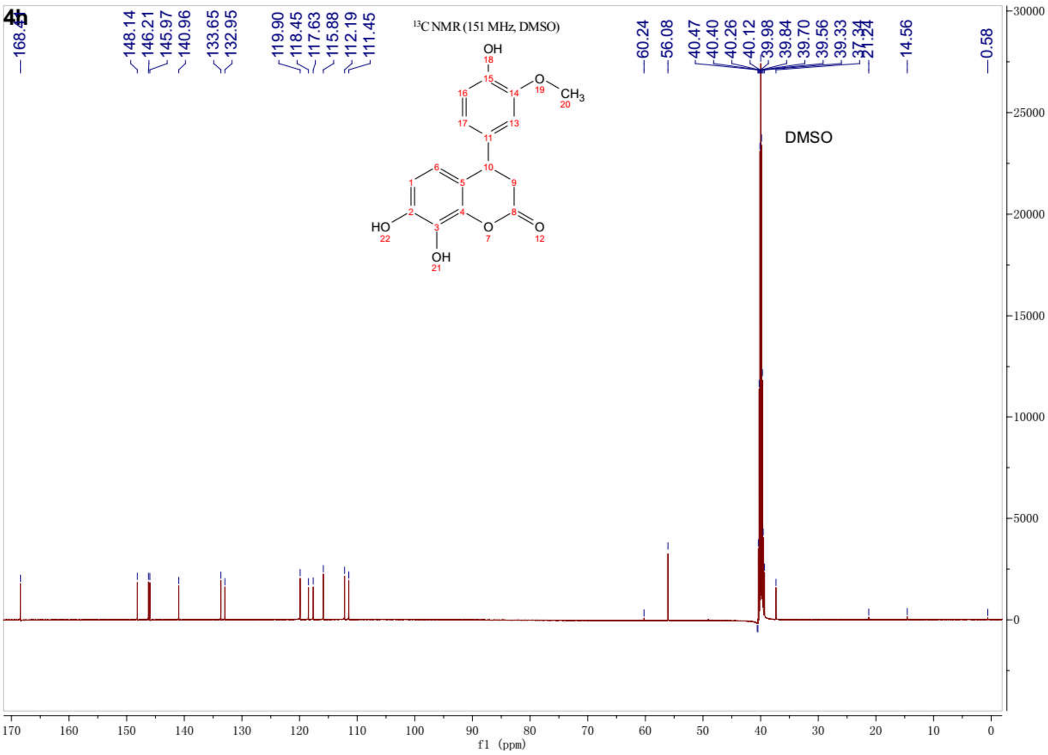


168.25
158.66
146.31
140.99
134.11
133.74
128.83
55.53
40.64
40.43
40.23
40.02
39.81
39.60
39.39
38.93
37.35
BRUKER
Current Data Parameters
NAME yky_m_280
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150909
Time 19.06
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 23434
SOLVENT DMSO
NS 8000
DS 4
SWH 26041.666 Hz
FIDRES 1.111277 Hz
AQ 0.4499328 sec
RG 206.13
DW 19.200 usec
DE 6.50 usec
TE 297.1 K
D1 0.50000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
SFO1 100.6233329 MHz
NUC1 13C
P1 12.20 usec
PLW1 46.00000000 W
CHANNEL f2
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 11.00000000 W
PLW12 0.22180000 W
PLW13 0.24195000 W
F2 - Processing parameters
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
ppm

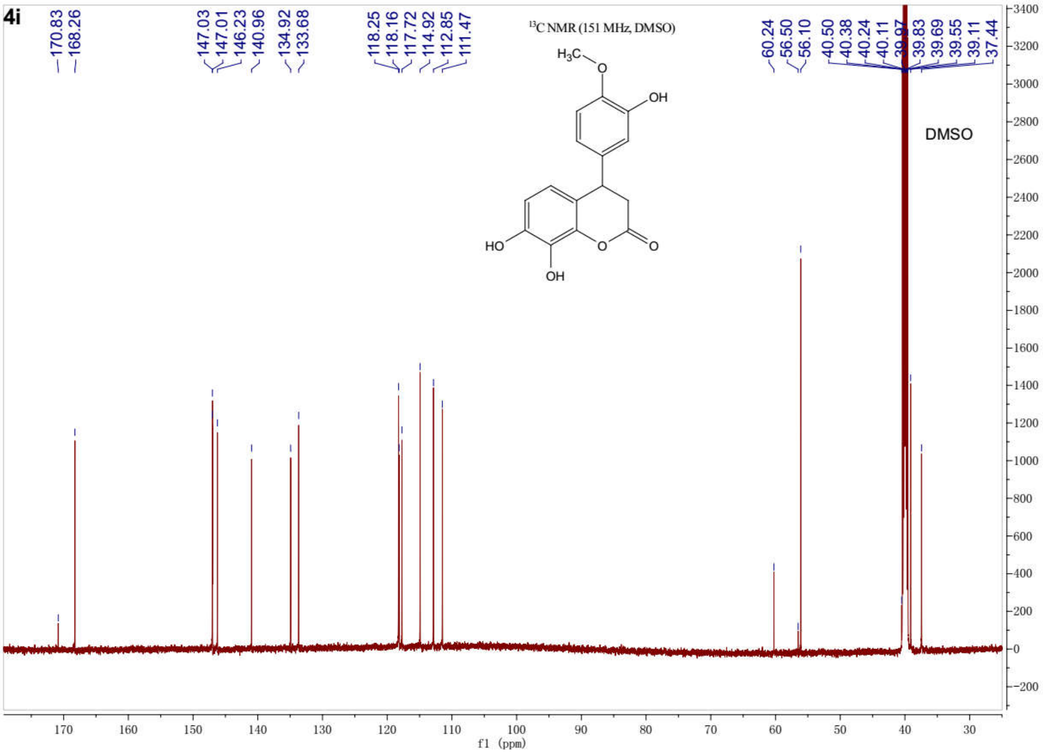
4g


13C NMR (151 MHz, DMSO)
DMSO
f1 (ppm)

4h

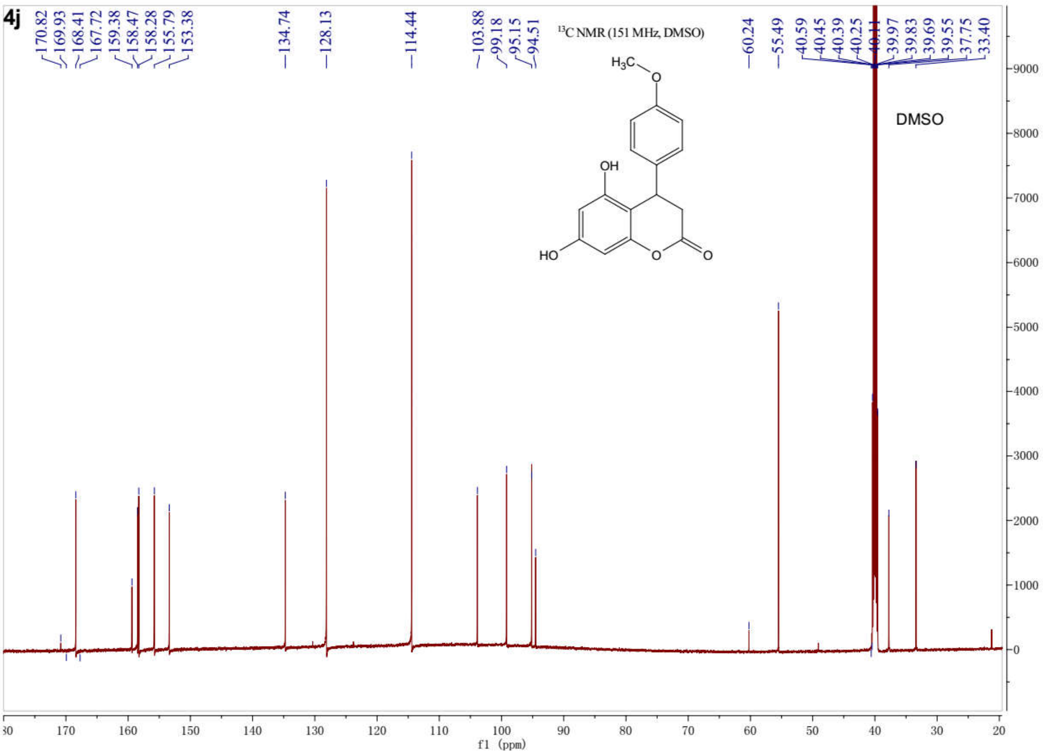

13C NMR (151 MHz, DMSO)
DMSO
f1 (ppm)

4i



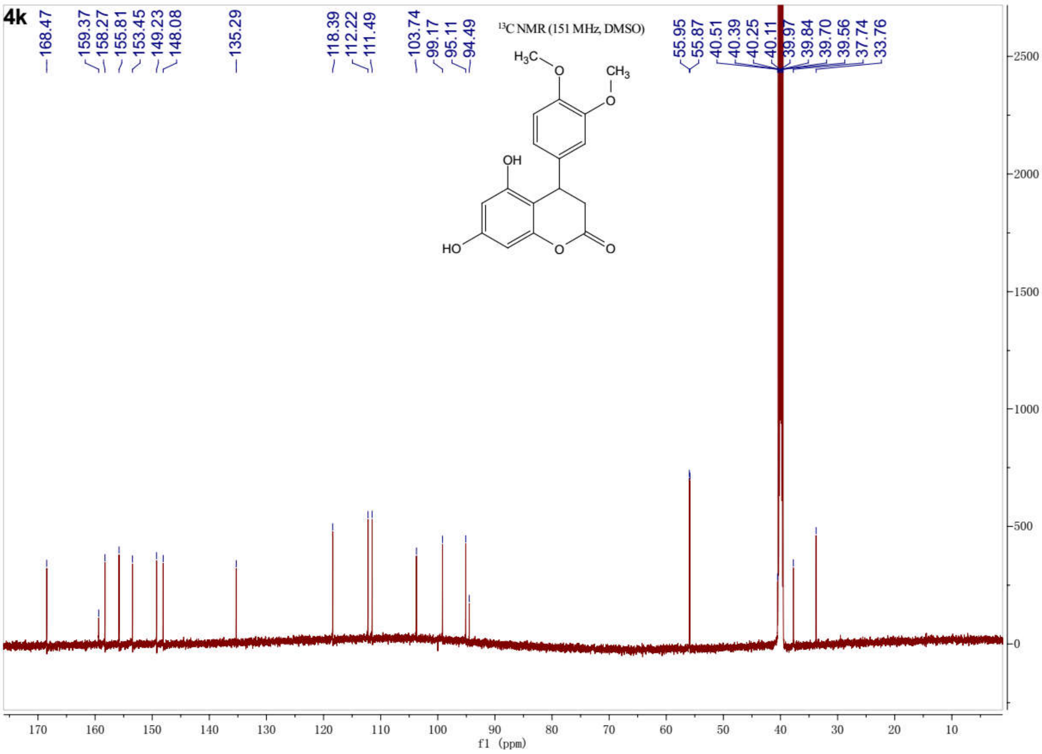
170.83
168.26
147.03
147.01
146.23
140.96
134.92
133.68
118.25
118.16
117.72
114.92
112.85
111.47
¹³C NMR (151 MHz, DMSO)
60.24
56.50
56.10
40.50
40.38
40.24
40.11
39.83
39.69
39.55
39.11
37.44
DMSO
f1 (ppm)

4j



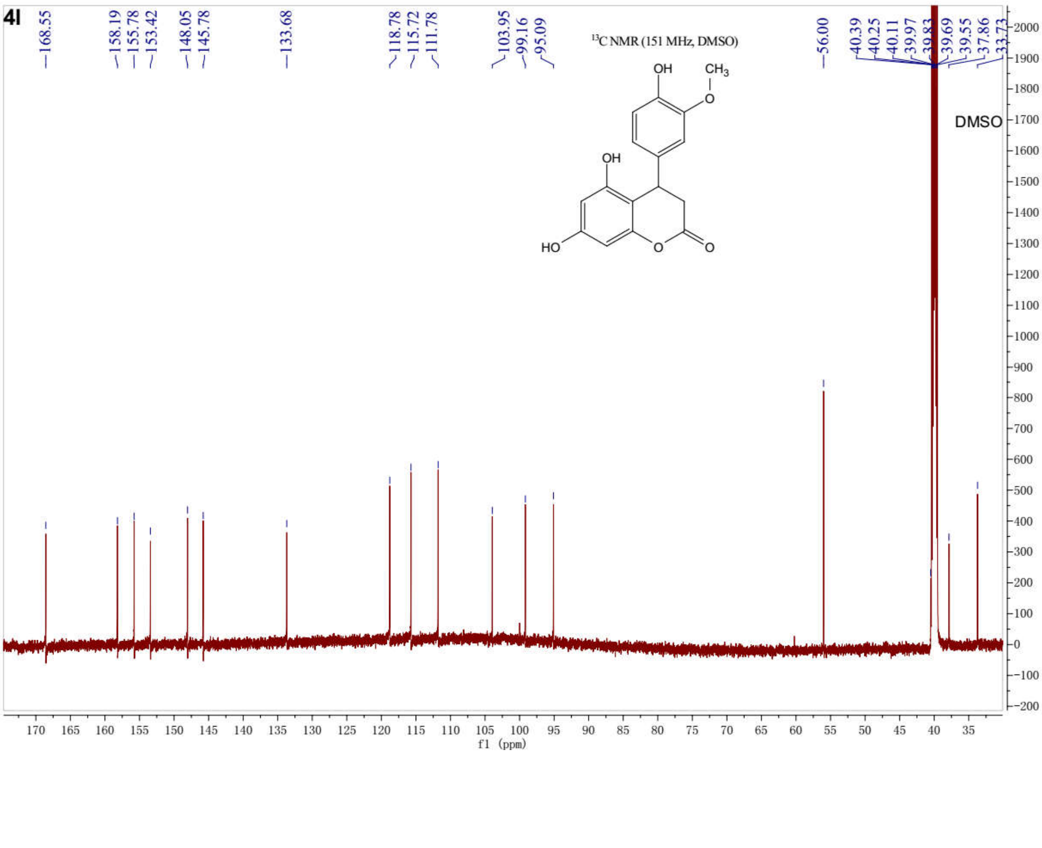
170.82
169.93
168.41
167.72
159.38
158.47
158.28
155.79
153.38
134.74
128.13
114.44
103.88
99.18
95.15
94.51
¹³C NMR (151 MHz, DMSO)
60.24
55.49
40.59
40.45
40.39
40.25
39.97
39.83
39.69
39.55
37.75
33.40
DMSO
f1 (ppm)

4k



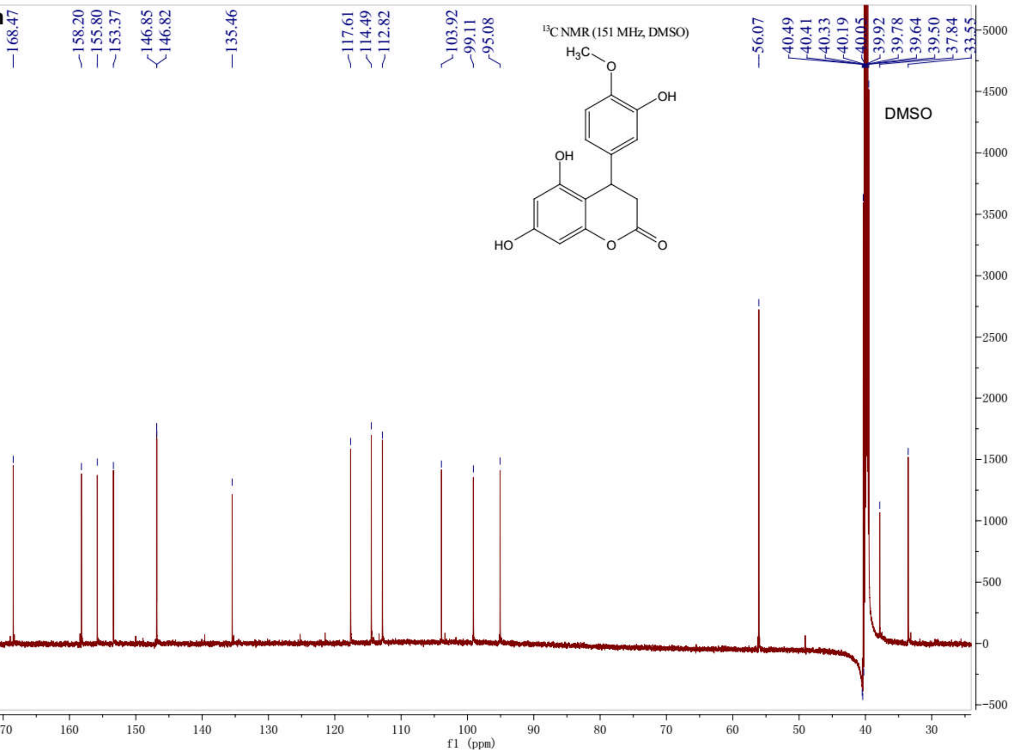
168.47
159.37
158.27
155.81
153.45
149.23
148.08
135.29
118.39
112.22
111.49
103.74
99.17
95.11
94.49
^{13}C NMR (151 MHz, DMSO)
55.95
55.87
40.51
40.39
40.25
40.11
39.97
39.84
39.70
39.56
37.74
33.76
f1 (ppm)

4l



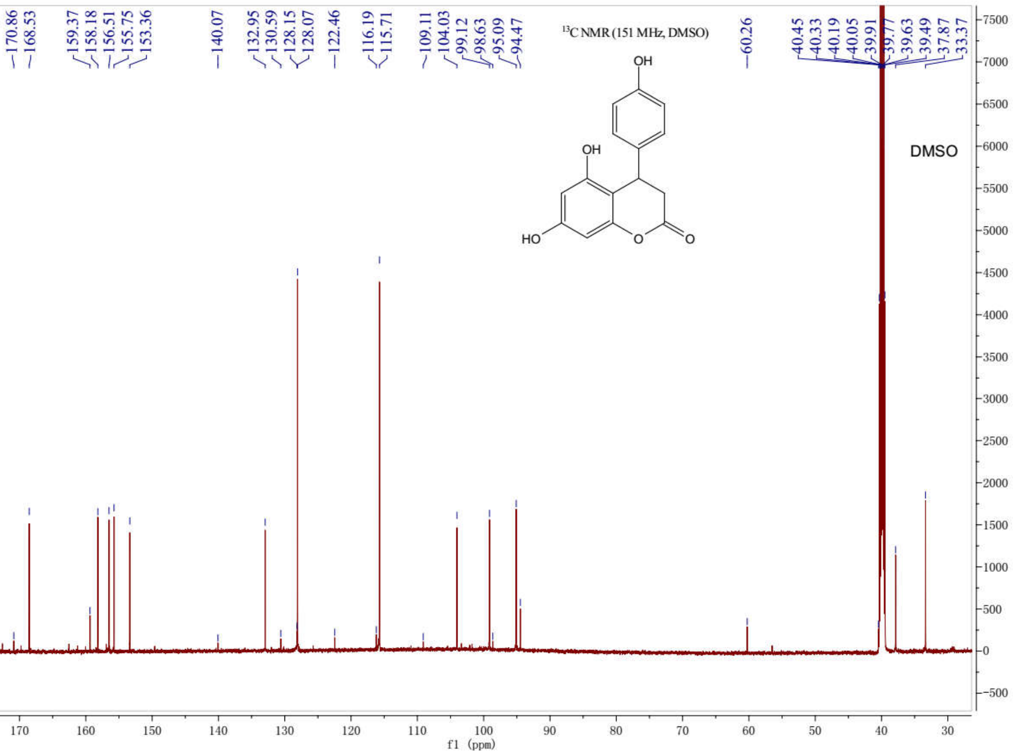
168.55
158.19
155.78
153.42
148.05
145.78
133.68
118.78
115.72
111.78
103.95
99.16
95.09
^{13}C NMR (151 MHz, DMSO)
56.00
40.39
40.25
40.11
39.97
39.83
39.69
39.55
37.86
33.73
DMSO
f1 (ppm)

4m



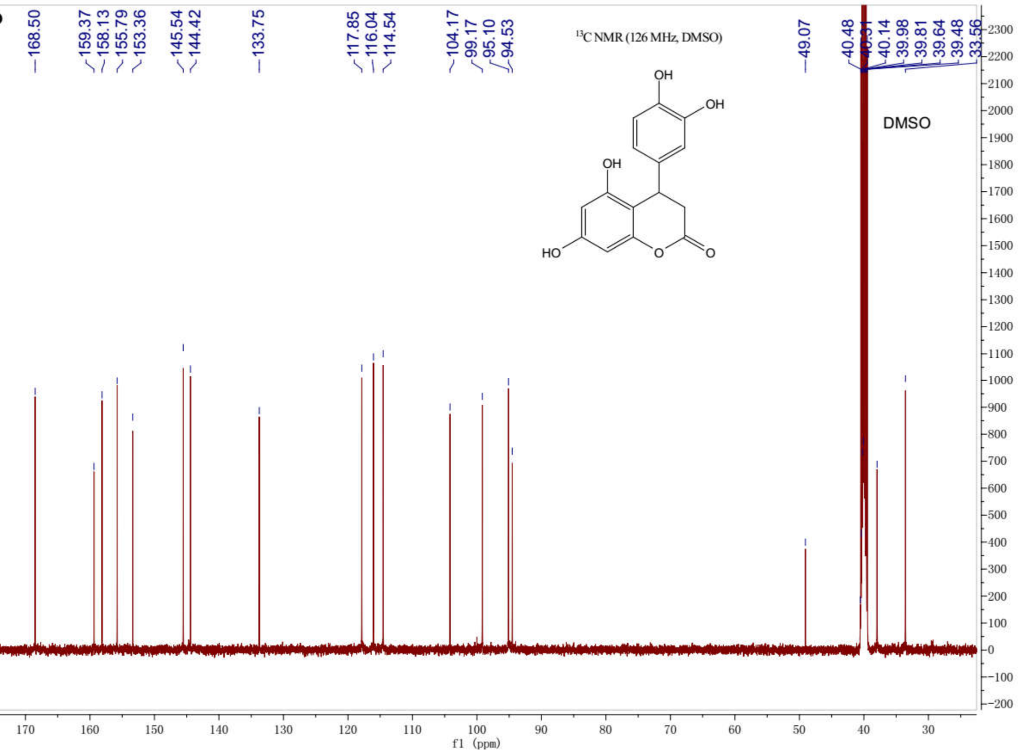
168.47
158.20
155.80
153.37
146.85
146.82
135.46
117.61
114.49
112.82
103.92
99.11
95.08
13C NMR (151 MHz, DMSO)
H3C
O
OH
OH
HO
O
O
56.07
40.49
40.41
40.33
40.19
40.05
39.92
39.78
39.64
39.50
37.84
33.55
DMSO
f1 (ppm)

4n



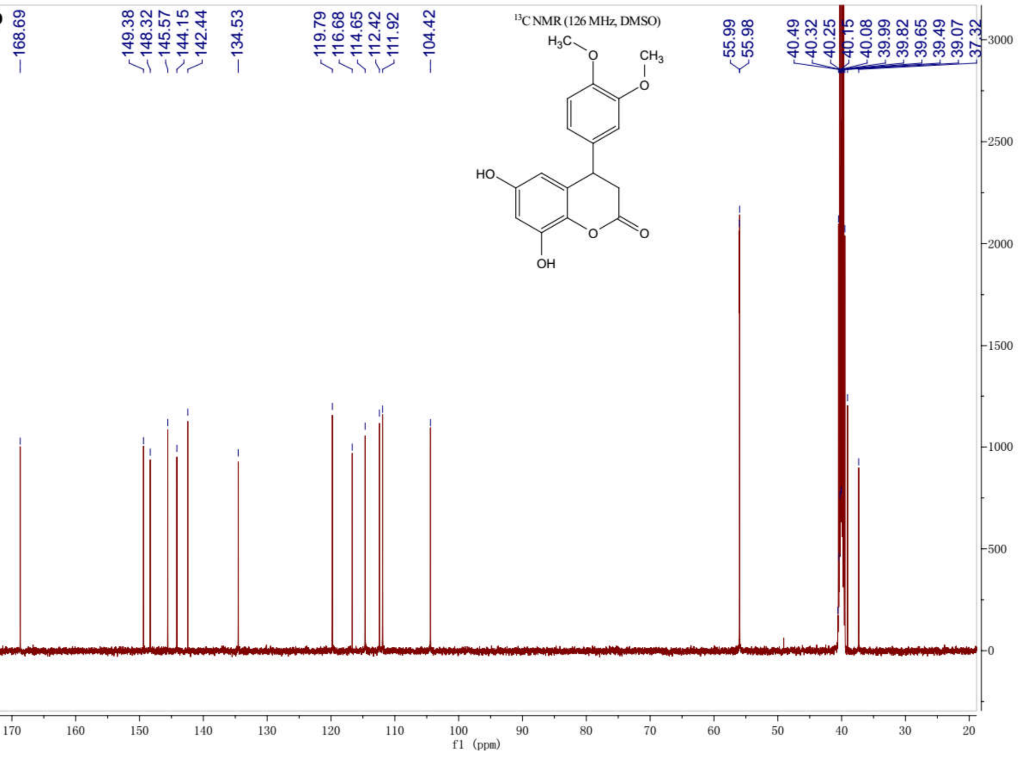
170.86
168.53
159.37
158.18
156.51
155.75
153.36
140.07
132.95
130.59
128.15
128.07
122.46
116.19
115.71
109.11
104.03
99.12
98.63
95.09
94.47
13C NMR (151 MHz, DMSO)
OH
OH
HO
O
O
60.26
40.45
40.33
40.19
40.05
39.91
39.77
39.63
39.49
37.87
33.37
DMSO
f1 (ppm)

4o

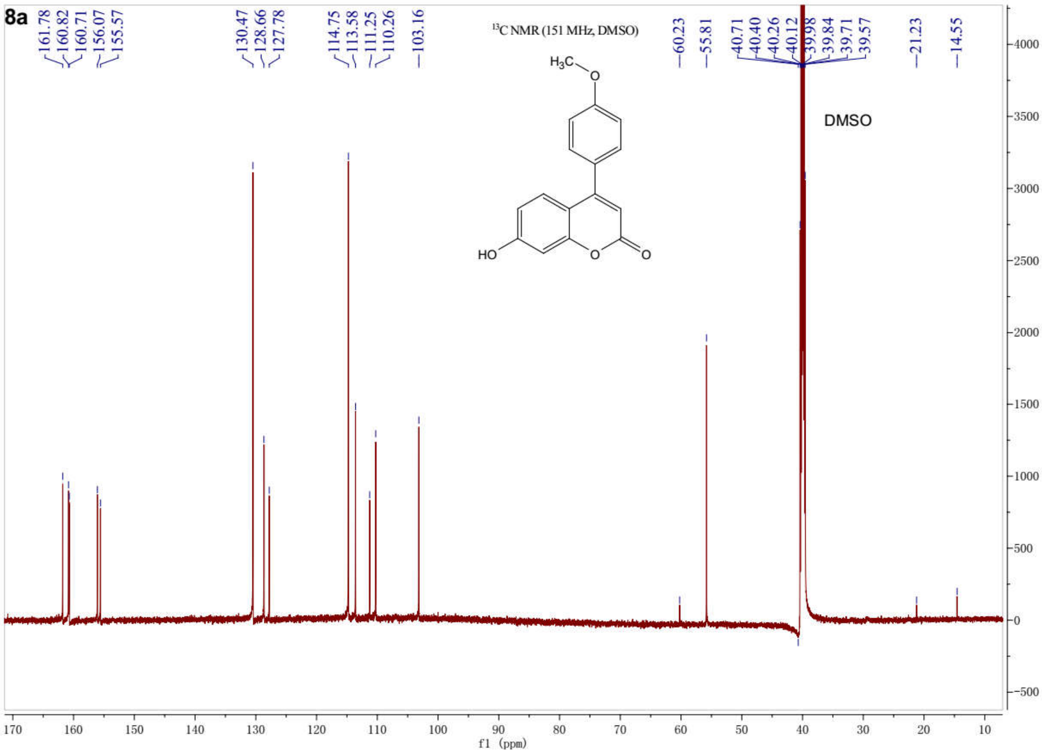


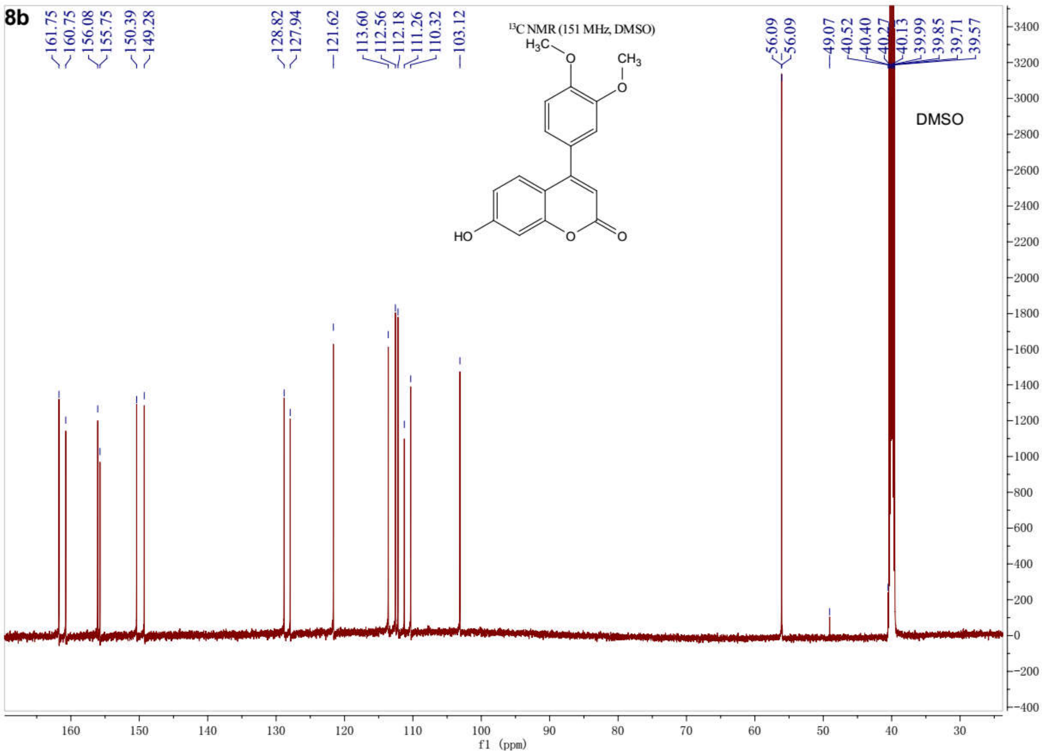
168.50
159.37
158.13
155.79
153.36
145.54
144.42
133.75
117.85
116.04
114.54
104.17
99.17
95.10
94.53
^{13}C NMR (126 MHz, DMSO)
49.07
40.48
40.31
40.14
39.98
39.81
39.64
39.48
33.56
DMSO
OH
OH
OH
HO
O
O
f1 (ppm)

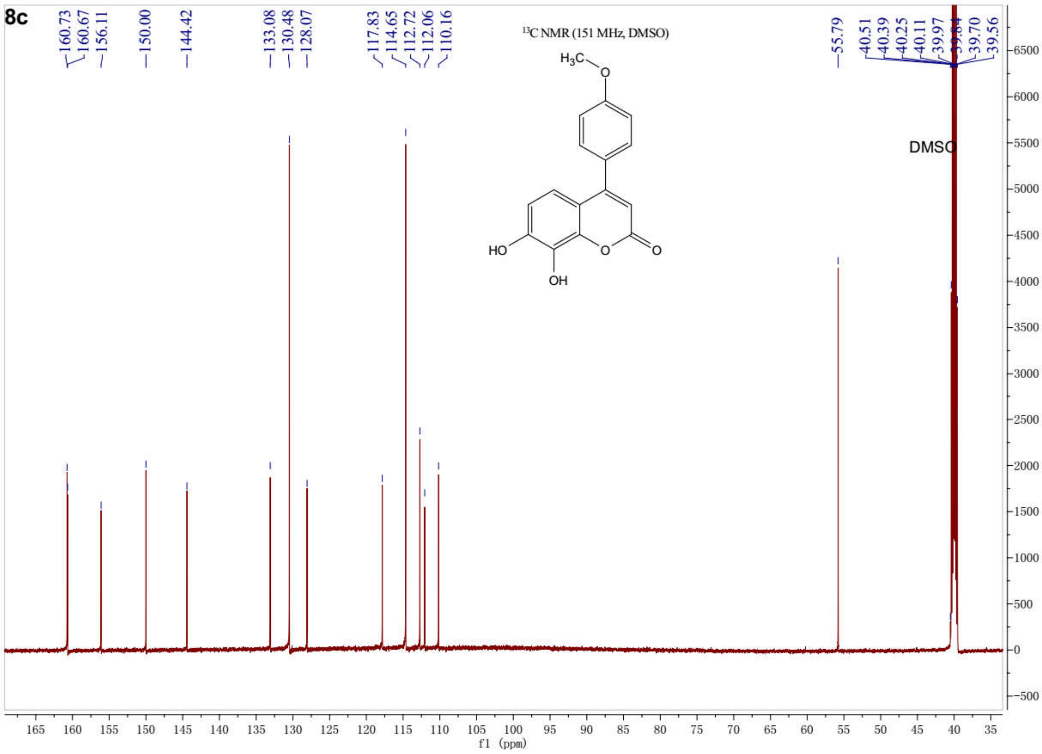
4p



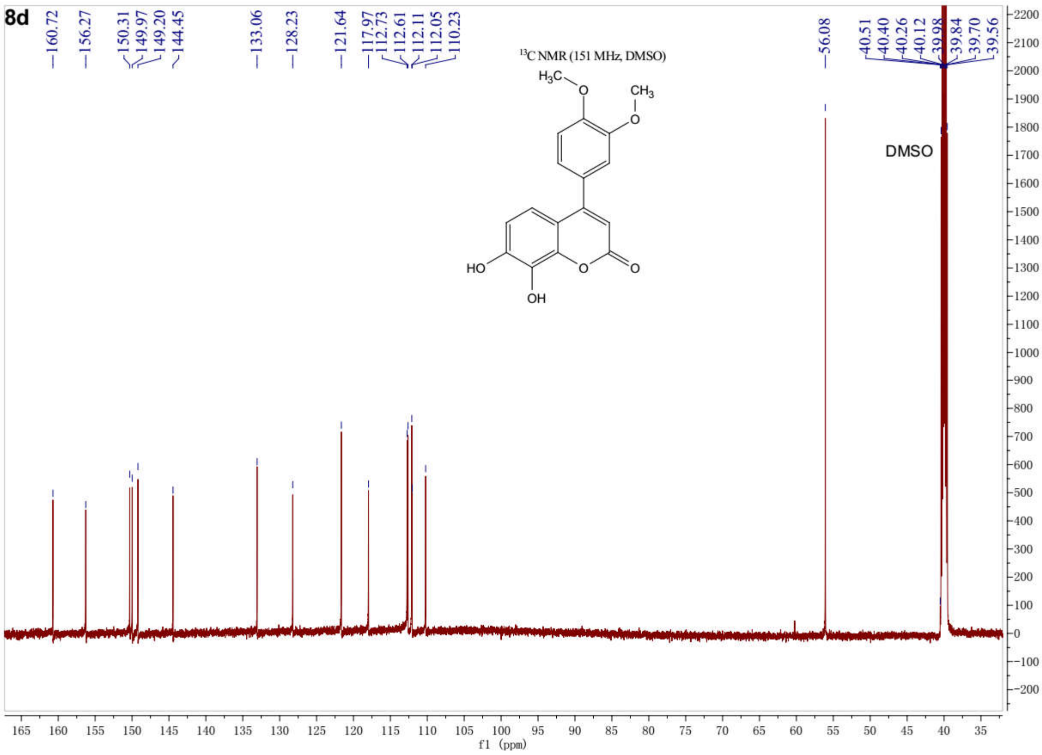
168.69
149.38
148.32
145.57
144.15
142.44
134.53
119.79
116.68
114.65
112.42
111.92
104.42
^{13}C NMR (126 MHz, DMSO)
55.99
55.98
40.49
40.32
40.25
40.15
40.08
39.99
39.82
39.65
39.49
39.07
37.32
H_3C
CH_3
O
O
HO
OH
O
O
f1 (ppm)


8a
161.78
160.82
160.71
156.07
155.57
130.47
128.66
127.78
114.75
113.58
111.25
110.26
103.16
13C NMR (151 MHz, DMSO)
60.23
55.81
40.71
40.40
40.26
40.12
39.98
39.84
39.71
39.57
21.23
14.55
DMSO
f1 (ppm)

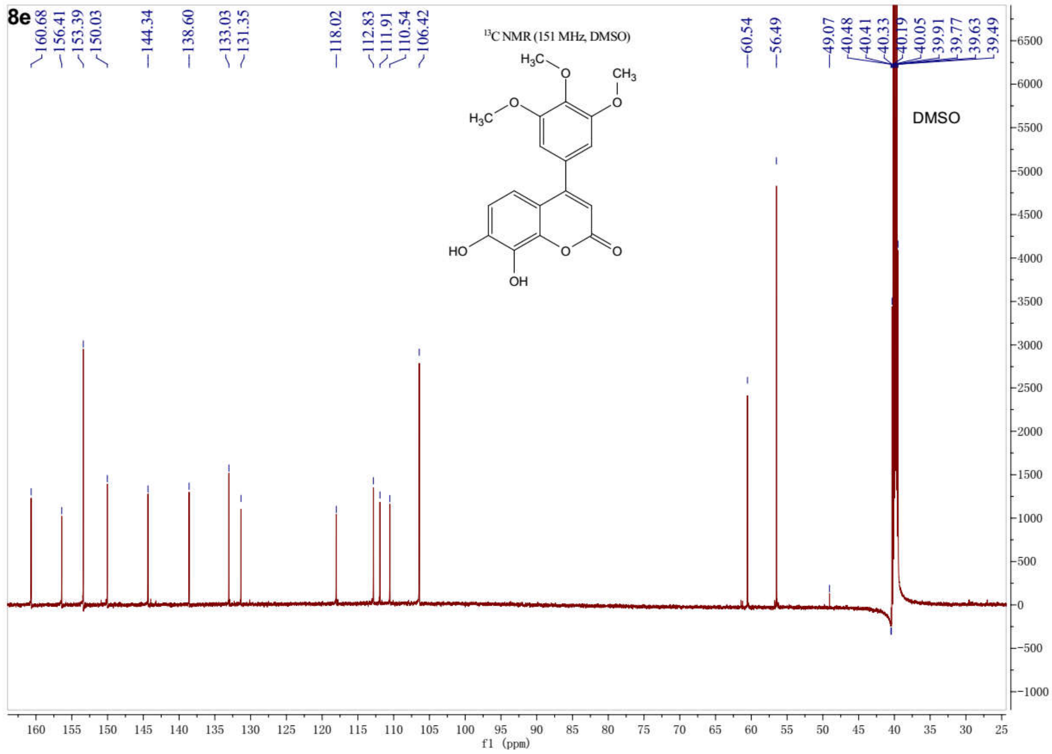

8b
161.75
160.75
156.08
155.75
150.39
149.28
128.82
127.94
121.62
113.60
112.56
112.18
111.26
110.32
103.12
13C NMR (151 MHz, DMSO)
56.09
56.09
49.07
40.52
40.40
40.27
40.13
39.99
39.85
39.71
39.57
DMSO
f1 (ppm)

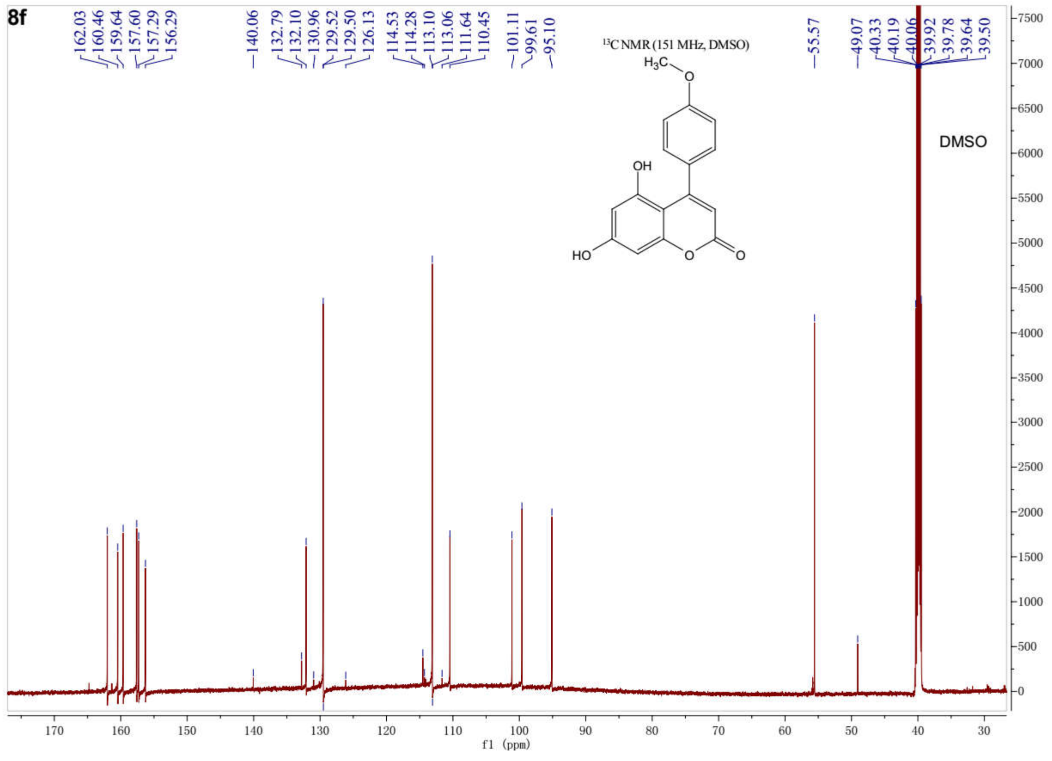


8c
160.73
160.67
156.11
150.00
144.42
133.08
130.48
128.07
117.83
114.65
112.72
112.06
110.16
13C NMR (151 MHz, DMSO)
55.79
40.51
40.39
40.25
40.11
39.97
39.84
39.70
39.56
DMSO
f1 (ppm)

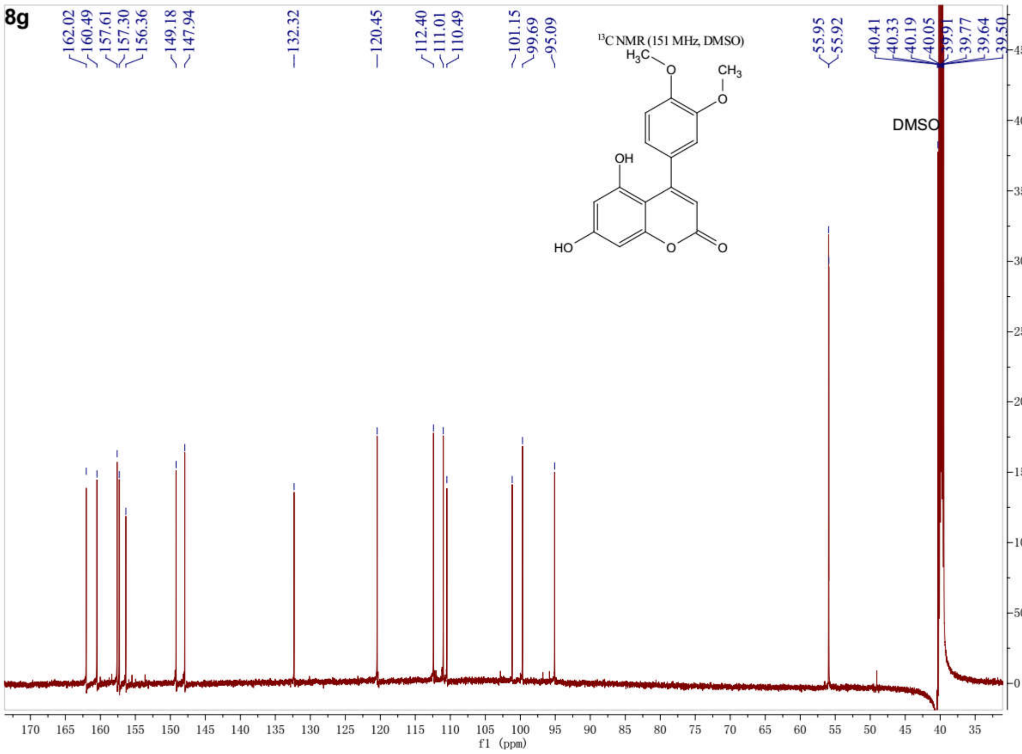


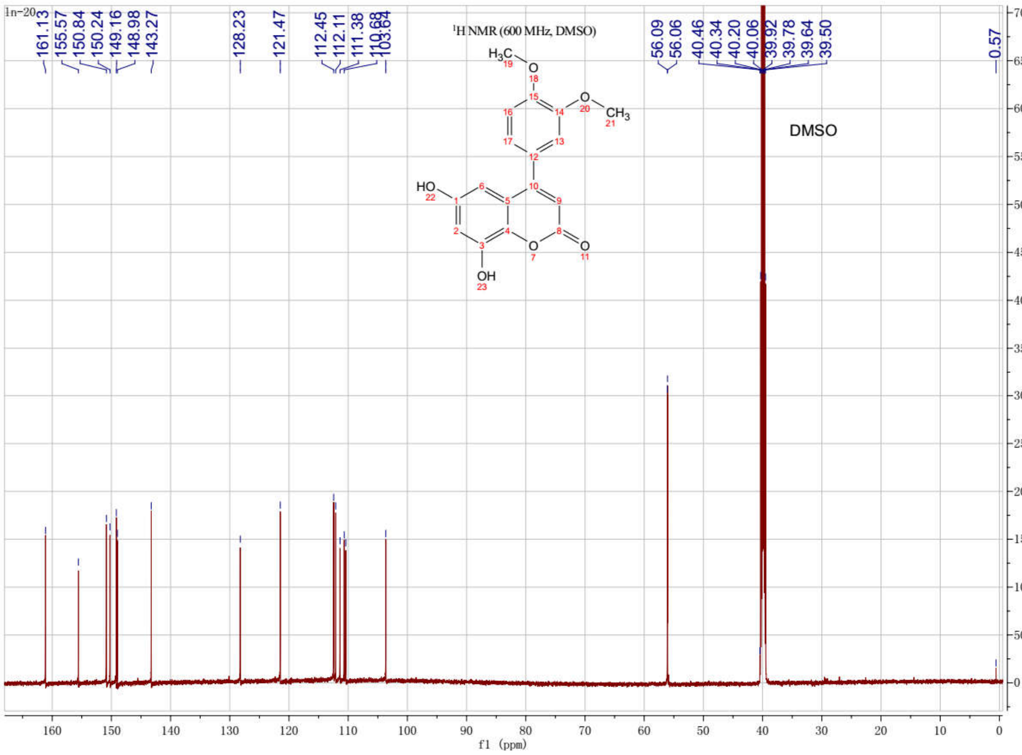
8d
160.72
156.27
150.31
149.97
149.20
144.45
133.06
128.23
121.64
117.97
112.73
112.61
112.11
112.05
110.23
13C NMR (151 MHz, DMSO)
56.08
40.51
40.40
40.26
40.12
39.98
39.84
39.70
39.56
DMSO
f1 (ppm)


8e
160.68
156.41
153.39
150.03
144.34
138.60
133.03
131.35
118.02
112.83
111.91
110.54
106.42
13C NMR (151 MHz, DMSO)
60.54
56.49
49.07
40.48
40.41
40.33
40.19
40.05
39.91
39.77
39.63
39.49
DMSO
HO
OH
O
O
f1 (ppm)

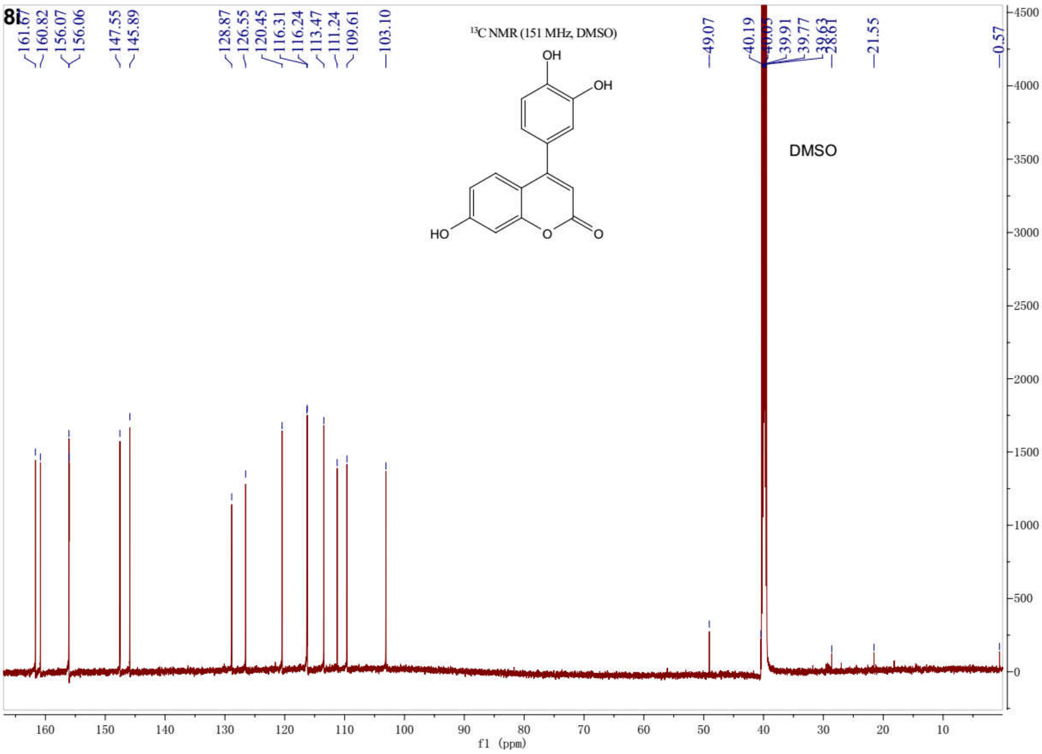

8f
162.03
160.46
159.64
157.60
157.29
156.29
140.06
132.79
132.10
130.96
129.52
129.50
126.13
114.53
114.28
113.10
113.06
111.64
110.45
101.11
99.61
95.10
13C NMR (151 MHz, DMSO)
55.57
49.07
40.33
40.19
40.06
39.92
39.78
39.64
39.50
DMSO
OH
HO
O
O
f1 (ppm)

8g

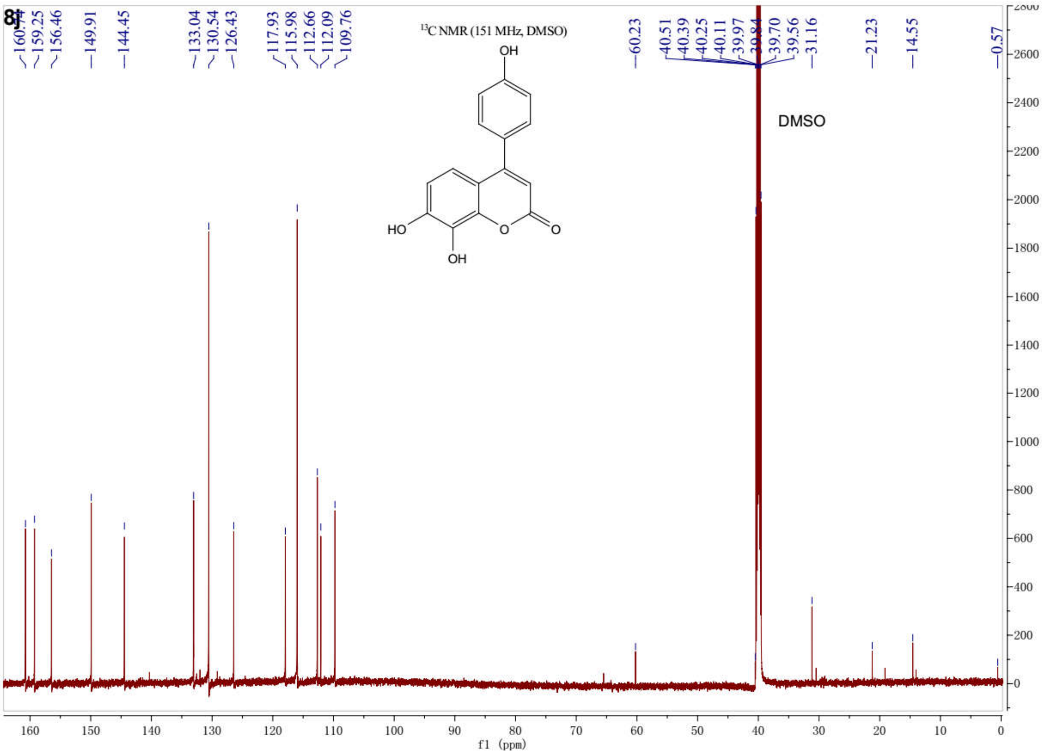

162.02
160.49
157.61
157.30
156.36
149.18
147.94
132.32
120.45
112.40
111.01
110.49
101.15
99.69
95.09
^{13}C NMR (151 MHz, DMSO)
55.95
55.92
40.41
40.33
40.19
40.05
39.91
39.77
39.64
39.50
DMSO
f1 (ppm)

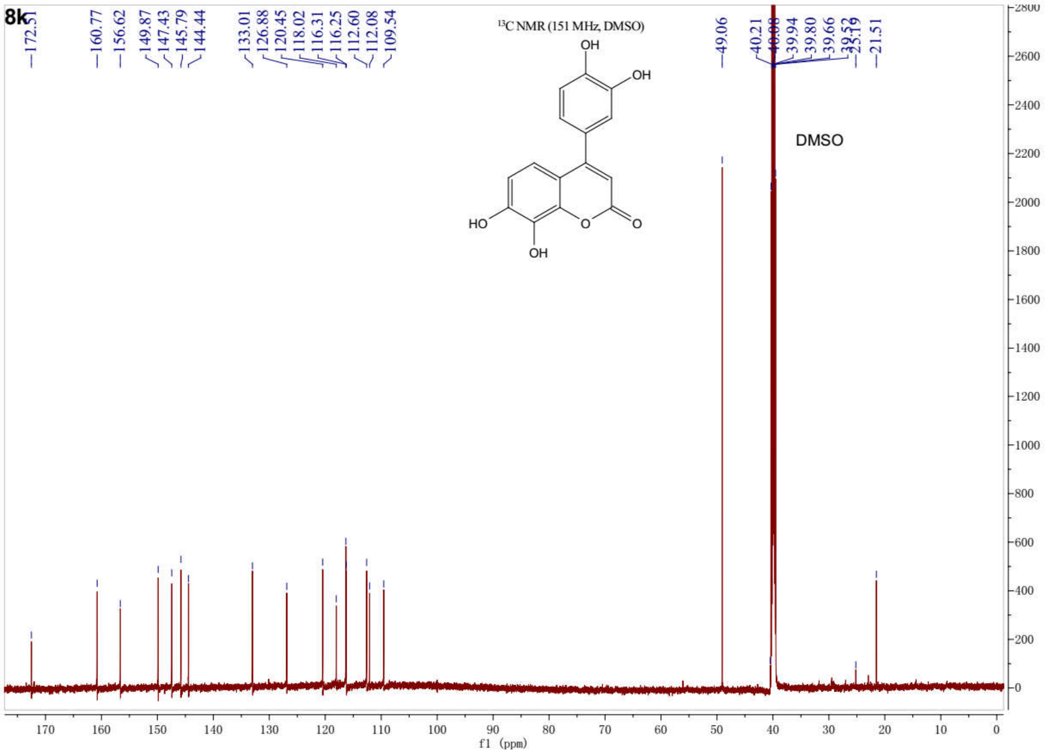

161.13
155.57
150.84
150.24
149.16
148.98
143.27
128.23
121.47
112.45
112.11
111.38
103.64
^{1}H NMR (600 MHz, DMSO)
56.09
56.06
40.46
40.34
40.20
40.06
39.92
39.78
39.64
39.50
0.57
DMSO
f1 (ppm)

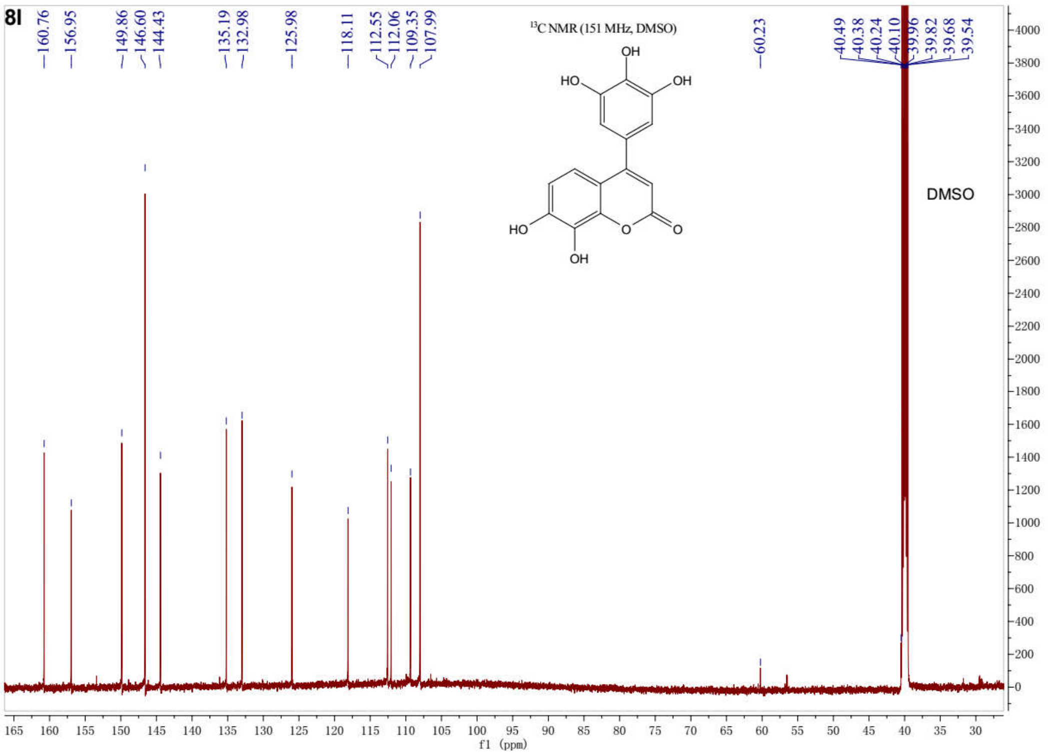
8i



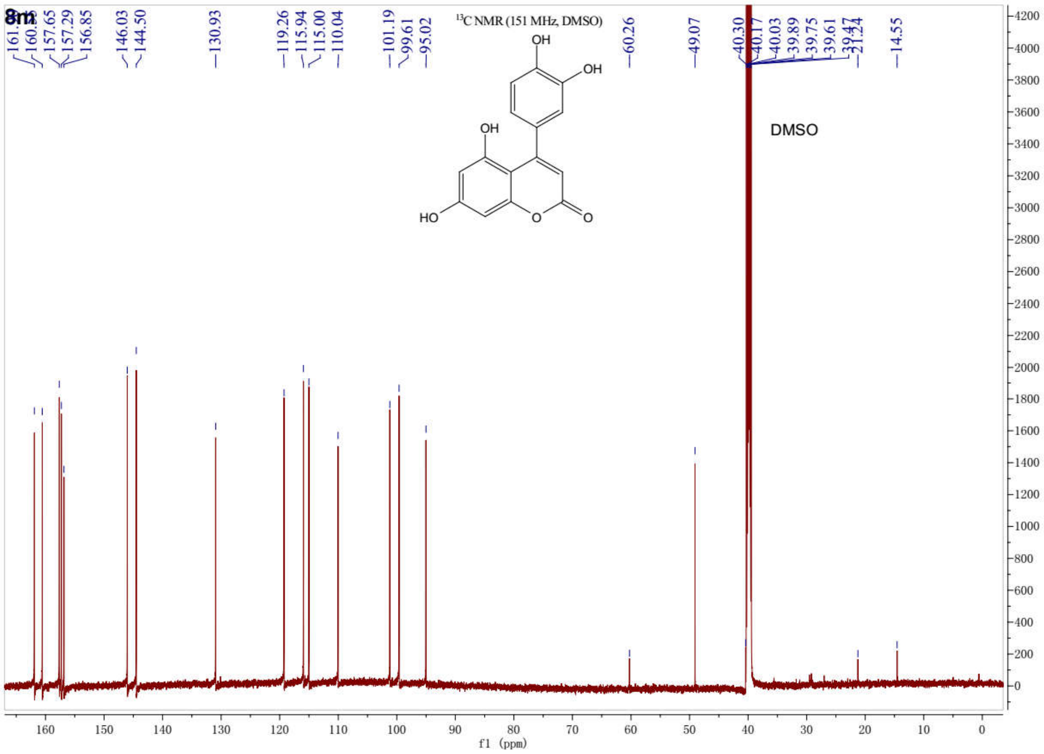
8j




8k
13C NMR (151 MHz, DMSO)
DMSO
172.51
160.77
156.62
149.87
147.43
145.79
144.44
133.01
126.88
120.45
118.02
116.31
116.25
112.60
112.08
109.54
49.06
40.21
40.08
39.94
39.80
39.66
39.52
25.19
21.51
f1 (ppm)

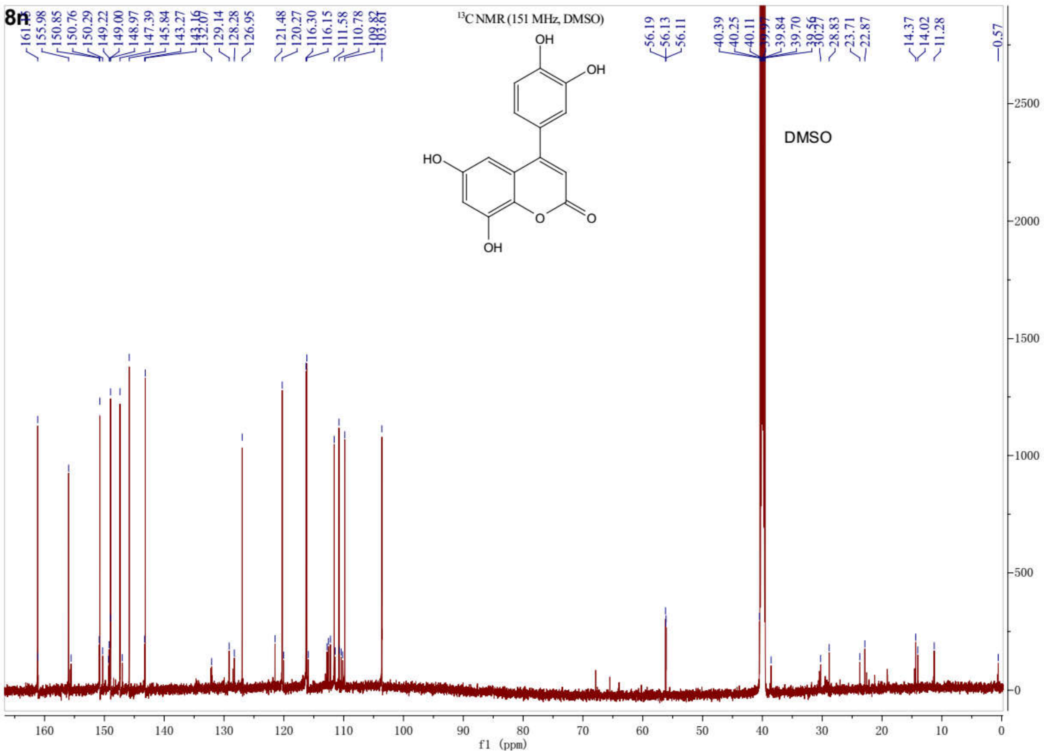

8l
13C NMR (151 MHz, DMSO)
DMSO
160.76
156.95
149.86
146.60
144.43
135.19
132.98
125.98
118.11
112.55
112.06
109.35
107.99
60.23
40.49
40.38
40.24
40.10
39.96
39.82
39.68
39.54
f1 (ppm)

8m



^{13}C NMR (151 MHz, DMSO)
DMSO
f1 (ppm)

8n



^{13}C NMR (151 MHz, DMSO)
DMSO
f1 (ppm)