Supporting Information

Synthesis, Structure-Activity Relationship Studies, and Antibacterial Evaluation of 4-Chromanones and Chalcones, as well as Olympicin A and Derivatives

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[#]M.M.M and Md.Z.A contributed equally to the work

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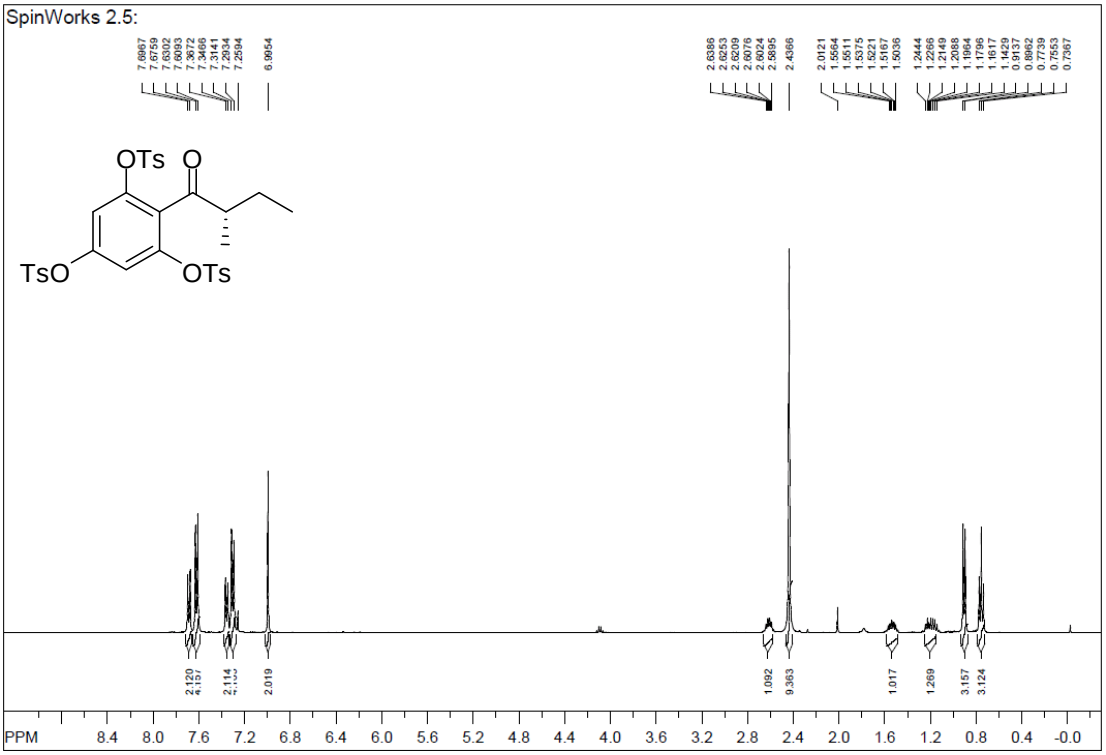
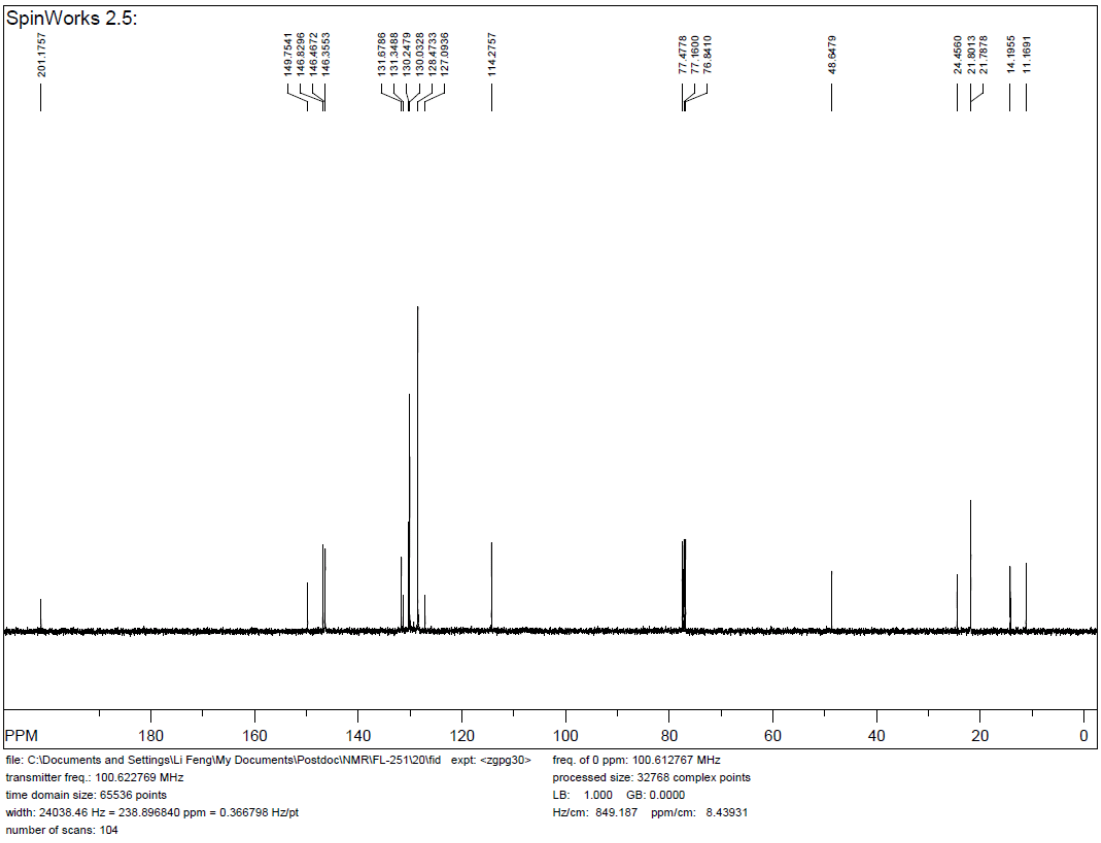
^{1}H and ^{13}C NMR spectra of **1b**





HPLC profile of **1b**

==== Shimadzu LCsolution Analysis Report ====

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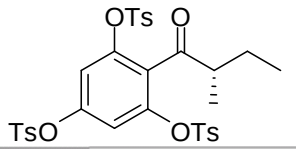

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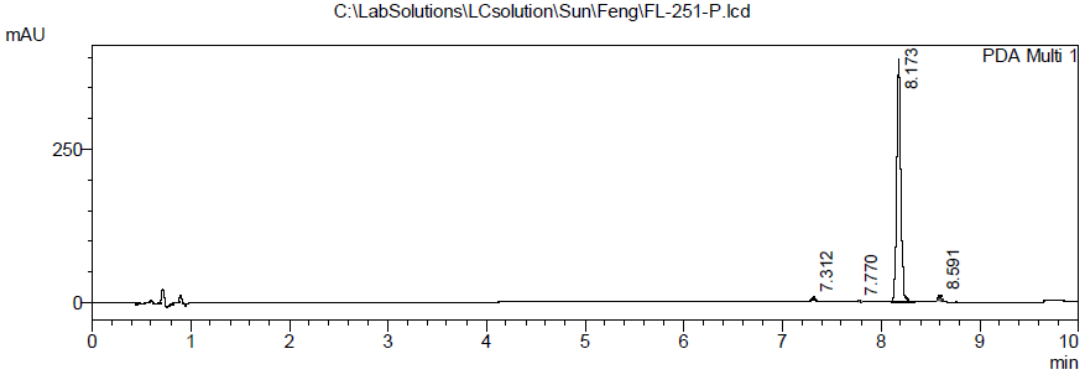

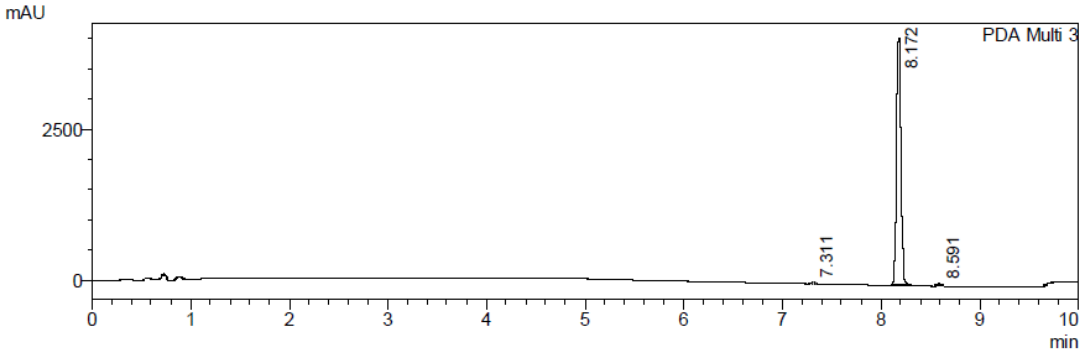

1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

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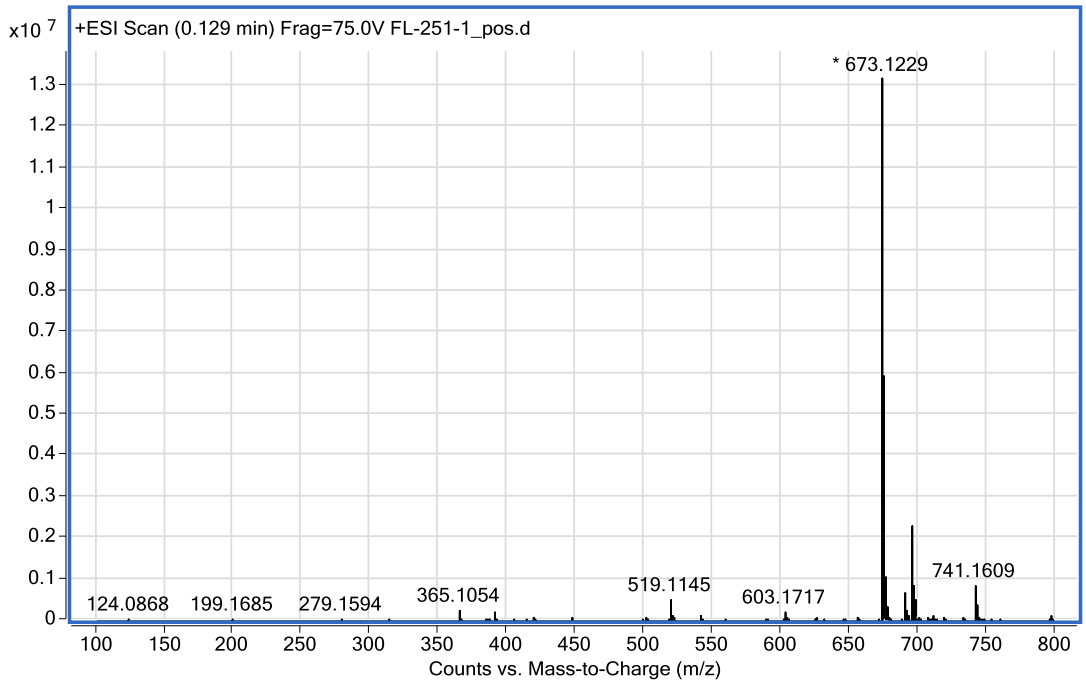
1	7.312	4791	3189	0.443	0.794
2	7.770	242	254	0.022	0.063
3	8.173	1065416	391979	98.558	97.564
4	8.591	10553	6343	0.976	1.579
Total		1081002	401764	100.000	100.000

PeakTable

PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.311	8966	6681	0.072	0.163
2	8.172	12363084	4070455	99.502	99.098
3	8.591	52881	30379	0.426	0.740
Total		12424931	4107515	100.000	100.000

HRMS of **1b**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* 673.1229
741.1609
519.1145
603.1717
365.1054
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199.1685
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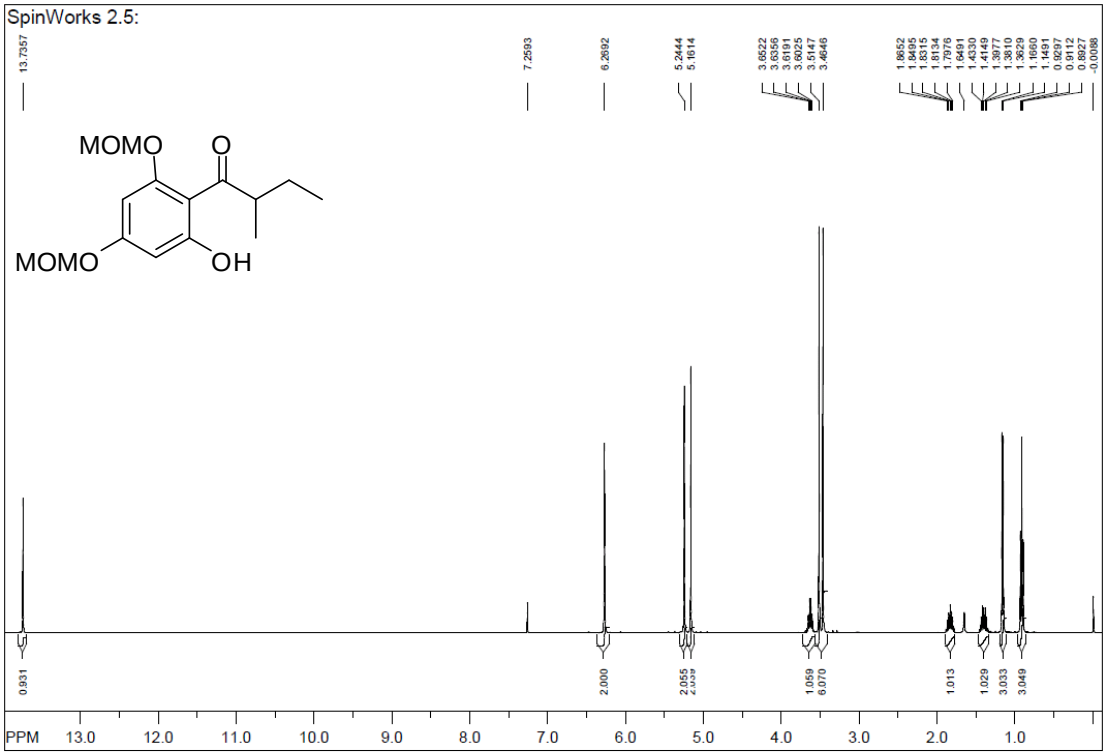
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **1c**



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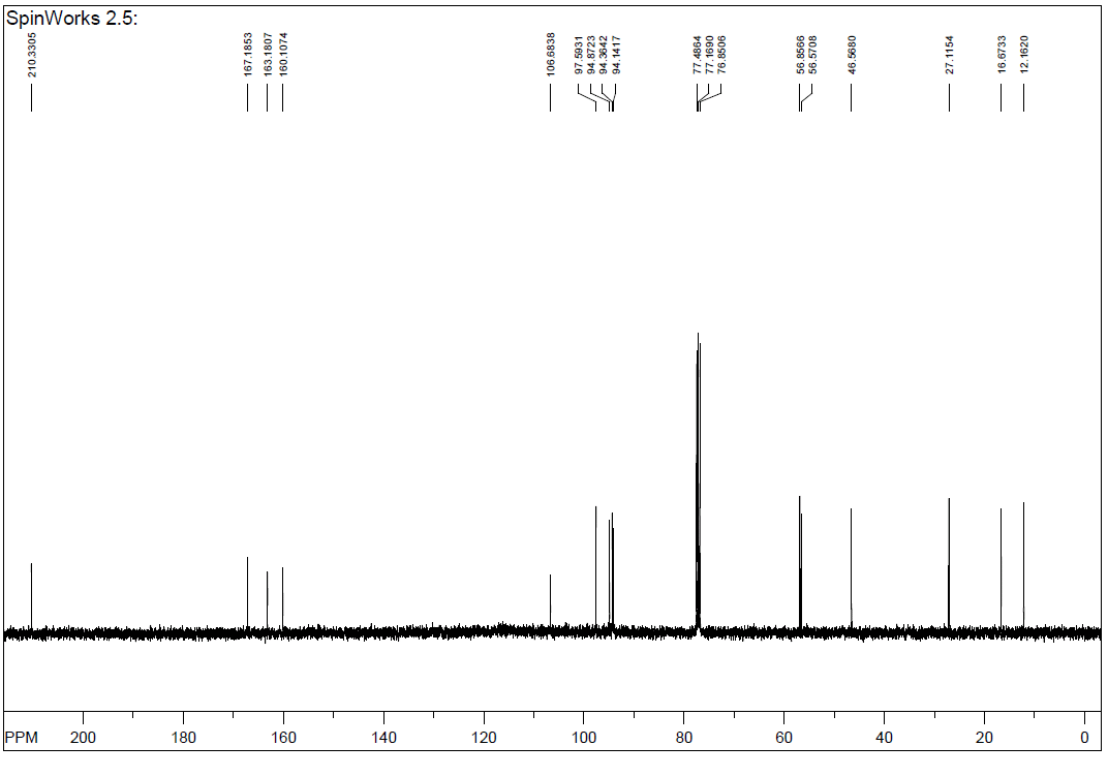

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number of scans: 292

freq. of 0 ppm: 100.612754 MHz
processed size: 32768 complex points
LB: 1.000 GB: 0.0000
Hz/cm: 882.272 ppm/cm: 8.76811

HPLC profile of **1c**

==== Shimadzu LCsolution Analysis Report ====

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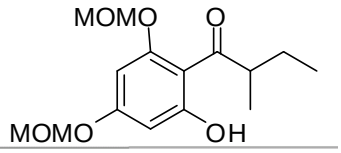

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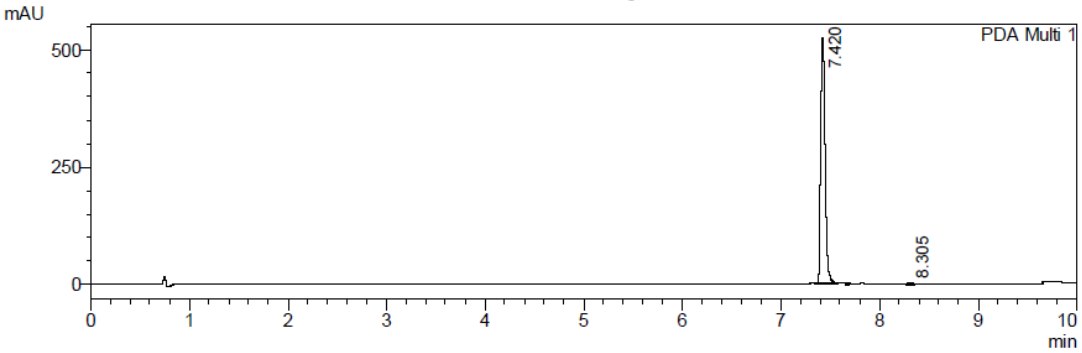
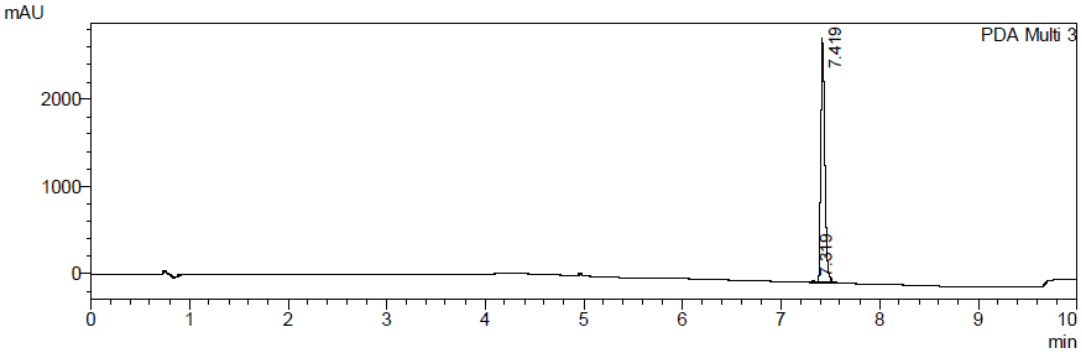




1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

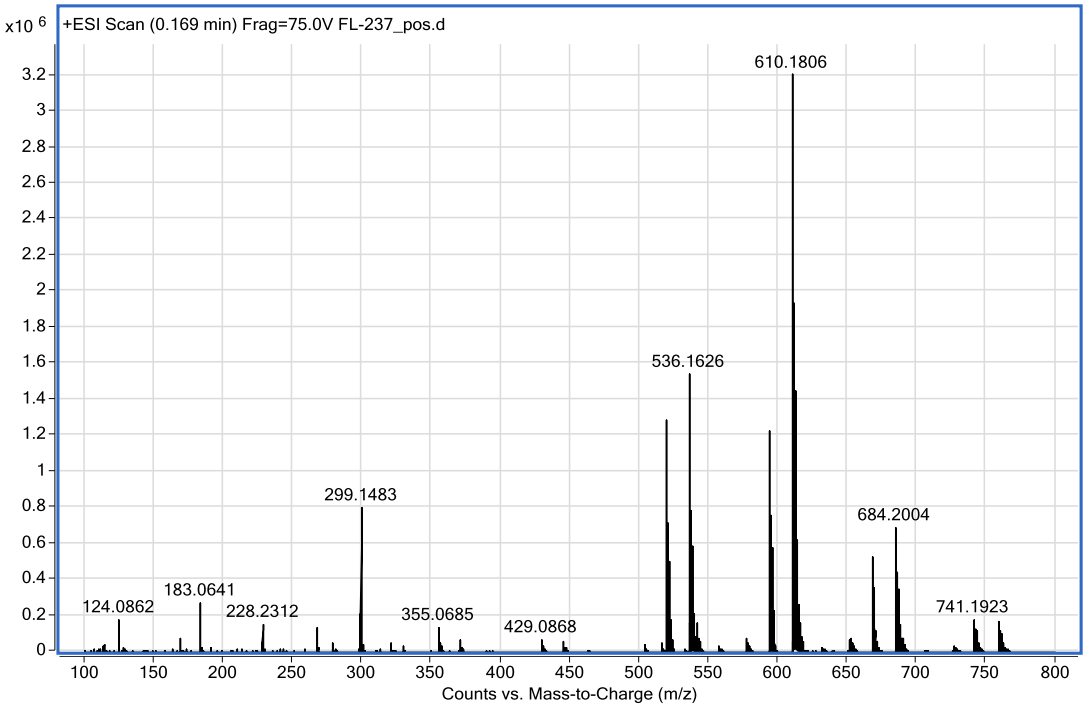
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.420	1519821	523211	99.824	99.768
2	8.305	2675	1217	0.176	0.232
Total		1522496	524428	100.000	100.000

PeakTable

PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.319	15979	7857	0.223	0.281
2	7.419	7142456	2788923	99.777	99.719
Total		7158435	2796779	100.000	100.000

HRMS of **1c**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124.0862
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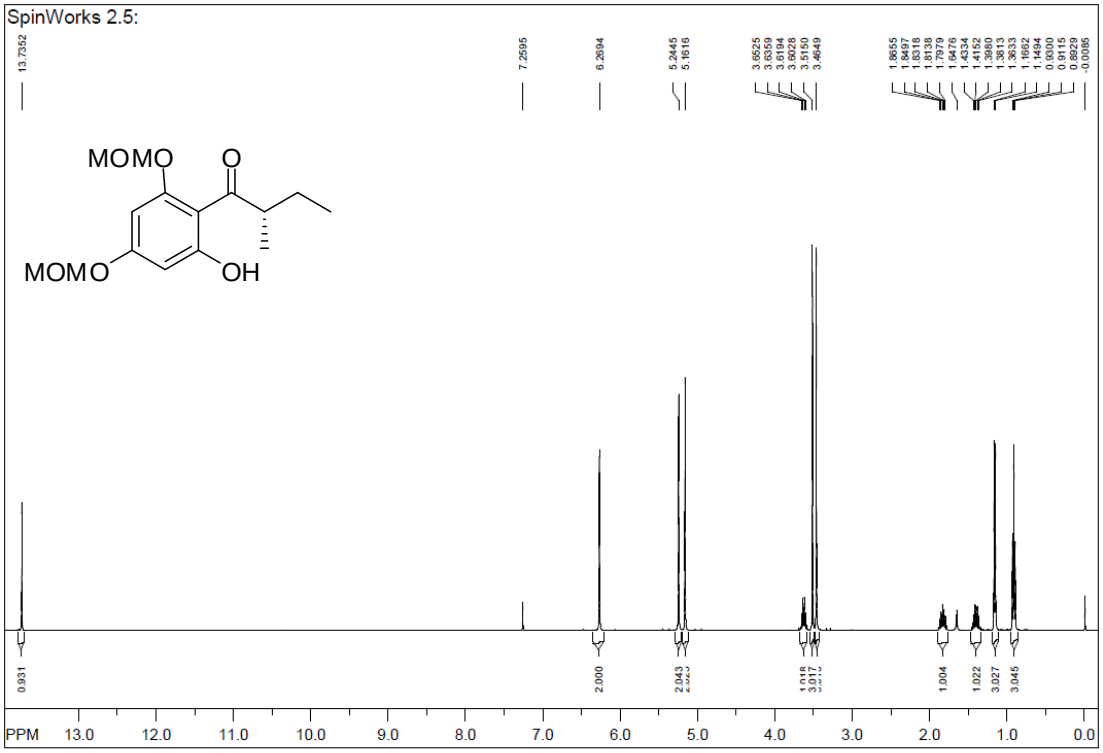
429.0868
741.1923
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **1c'**



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number of scans: 3

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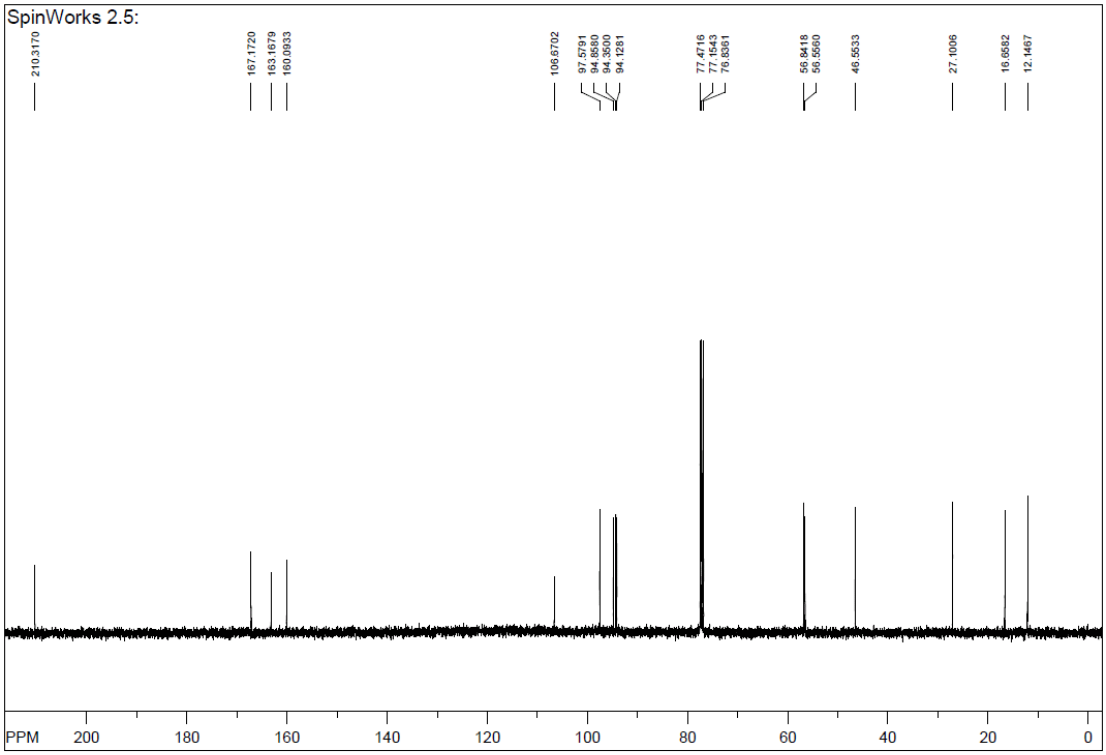

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number of scans: 425

freq. of 0 ppm: 100.612756 MHz
processed size: 32768 complex points
LB: 1.000 GB: 0.0000
Hz/cm: 882.272 ppm/cm: 8.76811

HPLC profile of **1c'**

==== Shimadzu LCsolution Analysis Report ====

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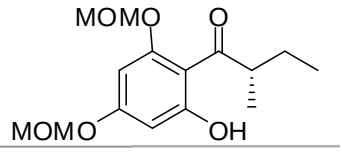

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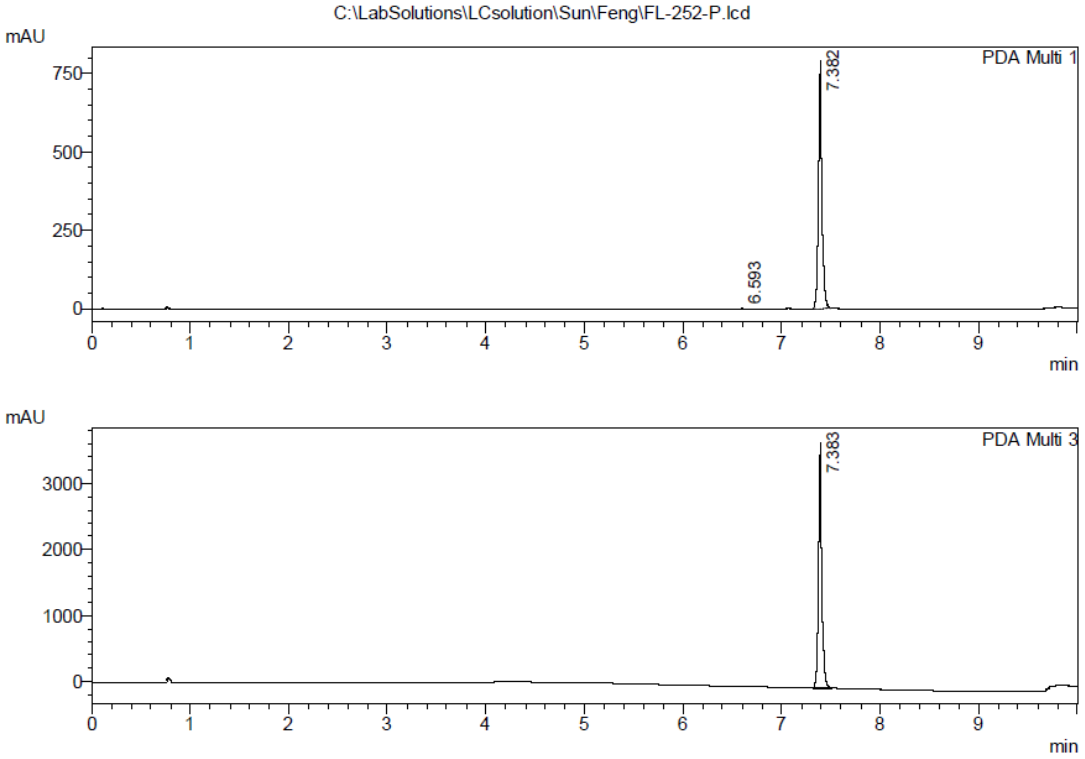

1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.593	866	435	0.038	0.056
2	7.382	2252220	781651	99.962	99.944
Total		2253086	782086	100.000	100.000

PeakTable

PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.383	10184818	3706299	100.000	100.000
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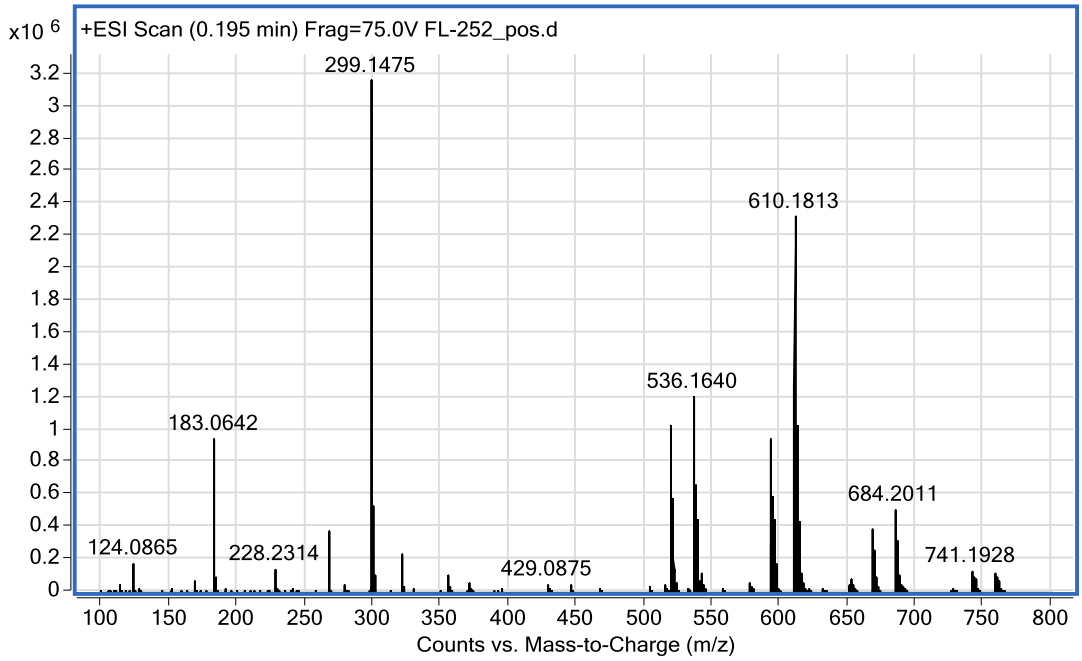
HRMS of **1c'**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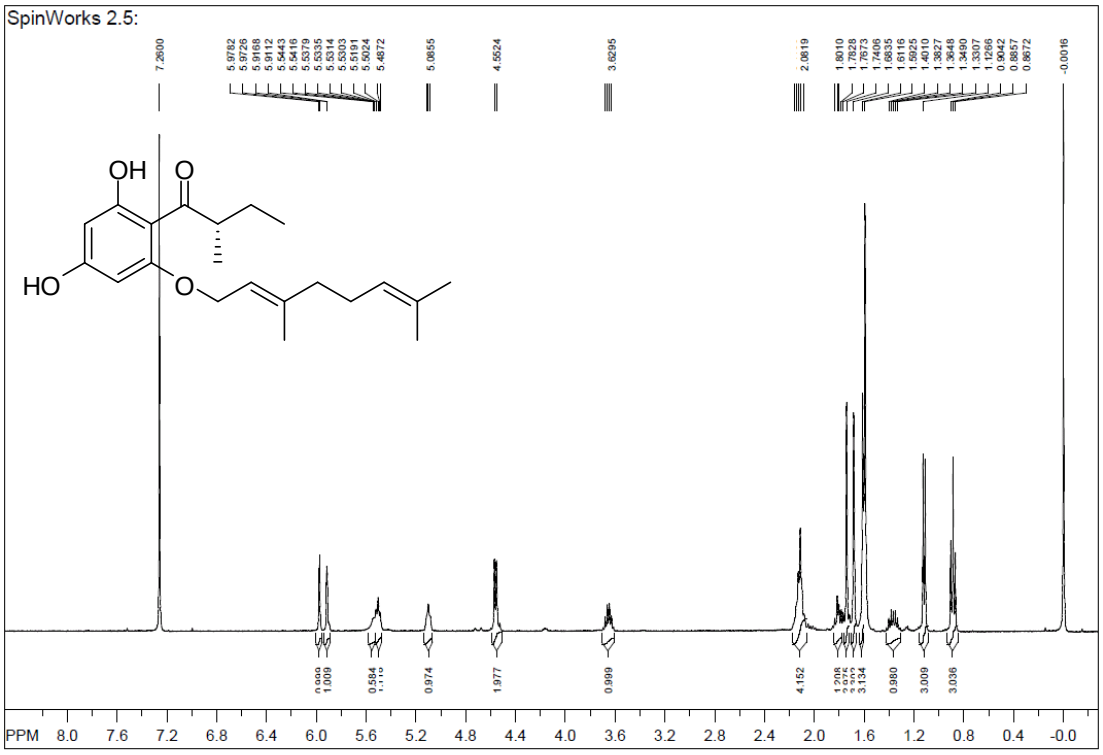
299.1475
610.1813
536.1640
183.0642
684.2011
124.0865
228.2314
429.0875
741.1928
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **2a**



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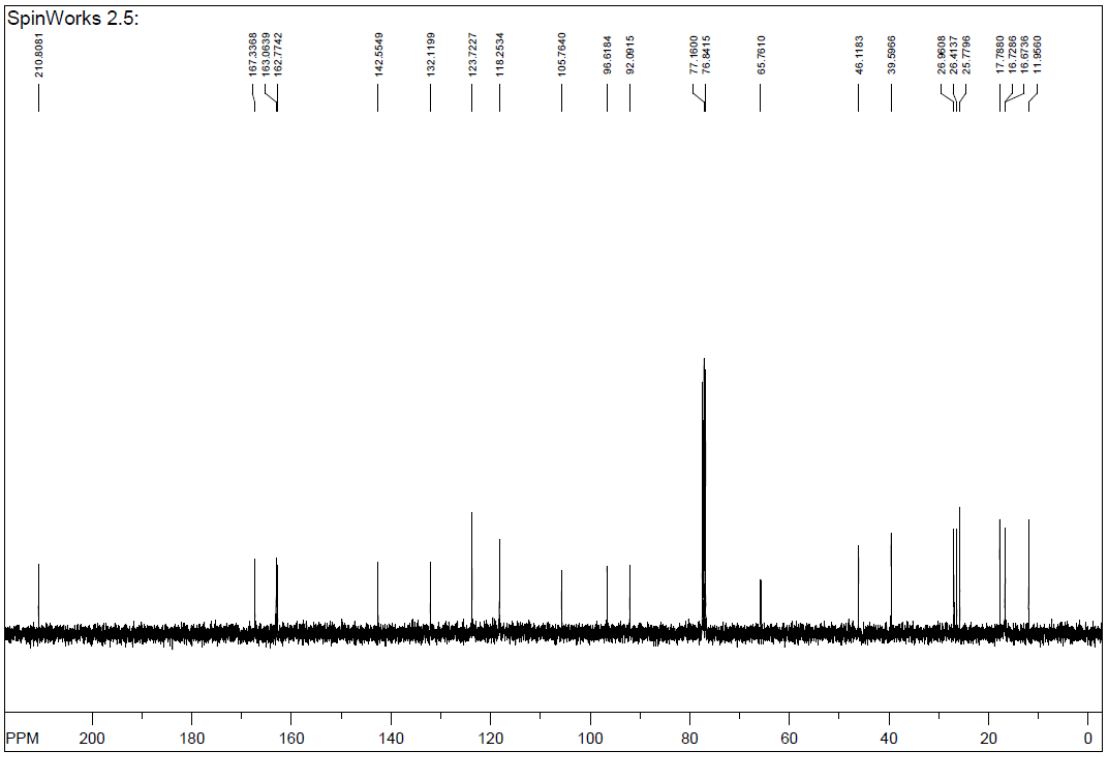

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number of scans: 94

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processed size: 32768 complex points
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Hz/cm: 887.097 ppm/cm: 8.81606

HPLC profile of **2a**

==== Shimadzu LCsolution Analysis Report ====

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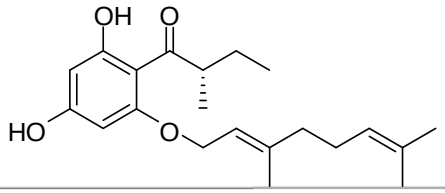

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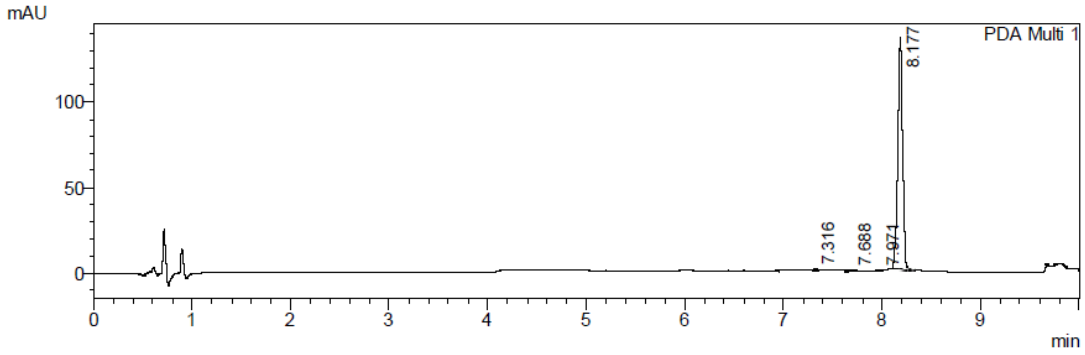

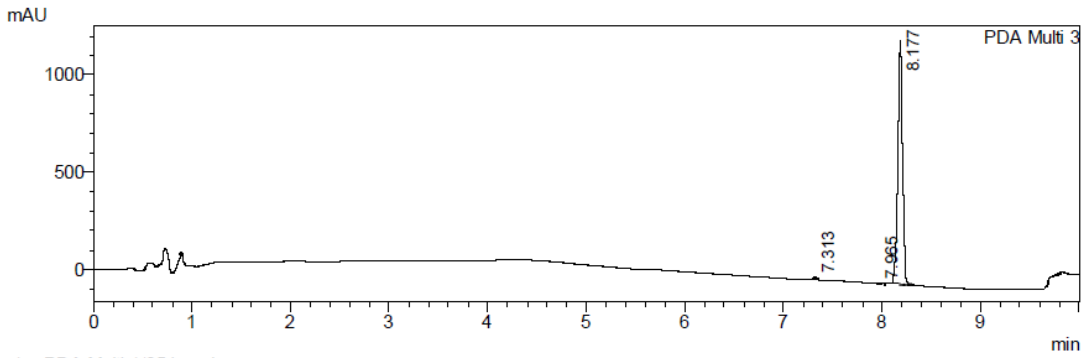

1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

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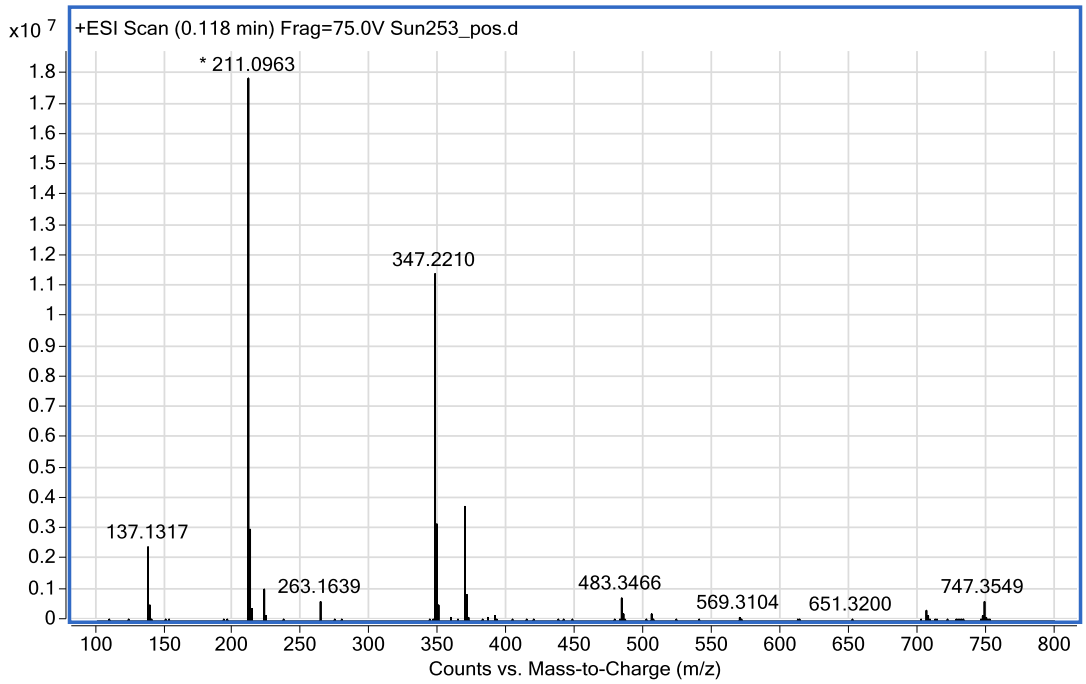
1	7.316	347	196	0.081	0.146
2	7.688	520	280	0.122	0.209
3	7.971	523	300	0.123	0.224
4	8.177	425020	133101	99.674	99.421
Total		426411	133877	100.000	100.000

PeakTable

PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.313	12194	5706	0.321	0.456
2	7.965	1316	1029	0.035	0.082
3	8.177	3779906	1243950	99.644	99.462
Total		3793416	1250684	100.000	100.000

HRMS of **2a**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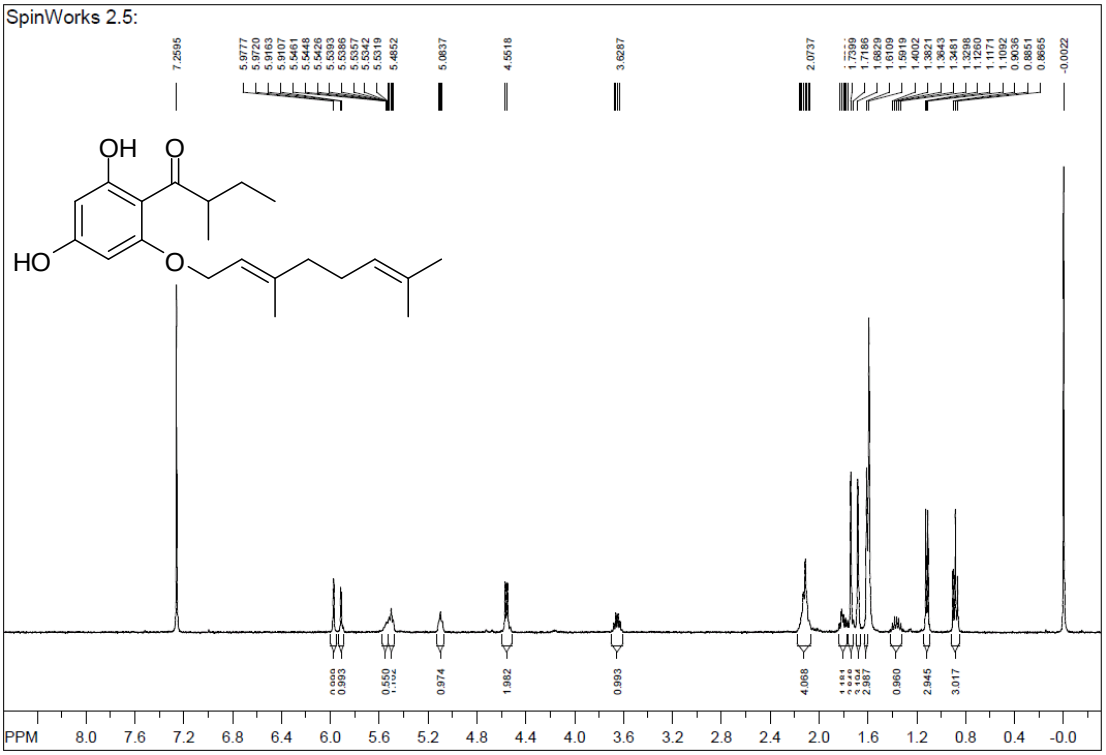
* 211.0963
347.2210
137.1317
263.1639
483.3466
569.3104
651.3200
747.3549
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **2b**



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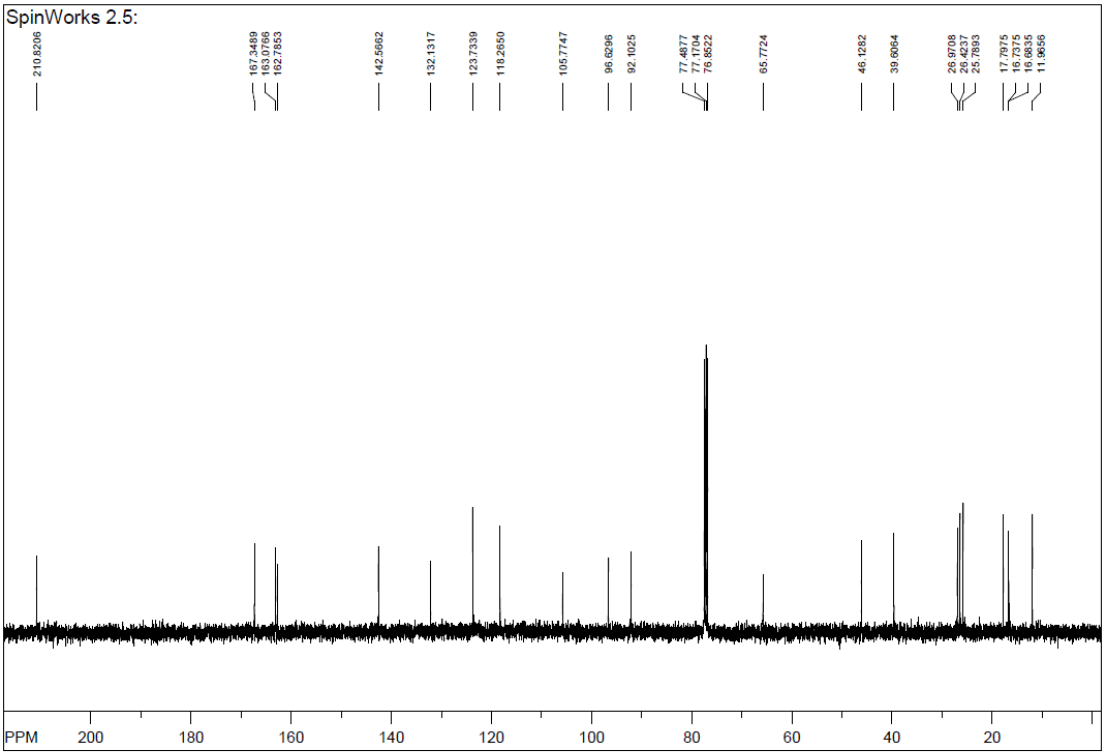

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number of scans: 116

freq. of 0 ppm: 100.612756 MHz
processed size: 32768 complex points
LB: 1.000 GB: 0.0000
Hz/cm: 882.272 ppm/cm: 8.76811

HPLC profile of **2b**

==== Shimadzu LCsolution Analysis Report ====

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Vail #	: 91
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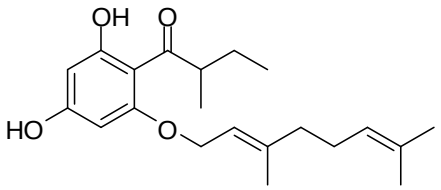

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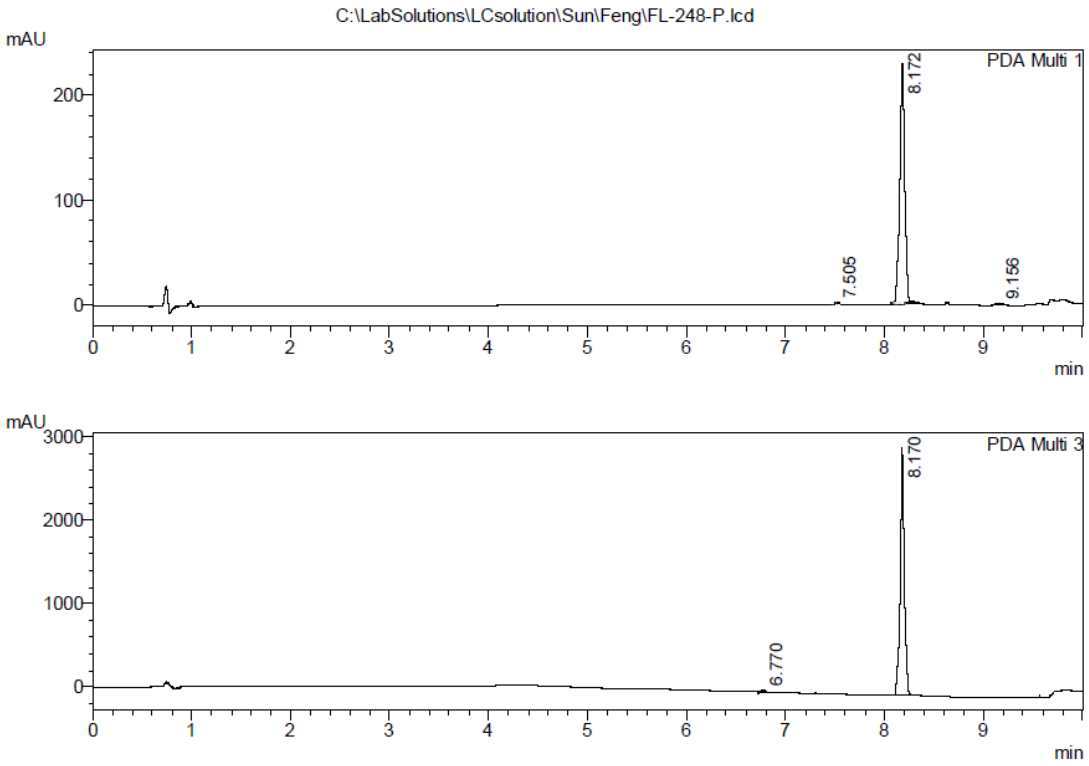


1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

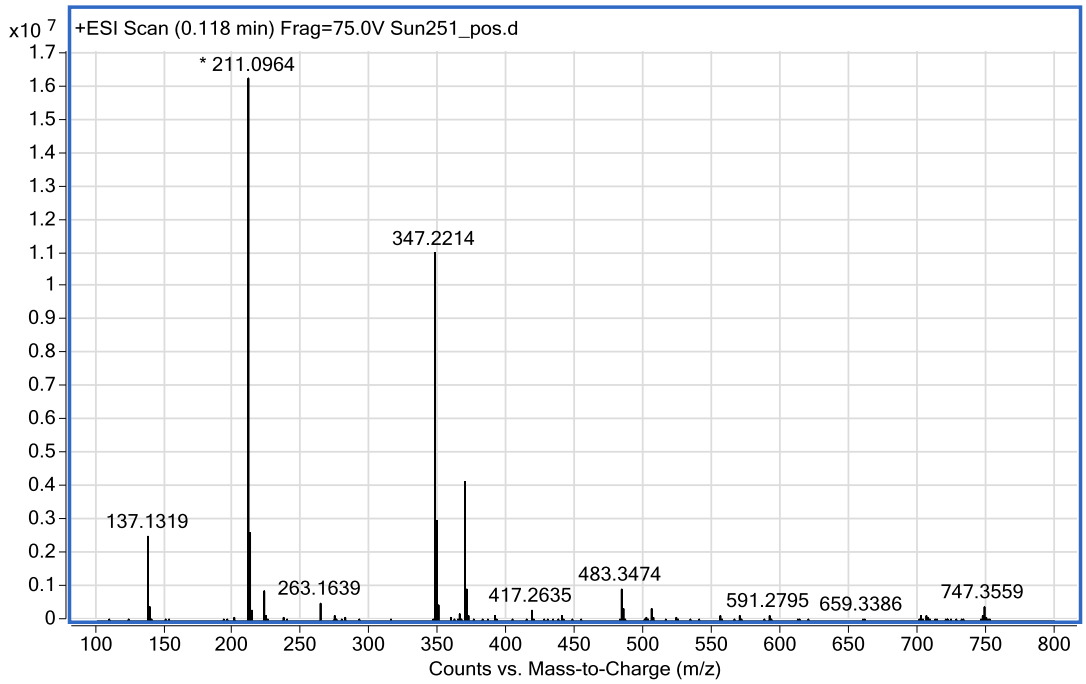
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.505	1320	506	0.177	0.222
2	8.172	741412	227279	99.650	99.573
3	9.156	1281	468	0.172	0.205
Total		744014	228253	100.000	100.000

PeakTable

PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.770	28572	14248	0.366	0.479
2	8.170	7787460	2959100	99.634	99.521
Total		7816033	2973348	100.000	100.000

HRMS of **2b**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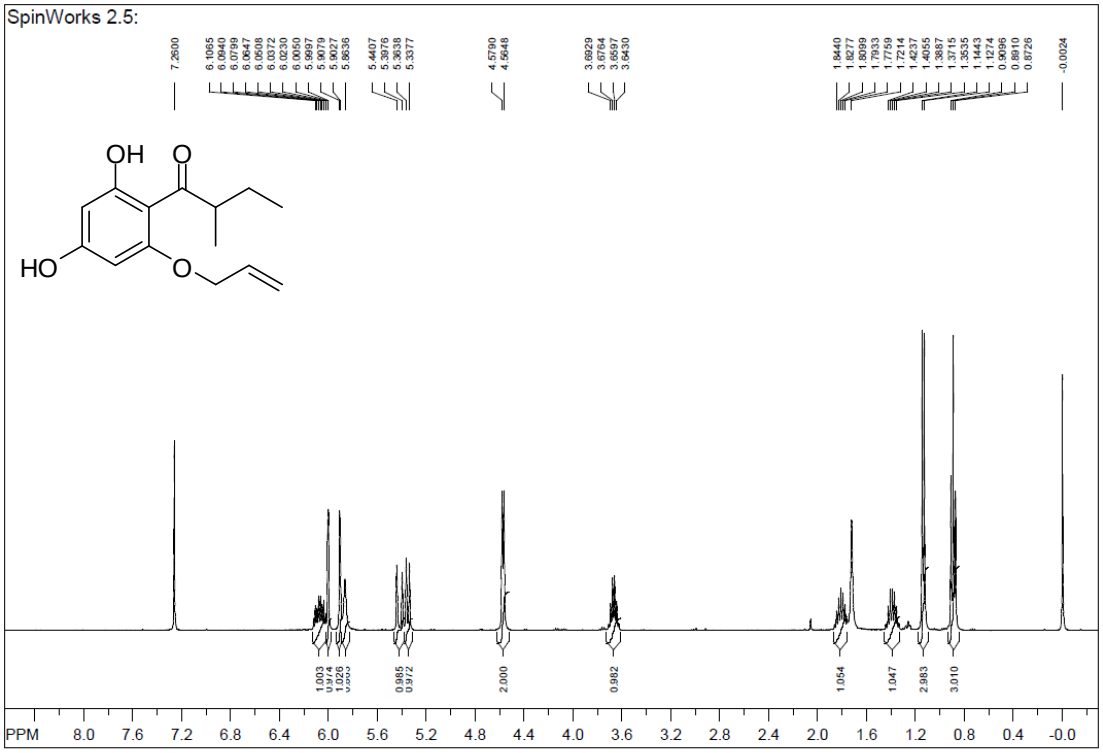
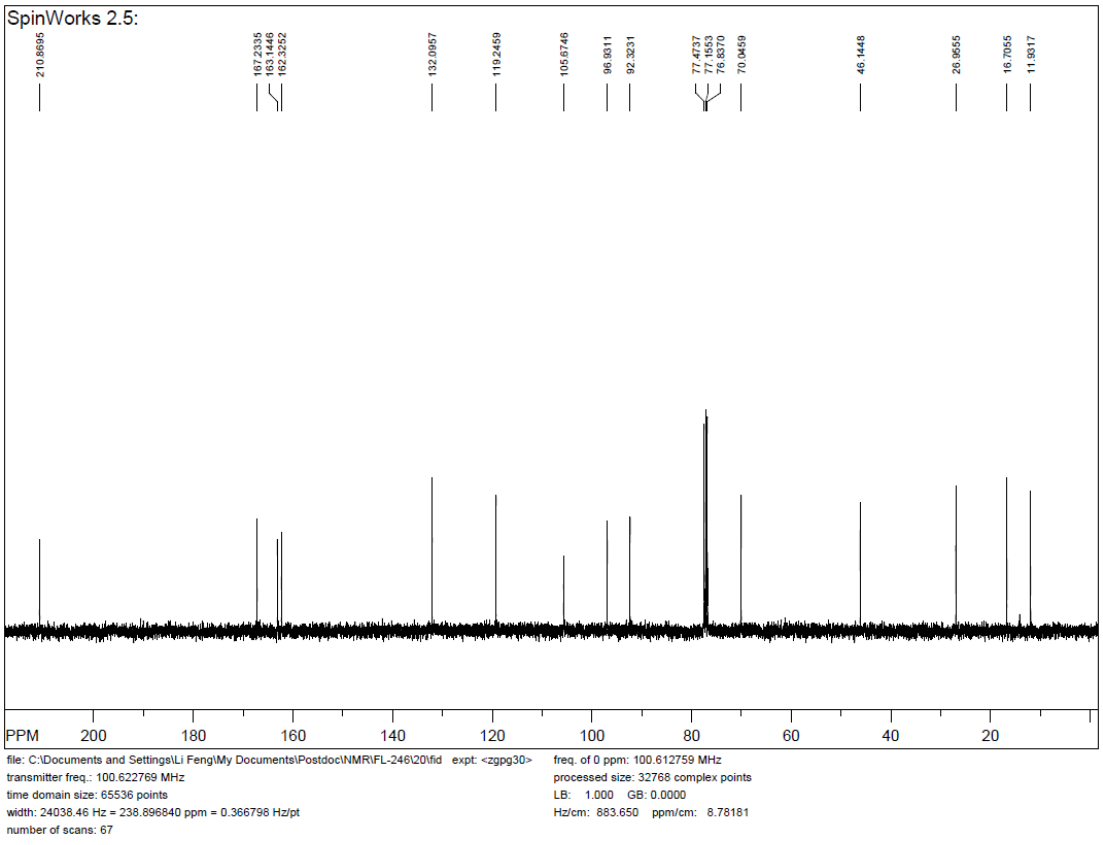
x10 7
* 211.0964
347.2214
137.1319
263.1639
417.2635
483.3474
591.2795
659.3386
747.3559
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **2c**





HPLC profile of **2c**

==== Shimadzu LCsolution Analysis Report ====

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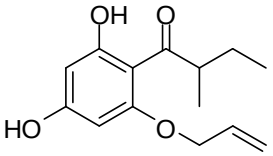
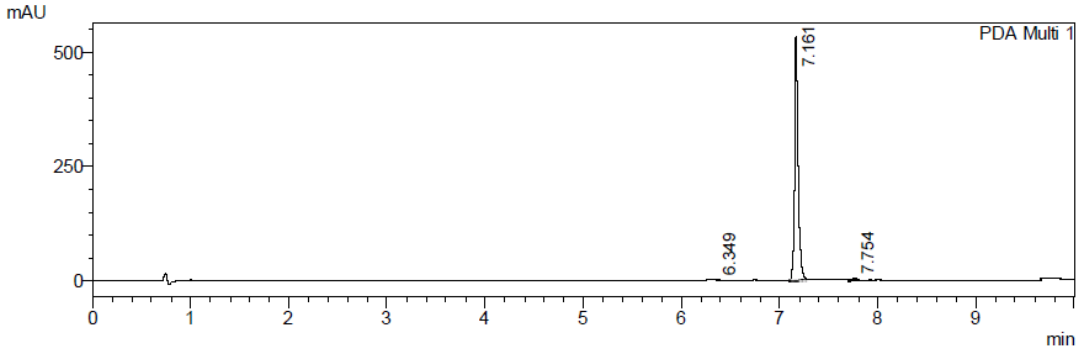
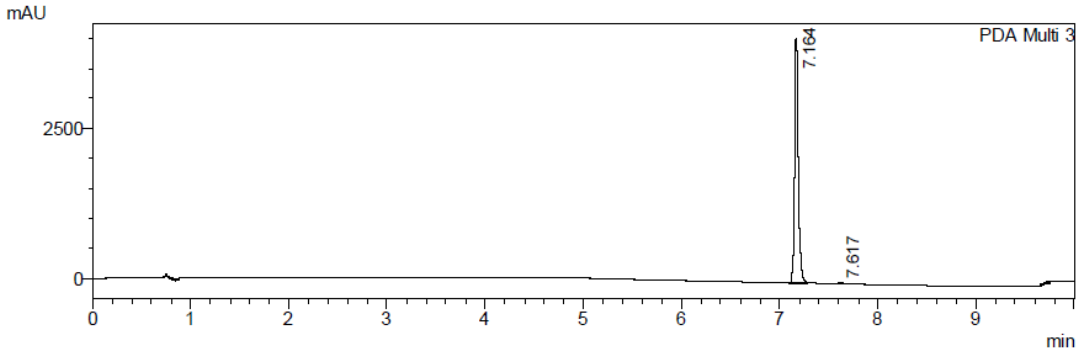
Sample Name	: FL-246-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 10 uL
Data File Name	: FL-246-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 6/1/2012 2:46:45 PM



<Chromatogram>

C:\LabSolutions\LCsolution\Sun\Feng\FL-246-P.lcd





1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

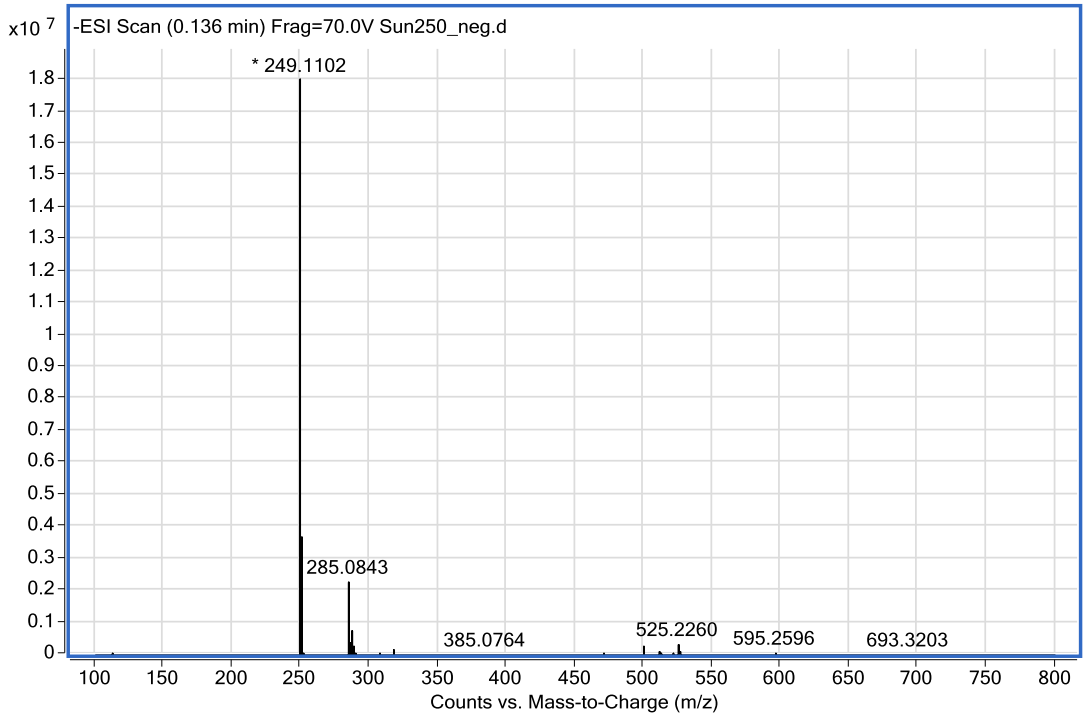
Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.349	631	503	0.042	0.096
2	7.161	1515756	521833	99.671	99.453
3	7.754	4375	2365	0.288	0.451
Total		1520762	524701	100.000	100.000

PeakTable

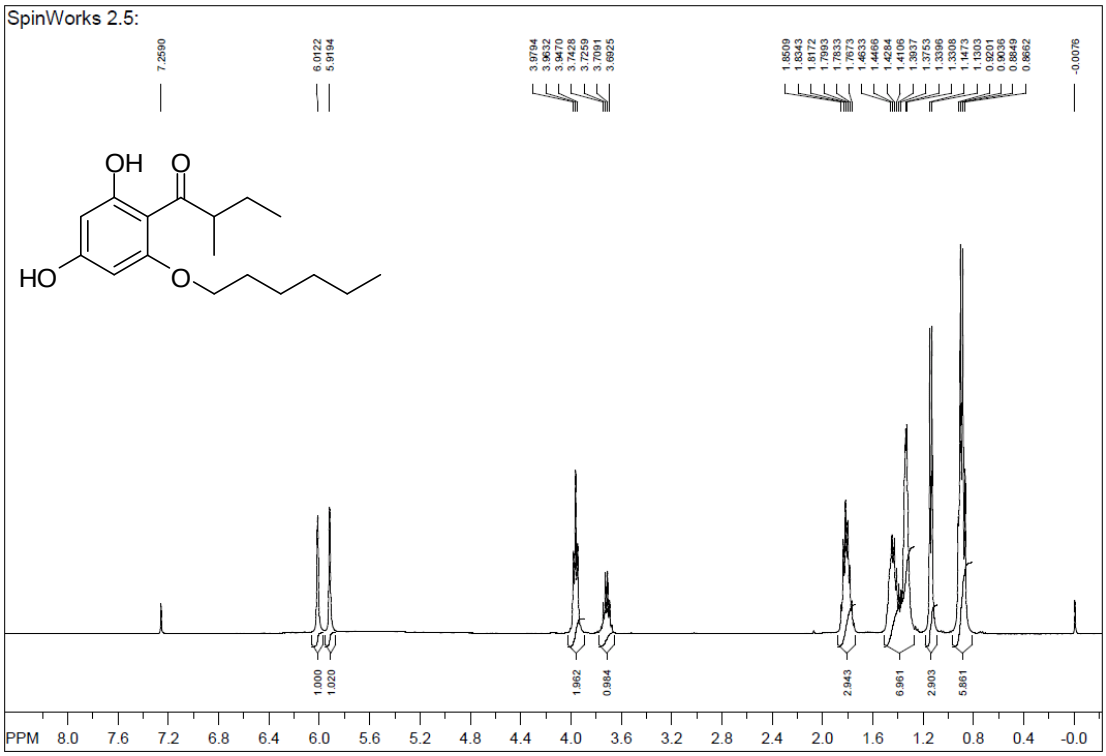
PDA Ch3 220nm 4nm

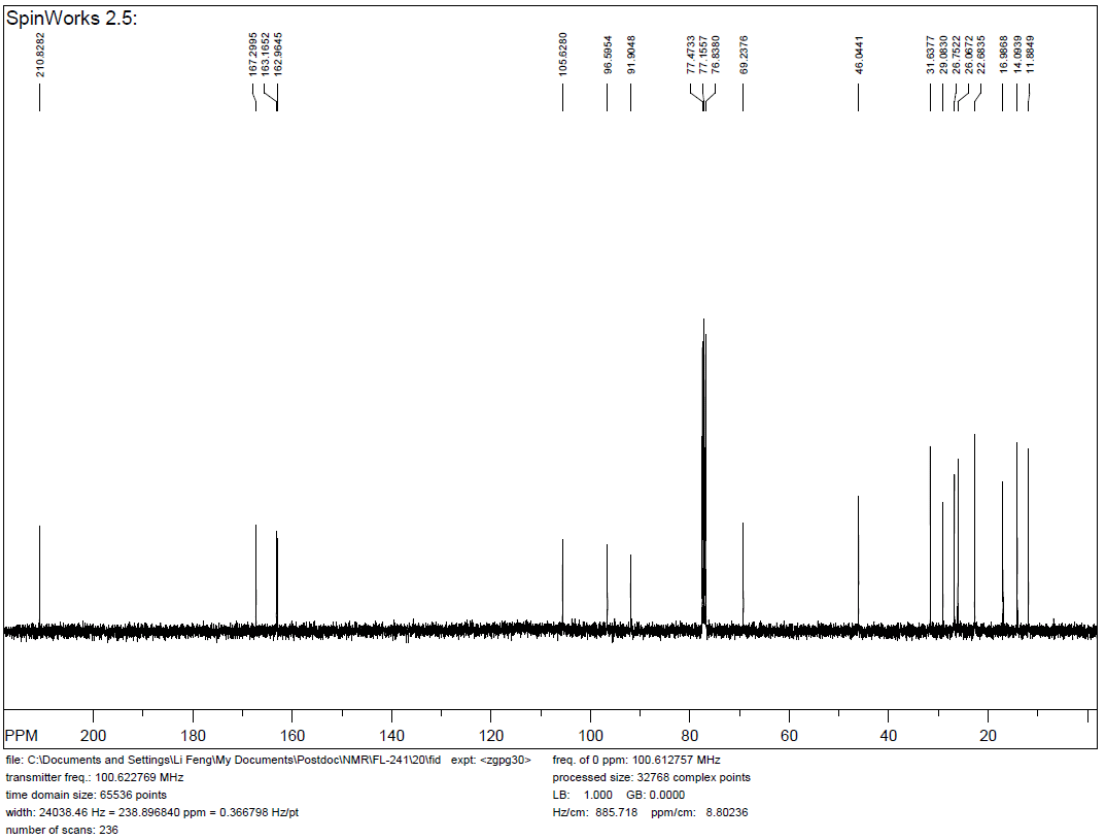
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.164	12501034	4065092	99.855	99.738
2	7.617	18210	10677	0.145	0.262
Total		12519244	4075768	100.000	100.000

HRMS of **2c**


x10 7
-ESI Scan (0.136 min) Frag=70.0V Sun250_neg.d
* 249.1102
285.0843
385.0764
525.2260
595.2596
693.3203
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **2d**



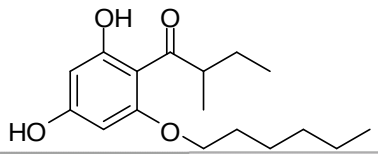


HPLC profile of **2d**

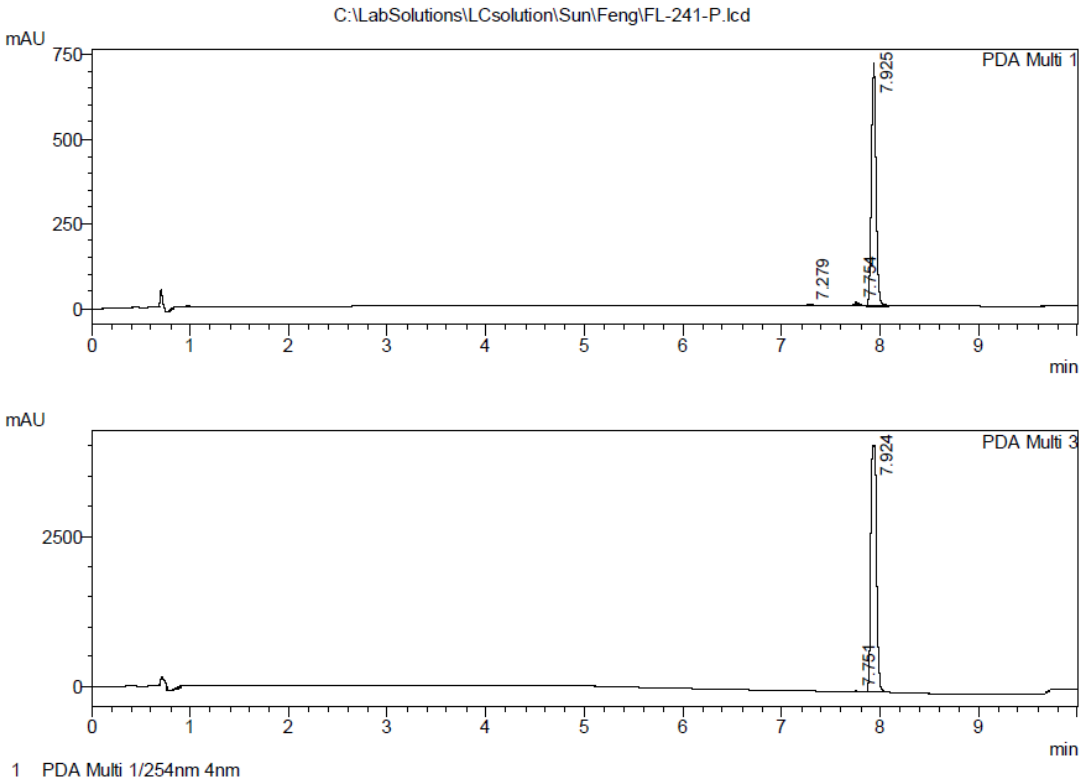
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\Feng\FL-241-P.lcd

Sample Name	: FL-241-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 18 uL
Data File Name	: FL-241-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 6/1/2012 4:28:09 PM



<Chromatogram>



1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

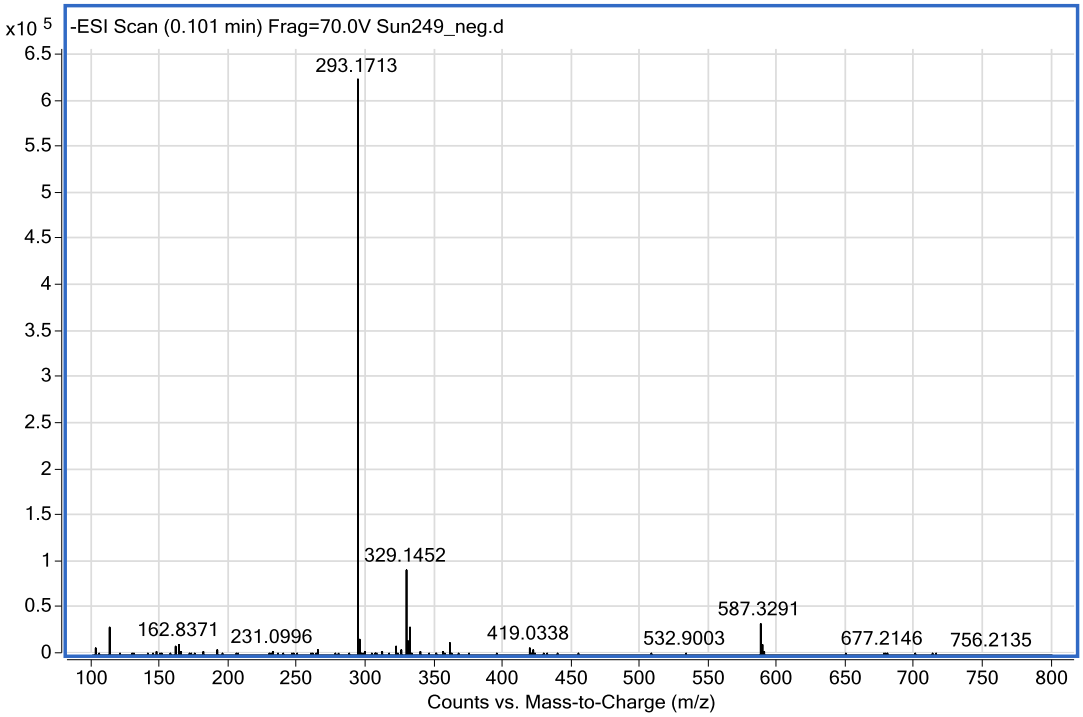
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.279	1687	1123	0.081	0.157
2	7.754	14637	6910	0.703	0.964
3	7.925	2064677	708547	99.216	98.879
Total		2081000	716580	100.000	100.000

PeakTable

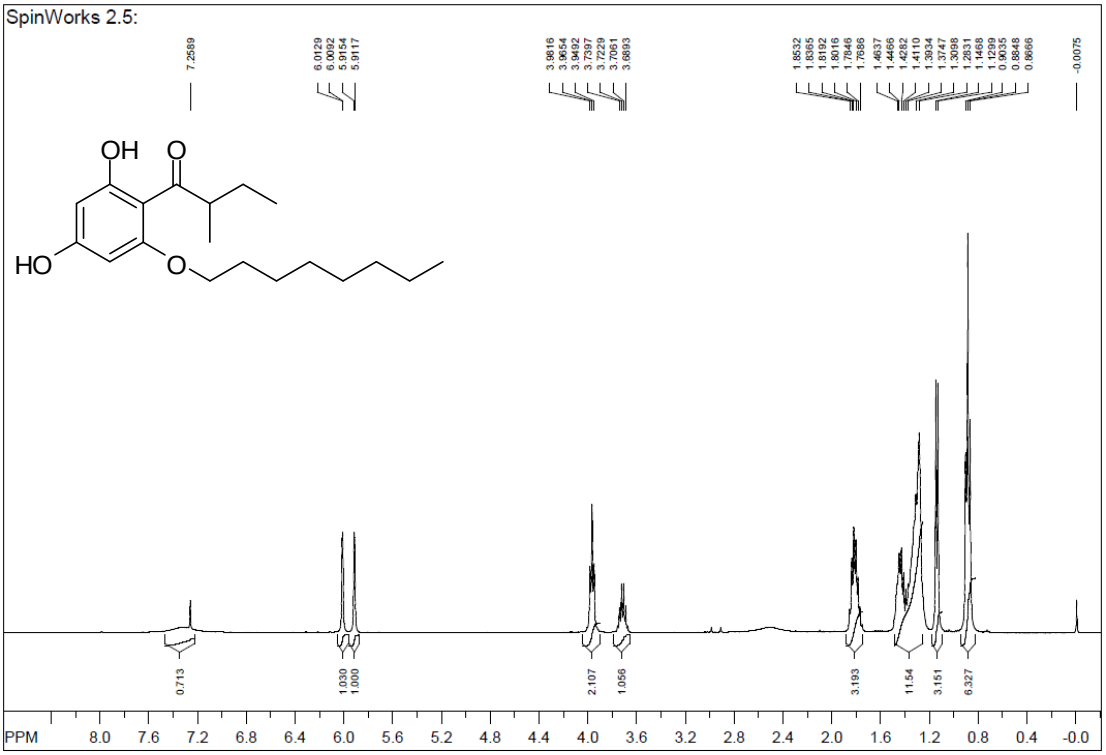
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.751	17290	9465	0.116	0.232
2	7.924	14885157	4069609	99.884	99.768
Total		14902447	4079075	100.000	100.000

HRMS of **2d**

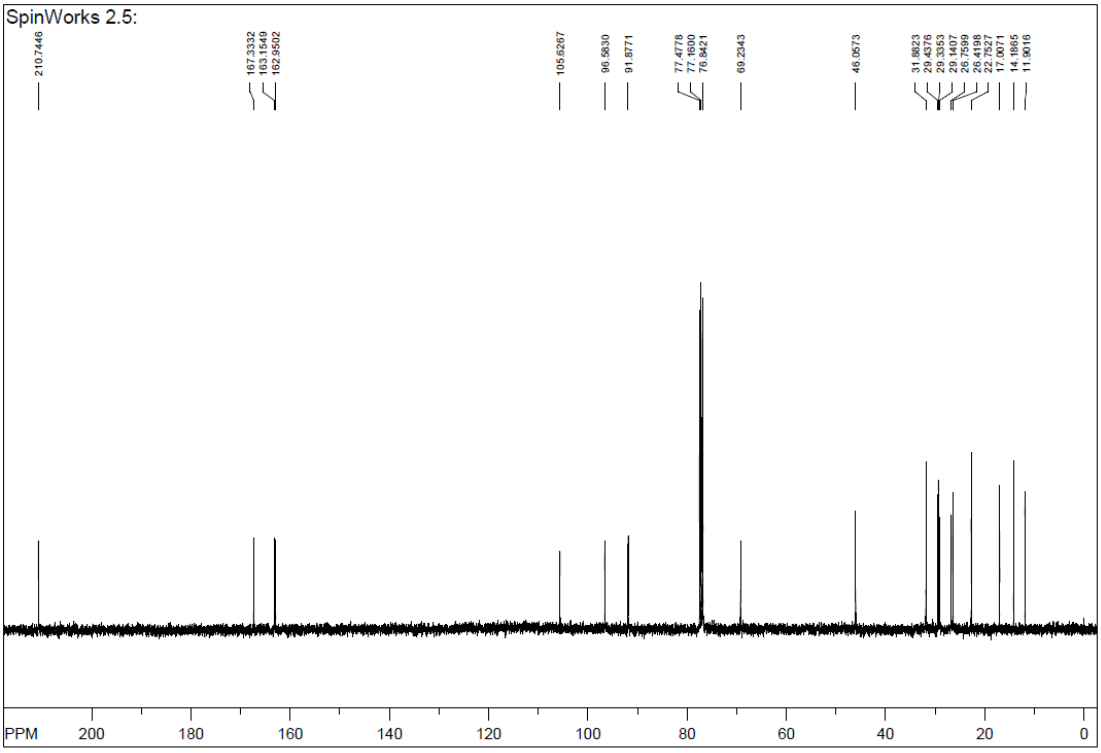

-ESI Scan (0.101 min) Frag=70.0V Sun249_neg.d
x10 5
293.1713
329.1452
587.3291
162.8371
231.0996
419.0338
532.9003
677.2146
756.2135
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **2e**



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-238\1\fid expt: <zg30>
transmitter freq.: 400.131600 MHz
time domain size: 65536 points
width: 8012.82 Hz = 20.025463 ppm = 0.122266 Hz/pt
number of scans: 3

freq. of 0 ppm: 400.130010 MHz
processed size: 32768 complex points
LB: 0.300 GB: 0.0000
Hz/cm: 144.058 ppm/cm: 0.36003



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-238\20\fid expt: <zgpg30>
transmitter freq.: 100.622769 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.896840 ppm = 0.366798 Hz/pt
number of scans: 390

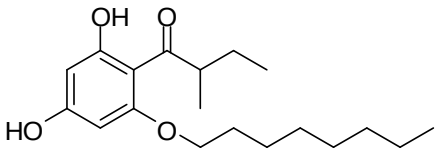
freq. of 0 ppm: 100.612756 MHz
processed size: 32768 complex points
LB: 1.000 GB: 0.0000
Hz/cm: 887.097 ppm/cm: 8.81606

HPLC profile of **2e**

==== Shimadzu LCsolution Analysis Report ====

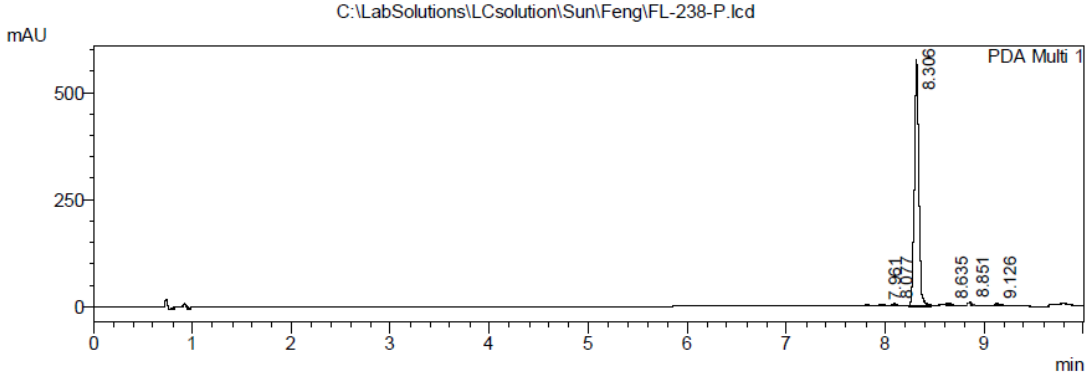
C:\LabSolutions\LCsolution\Sun\Feng\FL-238-P.lcd

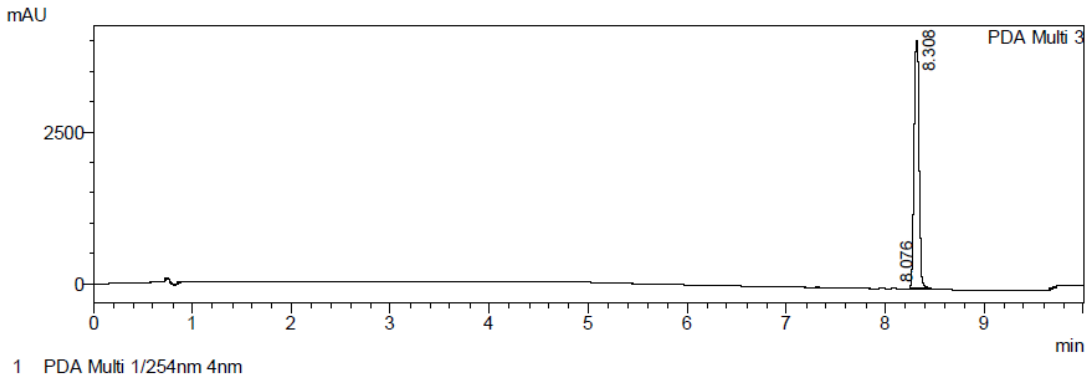
Sample Name	: FL-238-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 6 uL
Data File Name	: FL-238-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 5/29/2012 9:50:37 AM



<Chromatogram>

C:\LabSolutions\LCsolution\Sun\Feng\FL-238-P.lcd





1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

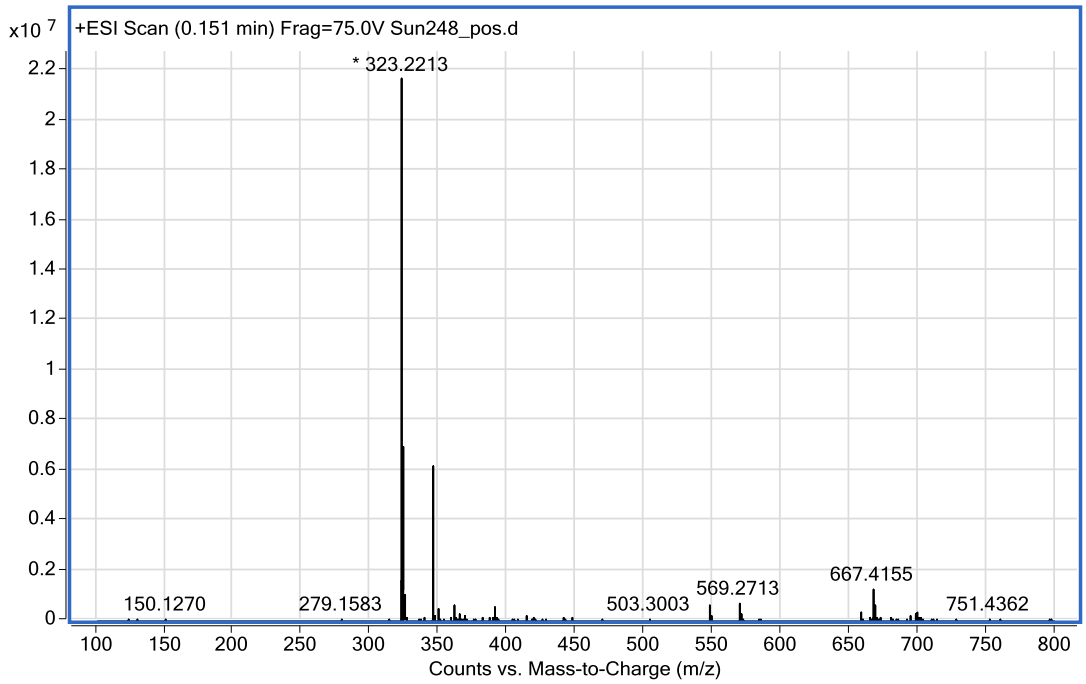
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.961	2986	1988	0.177	0.345
2	8.077	1801	1522	0.107	0.264
3	8.306	1669319	565216	98.768	98.072
4	8.635	4884	2071	0.289	0.359
5	8.851	6814	3447	0.403	0.598
6	9.126	4333	2087	0.256	0.362
Total		1690137	576330	100.000	100.000

PeakTable

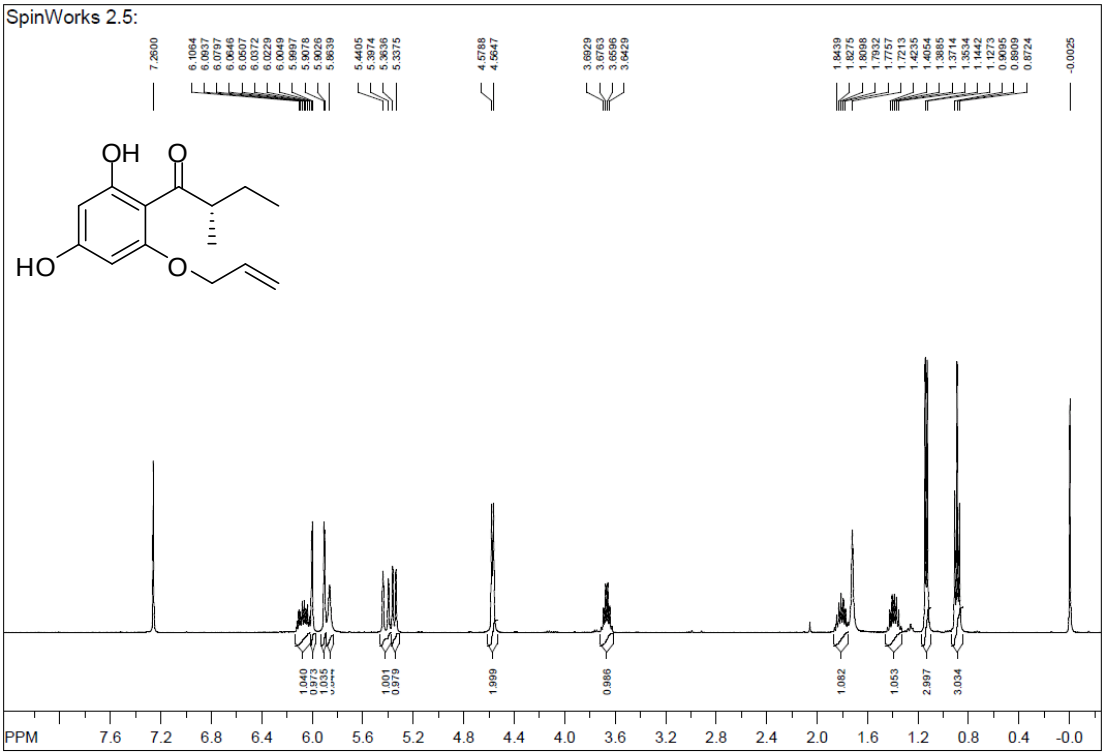
PDA Ch3 220nm 4nm

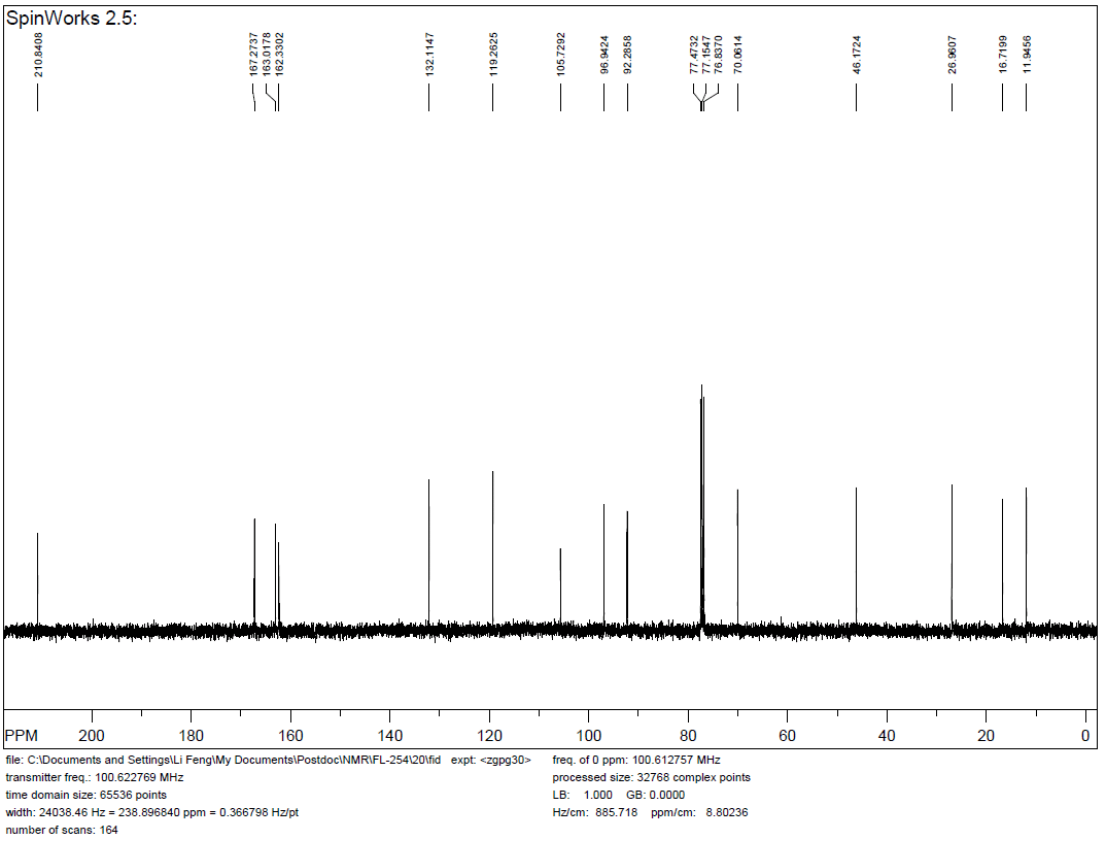
Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.076	5486	4481	0.040	0.110
2	8.308	13579648	4076754	99.960	99.890
Total		13585135	4081235	100.000	100.000

HRMS of **2e**


x10 7
+ESI Scan (0.151 min) Frag=75.0V Sun248_pos.d
* 323.2213
150.1270
279.1583
503.3003
569.2713
667.4155
751.4362
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **2f**



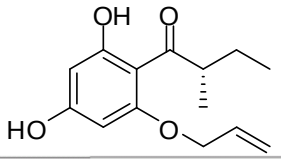


HPLC profile of **2f**

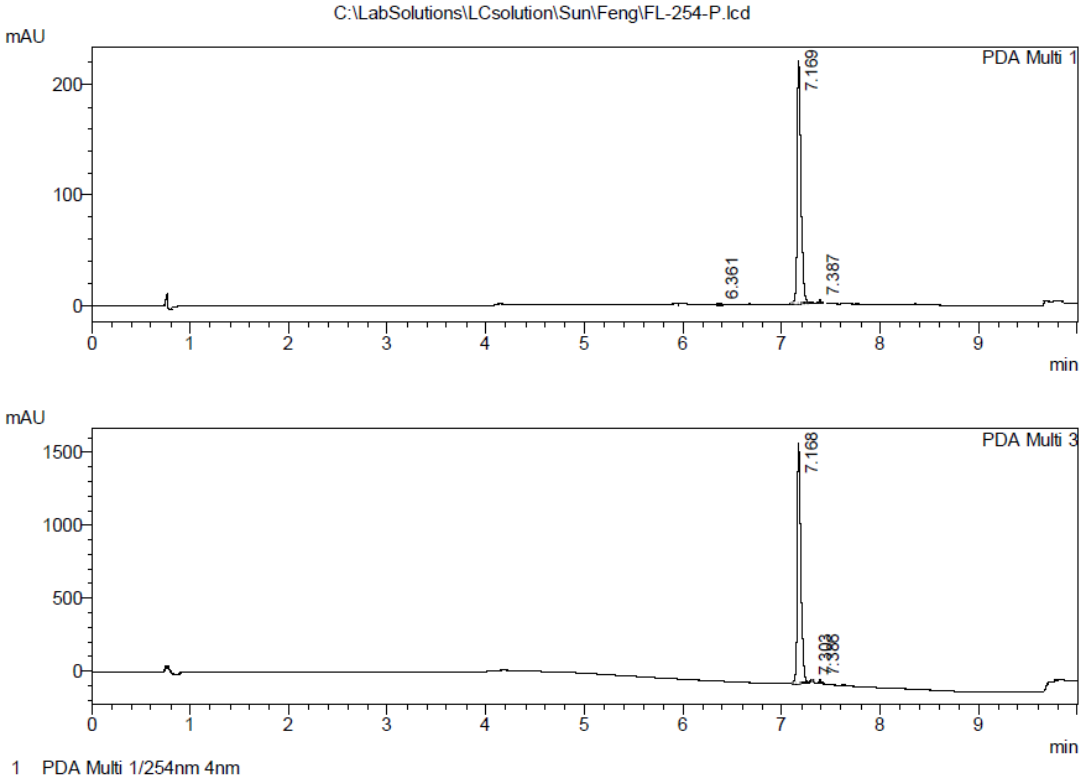
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\Feng\FL-254-P.lcd

Sample Name	: FL-254-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 8 uL
Data File Name	: FL-254-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 6/12/2012 12:12:11 PM



<Chromatogram>



1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

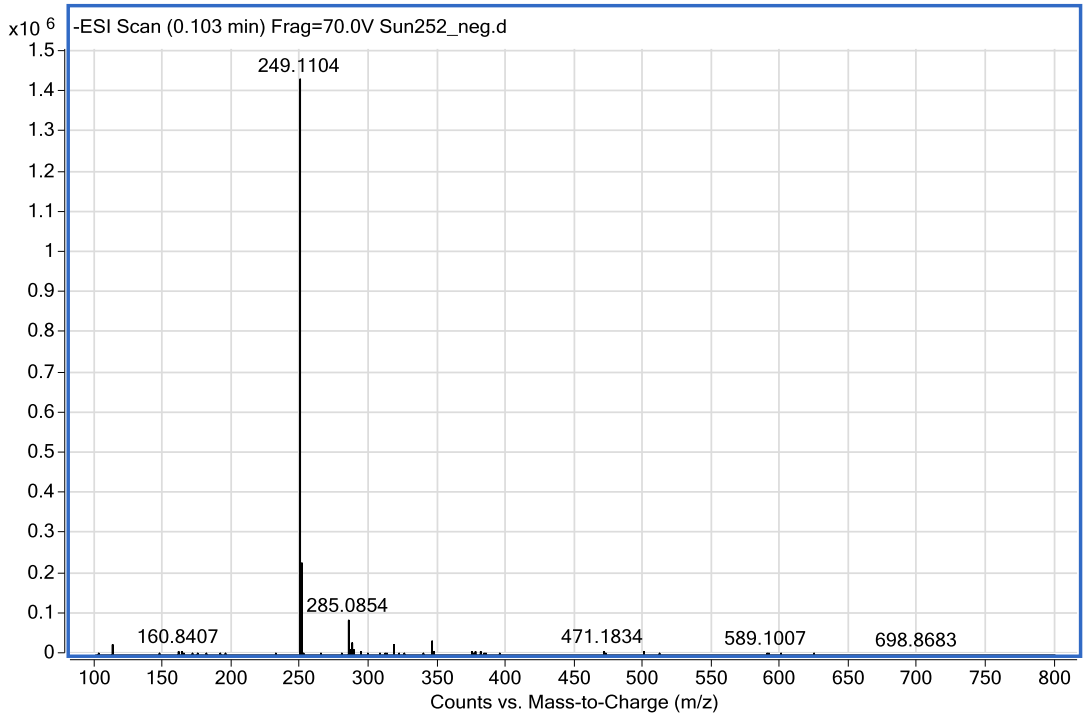
Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.361	1183	561	0.189	0.258
2	7.169	619052	214840	99.147	98.852
3	7.387	4143	1934	0.664	0.890
Total		624378	217334	100.000	100.000

PeakTable

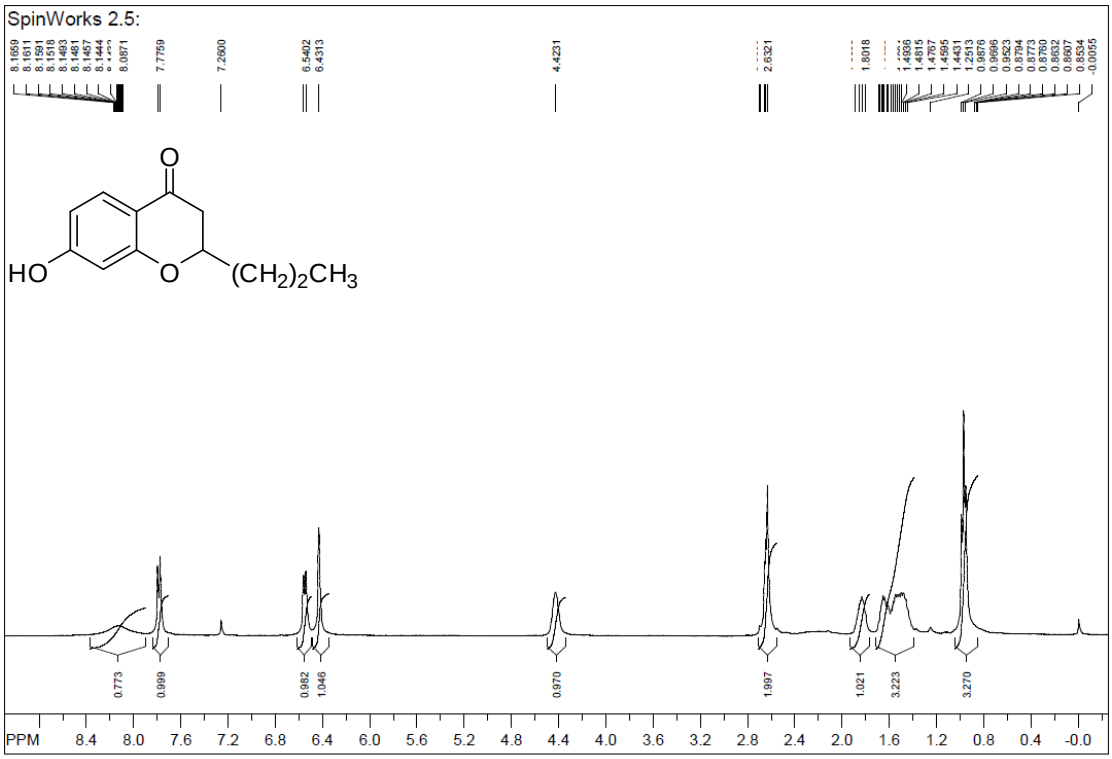
PDA Ch3 220nm 4nm

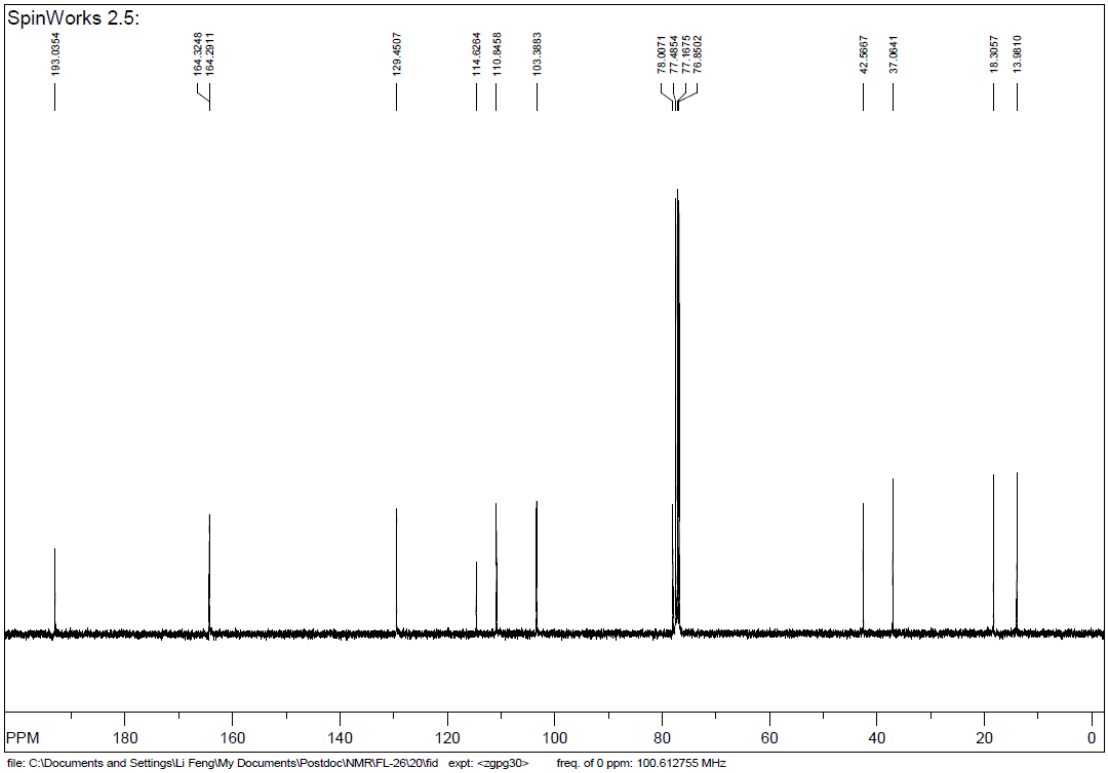
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.168	4451986	1645227	99.570	99.200
2	7.303	4346	3180	0.097	0.192
3	7.386	14859	10088	0.332	0.608
Total		4471191	1658495	100.000	100.000

HRMS of **2f**


x10 6
-ESI Scan (0.103 min) Frag=70.0V Sun252_neg.d
249.1104
285.0854
160.8407
471.1834
589.1007
698.8683
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **3a**



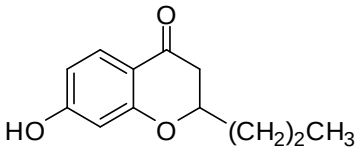


HPLC profile of **3a**

==== Shimadzu LCsolution Analysis Report ====

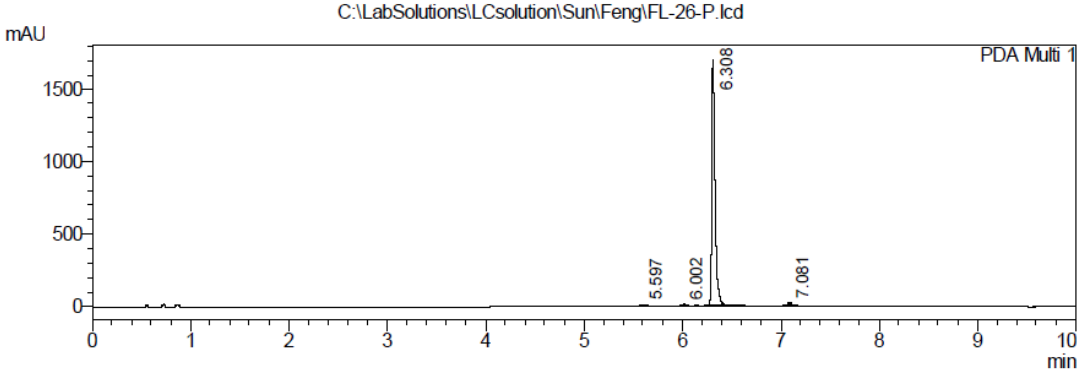
C:\LabSolutions\LCsolution\Sun\Feng\FL-26-P.lcd

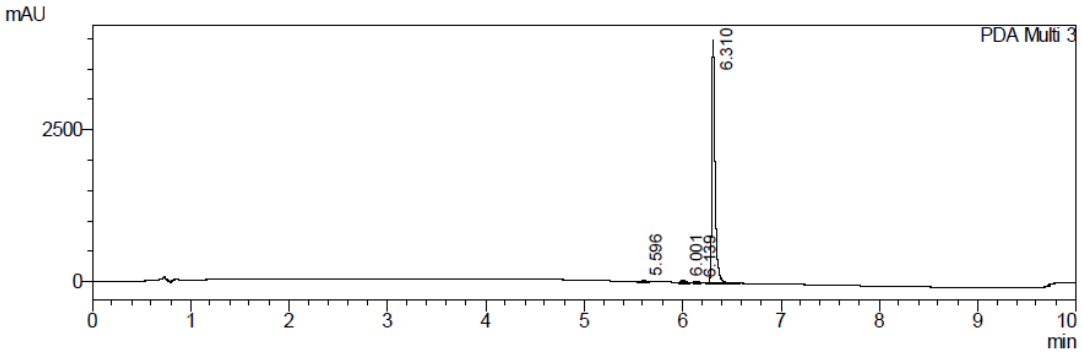
Sample Name	: FL-26-P
Tray#	: 1
Vail #	: 93
Injection Volume	: 5 uL
Data File Name	: FL-26-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	: Batch 1.lcb
Data Acquired	: 12/2/2011 11:40:37 AM



<Chromatogram>

C:\LabSolutions\LCsolution\Sun\Feng\FL-26-P.lcd





1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

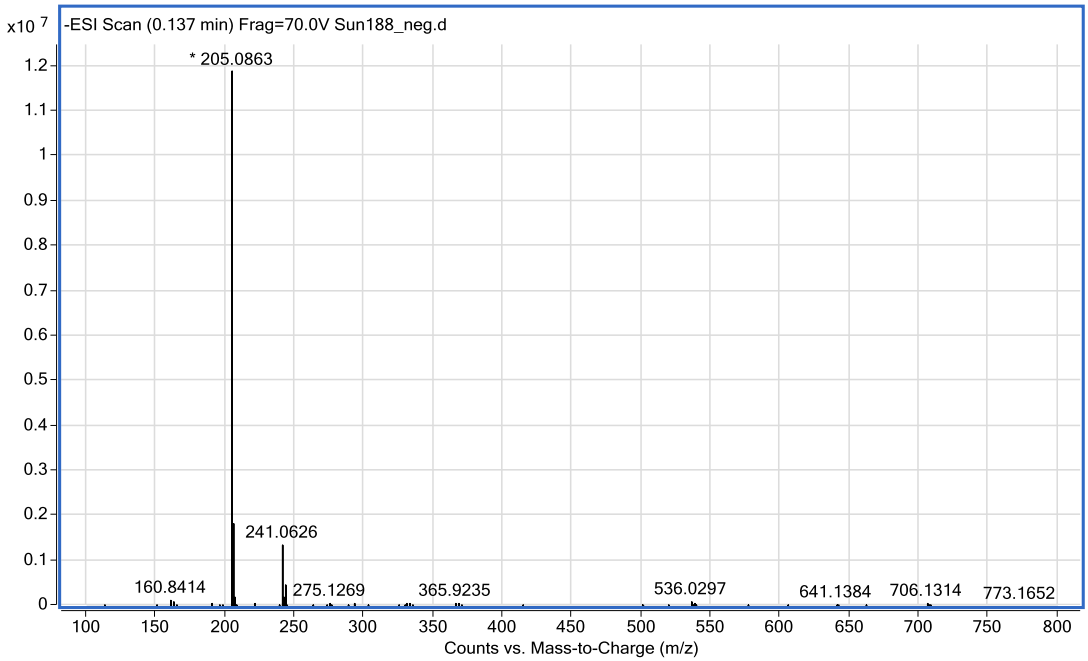
Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.597	19719	9009	0.448	0.516
2	6.002	36266	15648	0.825	0.896
3	6.308	4280075	1695387	97.328	97.133
4	7.081	61502	25380	1.399	1.454
Total		4397562	1745423	100.000	100.000

PeakTable

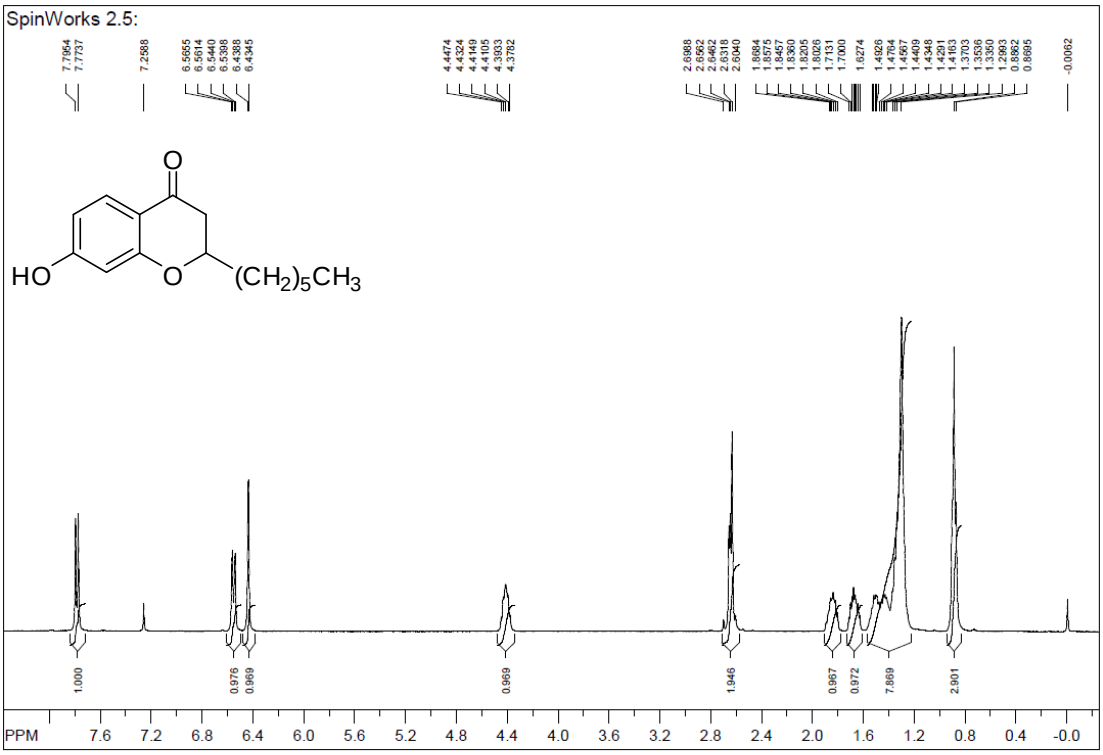
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.596	42874	17638	0.426	0.434
2	6.001	70281	30111	0.698	0.741
3	6.139	30787	16697	0.306	0.411
4	6.310	9926608	4000820	98.571	98.415
Total		10070551	4065266	100.000	100.000

HRMS of **3a**

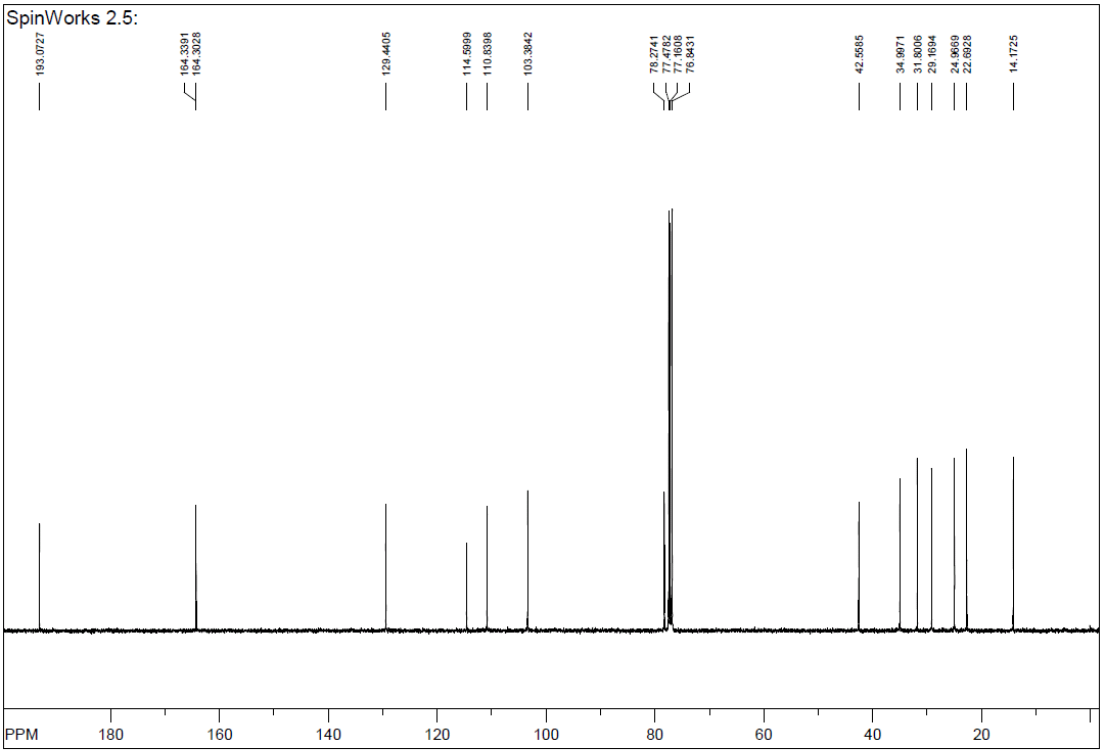

x10 7
-ESI Scan (0.137 min) Frag=70.0V Sun188_neg.d
* 205.0863
241.0626
160.8414
275.1269
365.9235
536.0297
641.1384
706.1314
773.1652
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **3b**



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-24\2\fid expt: <zg30>
transmitter freq.: 400.131600 MHz
time domain size: 65536 points
width: 8012.82 Hz = 20.025463 ppm = 0.122266 Hz/pt
number of scans: 8

freq. of 0 ppm: 400.130010 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 137.855 ppm/cm: 0.34452



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-24\20\fid expt: <zgpg30>
transmitter freq.: 100.622769 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.896840 ppm = 0.366798 Hz/pt
number of scans: 2454

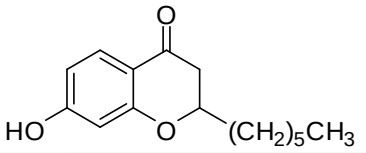
freq. of 0 ppm: 100.612756 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 809.817 ppm/cm: 8.04805

HPLC profile of **3b**

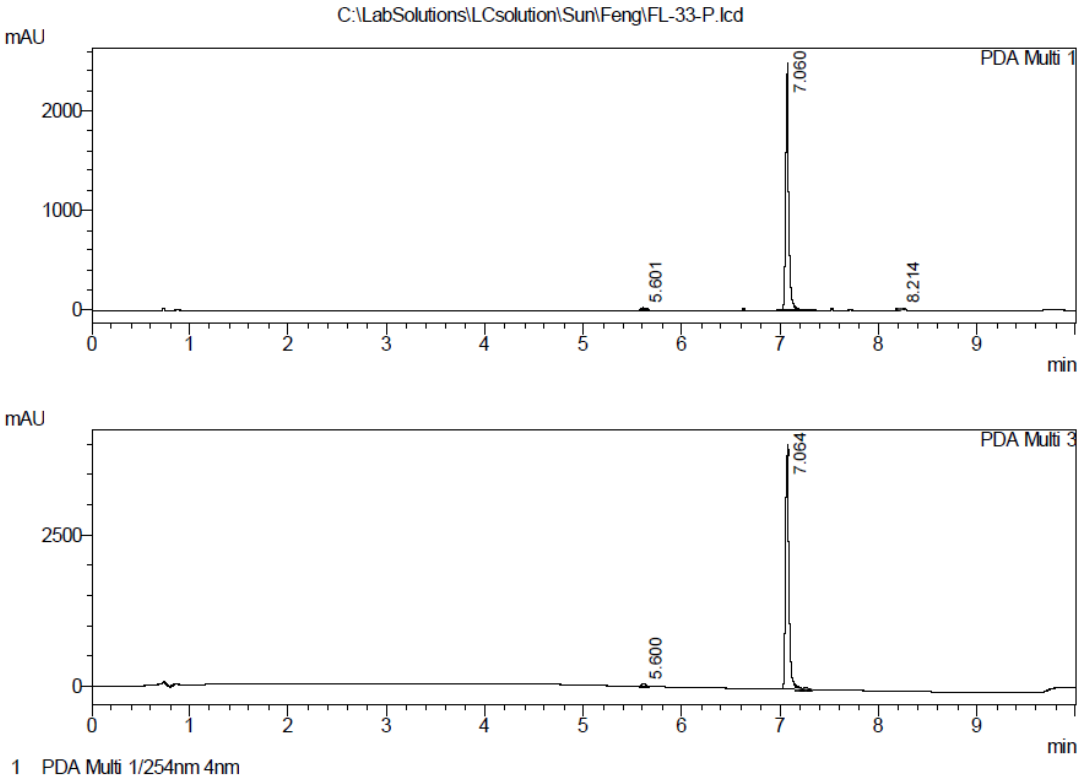
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\Feng\FL-33-P.lcd

Sample Name	: FL-33-P
Tray#	: 1
Vail #	: 94
Injection Volume	: 5 uL
Data File Name	: FL-33-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	: Batch 1.lcb
Data Acquired	: 12/2/2011 11:51:06 AM



<Chromatogram>



1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

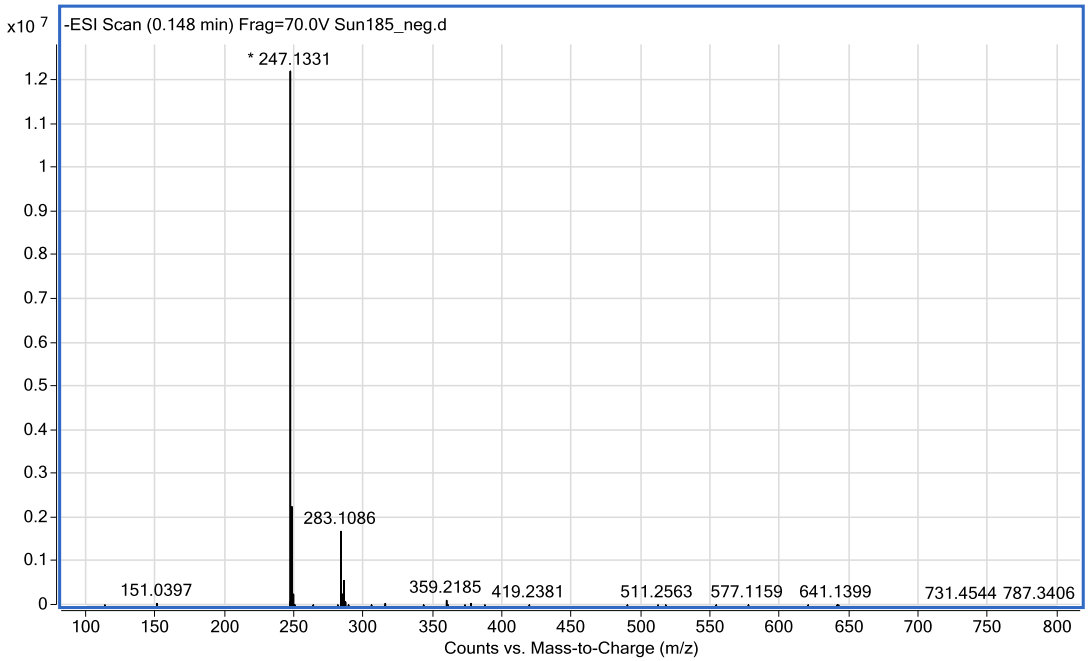
Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.601	59260	24157	0.995	0.962
2	7.060	5860048	2472339	98.422	98.414
3	8.214	34698	15694	0.583	0.625
Total		5954005	2512190	100.000	100.000

PeakTable

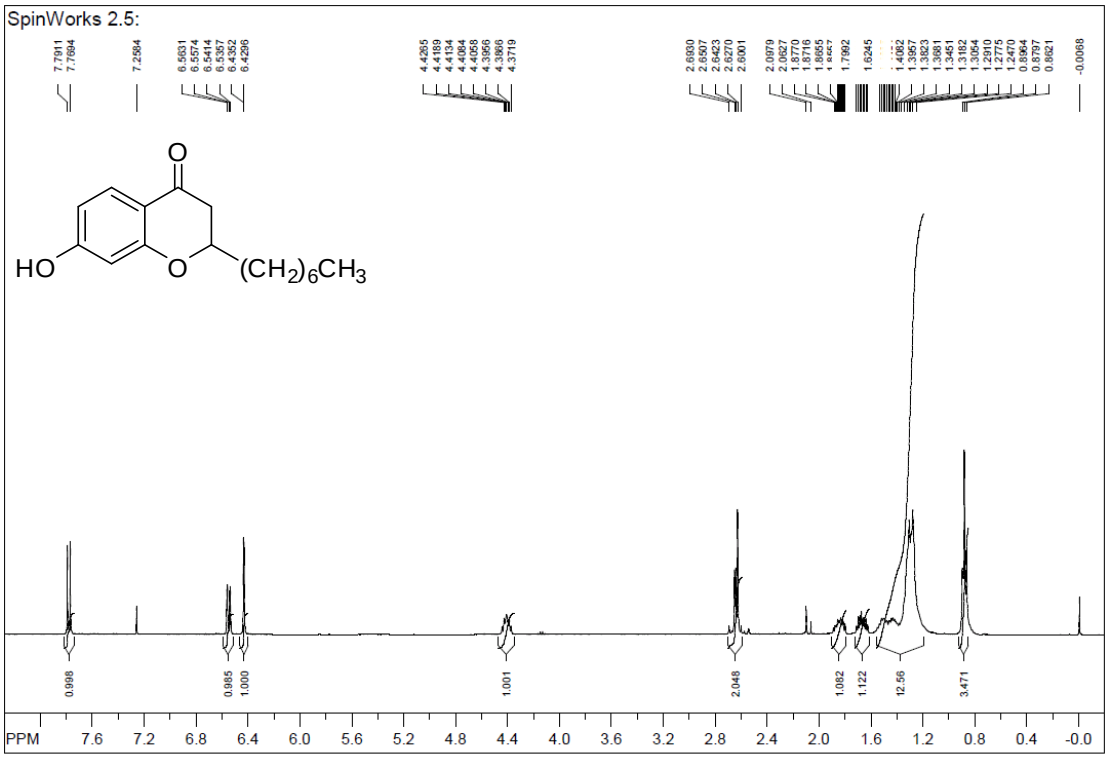
PDA Ch3 220nm 4nm

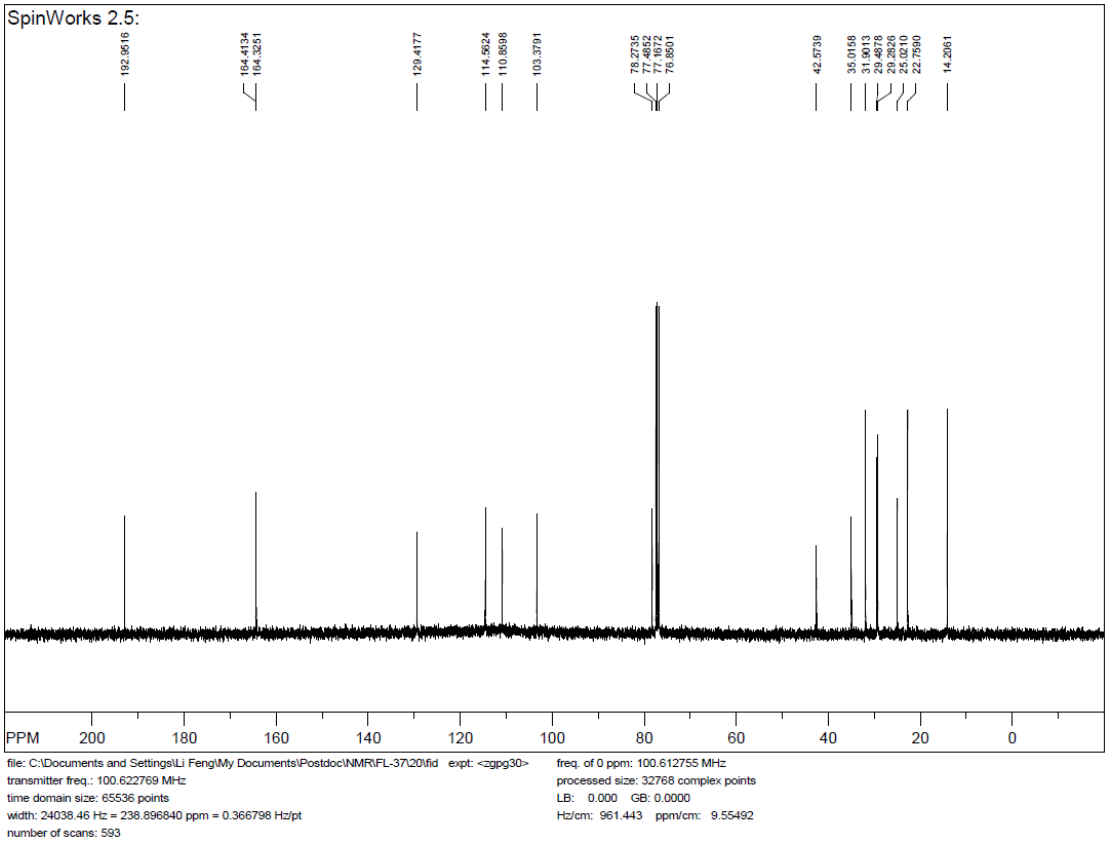
Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.600	105419	44395	0.940	1.088
2	7.064	11111850	4036335	99.060	98.912
Total		11217269	4080730	100.000	100.000

HRMS of **3b**


x10 7
-ESI Scan (0.148 min) Frag=70.0V Sun185_neg.d
* 247.1331
283.1086
151.0397
359.2185
419.2381
511.2563
577.1159
641.1399
731.4544
787.3406
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **3c**



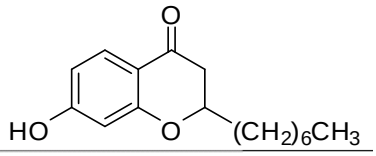


HPLC profile of **3c**

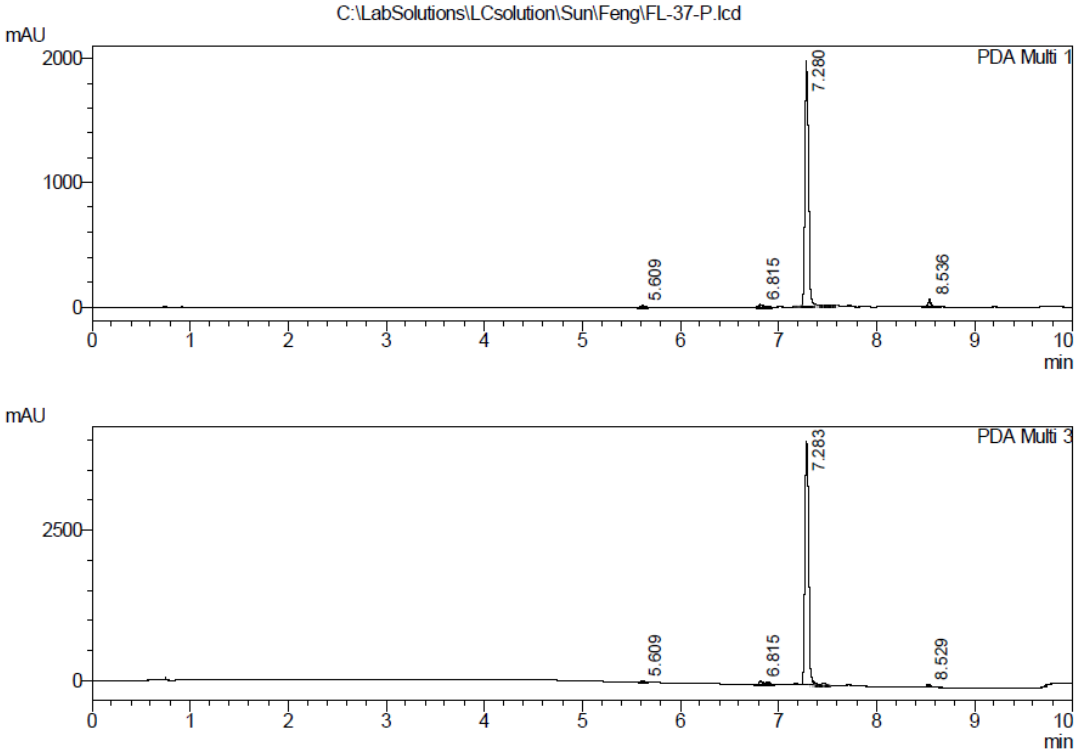
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\Feng\FL-37-P.lcd

Sample Name	: FL-37-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 5 uL
Data File Name	: FL-37-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 12/2/2011 12:58:42 PM



<Chromatogram>



1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

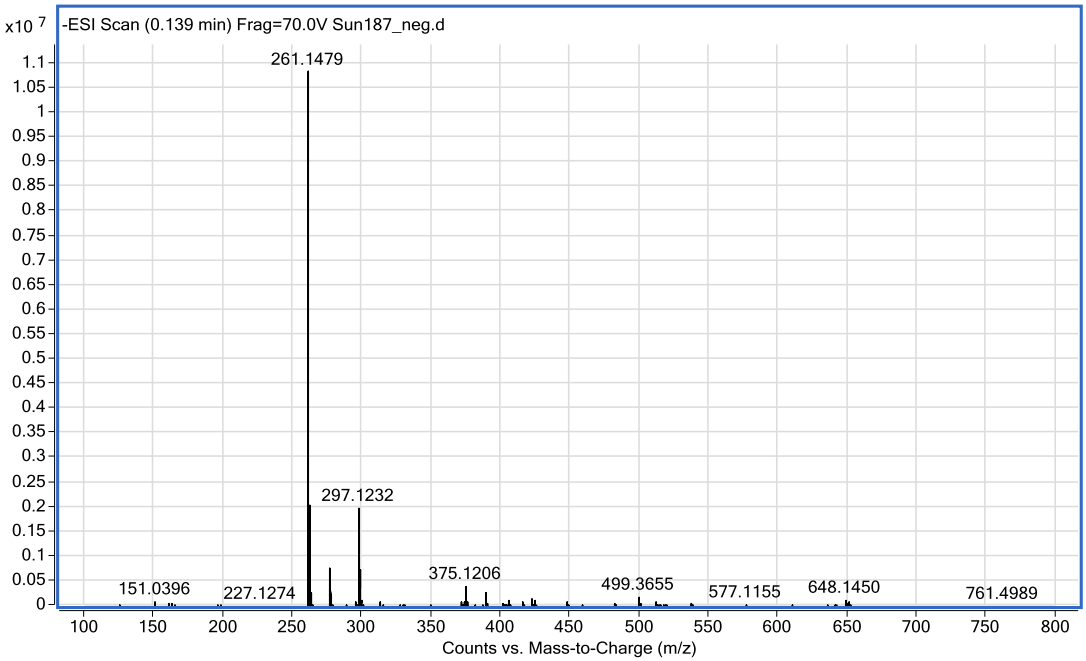
Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.609	29157	12173	0.598	0.613
2	6.815	58390	18377	1.197	0.926
3	7.280	4634568	1896096	94.985	95.496
4	8.536	157136	58876	3.220	2.965
Total		4879251	1985523	100.000	100.000

PeakTable

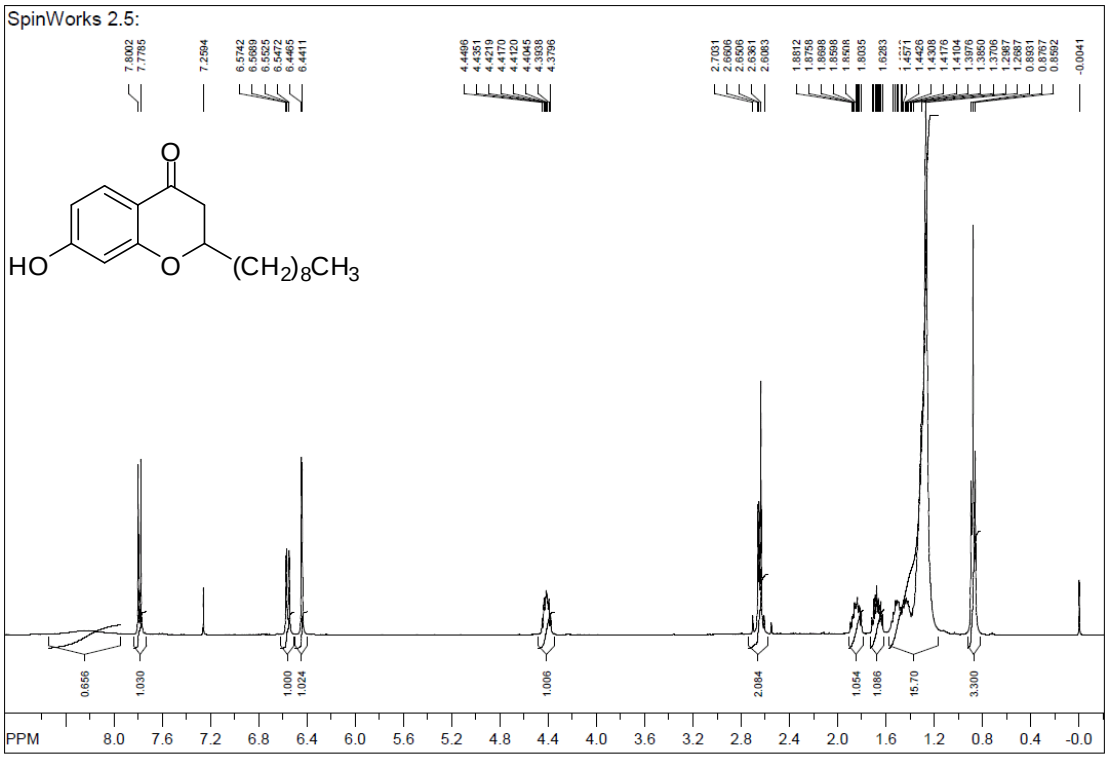
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.609	51553	22300	0.482	0.537
2	6.815	226513	50722	2.118	1.220
3	7.283	10280614	4044804	96.138	97.327
4	8.529	134933	38045	1.262	0.915
Total		10693613	4155871	100.000	100.000

HRMS of **3c**

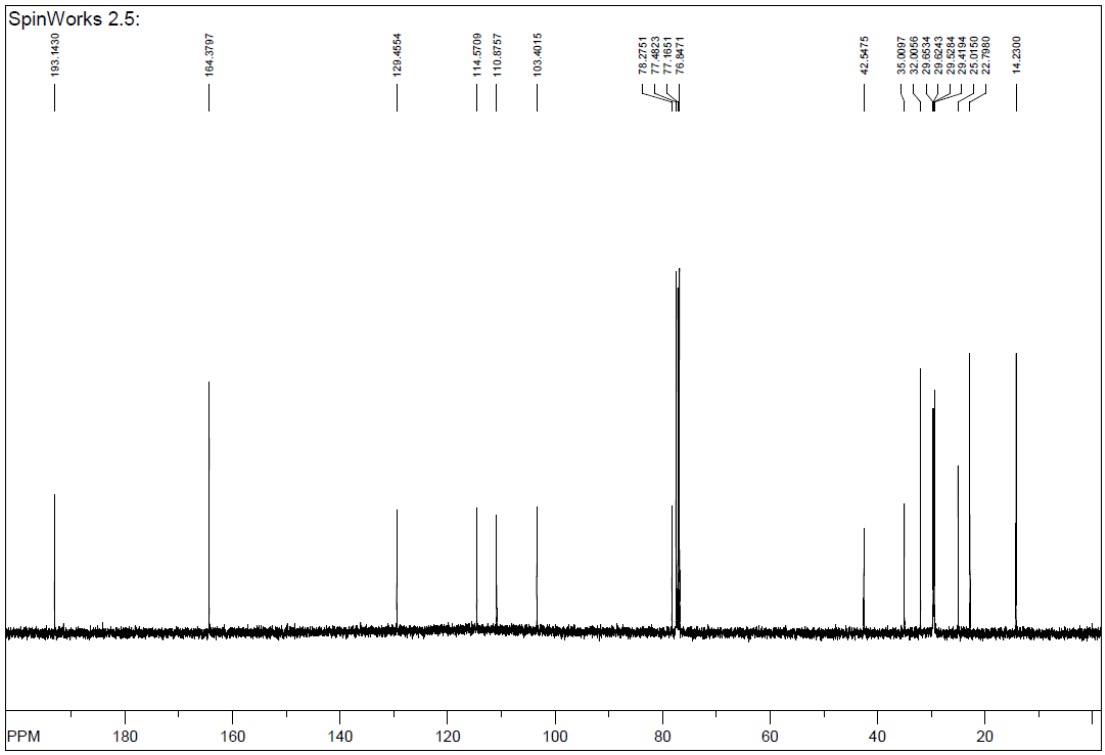

x10 7
-ESI Scan (0.139 min) Frag=70.0V Sun187_neg.d
261.1479
297.1232
375.1206
151.0396
227.1274
499.3655
577.1155
648.1450
761.4989
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **3d**



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-36\1\fid expt: <zg30>
transmitter freq.: 400.131600 MHz
time domain size: 65536 points
width: 8012.82 Hz = 20.025463 ppm = 0.122266 Hz/pt
number of scans: 8

freq. of 0 ppm: 400.130009 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 145.897 ppm/cm: 0.36462



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-36\20\fid expt: <zgpg30>
transmitter freq.: 100.622769 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.896840 ppm = 0.366798 Hz/pt
number of scans: 743

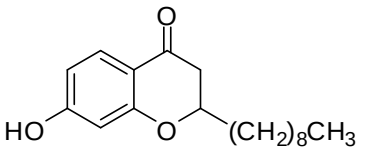
freq. of 0 ppm: 100.612756 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 820.155 ppm/cm: 8.15079

HPLC profile of **3d**

==== Shimadzu LCsolution Analysis Report ====

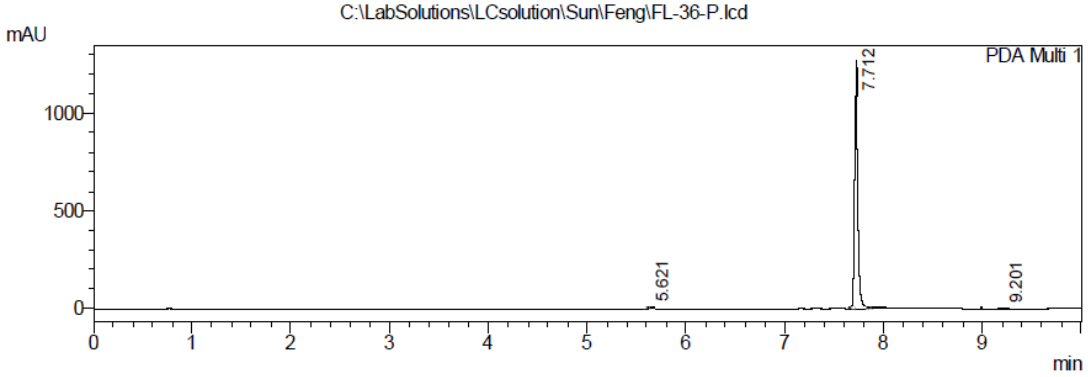
C:\LabSolutions\LCsolution\Sun\Feng\FL-36-P.lcd

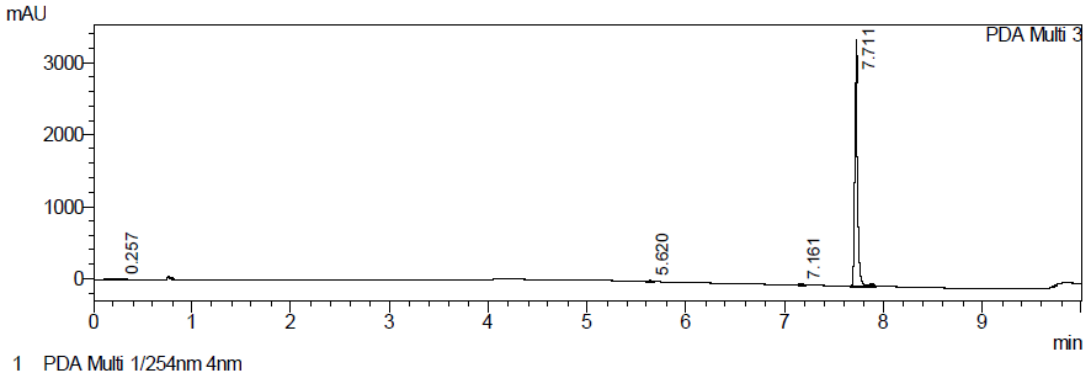
Sample Name	: FL-36-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 5 uL
Data File Name	: FL-36-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 12/2/2011 12:03:09 PM



<Chromatogram>

C:\LabSolutions\LCsolution\Sun\Feng\FL-36-P.lcd





1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

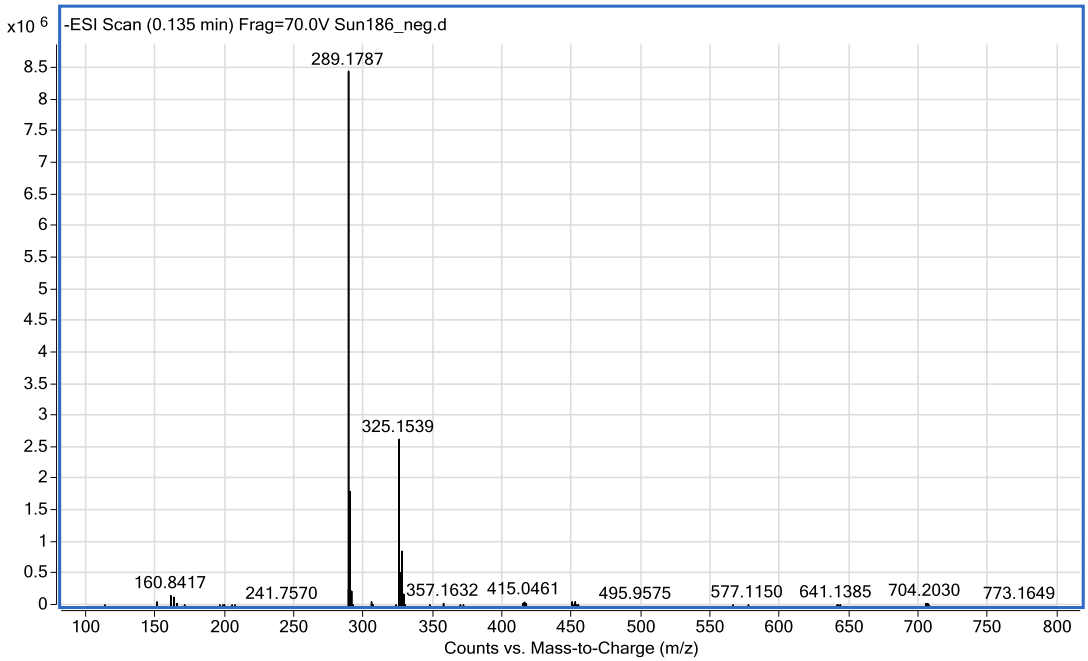
Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.621	16504	7168	0.513	0.582
2	7.712	3191912	1220214	99.149	99.100
3	9.201	10889	3915	0.338	0.318
Total		3219305	1231297	100.000	100.000

PeakTable

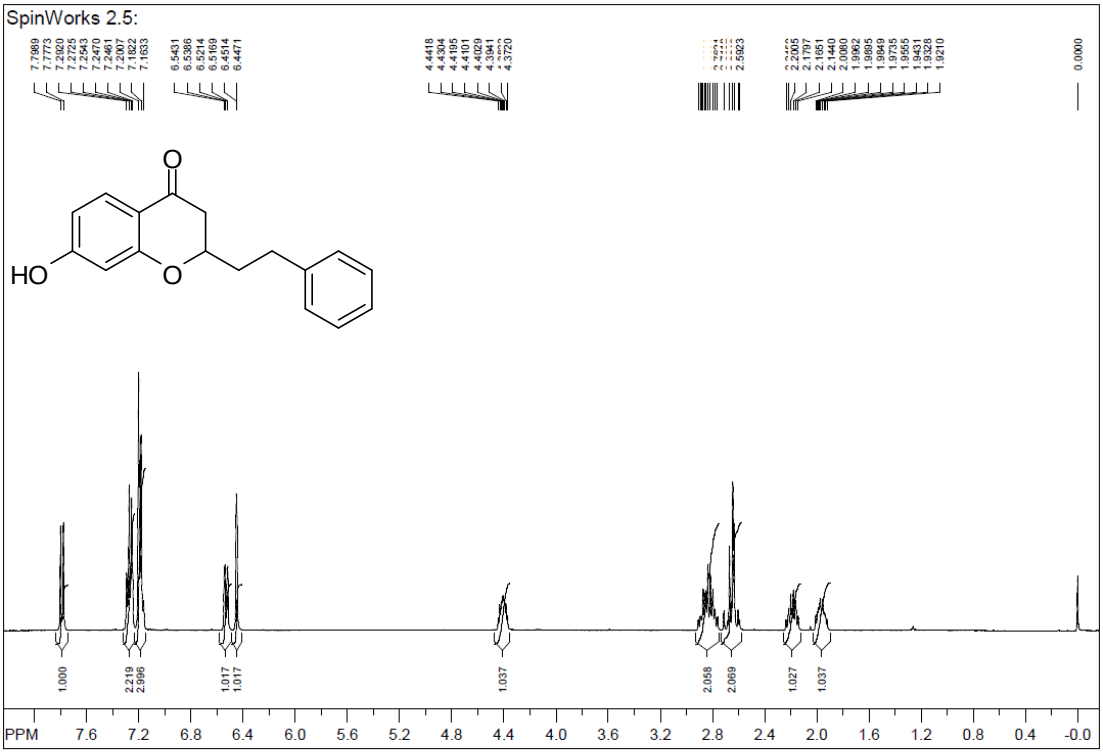
PDA Ch3 220nm 4nm

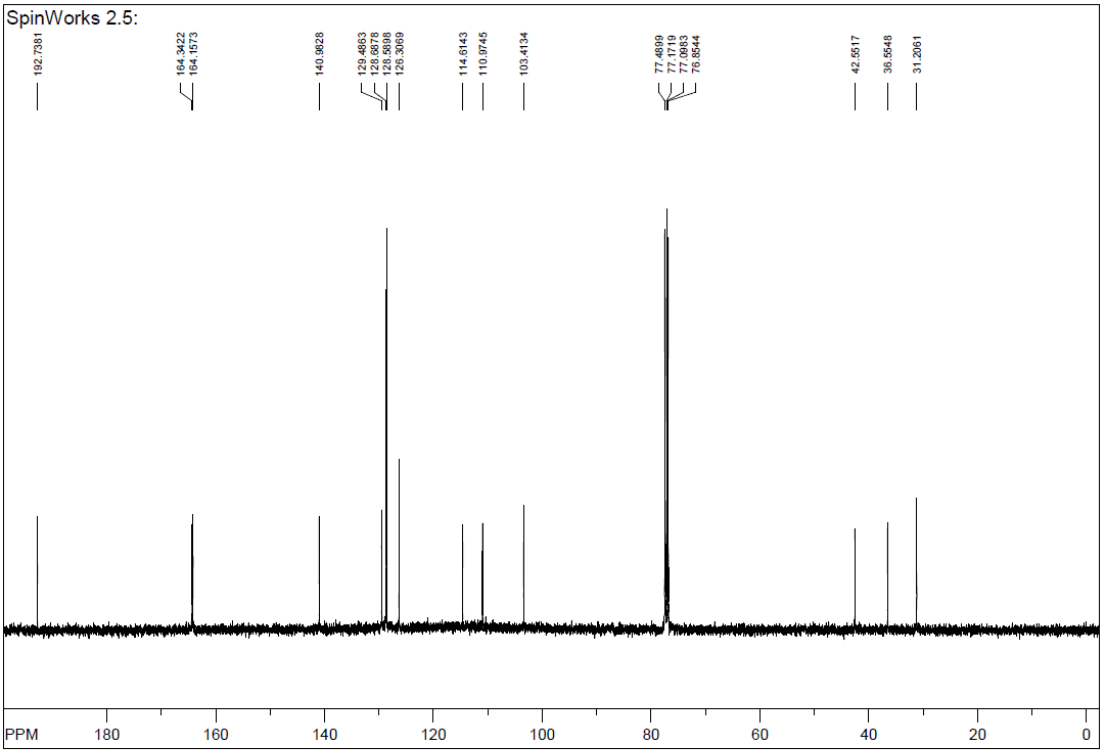
Peak#	Ret. Time	Area	Height	Area %	Height %
1	0.257	2074	255	0.028	0.007
2	5.620	29178	12902	0.390	0.375
3	7.161	23350	10158	0.312	0.295
4	7.711	7422250	3420679	99.270	99.323
Total		7476852	3443994	100.000	100.000

HRMS of **3d**


x10 6
-ESI Scan (0.135 min) Frag=70.0V Sun186_neg.d
289.1787
325.1539
160.8417
241.7570
357.1632
415.0461
495.9575
577.1150
641.1385
704.2030
773.1649
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **3e**



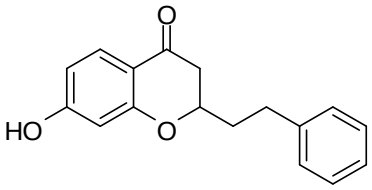


HPLC profile of **3e**

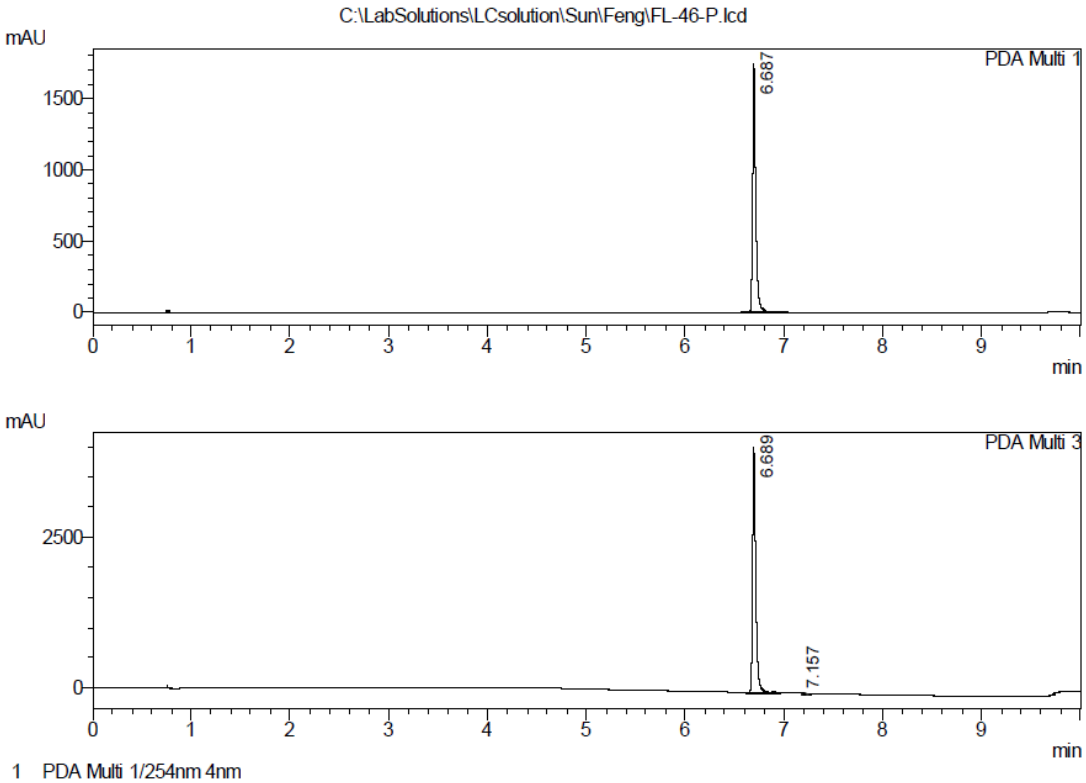
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\Feng\FL-46-P.lcd

Sample Name	: FL-46-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 5 uL
Data File Name	: FL-46-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	: Batch 1.lcb
Data Acquired	: 12/2/2011 1:35:47 PM



<Chromatogram>



1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

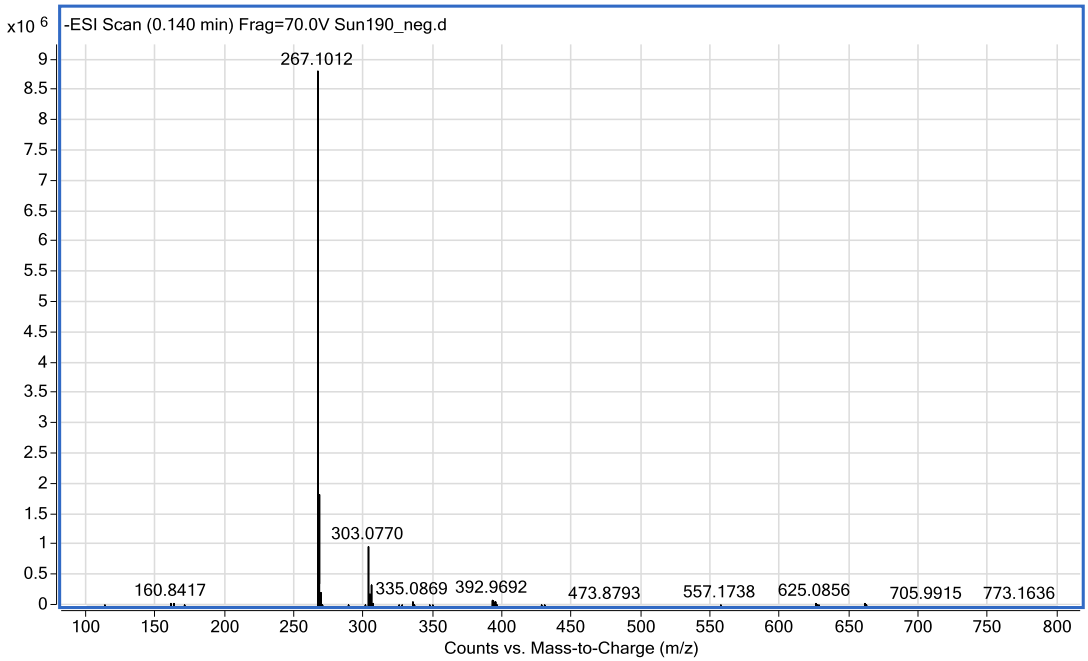
Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.687	4335892	1710572	100.000	100.000
Total		4335892	1710572	100.000	100.000

PeakTable

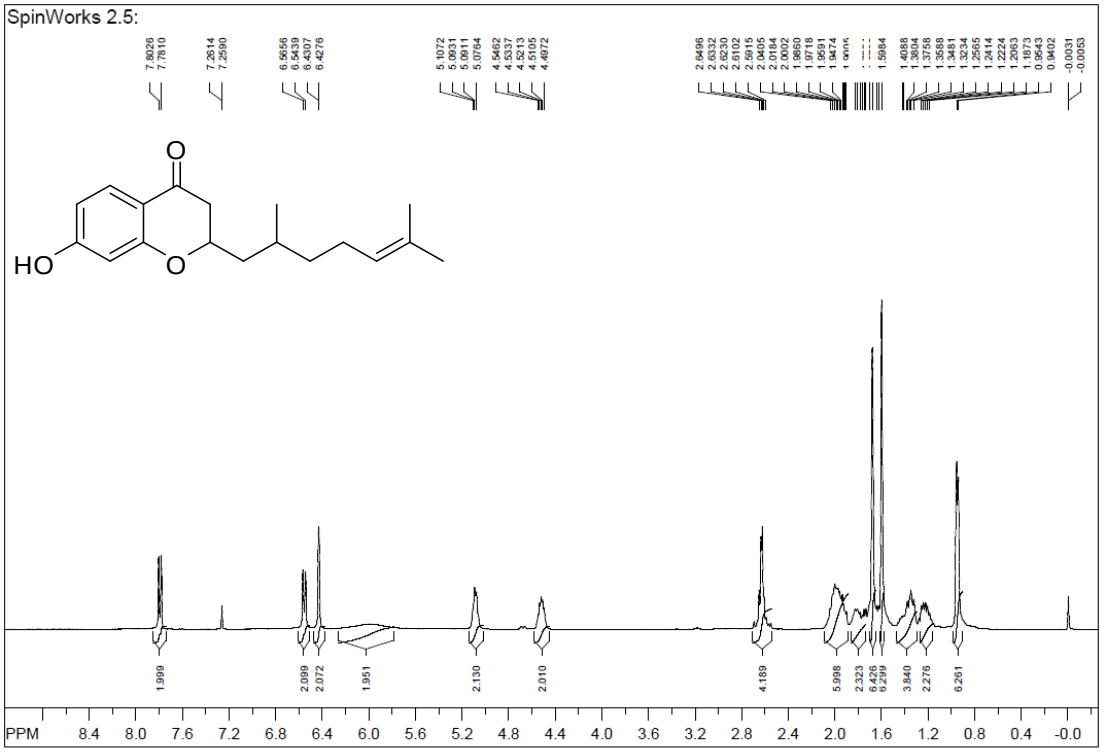
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.689	10422186	4069912	99.500	99.614
2	7.157	52372	15764	0.500	0.386
Total		10474558	4085676	100.000	100.000

HRMS of **3e**


x10 6
-ESI Scan (0.140 min) Frag=70.0V Sun190_neg.d
267.1012
303.0770
160.8417
335.0869
392.9692
473.8793
557.1738
625.0856
705.9915
773.1636
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **3f**



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-67\1\fid expt: <zg30>
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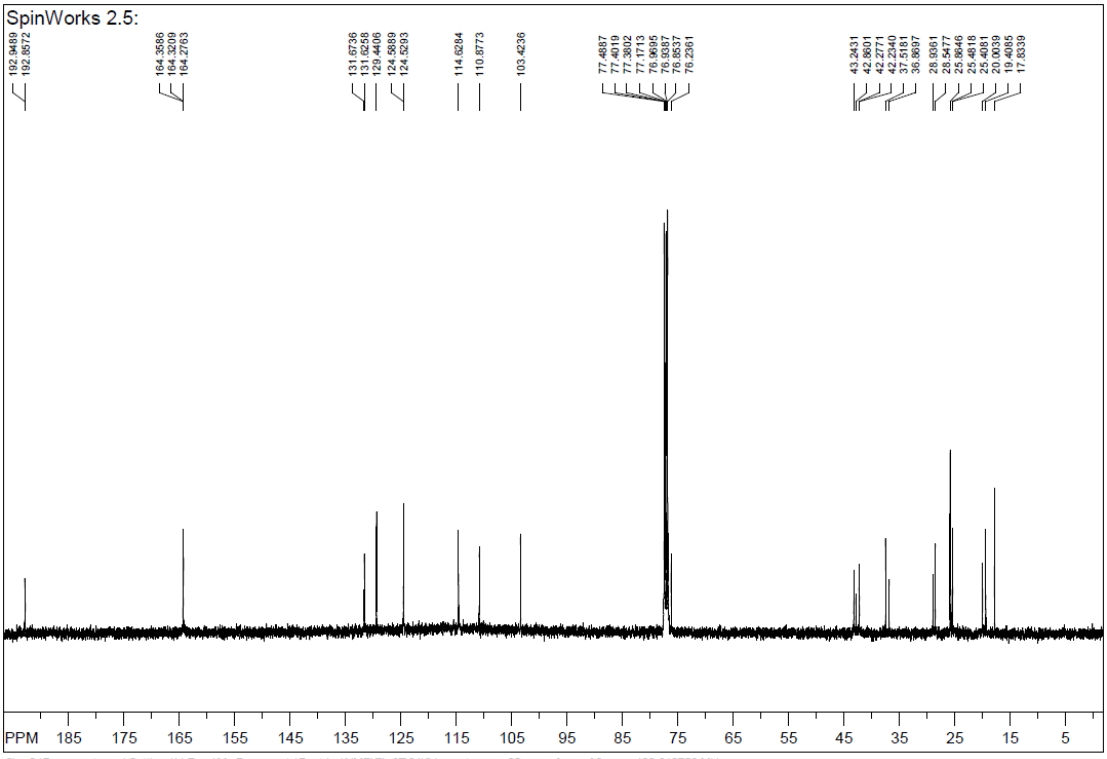
time domain size: 65536 points
width: 8012.82 Hz = 20.025463 ppm = 0.122266 Hz/pt
number of scans: 4

freq. of 0 ppm: 400.130007 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 150.262 ppm/cm: 0.37553



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-67\21\fid expt: <zgpg30>
transmitter freq.: 100.622769 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.896840 ppm = 0.366798 Hz/pt
number of scans: 1240

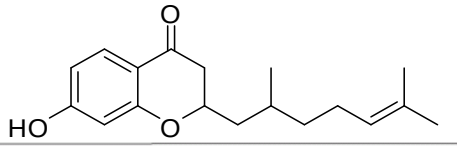
freq. of 0 ppm: 100.612756 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 798.790 ppm/cm: 7.93846

HPLC profile of **3f**

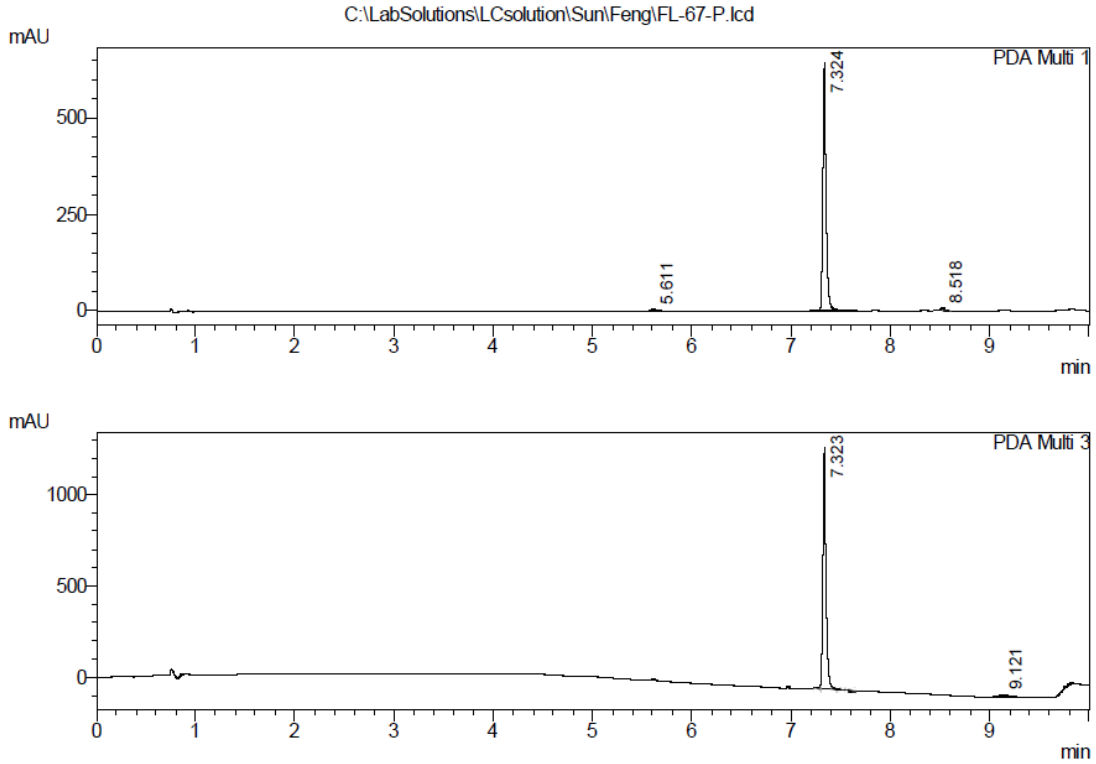
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\Feng\FL-67-P.lcd

Sample Name	: FL-67-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 3 uL
Data File Name	: FL-67-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 11/28/2011 5:12:41 PM



<Chromatogram>



1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

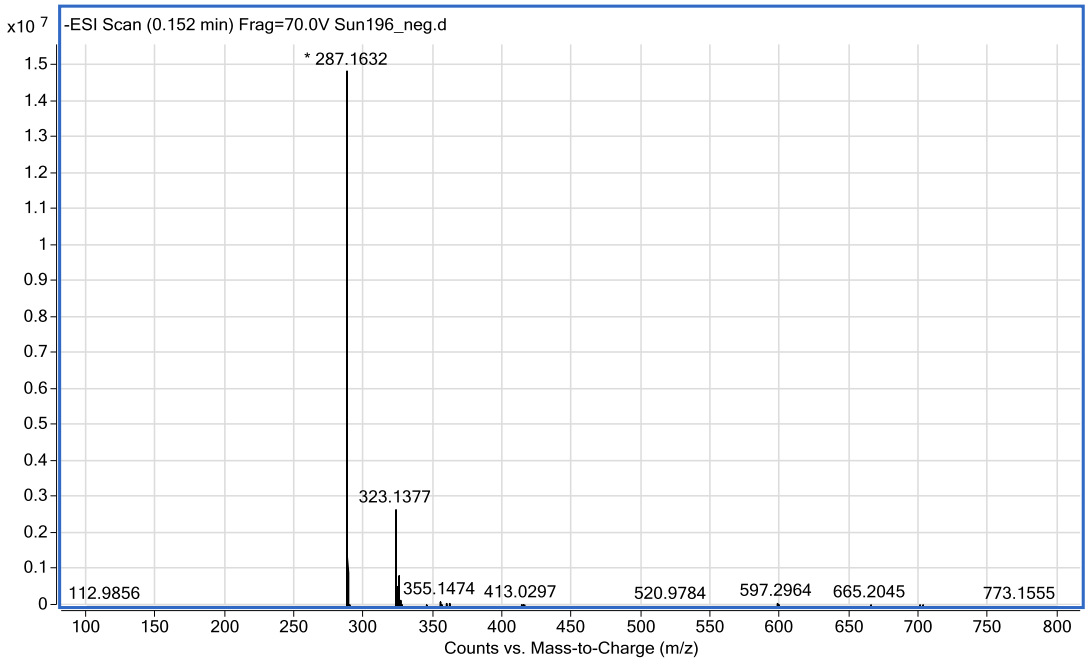
Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.611	14238	5819	0.838	0.889
2	7.324	1660986	640346	97.755	97.837
3	8.518	23900	8340	1.407	1.274
Total		1699124	654505	100.000	100.000

PeakTable

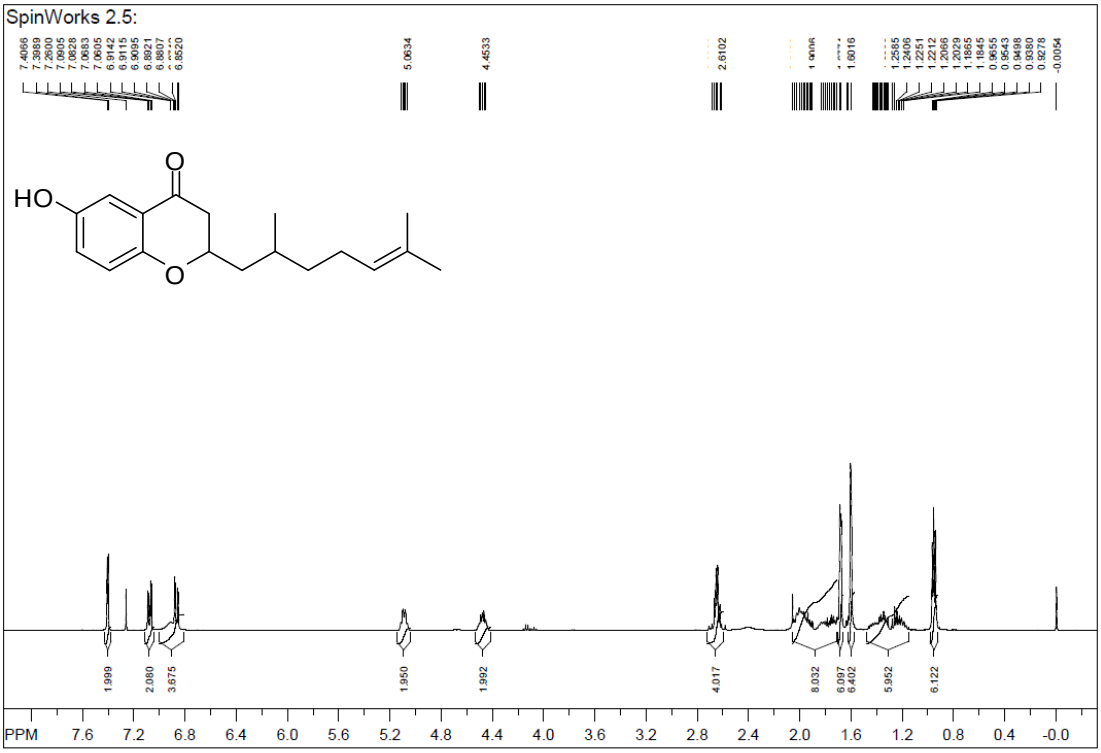
PDA Ch3 220nm 4nm

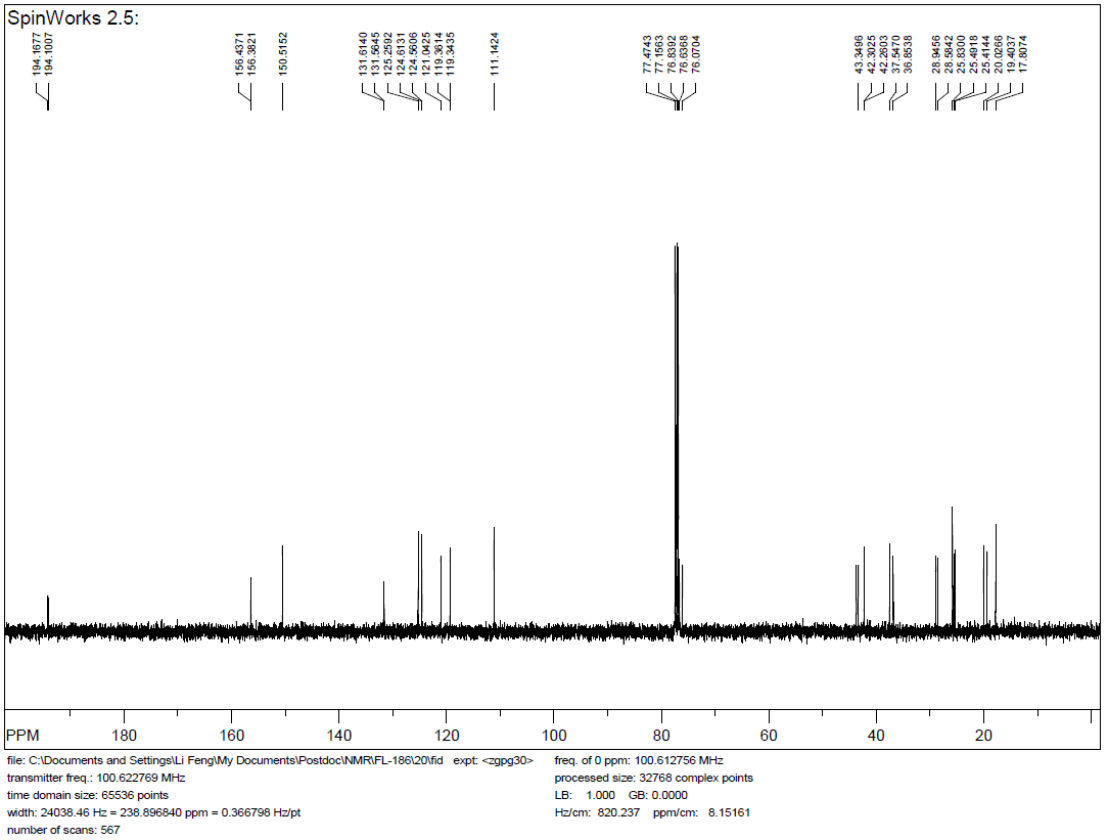
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.323	3281170	1325083	97.953	99.278
2	9.121	68574	9637	2.047	0.722
Total		3349744	1334720	100.000	100.000

HRMS of **3f**


x10 7
-ESI Scan (0.152 min) Frag=70.0V Sun196_neg.d
* 287.1632
323.1377
355.1474
413.0297
112.9856
520.9784
597.2964
665.2045
773.1555
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **3k**



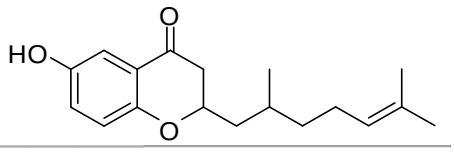


HPLC profile of **3k**

==== Shimadzu LCsolution Analysis Report ====

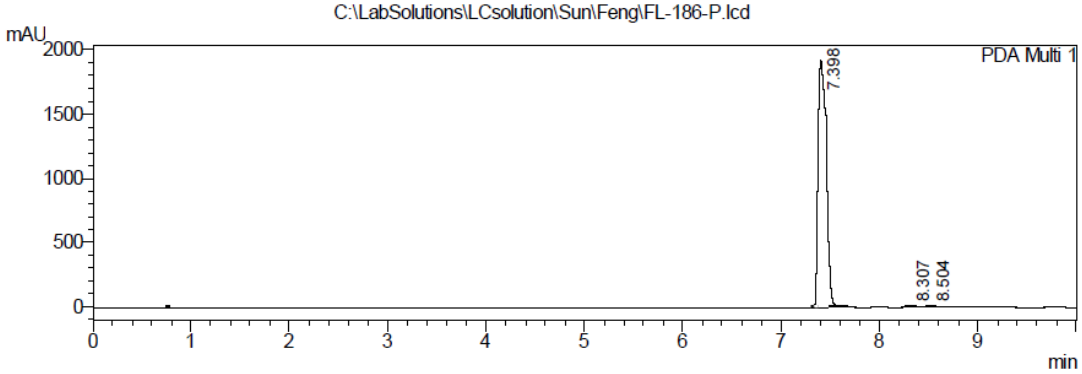
C:\LabSolutions\LCsolution\Sun\Feng\FL-186-P.lcd

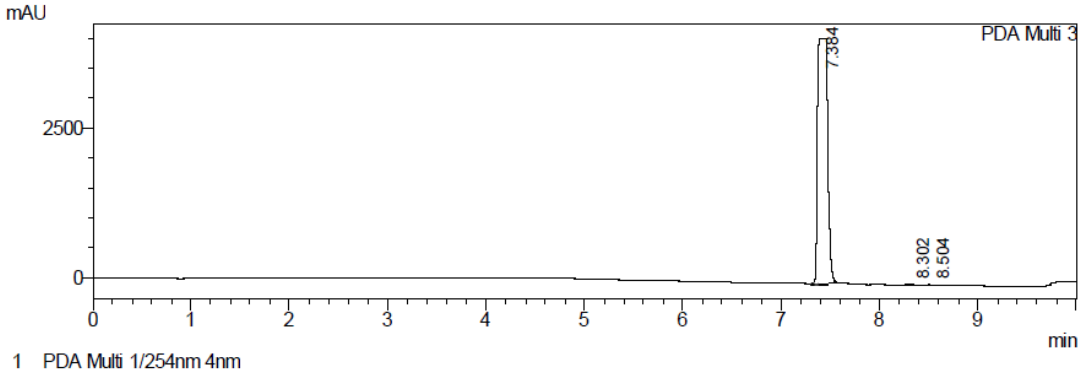
Sample Name	: FL-186-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 10 uL
Data File Name	: FL-186-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 3/12/2012 2:17:22 PM



<Chromatogram>

C:\LabSolutions\LCsolution\Sun\Feng\FL-186-P.lcd





1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

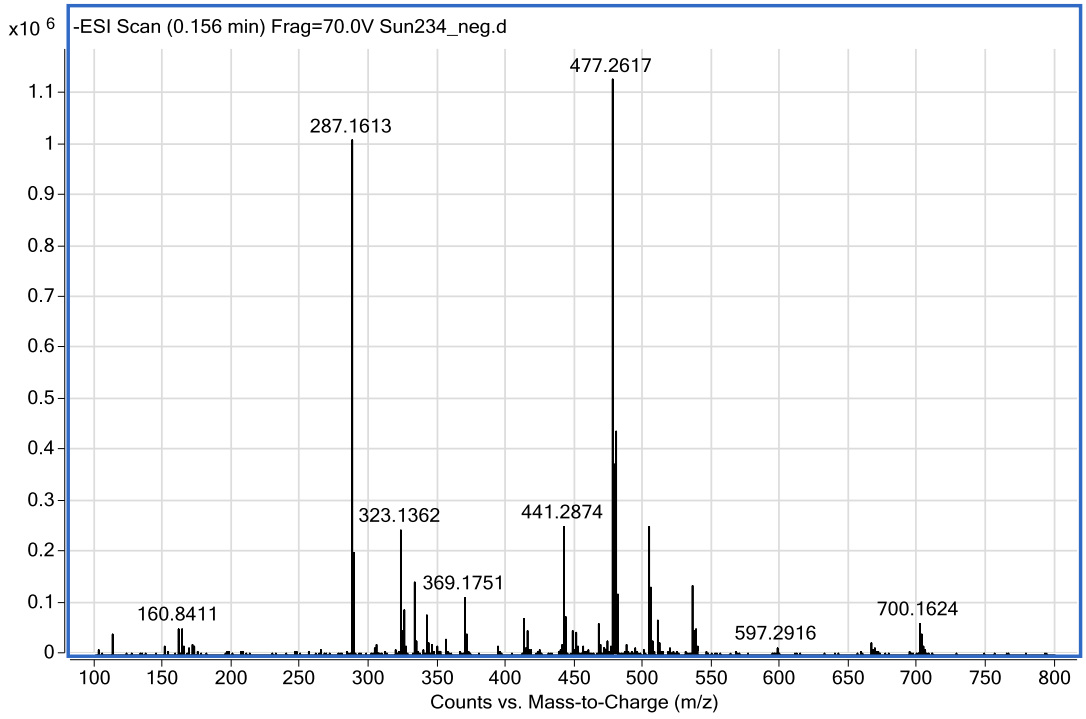
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.398	11218053	1908614	99.758	99.620
2	8.307	13698	3564	0.122	0.186
3	8.504	13466	3711	0.120	0.194
Total		11245217	1915890	100.000	100.000

PeakTable

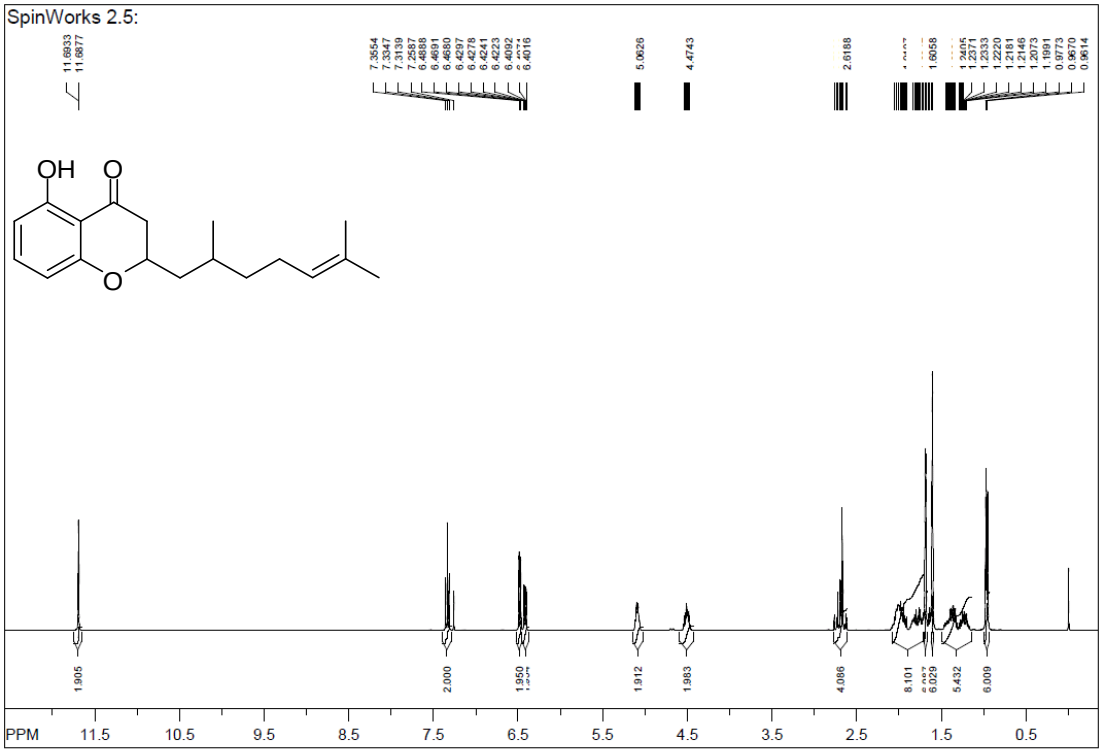
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.384	29465755	4083768	99.711	99.564
2	8.302	58447	11464	0.198	0.280
3	8.504	26810	6400	0.091	0.156
Total		29551012	4101632	100.000	100.000

HRMS of **3k**

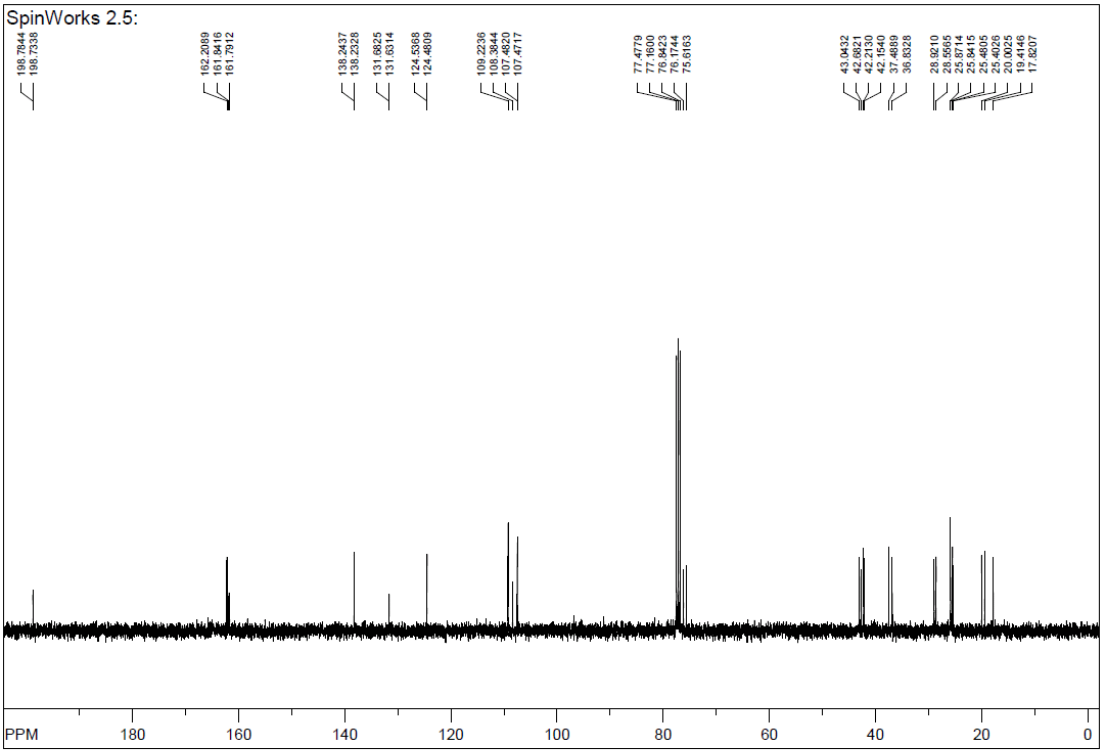

x10 6
-ESI Scan (0.156 min) Frag=70.0V Sun234_neg.d
477.2617
287.1613
323.1362
441.2874
369.1751
160.8411
597.2916
700.1624
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **3l**



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-187\1\fid expt: <zg30>
transmitter freq.: 400.131600 MHz
time domain size: 65536 points
width: 8012.82 Hz = 20.025463 ppm = 0.122266 Hz/pt
number of scans: 4

freq. of 0 ppm: 400.130010 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 206.782 ppm/cm: 0.51679



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-187\20\fid expt: <zgpg30>
transmitter freq.: 100.622769 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.896840 ppm = 0.366798 Hz/pt
number of scans: 448

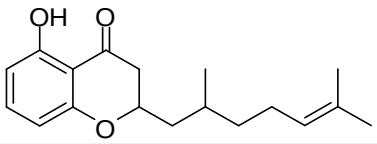
freq. of 0 ppm: 100.612755 MHz
processed size: 32768 complex points
LB: 1.000 GB: 0.0000
Hz/cm: 830.576 ppm/cm: 8.25436

HPLC profile of **3l**

==== Shimadzu LCsolution Analysis Report ====

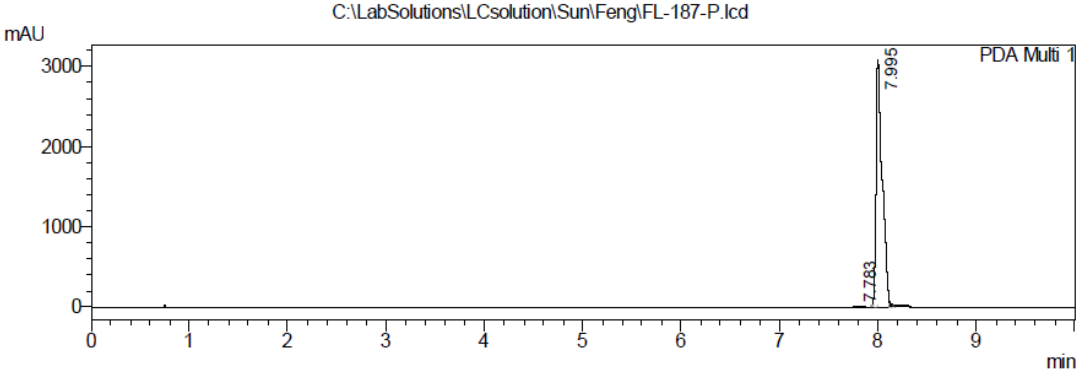
C:\LabSolutions\LCsolution\Sun\Feng\FL-187-P.lcd

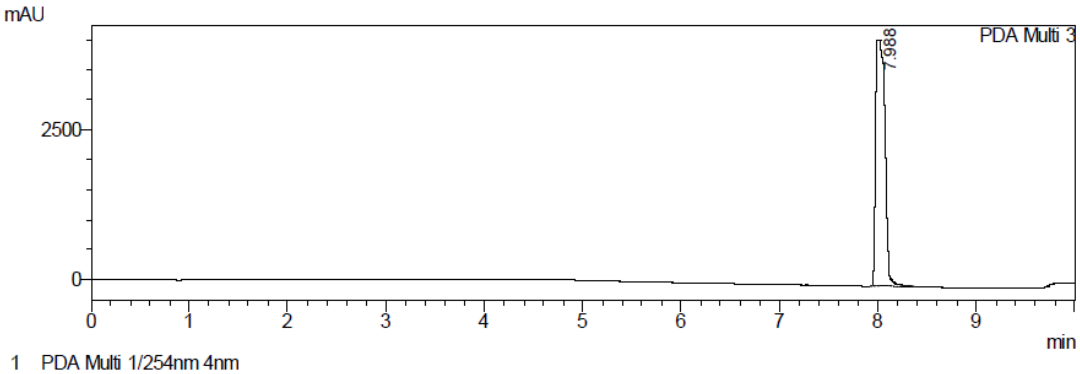
Sample Name	: FL-187-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 10 uL
Data File Name	: FL-187-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 3/13/2012 2:06:54 PM



<Chromatogram>

C:\LabSolutions\LCsolution\Sun\Feng\FL-187-P.lcd





1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

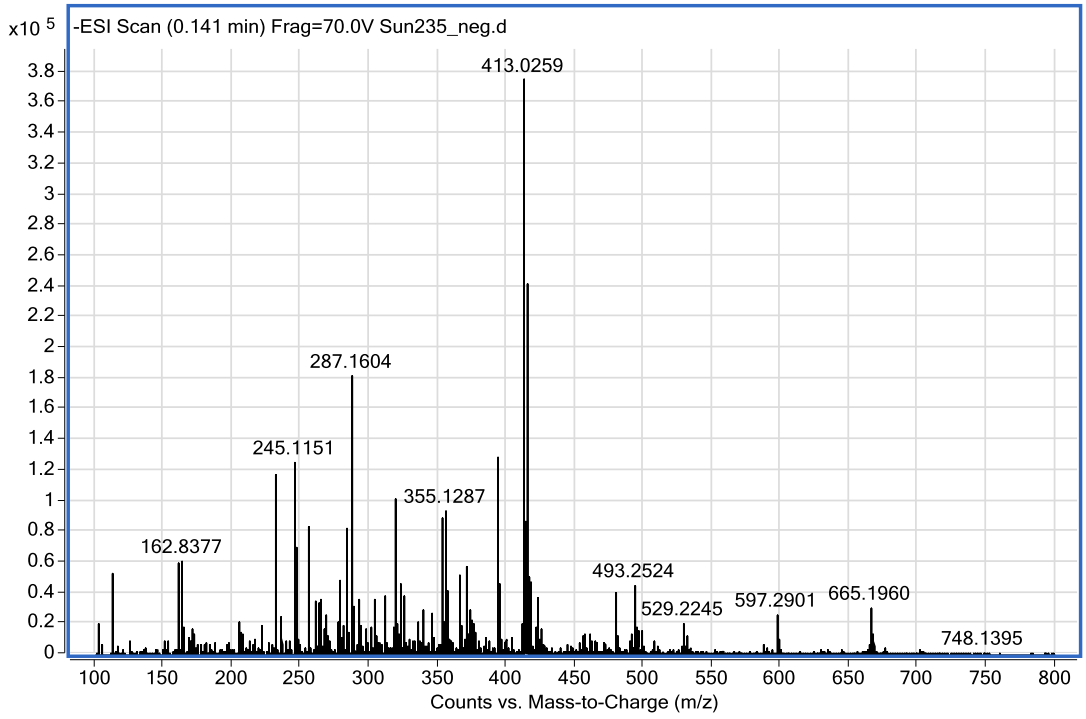
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.783	16231	4167	0.116	0.136
2	7.995	14010644	3070812	99.884	99.864
Total		14026875	3074979	100.000	100.000

PeakTable

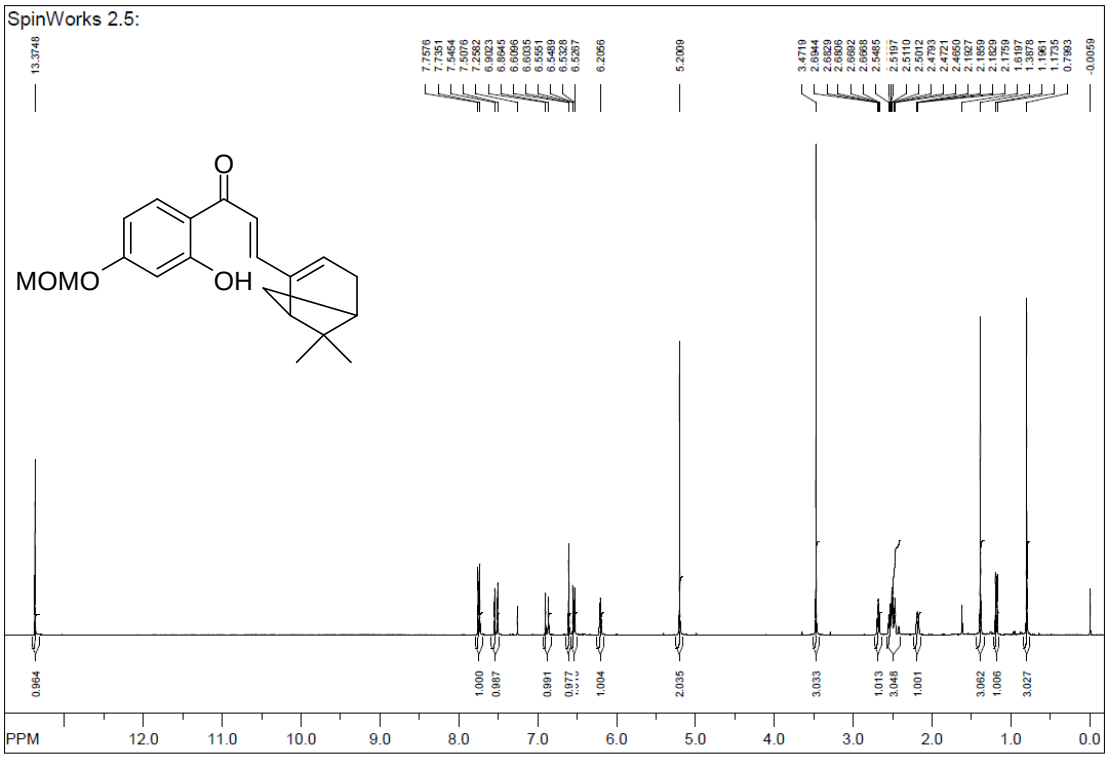
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.988	27678026	4099350	100.000	100.000
Total		27678026	4099350	100.000	100.000

HRMS of **3l**

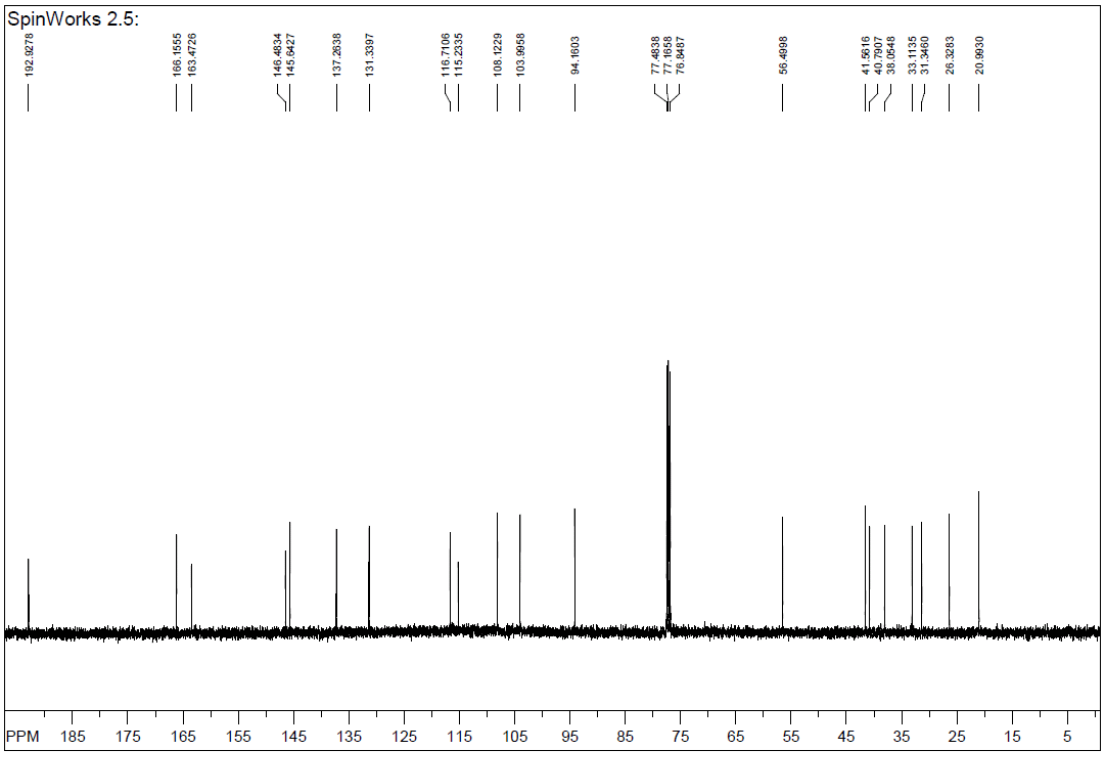

x10 5
-ESI Scan (0.141 min) Frag=70.0V Sun235_neg.d
413.0259
287.1604
245.1151
355.1287
162.8377
493.2524
529.2245
597.2901
665.1960
748.1395
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **3h**



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-57\3\fid expt: <zg30>
transmitter freq.: 400.131600 MHz
time domain size: 65536 points
width: 8012.82 Hz = 20.025463 ppm = 0.122266 Hz/pt
number of scans: 8

freq. of 0 ppm: 400.130010 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 223.095 ppm/cm: 0.55755



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-57\20\fid expt: <zgpg30>
transmitter freq.: 100.622769 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.896840 ppm = 0.366798 Hz/pt
number of scans: 431

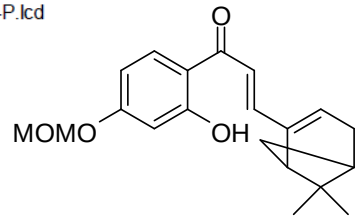
freq. of 0 ppm: 100.612756 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 797.412 ppm/cm: 7.92476

HPLC profile of **3h**

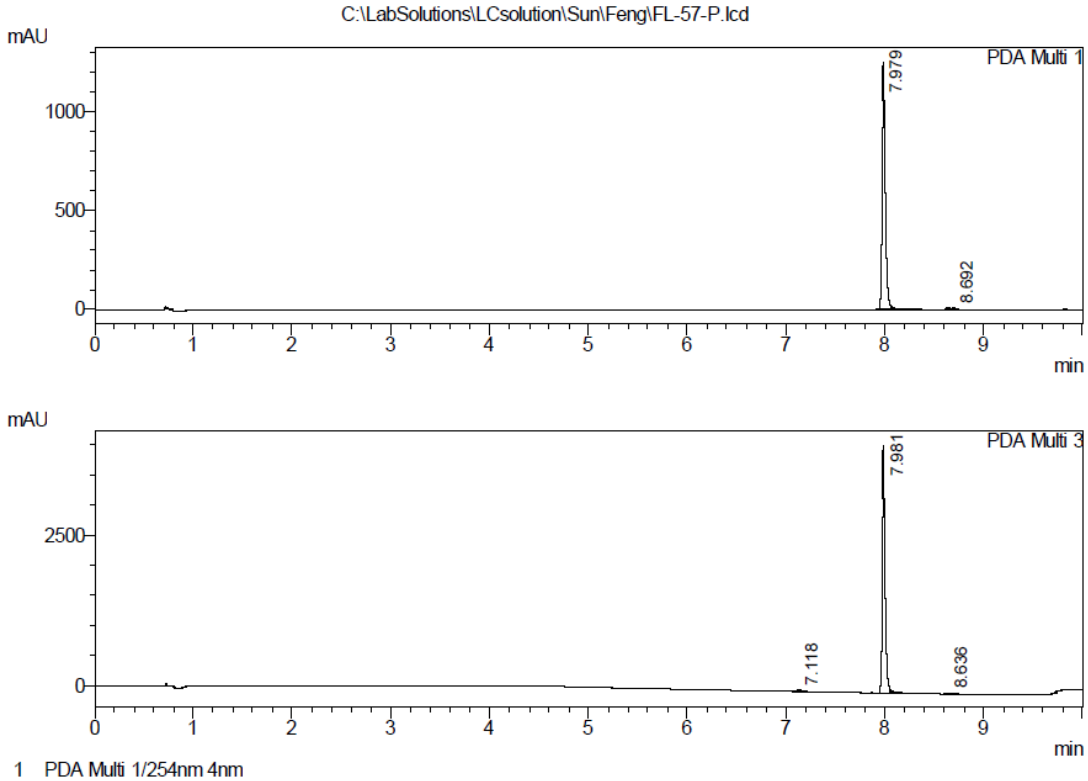
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\Feng\FL-57-P.lcd

Sample Name	: FL-57-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 20 uL
Data File Name	: FL-57-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 12/2/2011 4:46:07 PM



<Chromatogram>



1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

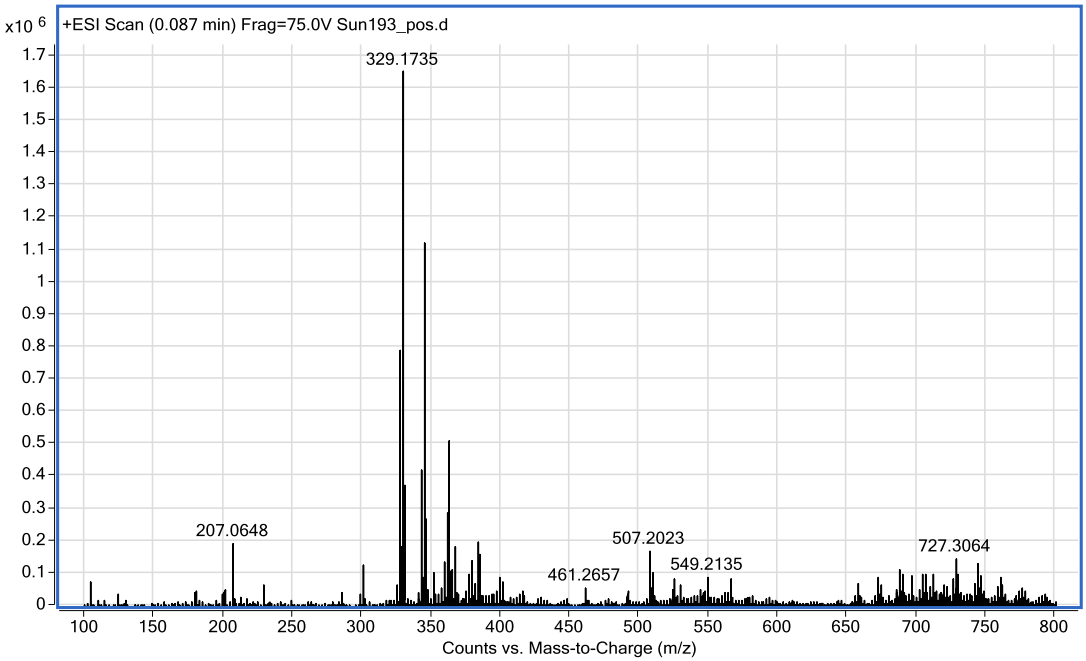
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.979	3105651	1235106	98.809	99.251
2	8.692	37427	9324	1.191	0.749
Total		3143078	1244430	100.000	100.000

PeakTable

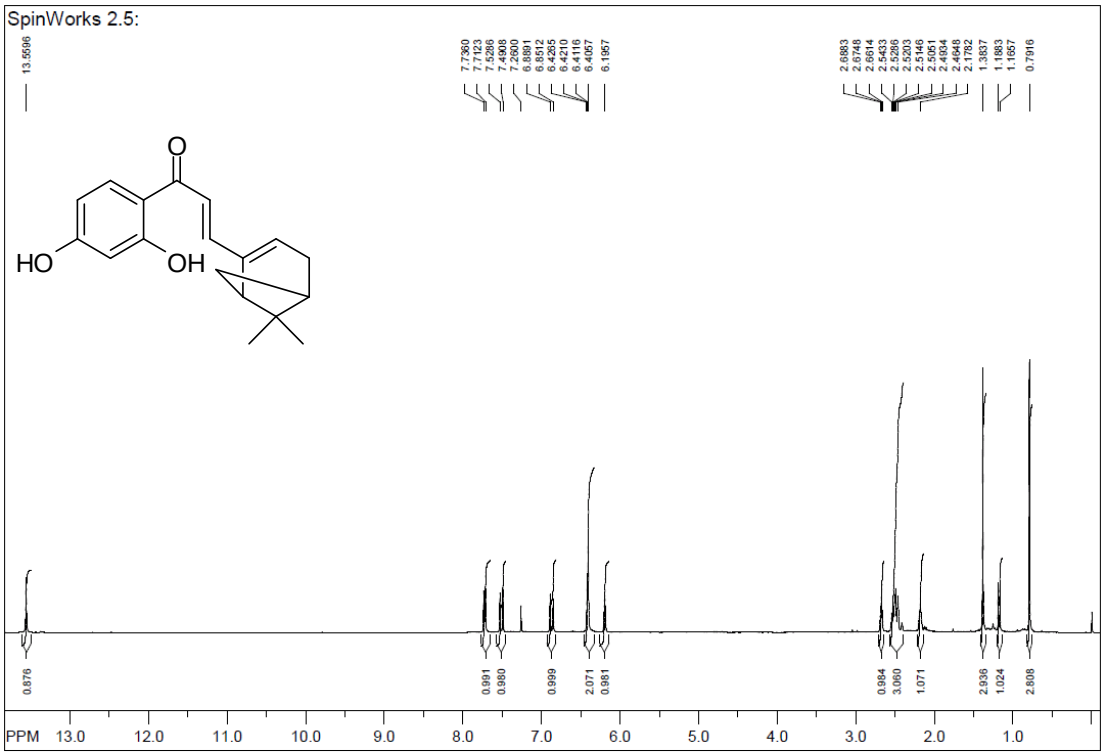
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.118	88162	20061	0.971	0.486
2	7.981	8949523	4096692	98.543	99.283
3	8.636	44145	9517	0.486	0.231
Total		9081831	4126270	100.000	100.000

HRMS of **3h**

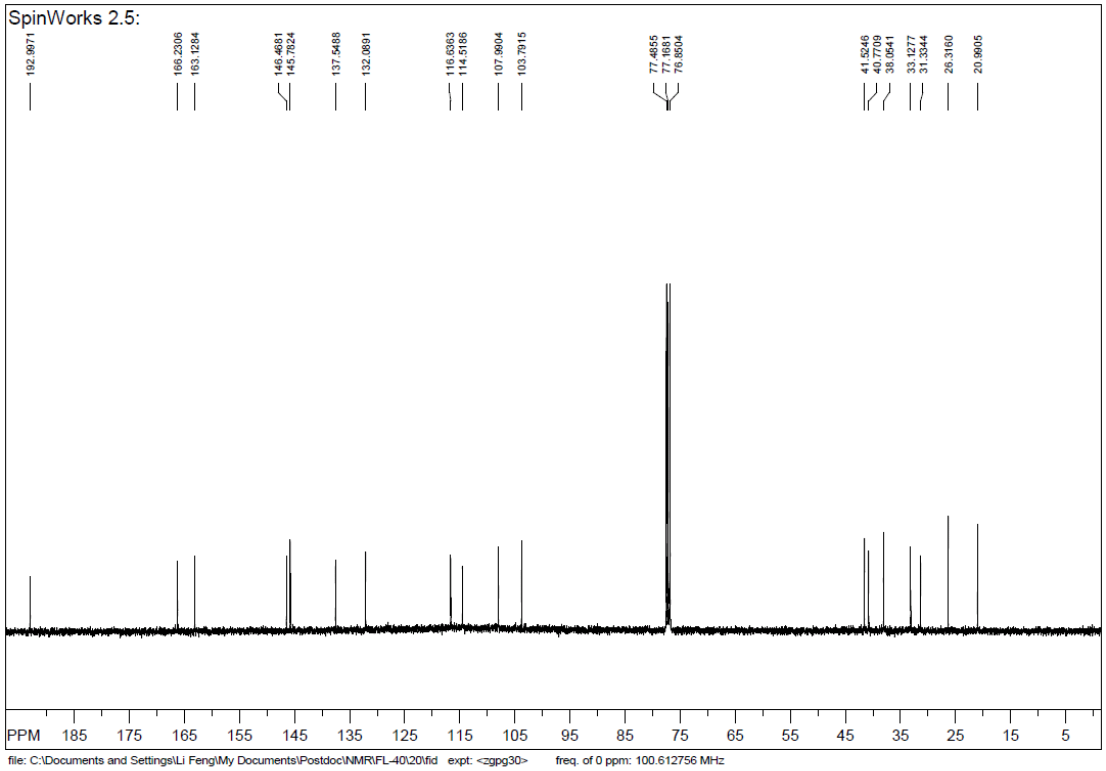

x10 6
+ESI Scan (0.087 min) Frag=75.0V Sun193_pos.d
329.1735
207.0648
507.2023
549.2135
461.2657
727.3064
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **3g**



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-40\1\fid expt: <zg30>
transmitter freq.: 400.131600 MHz
time domain size: 65536 points
width: 8012.82 Hz = 20.025463 ppm = 0.122266 Hz/pt
number of scans: 16

freq. of 0 ppm: 400.130009 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 223.095 ppm/cm: 0.55755



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-40\20\fid expt: <zgpg30>
transmitter freq.: 100.622769 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.896840 ppm = 0.366798 Hz/pt
number of scans: 1522

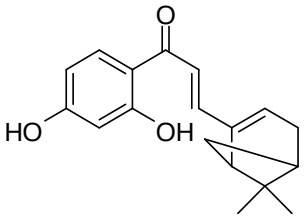
freq. of 0 ppm: 100.612756 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 800.169 ppm/cm: 7.95216

HPLC profile of **3g**

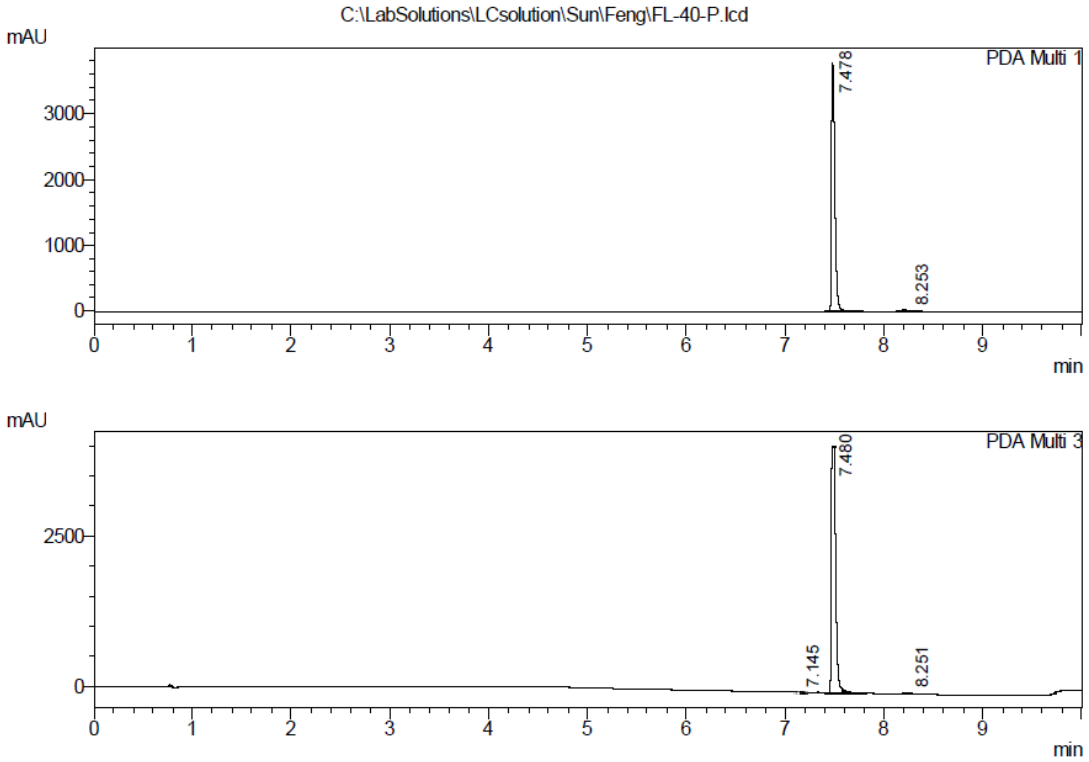
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\Feng\FL-40-P.lcd

Sample Name	: FL-40-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 3 uL
Data File Name	: FL-40-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 12/6/2011 3:40:08 PM



<Chromatogram>



1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

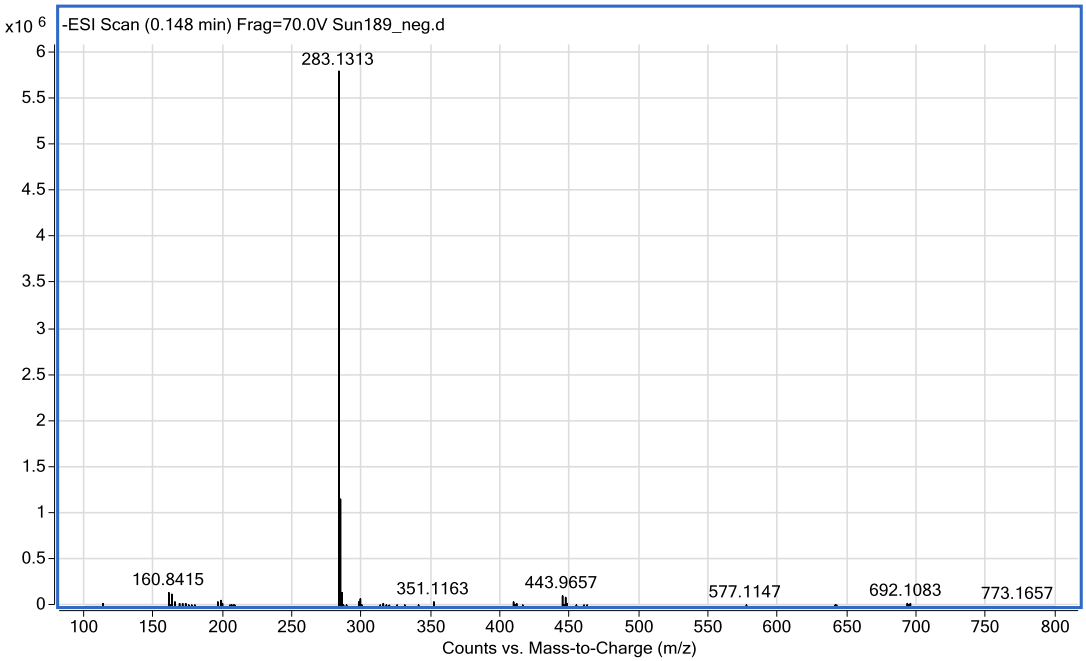
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.478	8505954	3643264	99.296	99.679
2	8.253	60315	11737	0.704	0.321
Total		8566269	3655001	100.000	100.000

PeakTable

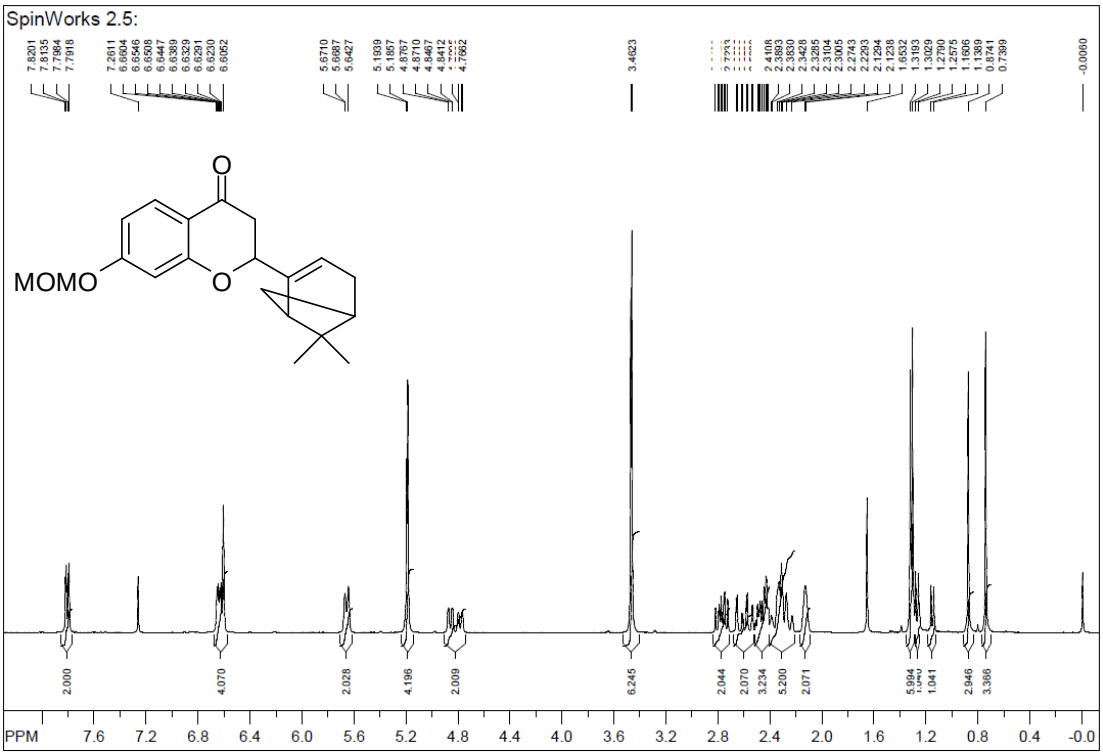
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.145	55275	16808	0.429	0.408
2	7.480	12782274	4093945	99.159	99.313
3	8.251	53176	11505	0.413	0.279
Total		12890725	4122258	100.000	100.000

HRMS of **3g**

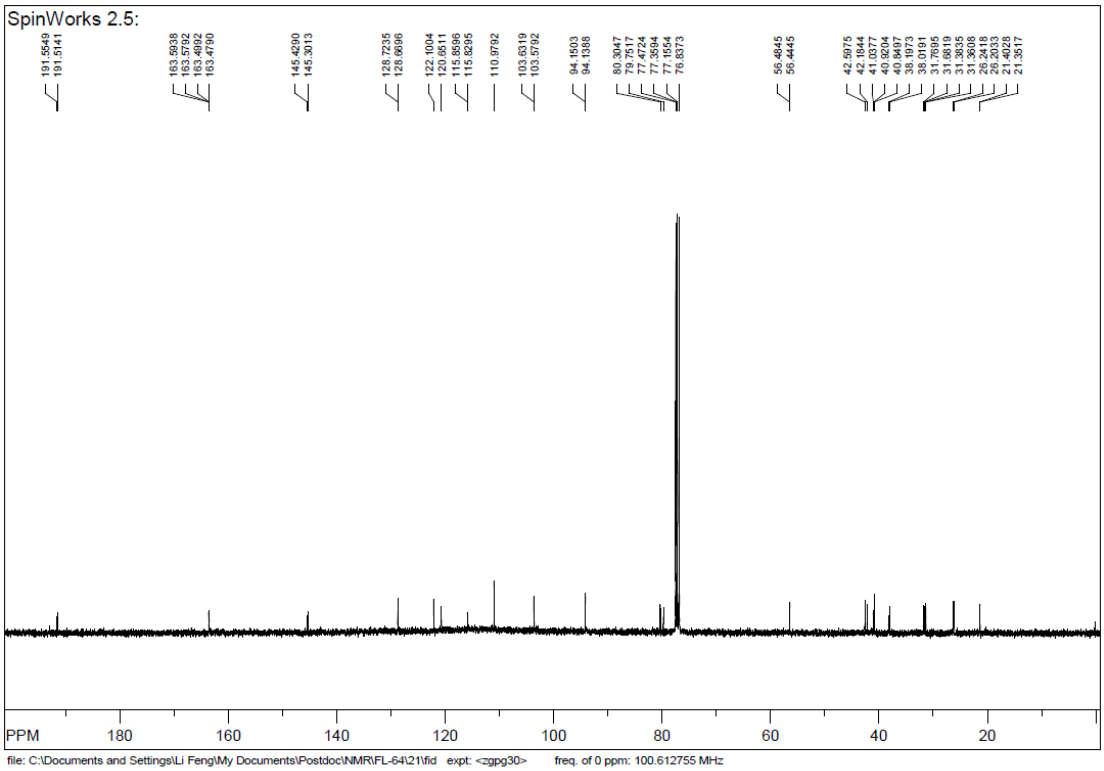

x10 6
-ESI Scan (0.148 min) Frag=70.0V Sun189_neg.d
283.1313
160.8415
351.1163
443.9657
577.1147
692.1083
773.1657
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **3i**



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-64\1\1\fid expt: <zg30>
transmitter freq.: 400.131600 MHz
time domain size: 65536 points
width: 8012.82 Hz = 20.025463 ppm = 0.122266 Hz/pt
number of scans: 8

freq. of 0 ppm: 400.130007 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 134.868 ppm/cm: 0.33706



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-64\21\1\fid expt: <zgpg30>
transmitter freq.: 100.622769 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.896840 ppm = 0.366798 Hz/pt
number of scans: 2274

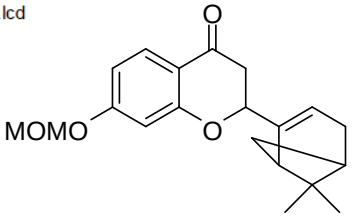
freq. of 0 ppm: 100.612755 MHz
processed size: 32768 complex points
LB: 1.000 GB: 0.0000
Hz/cm: 812.655 ppm/cm: 8.07625

HPLC profile of **3i**

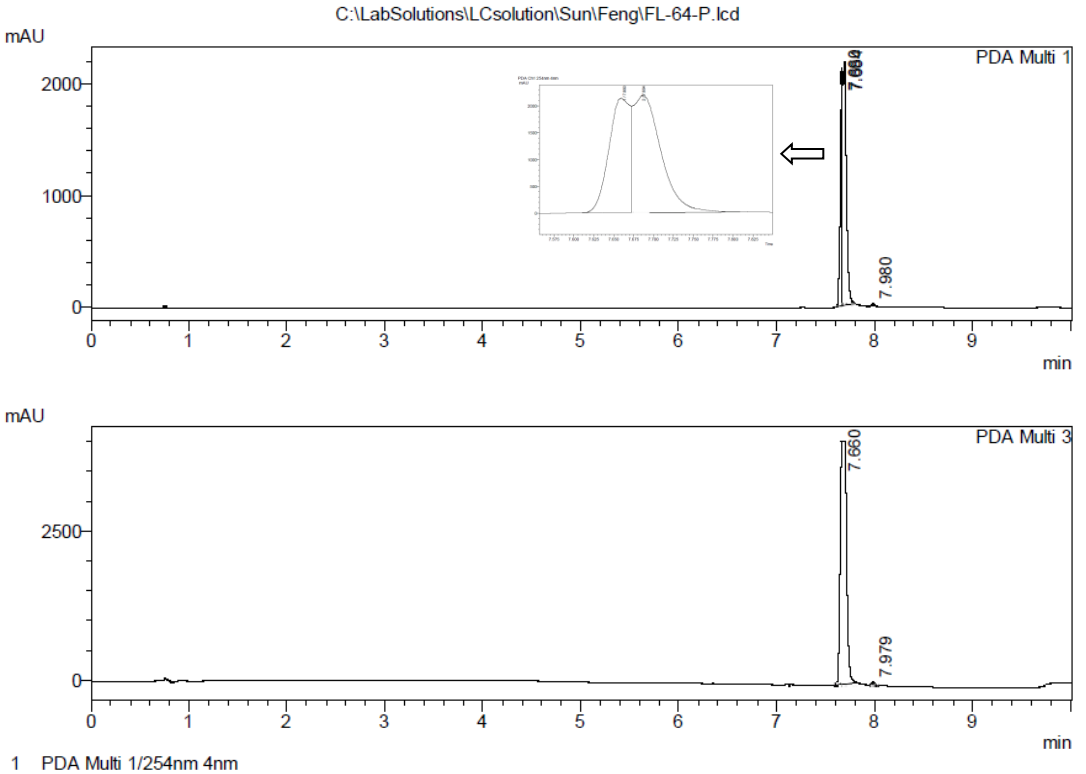
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\Feng\FL-64-P.lcd

Sample Name	: FL-64-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 5 uL
Data File Name	: FL-64-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 11/28/2011 5:36:07 PM



<Chromatogram>



1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.660	4084107	2103162	44.665	49.005
2	7.684	5029259	2170121	55.002	50.565
3	7.980	30472	18483	0.333	0.431
Total		9143837	4291766	100.000	100.000

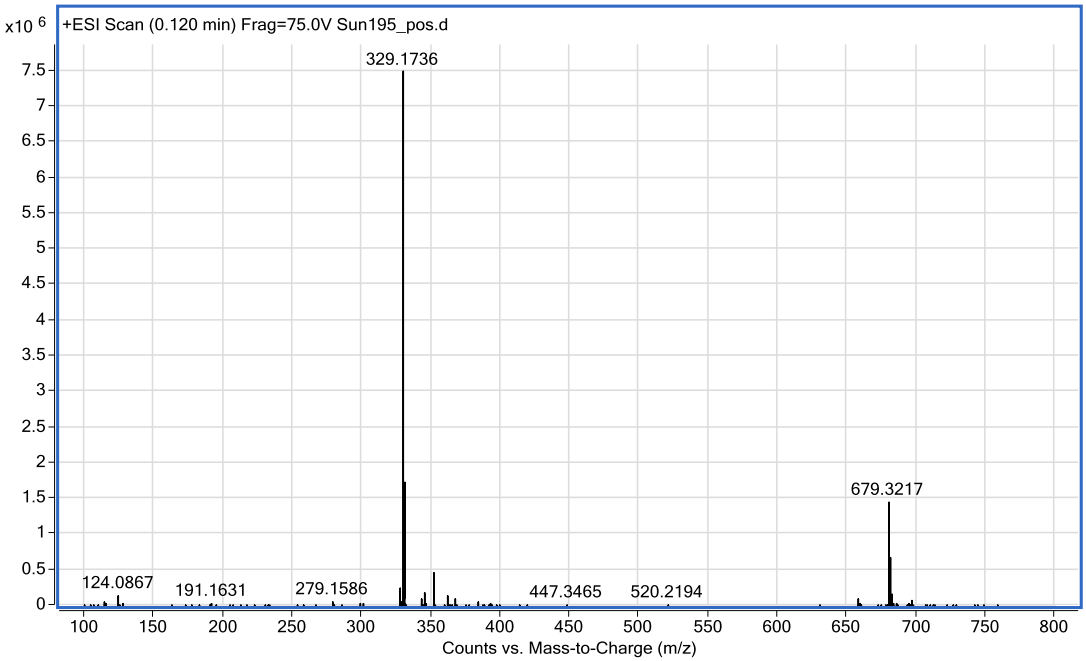
PeakTable

PDA Ch3 220nm 4nm

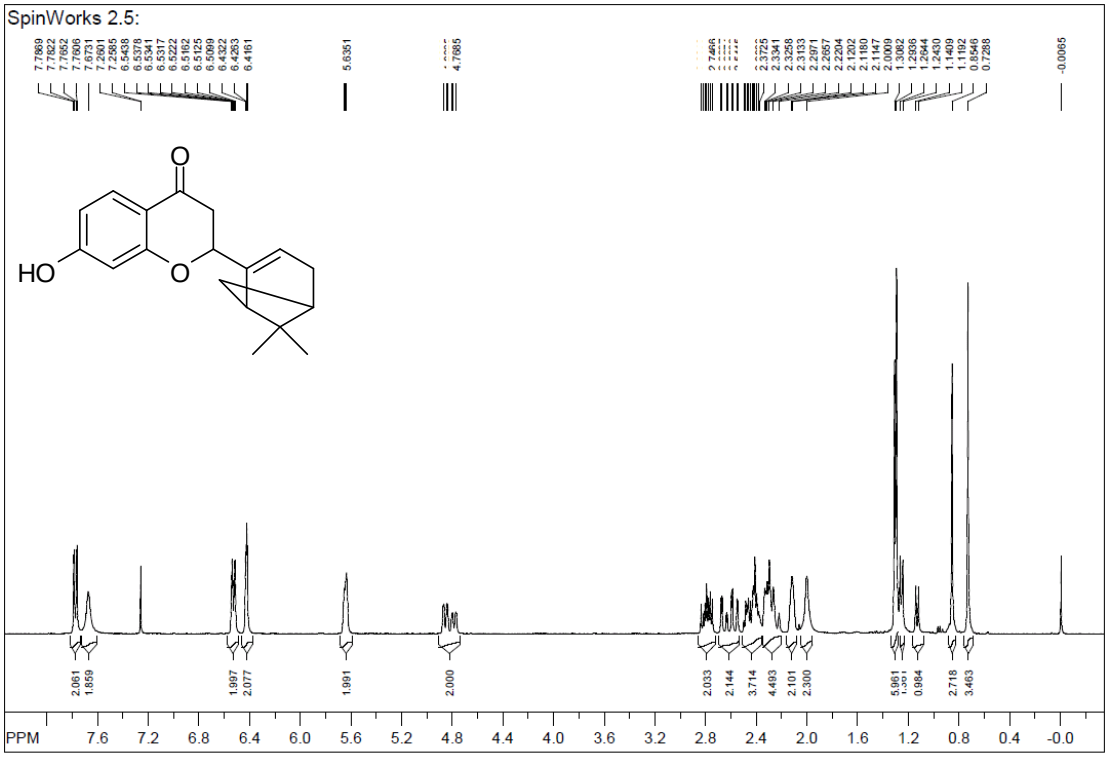
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.660	19071139	4051657	99.455	98.799
2	7.979	104542	49253	0.545	1.201
Total		19175681	4100910	100.000	100.000

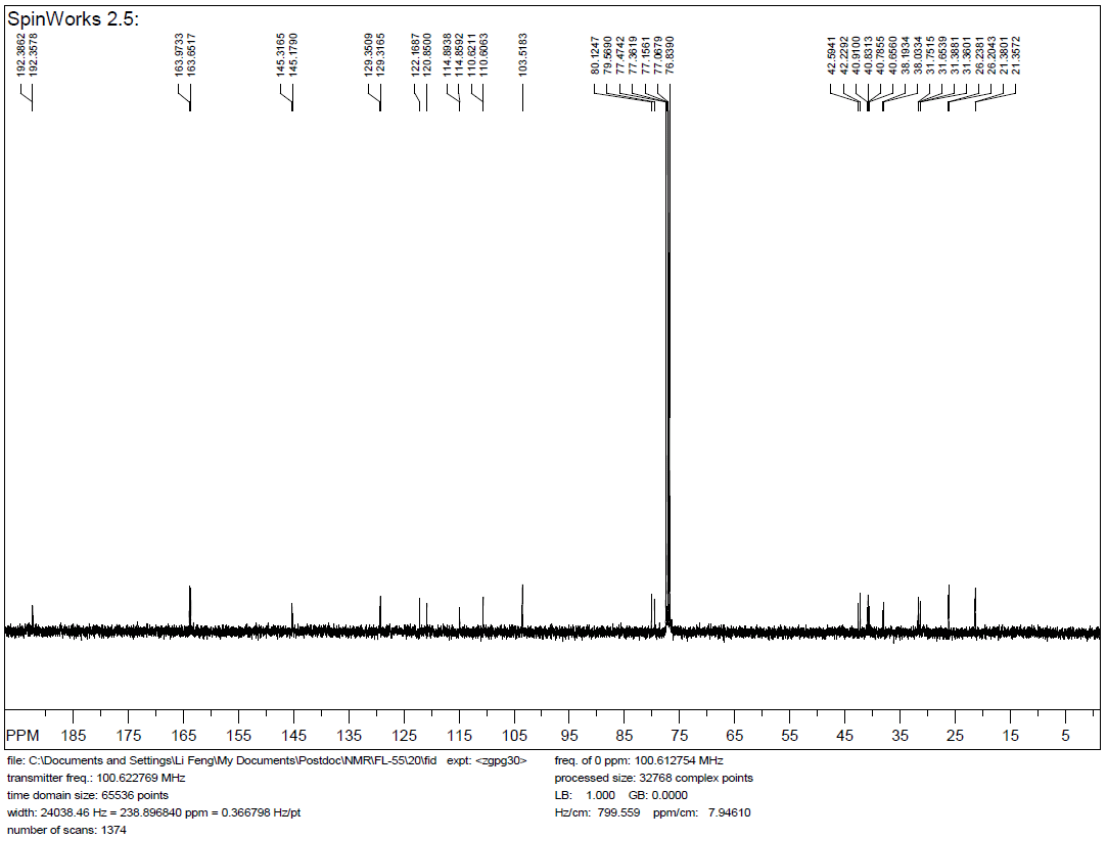
*A split HPLC trace (7.66 min and 7.68 min) under 254 nm further supported that the product was formed as a mixture of two diastereomers.

HRMS of **3i**


x10 6
+ESI Scan (0.120 min) Frag=75.0V Sun195_pos.d
329.1736
679.3217
124.0867
191.1631
279.1586
447.3465
520.2194
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **3j**



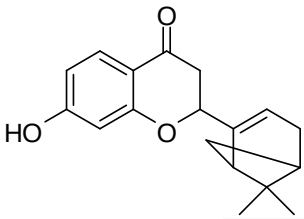


HPLC profile of **3j**

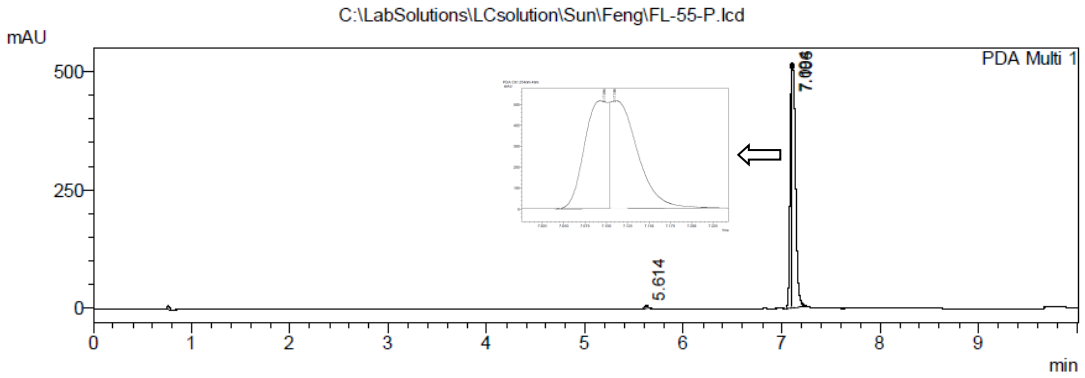
==== Shimadzu LCsolution Analysis Report ====

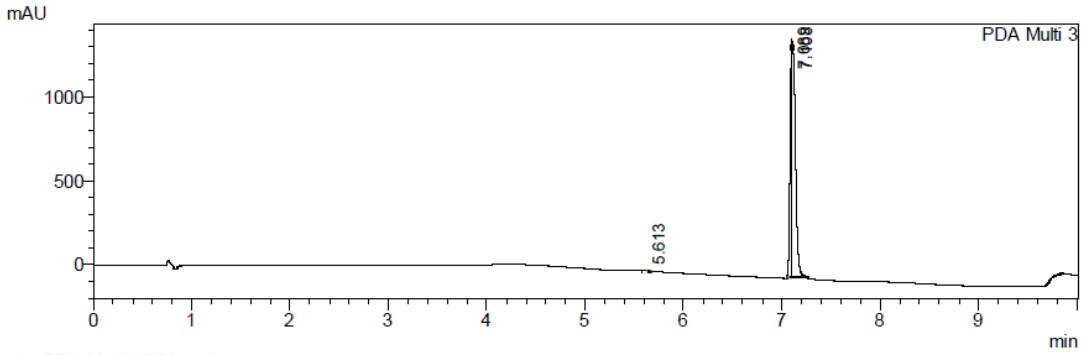
C:\LabSolutions\LCsolution\Sun\Feng\FL-55-P.lcd

Sample Name	: FL-55-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 5 uL
Data File Name	: FL-55-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 11/28/2011 5:25:06 PM



<Chromatogram>





1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.614	12167	6040	0.565	0.584
2	7.094	1060621	513987	49.280	49.684
3	7.106	1079451	514480	50.155	49.732
Total		2152239	1034507	100.000	100.000

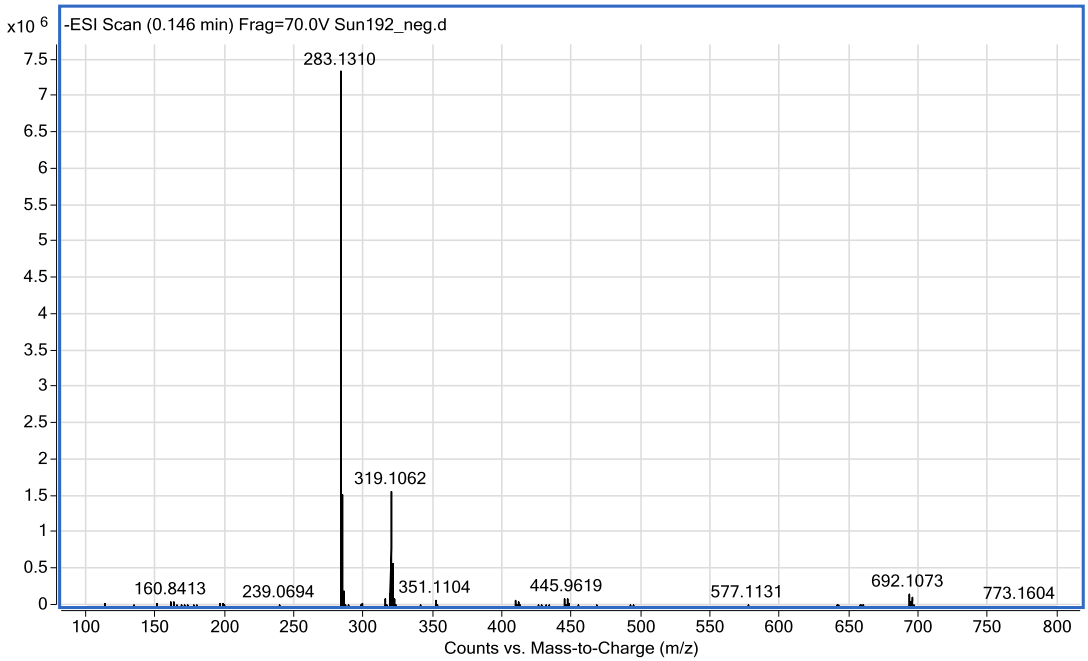
PeakTable

PDA Ch3 220nm 4nm

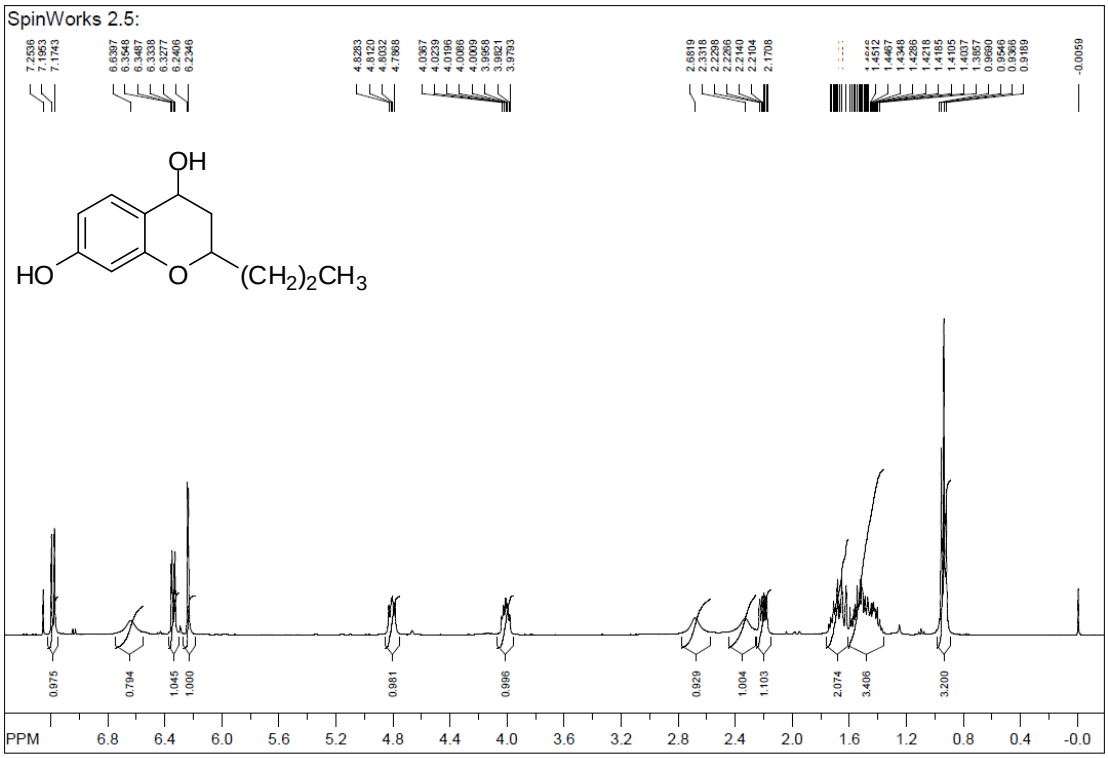
Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.613	24787	11545	0.431	0.409
2	7.089	2893672	1428123	50.335	50.591
3	7.108	2830365	1383196	49.234	49.000
Total		5748824	2822864	100.000	100.000

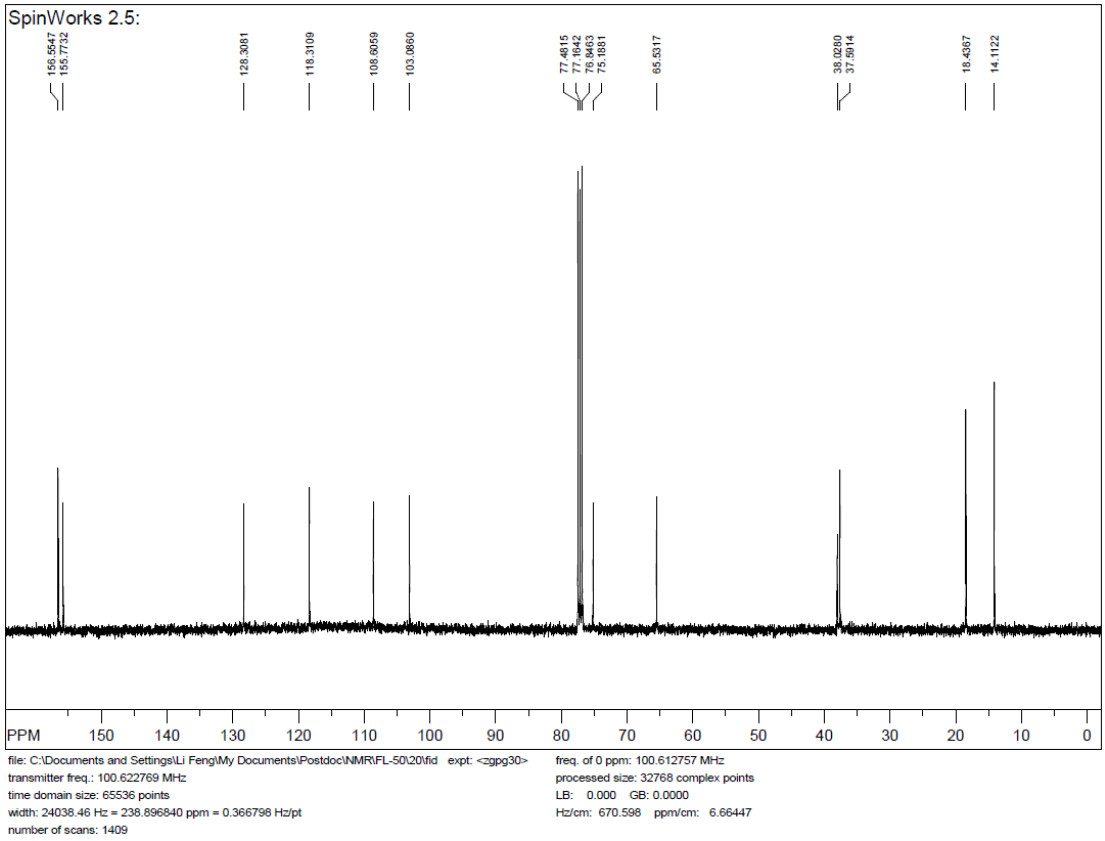
*A split HPLC trace (7.09 min and 7.11 min) further supported that the product was formed as a mixture of two diastereomers.

HRMS of **3j**


x10 6
-ESI Scan (0.146 min) Frag=70.0V Sun192_neg.d
283.1310
319.1062
160.8413
239.0694
351.1104
445.9619
577.1131
692.1073
773.1604
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **4a**



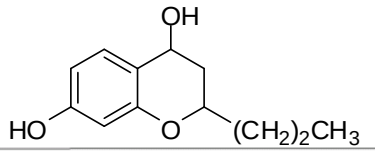


HPLC profile of **4a**

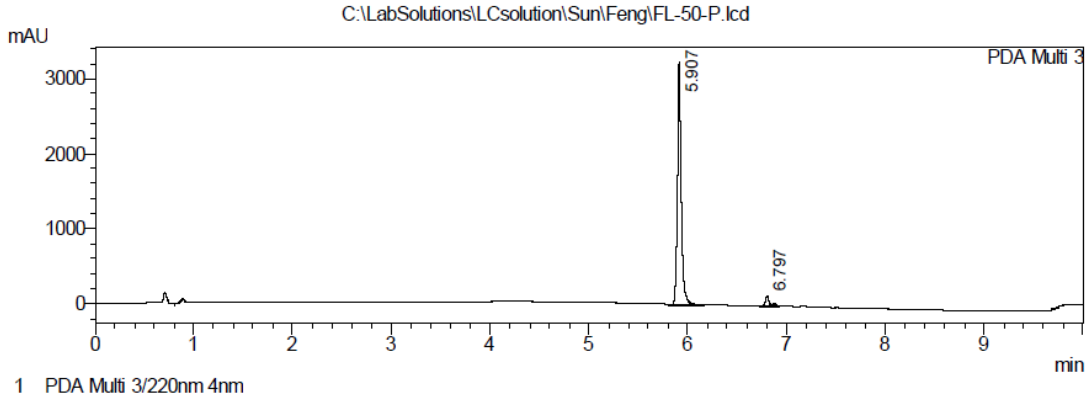
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\Feng\FL-50-P.lcd

Sample Name	: FL-50-P
Tray#	: 1
Vail #	: 93
Injection Volume	: 15 uL
Data File Name	: FL-50-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	: Batch 1.lcb
Data Acquired	: 11/9/2011 3:48:36 PM



<Chromatogram>



1 PDA Multi 3/220nm 4nm

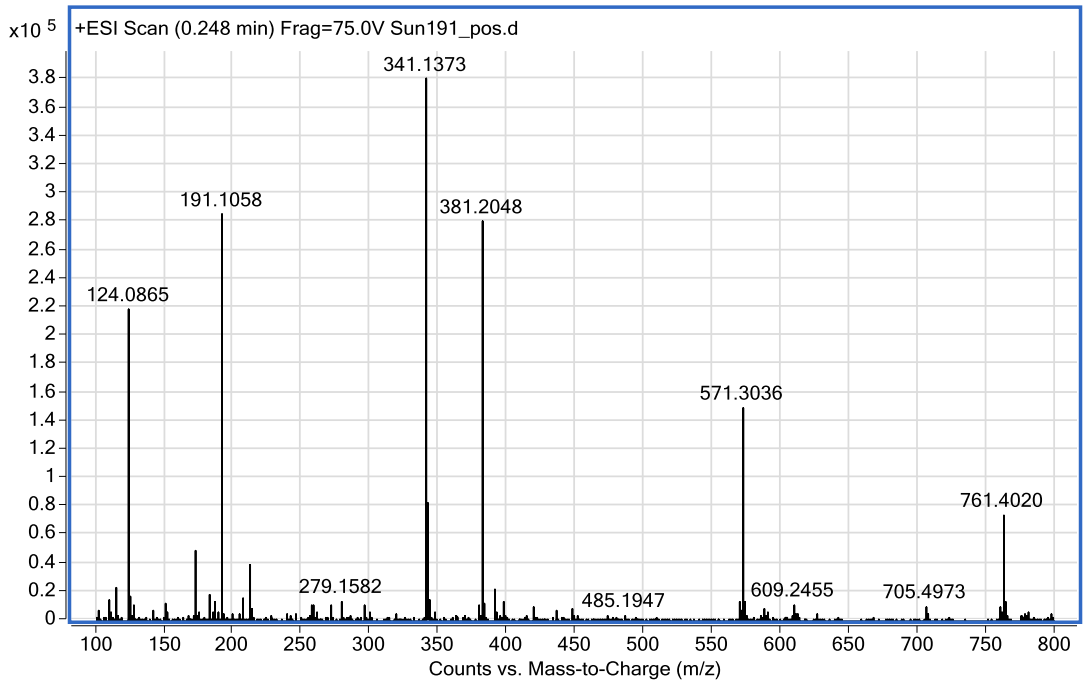
PeakTable

PDA Ch3 220nm 4nm

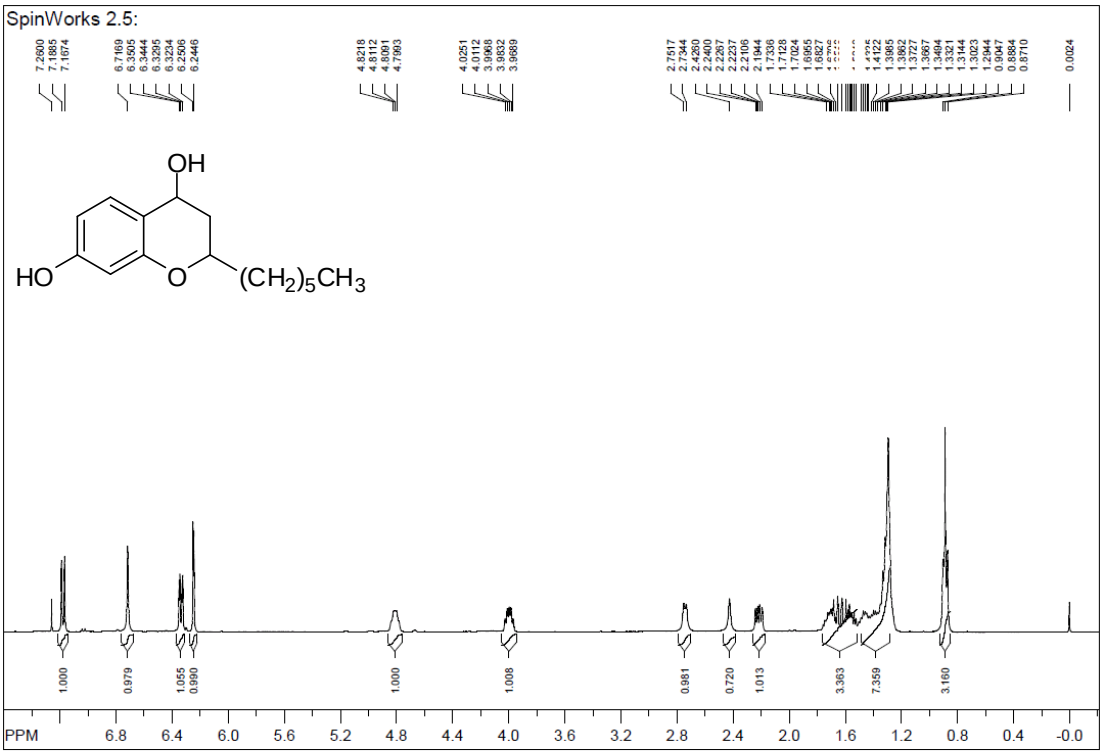
Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.907	9445358	3235926	95.250	95.844
2	6.797	471019	140322	4.750	4.156
Total		9916377	3376248	100.000	100.000

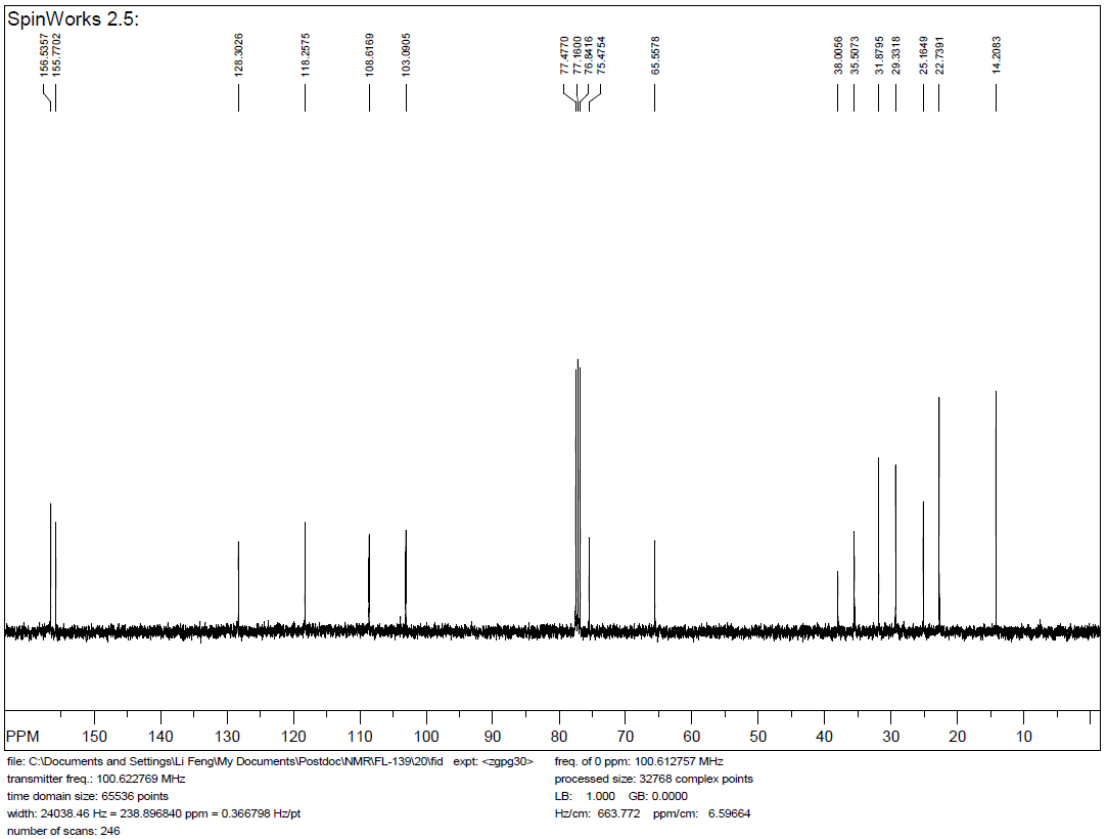
*The HPLC trace at 254 nm of the product is not shown because of the very weak UV-absorption of the product.

HRMS of **4a**


x10 5
+ESI Scan (0.248 min) Frag=75.0V Sun191_pos.d
341.1373
191.1058
381.2048
124.0865
571.3036
761.4020
279.1582
485.1947
609.2455
705.4973
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **4b**



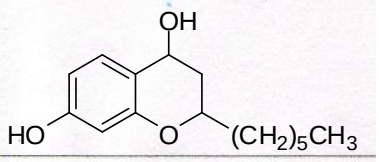


HPLC profile of **4b**

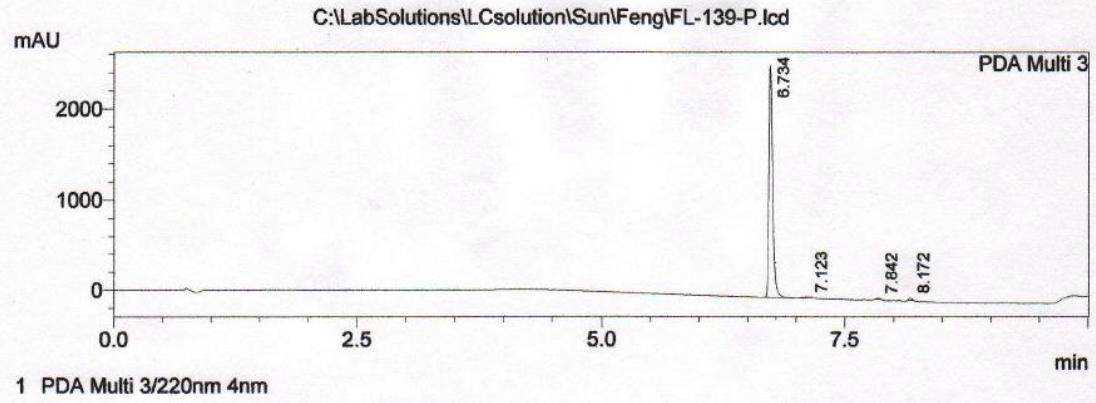
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\Feng\FL-139-P.lcd

Sample Name	: FL-139-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 10 uL
Data File Name	: FL-139-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 2/6/2012 1:26:35 PM



<Chromatogram>



1 PDA Multi 3/220nm 4nm

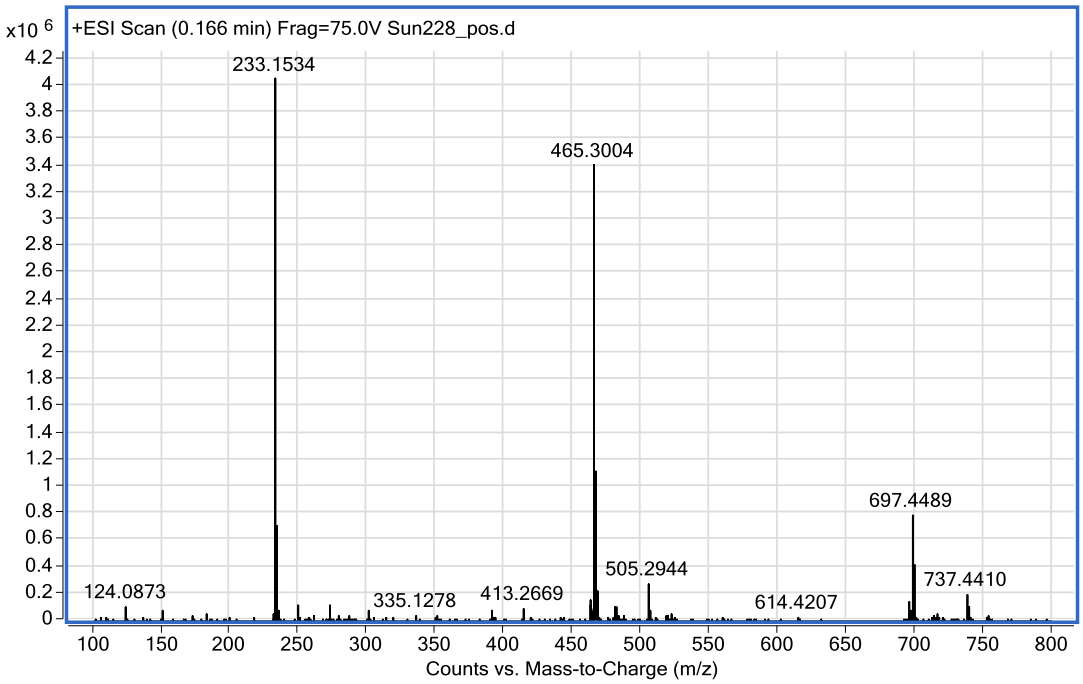
PeakTable

PDA Ch3 220nm 4nm

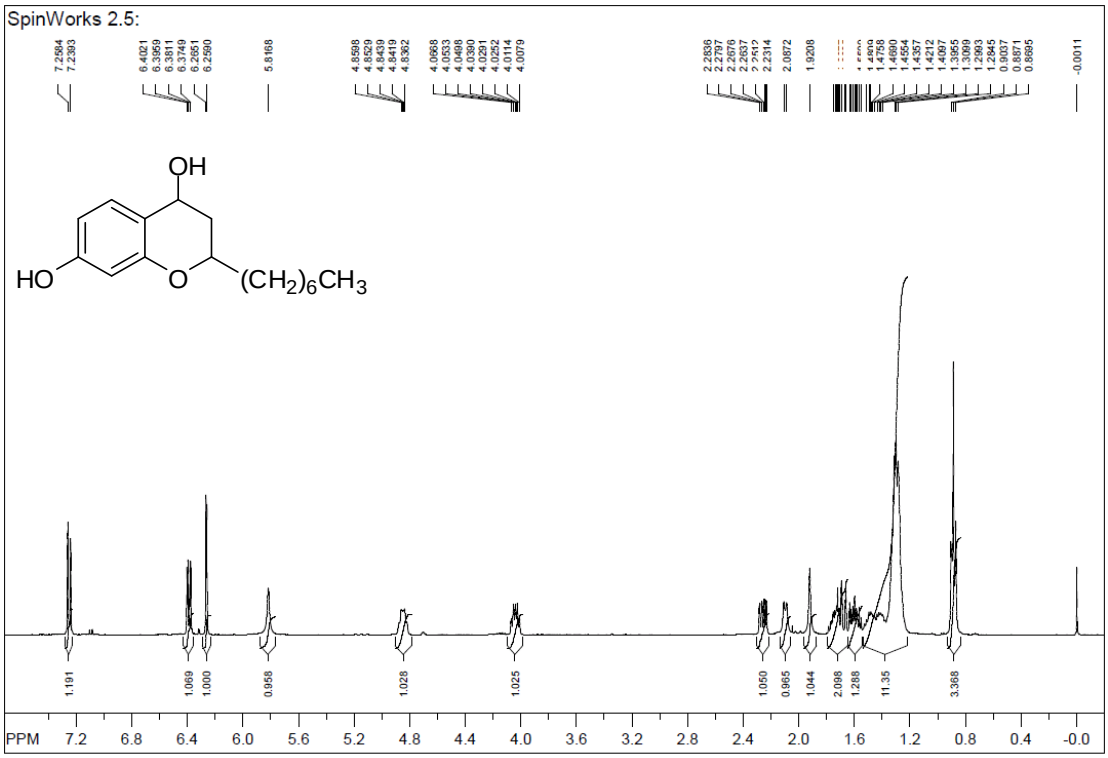
Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.734	6753668	2558960	97.814	98.128
2	7.123	59055	10437	0.855	0.400
3	7.842	31683	11889	0.459	0.456
4	8.172	60211	26501	0.872	1.016
Total		6904617	2607788	100.000	100.000

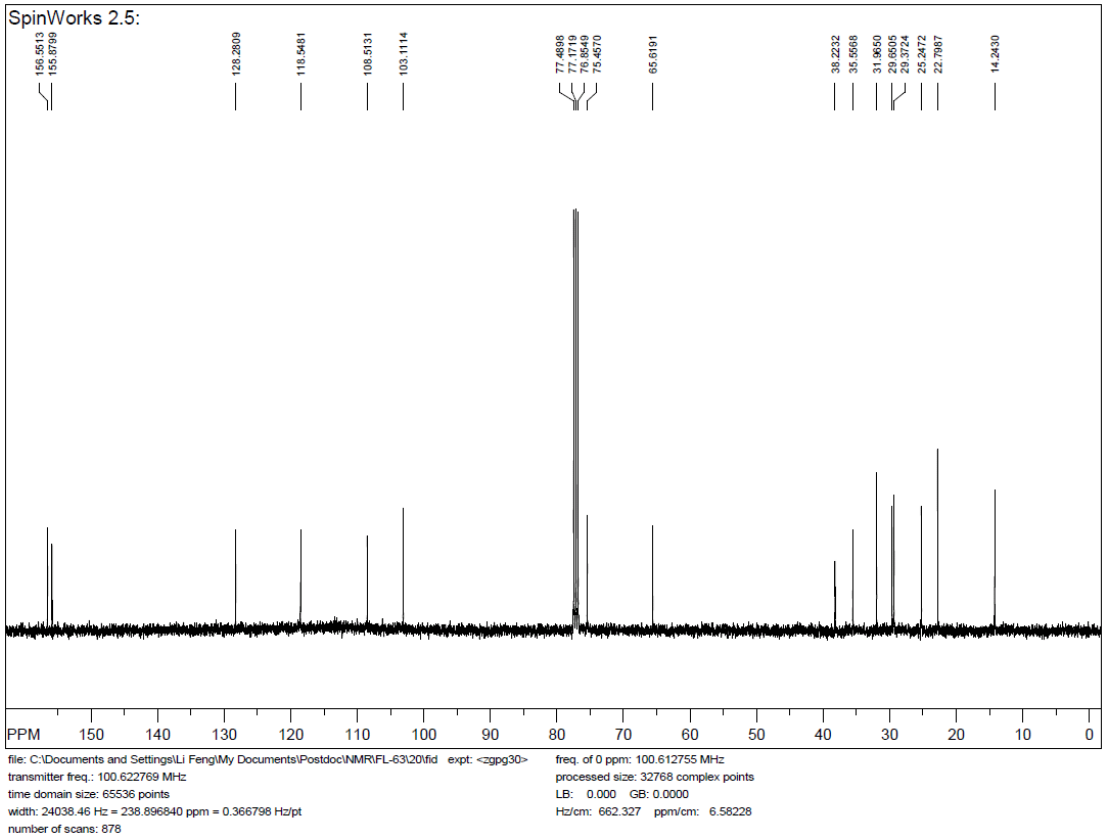
*The HPLC trace at 254 nm of the product is not shown because of the very weak UV-absorption of the product.

HRMS of **4b**


x10 6
+ESI Scan (0.166 min) Frag=75.0V Sun228_pos.d
233.1534
465.3004
697.4489
505.2944
737.4410
124.0873
335.1278
413.2669
614.4207
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **4c**



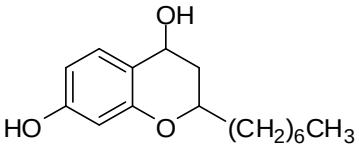


HPLC profile of **4c**

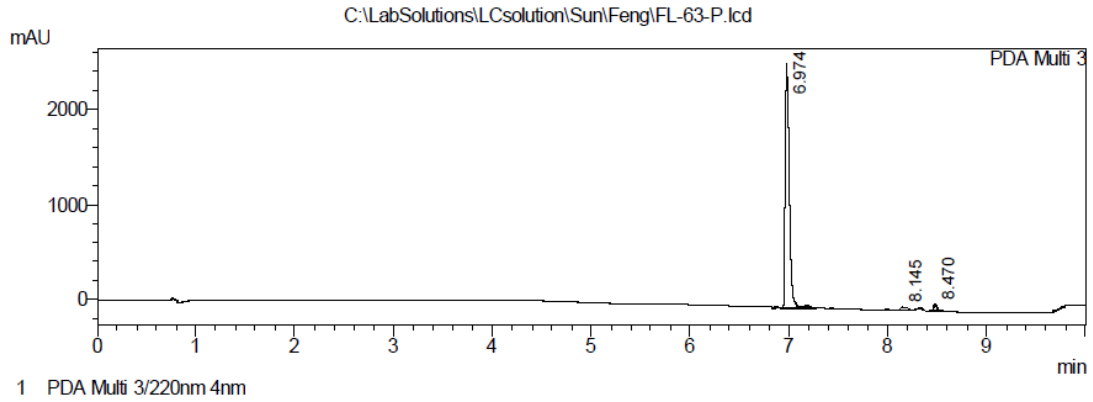
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\Feng\FL-63-P.lcd

Sample Name	: FL-63-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 5 uL
Data File Name	: FL-63-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 11/18/2011 9:31:24 AM



<Chromatogram>



1 PDA Multi 3/220nm 4nm

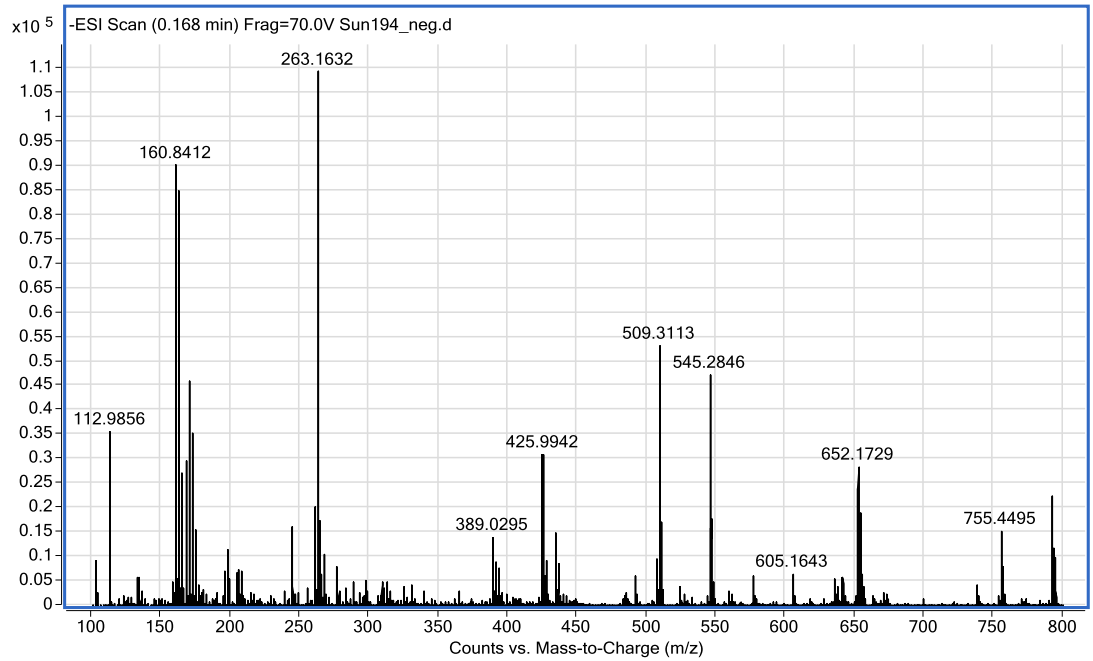
PeakTable

PDA Ch3 220nm 4nm

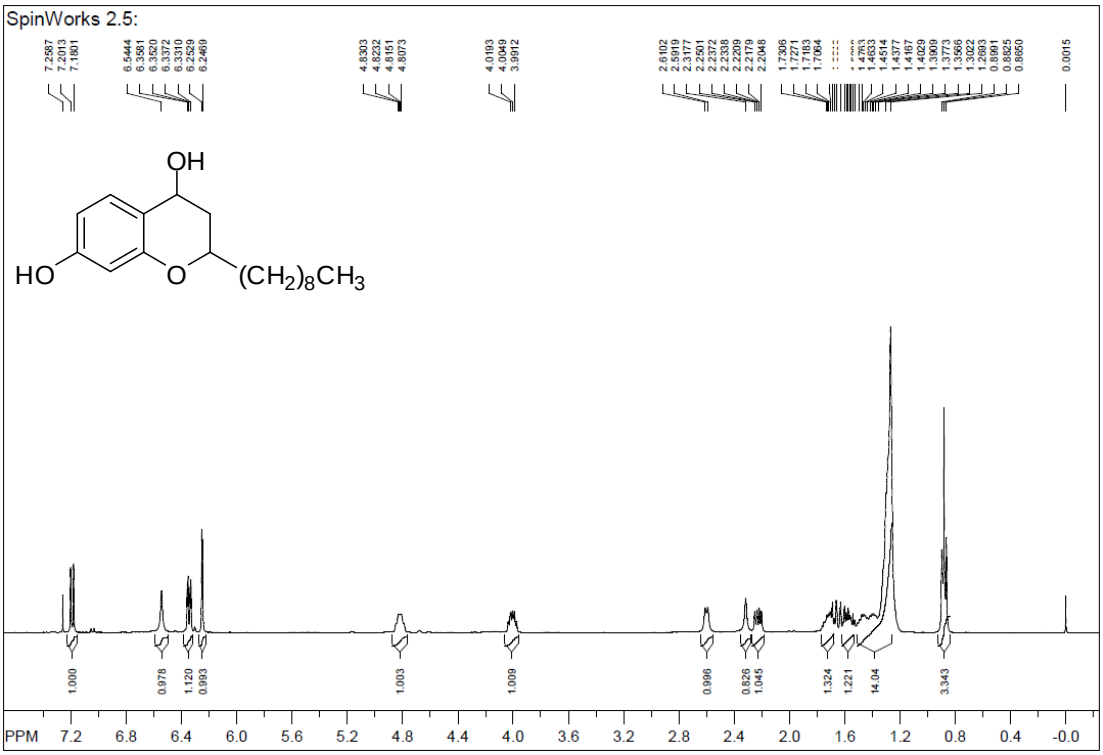
Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.974	6713802	2556564	95.746	96.356
2	8.145	117428	29492	1.675	1.112
3	8.470	180839	67198	2.579	2.533
Total		7012069	2653254	100.000	100.000

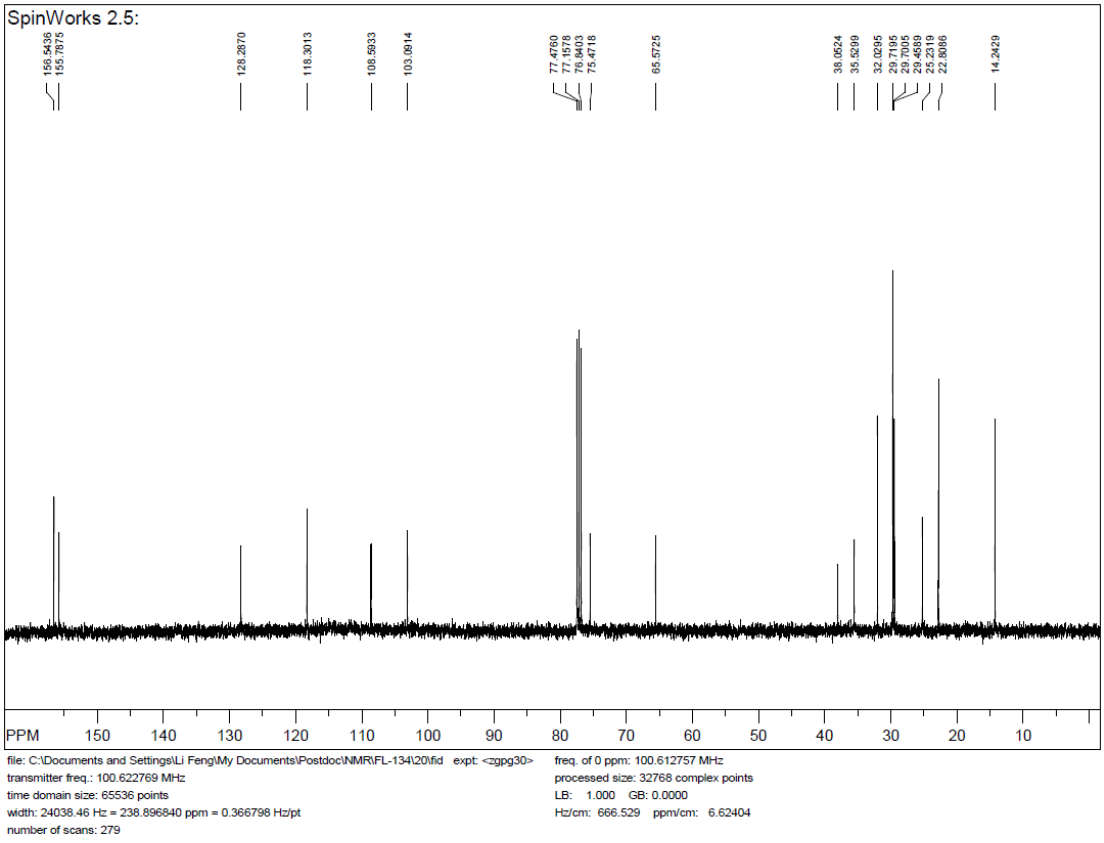
*The HPLC trace at 254 nm of the product is not shown because of the very weak UV-absorption of the product.

HRMS of **4c**


x10 5
-ESI Scan (0.168 min) Frag=70.0V Sun194_neg.d
263.1632
160.8412
509.3113
545.2846
112.9856
425.9942
652.1729
389.0295
755.4495
605.1643
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **4d**



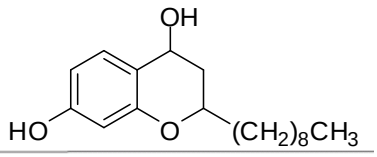


HPLC profile of **4d**

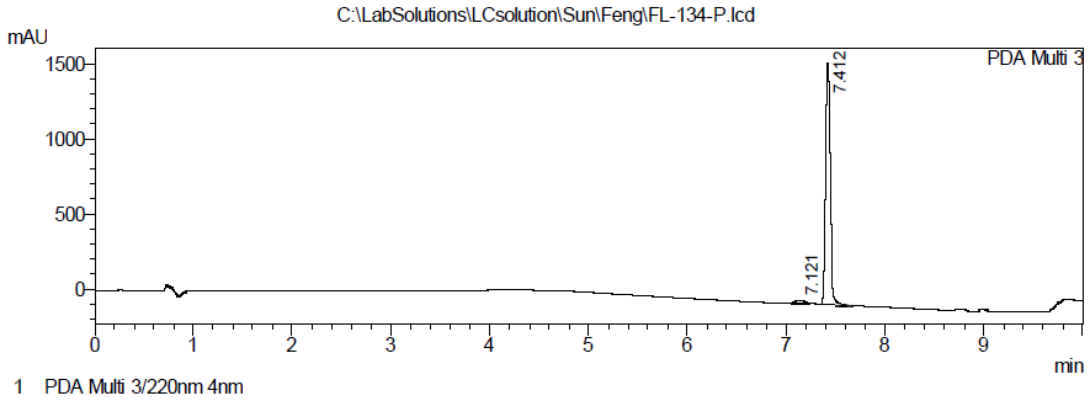
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\Feng\FL-134-P.lcd

Sample Name	: FL-134-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 20 uL
Data File Name	: FL-134-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 2/3/2012 2:21:54 PM



<Chromatogram>



1 PDA Multi 3/220nm 4nm

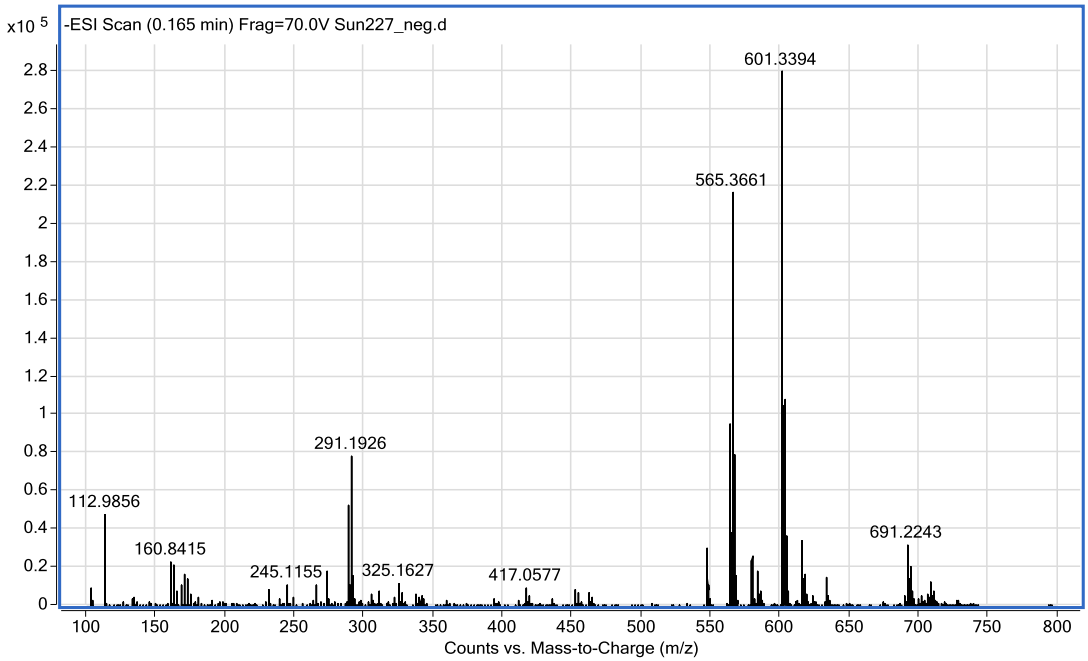
PeakTable

PDA Ch3 220nm 4nm

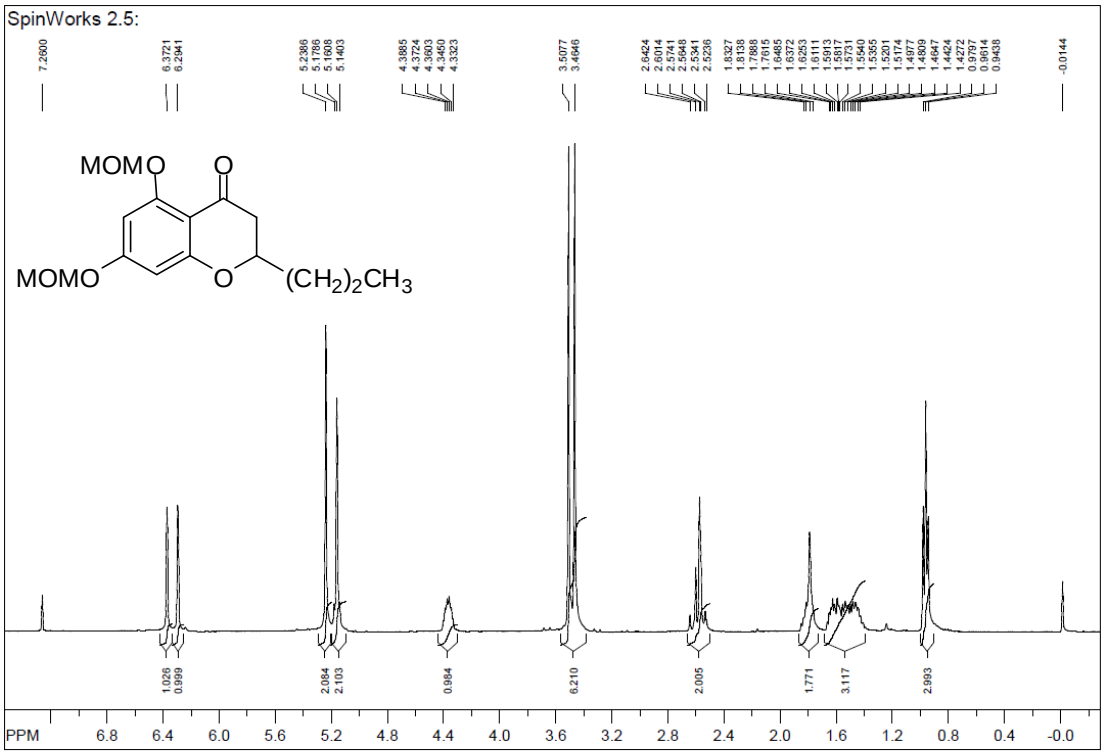
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.121	116882	23087	2.295	1.416
2	7.412	4976957	1607200	97.705	98.584
Total		5093839	1630287	100.000	100.000

*The HPLC trace at 254 nm of the product is not shown because of the very weak UV-absorption of the product.

HRMS of **4d**

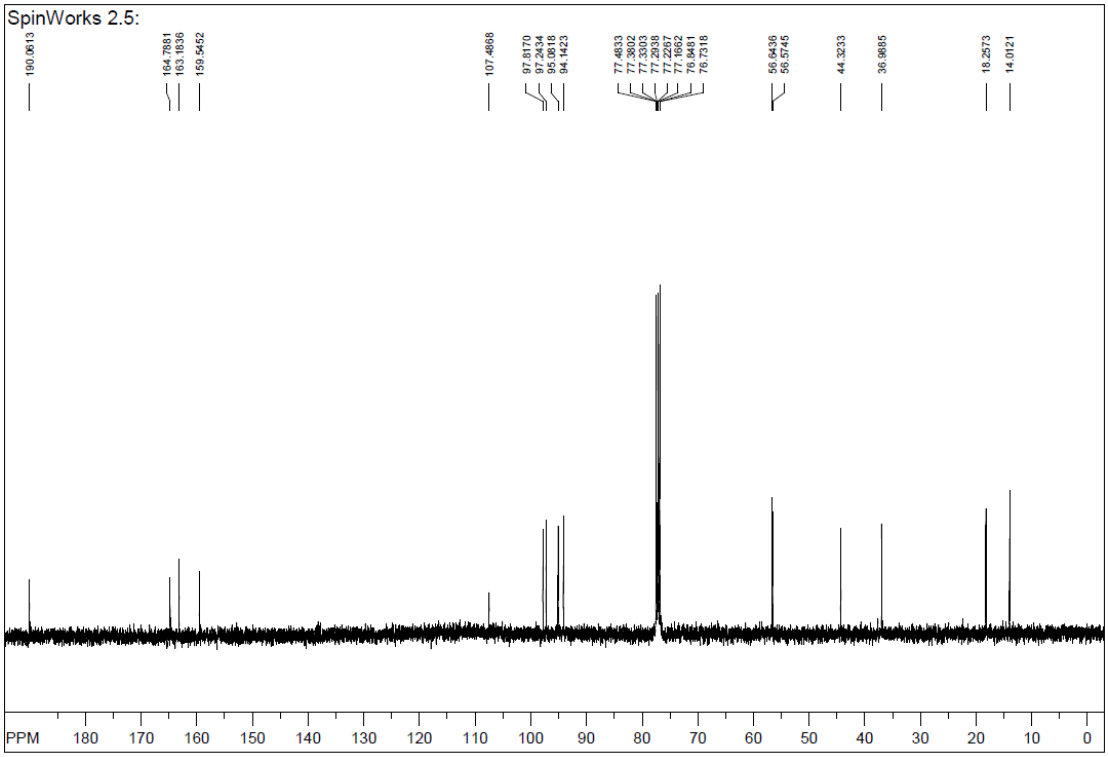

x10 5
-ESI Scan (0.165 min) Frag=70.0V Sun227_neg.d
601.3394
565.3661
291.1926
112.9856
160.8415
245.1155
325.1627
417.0577
691.2243
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **5a**



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-72\2\fid expt: <zg30>
transmitter freq.: 400.131600 MHz
time domain size: 65536 points
width: 8012.82 Hz = 20.025463 ppm = 0.122266 Hz/pt
number of scans: 4

freq. of 0 ppm: 400.130009 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 124.989 ppm/cm: 0.31237



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-72\20\fid expt: <zgpg30>
transmitter freq.: 100.622769 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.896840 ppm = 0.366798 Hz/pt
number of scans: 469

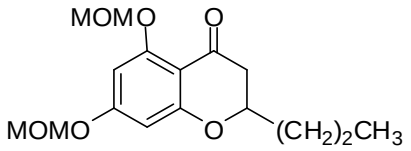
freq. of 0 ppm: 100.612758 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 794.655 ppm/cm: 7.89737

HPLC profile of **5a**

==== Shimadzu LCsolution Analysis Report ====

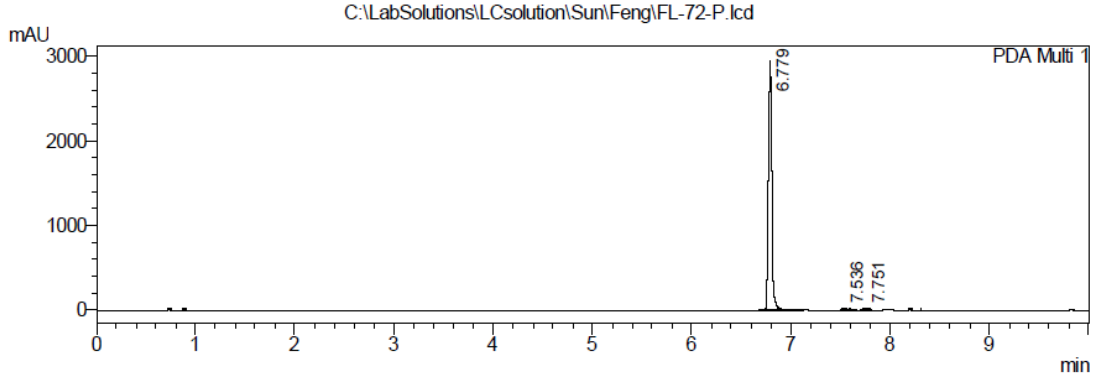
C:\LabSolutions\LCsolution\Sun\Feng\FL-72-P.lcd

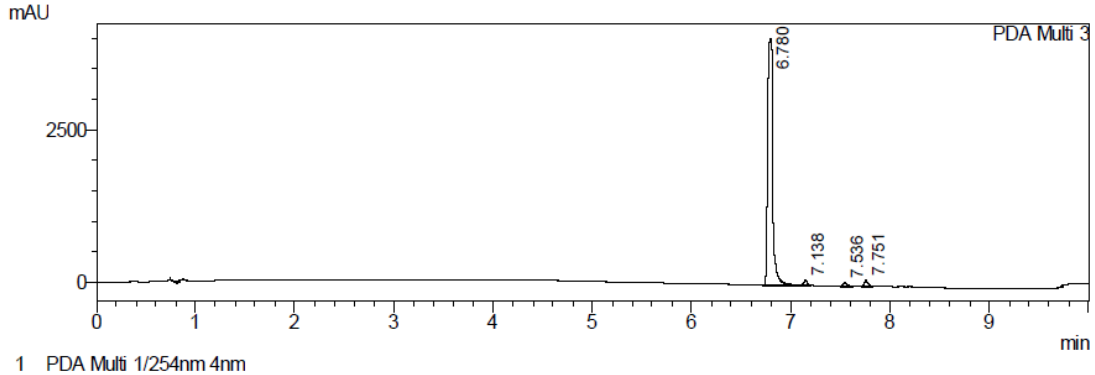
Sample Name	: FL-72-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 5 uL
Data File Name	: FL-72-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 11/28/2011 12:56:43 PM



<Chromatogram>

C:\LabSolutions\LCsolution\Sun\Feng\FL-72-P.lcd





1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

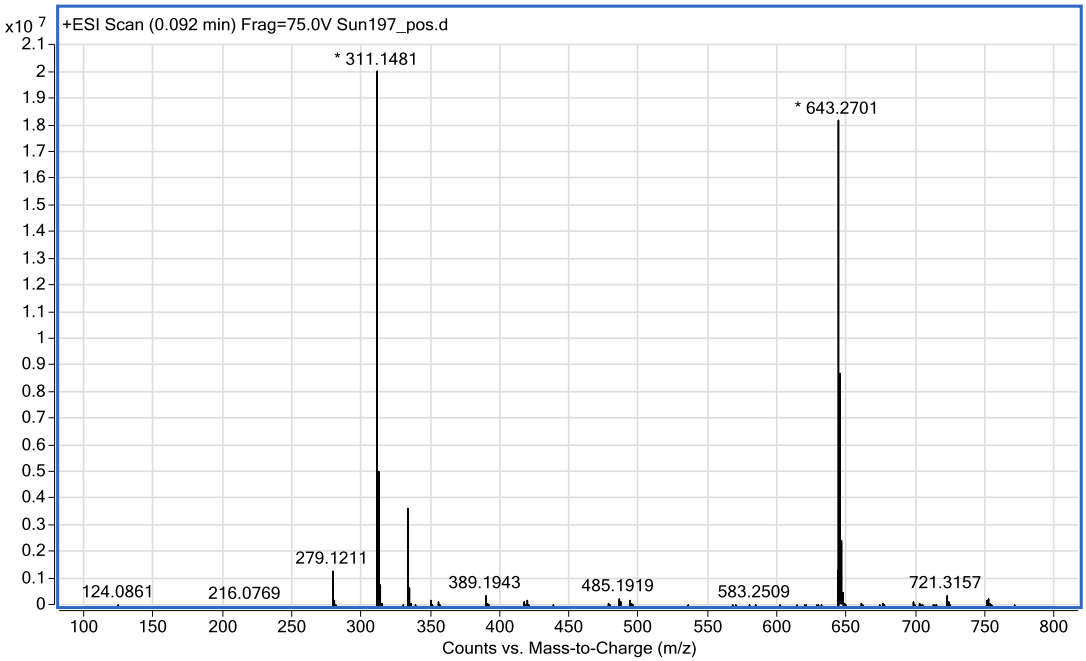
Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.779	6987339	2913639	97.961	98.465
2	7.536	91645	22337	1.285	0.755
3	7.751	53777	23096	0.754	0.781
Total		7132762	2959071	100.000	100.000

PeakTable

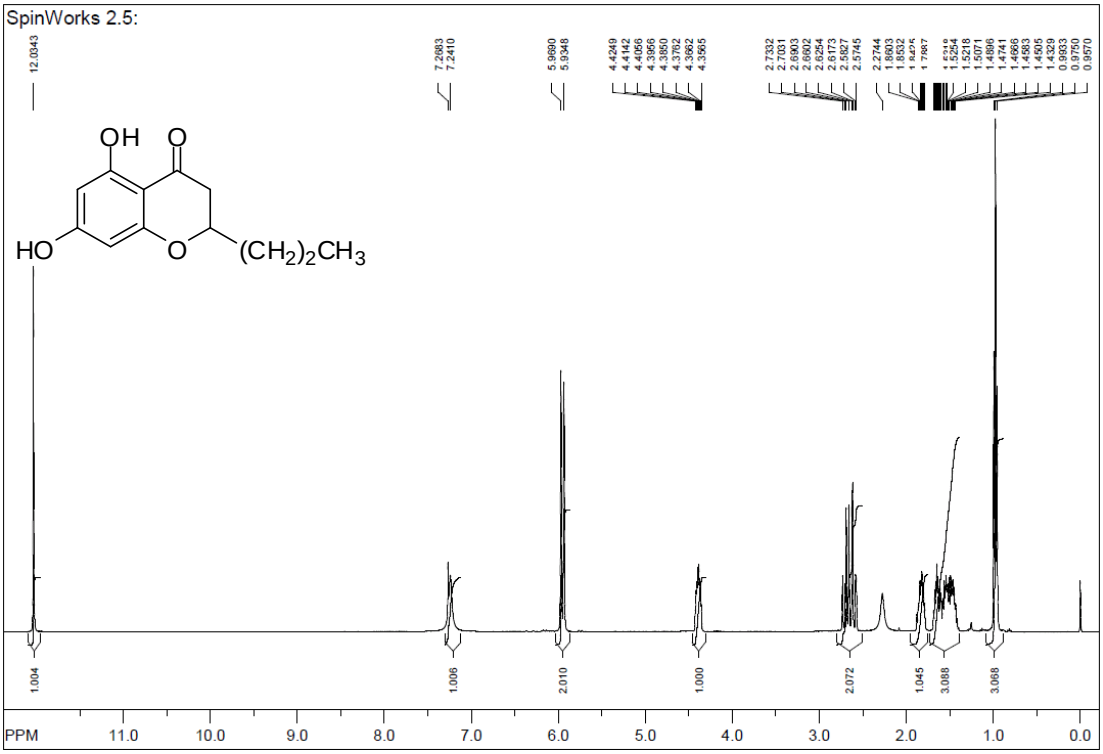
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.780	14459718	4034386	96.255	94.390
2	7.138	182246	78697	1.213	1.841
3	7.536	149550	60636	0.996	1.419
4	7.751	230810	100458	1.536	2.350
Total		15022323	4274175	100.000	100.000

HRMS of **5a**

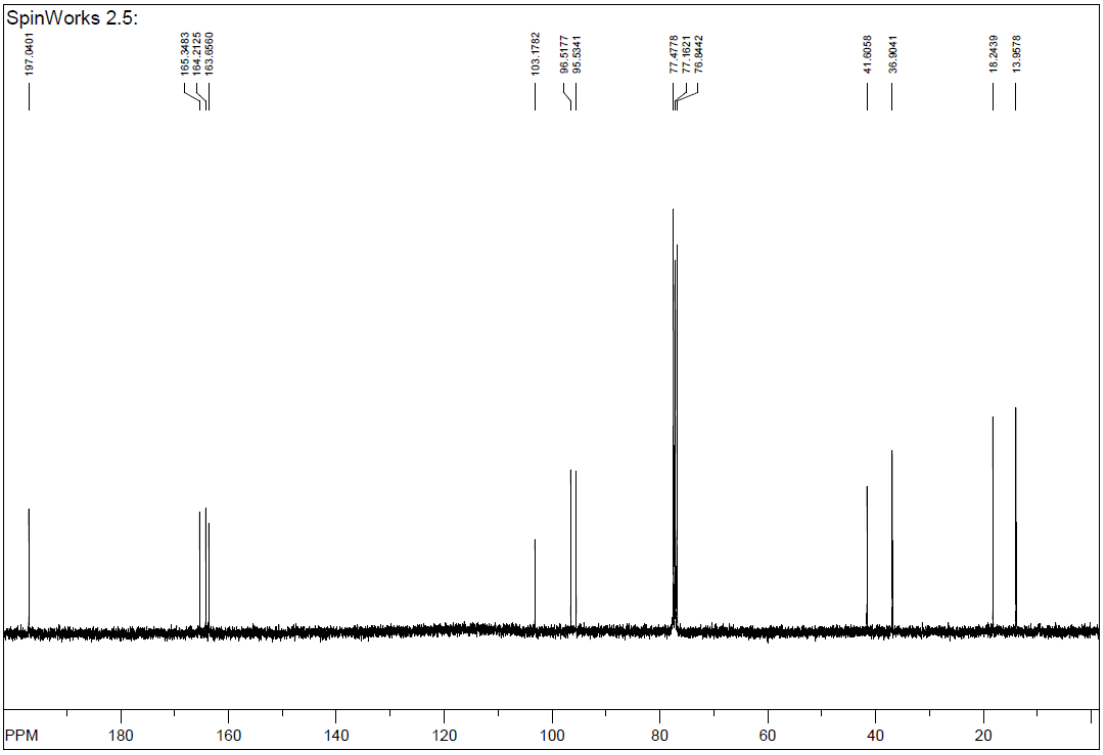

+ESI Scan (0.092 min) Frag=75.0V Sun197_pos.d
x10 7
* 311.1481
* 643.2701
279.1211
124.0861
216.0769
389.1943
485.1919
583.2509
721.3157
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **5b**



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-73\1\fid expt: <zg30>
transmitter freq.: 400.131600 MHz
time domain size: 65536 points
width: 8012.82 Hz = 20.025463 ppm = 0.122266 Hz/pt
number of scans: 8

freq. of 0 ppm: 400.130006 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 201.498 ppm/cm: 0.50358



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-73\20\fid expt: <zgpg30>
transmitter freq.: 100.622769 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.896840 ppm = 0.366798 Hz/pt
number of scans: 744

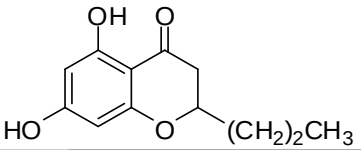
freq. of 0 ppm: 100.612758 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 817.399 ppm/cm: 8.12340

HPLC profile of **5b**

==== Shimadzu LCsolution Analysis Report ====

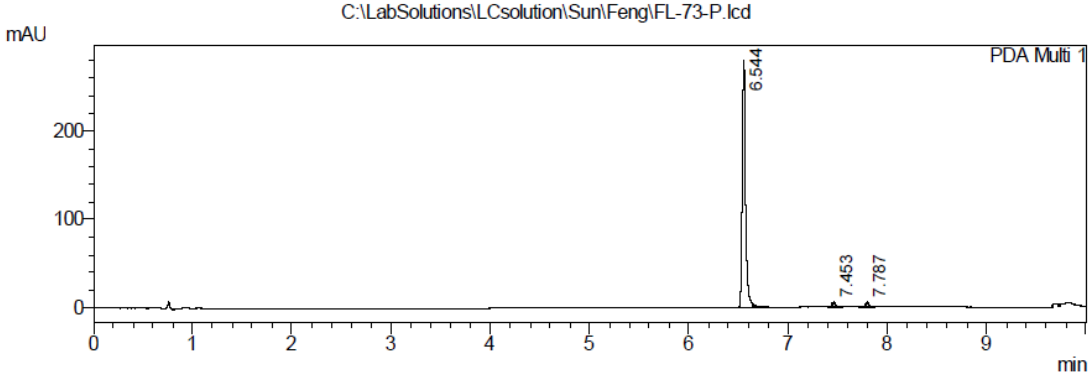
C:\LabSolutions\LCsolution\Sun\Feng\FL-73-P.lcd

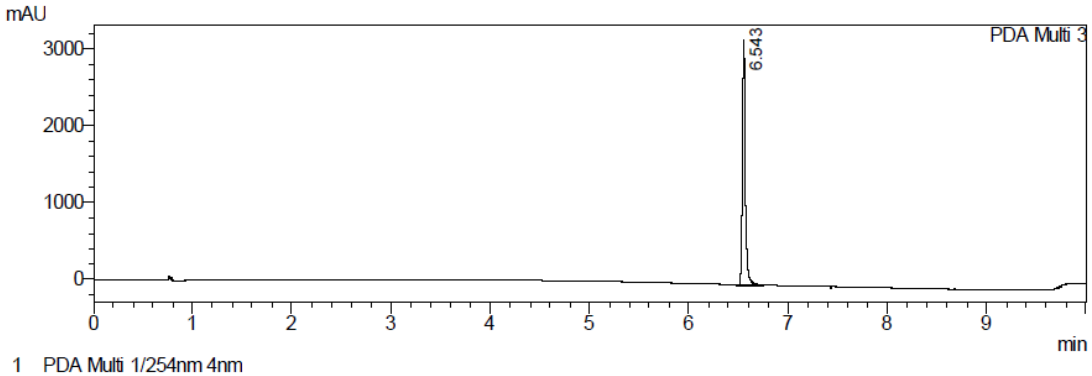
Sample Name	: FL-73-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 4 uL
Data File Name	: FL-73-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 11/28/2011 1:58:09 PM



<Chromatogram>

C:\LabSolutions\LCsolution\Sun\Feng\FL-73-P.lcd





1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

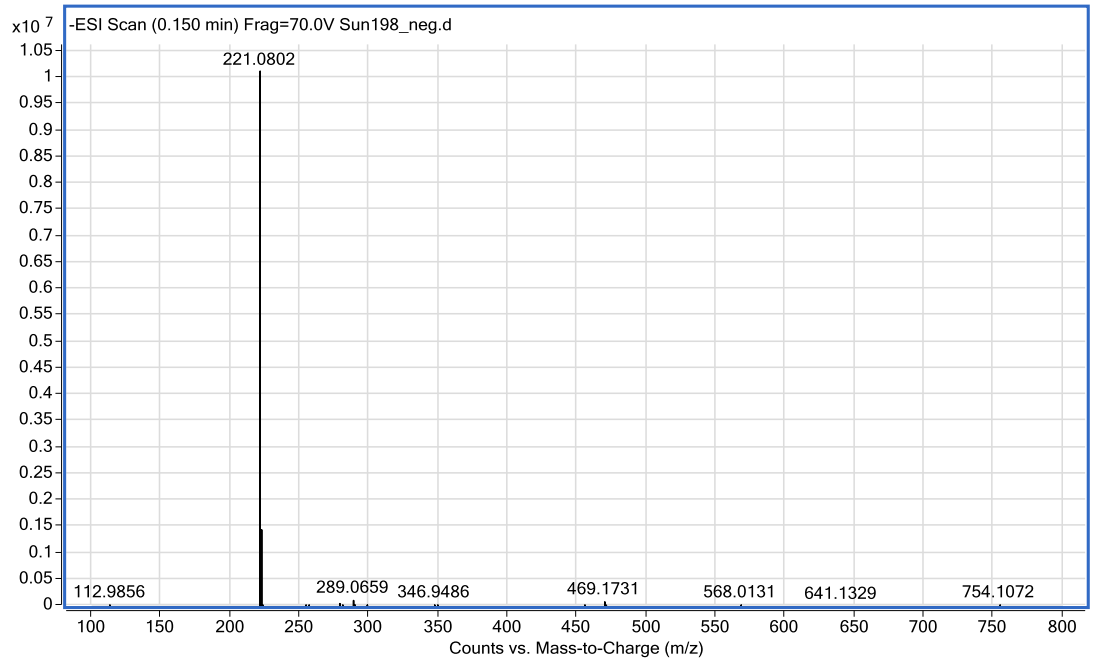
Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.544	724978	271529	96.722	96.436
2	7.453	13660	5212	1.822	1.851
3	7.787	10910	4822	1.456	1.713
Total		749548	281563	100.000	100.000

PeakTable

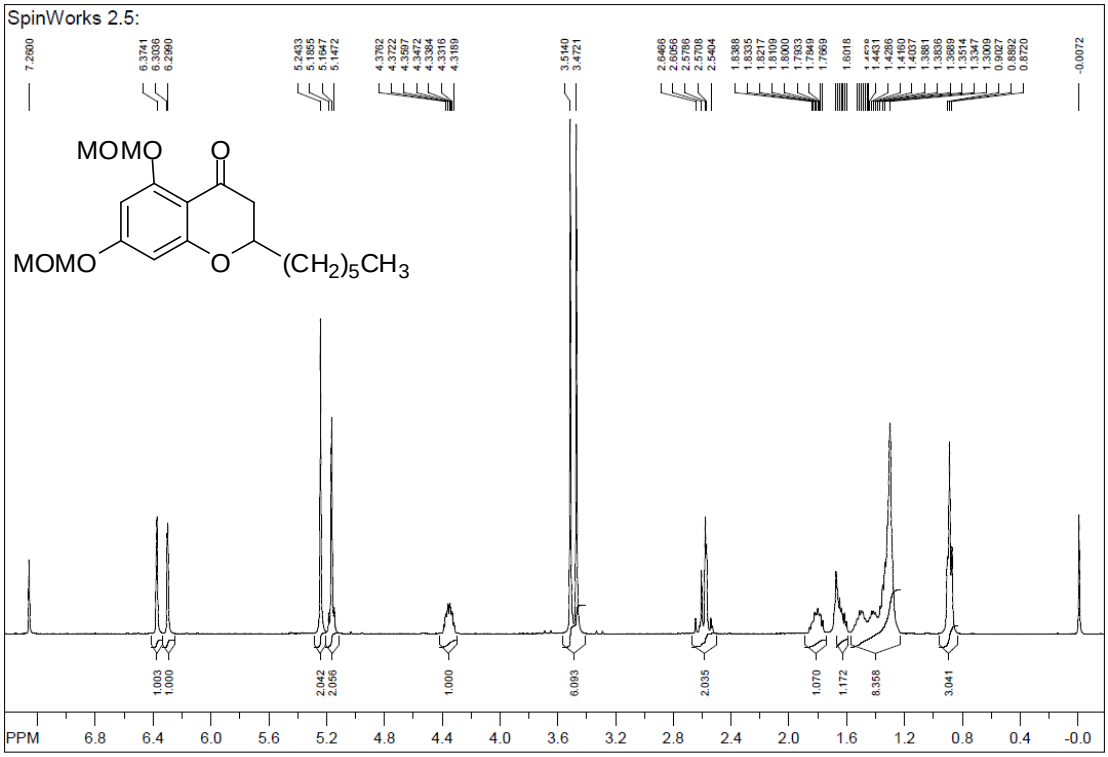
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.543	7072564	3186261	100.000	100.000
Total		7072564	3186261	100.000	100.000

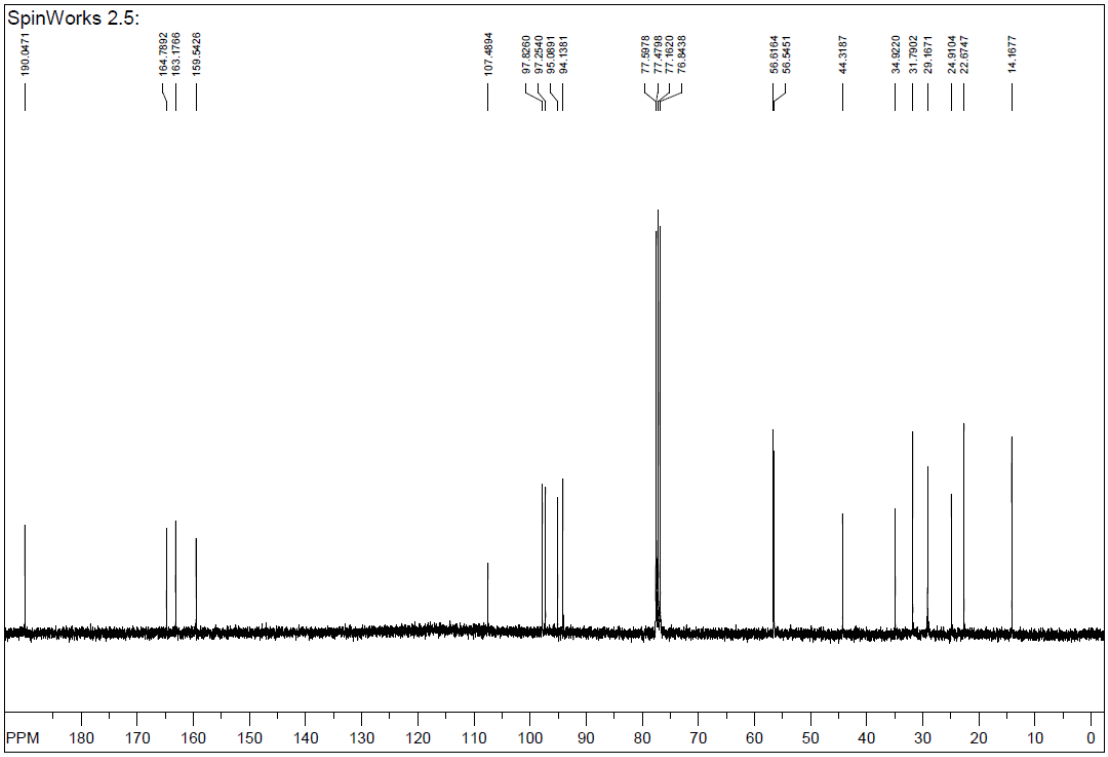
HRMS of **5b**


-ESI Scan (0.150 min) Frag=70.0V Sun198_neg.d
x10 7
221.0802
112.9856
289.0659
346.9486
469.1731
568.0131
641.1329
754.1072
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **5c**



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-76\3\fid expt: <zg30>
transmitter freq.: 400.131600 MHz
time domain size: 65536 points
width: 8012.82 Hz = 20.025463 ppm = 0.122266 Hz/pt
number of scans: 2
freq. of 0 ppm: 400.130010 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 121.772 ppm/cm: 0.30433



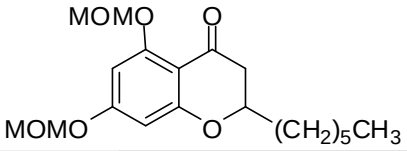
file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-76\20\fid expt: <zgpg30>
transmitter freq.: 100.622769 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.896840 ppm = 0.366798 Hz/pt
number of scans: 812
freq. of 0 ppm: 100.612758 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 788.452 ppm/cm: 7.83572

HPLC profile of **5c**

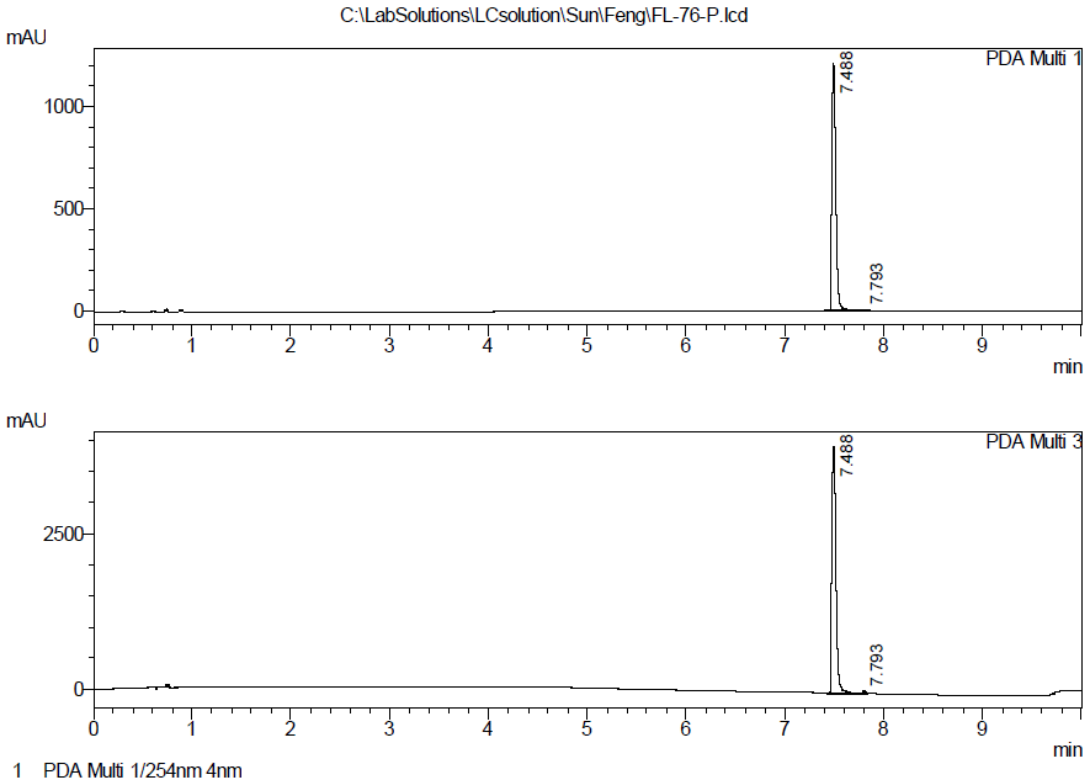
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\Feng\FL-76-P.lcd

Sample Name	: FL-76-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 4 uL
Data File Name	: FL-76-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	: Batch 1.lcb
Data Acquired	: 11/30/2011 2:32:44 PM



<Chromatogram>



1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

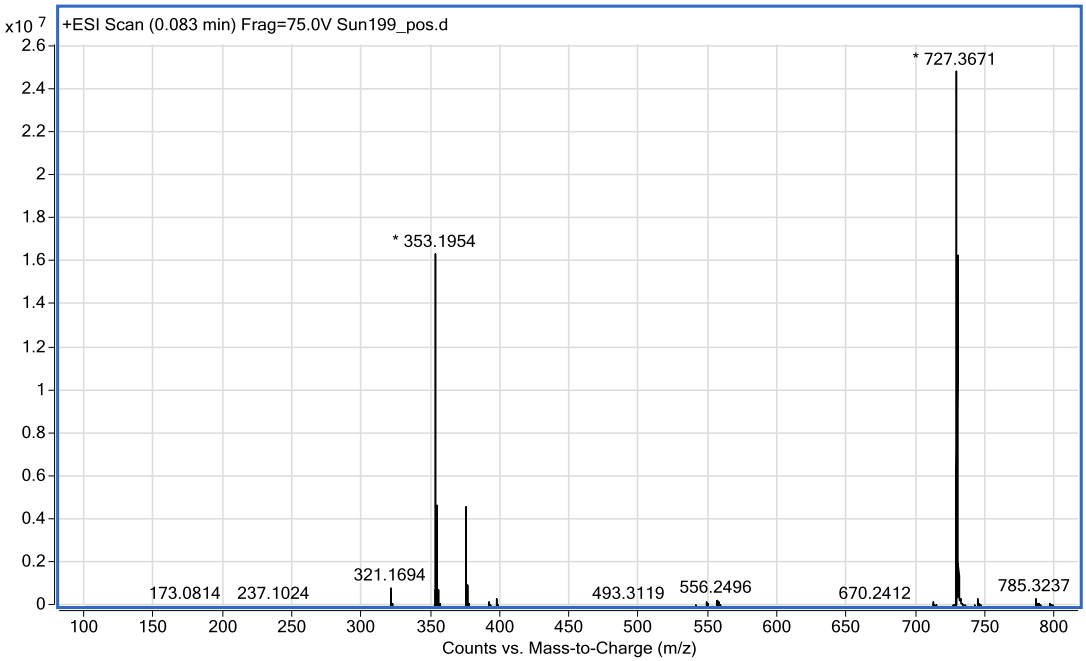
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.488	3031043	1173781	99.515	99.480
2	7.793	14779	6139	0.485	0.520
Total		3045821	1179920	100.000	100.000

PeakTable

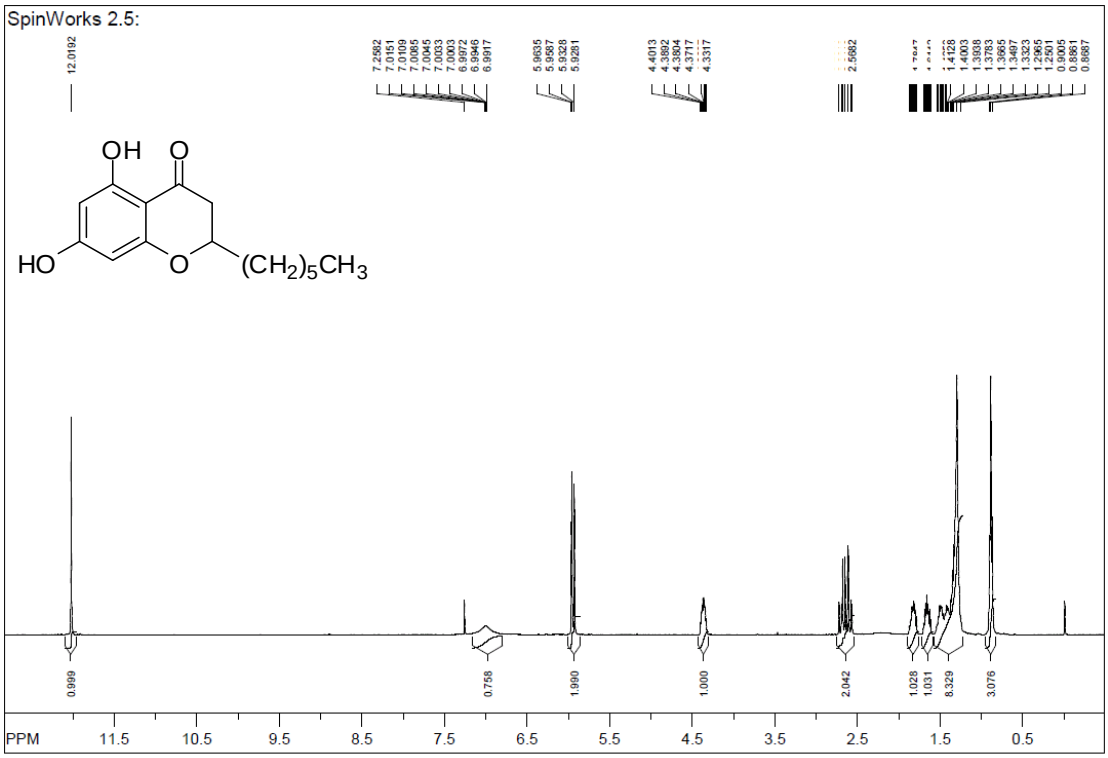
PDA Ch3 220nm 4nm

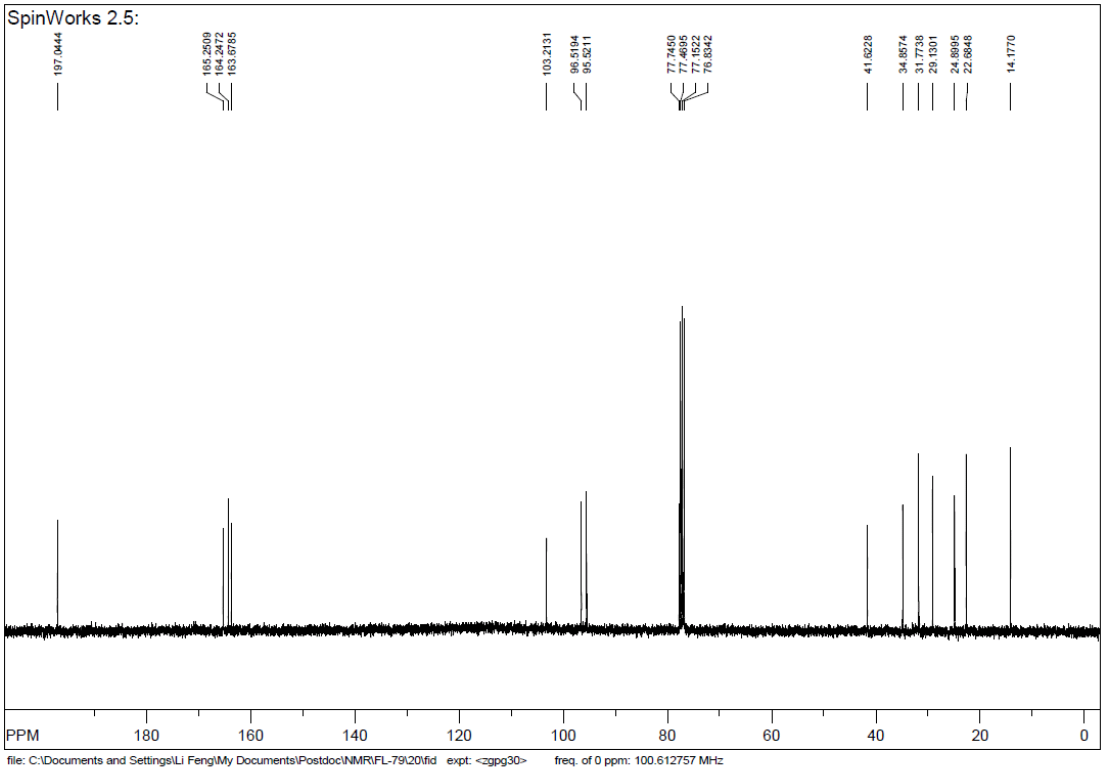
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.488	10532044	3965245	99.289	99.075
2	7.793	75417	37026	0.711	0.925
Total		10607461	4002271	100.000	100.000

HRMS of **5c**


x10 7
+ESI Scan (0.083 min) Frag=75.0V Sun199_pos.d
* 727.3671
* 353.1954
321.1694
173.0814
237.1024
493.3119
556.2496
670.2412
785.3237
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **5d**



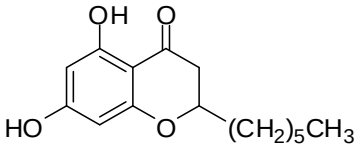


HPLC profile of **5d**

==== Shimadzu LCsolution Analysis Report ====

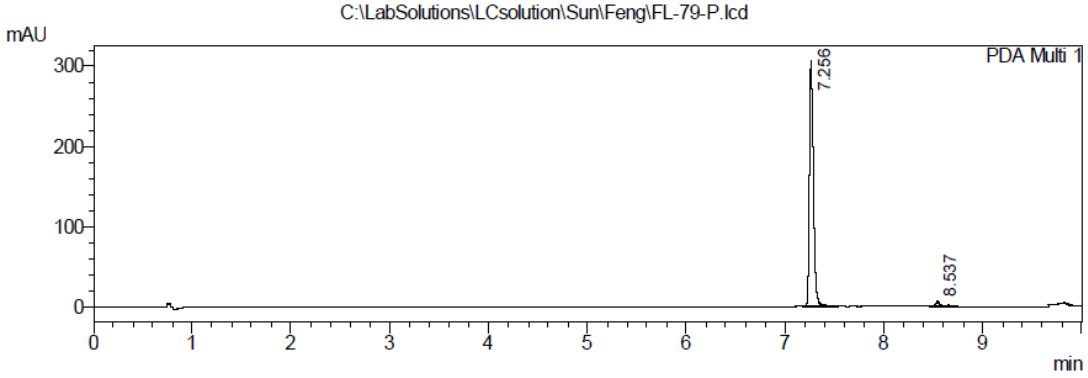
C:\LabSolutions\LCsolution\Sun\Feng\FL-79-P.lcd

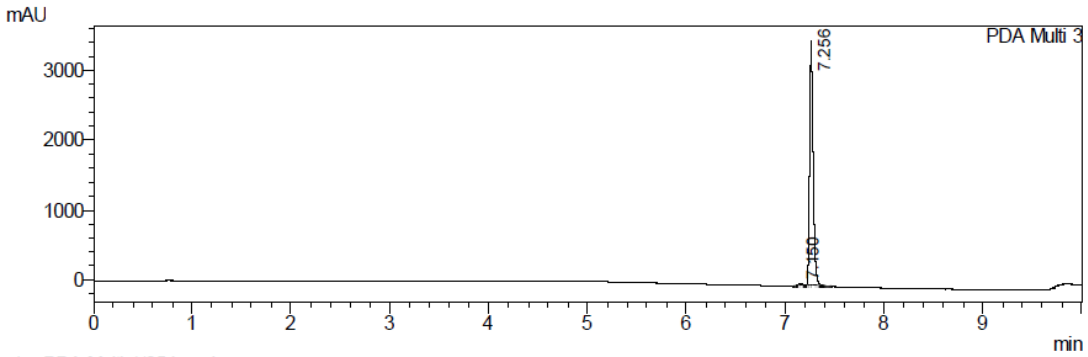
Sample Name	: FL-79-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 8 uL
Data File Name	: FL-79-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 12/1/2011 11:22:33 AM



<Chromatogram>

C:\LabSolutions\LCsolution\Sun\Feng\FL-79-P.lcd





1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

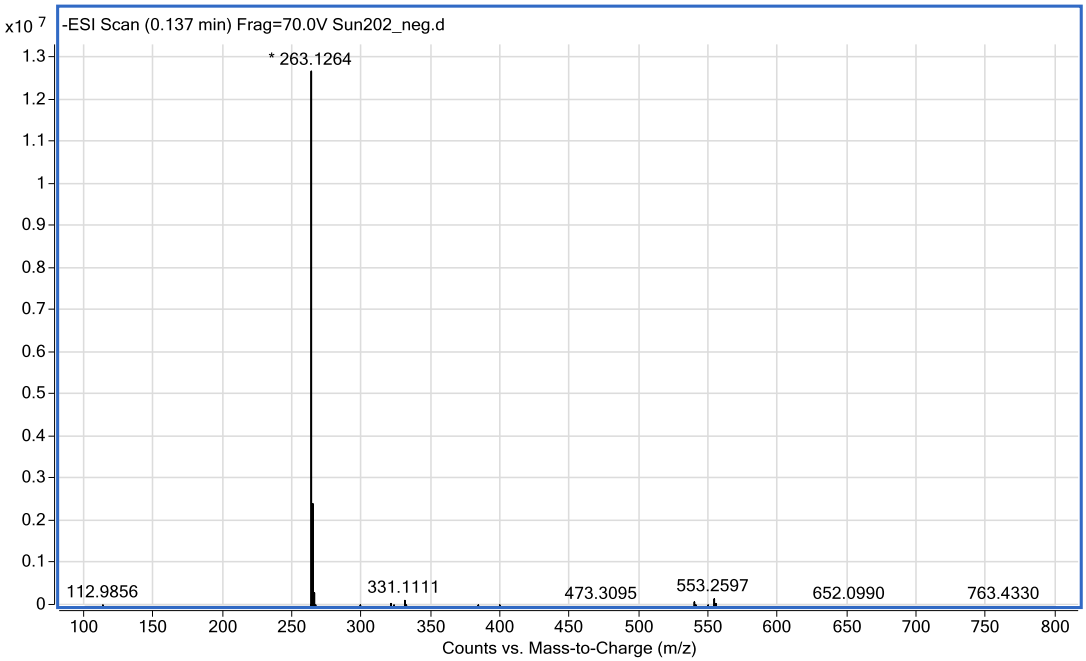
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.256	766277	294534	97.854	98.234
2	8.537	16808	5295	2.146	1.766
Total		783086	299829	100.000	100.000

PeakTable

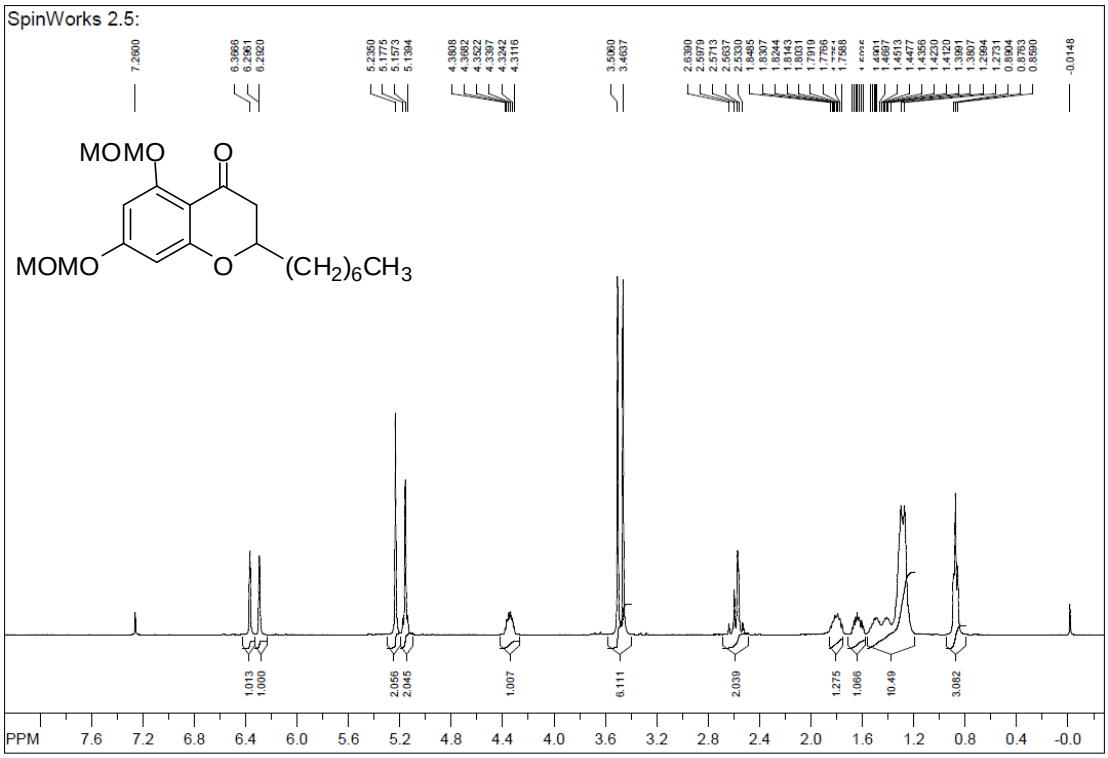
PDA Ch3 220nm 4nm

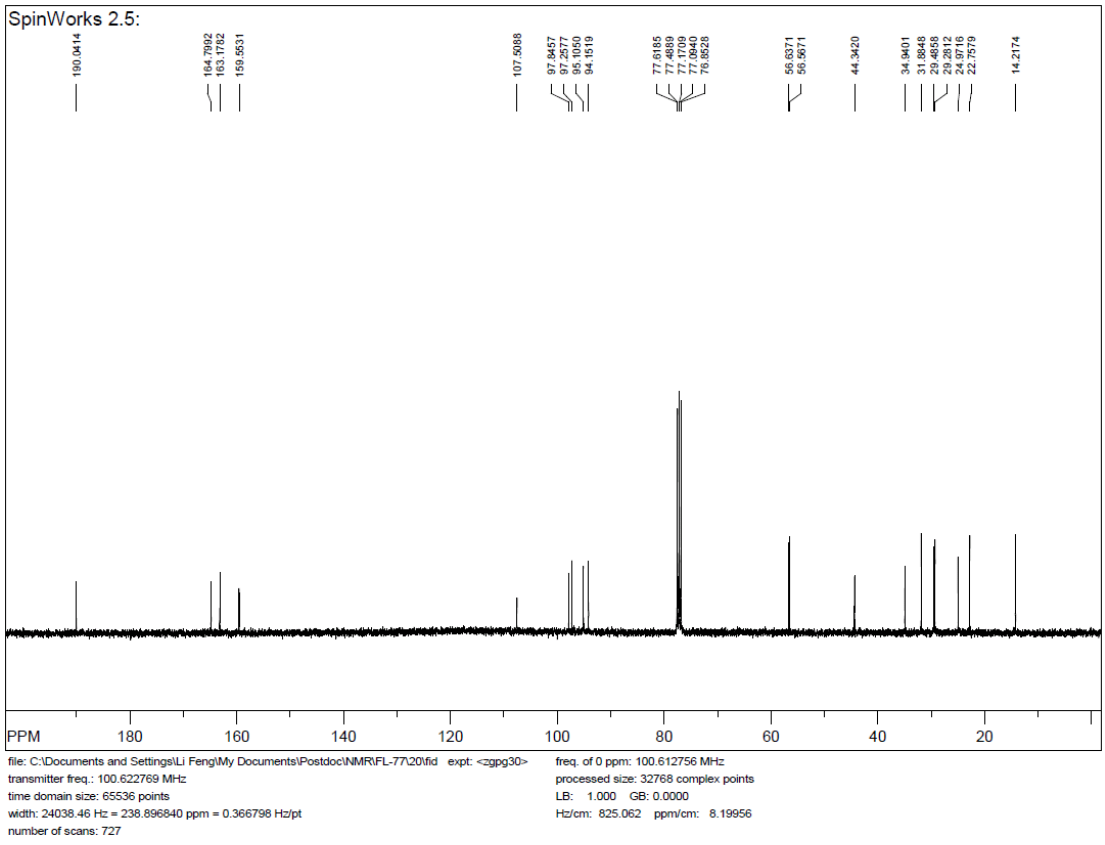
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.150	67014	23159	0.857	0.657
2	7.256	7752668	3500378	99.143	99.343
Total		7819682	3523536	100.000	100.000

HRMS of **5d**


x10 7
-ESI Scan (0.137 min) Frag=70.0V Sun202_neg.d
* 263.1264
112.9856
331.1111
473.3095
553.2597
652.0990
763.4330
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **5e**



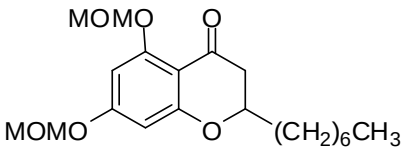


HPLC profile of **5e**

==== Shimadzu LCsolution Analysis Report ====

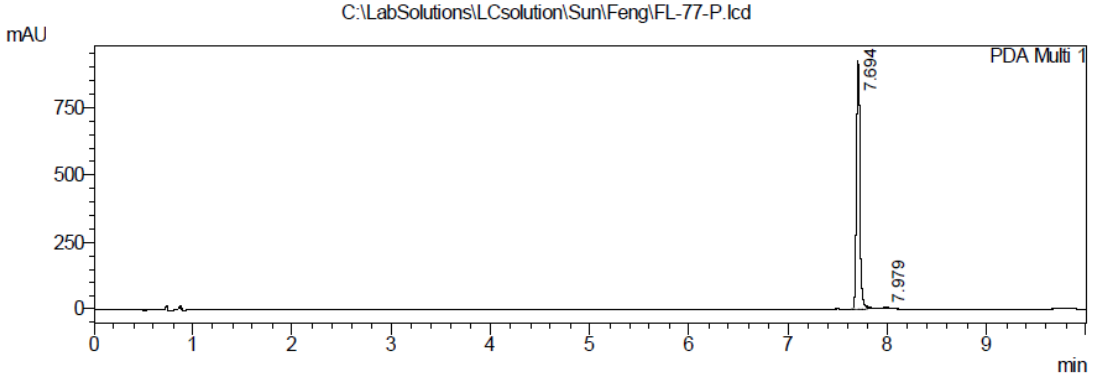
C:\LabSolutions\LCsolution\Sun\Feng\FL-77-P.lcd

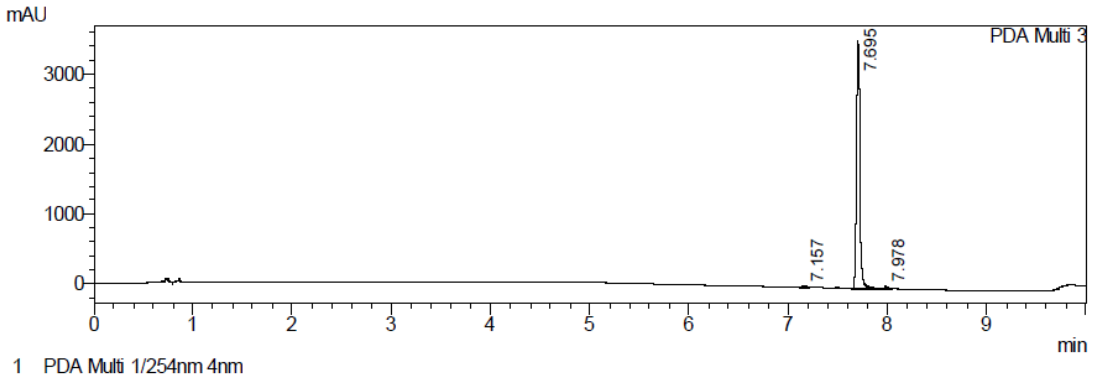
Sample Name	: FL-77-P
Tray#	: 1
Vail #	: 92
Injection Volume	: 4 uL
Data File Name	: FL-77-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	: Batch 1.lcb
Data Acquired	: 11/30/2011 2:43:11 PM



<Chromatogram>

C:\LabSolutions\LCsolution\Sun\Feng\FL-77-P.lcd





1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

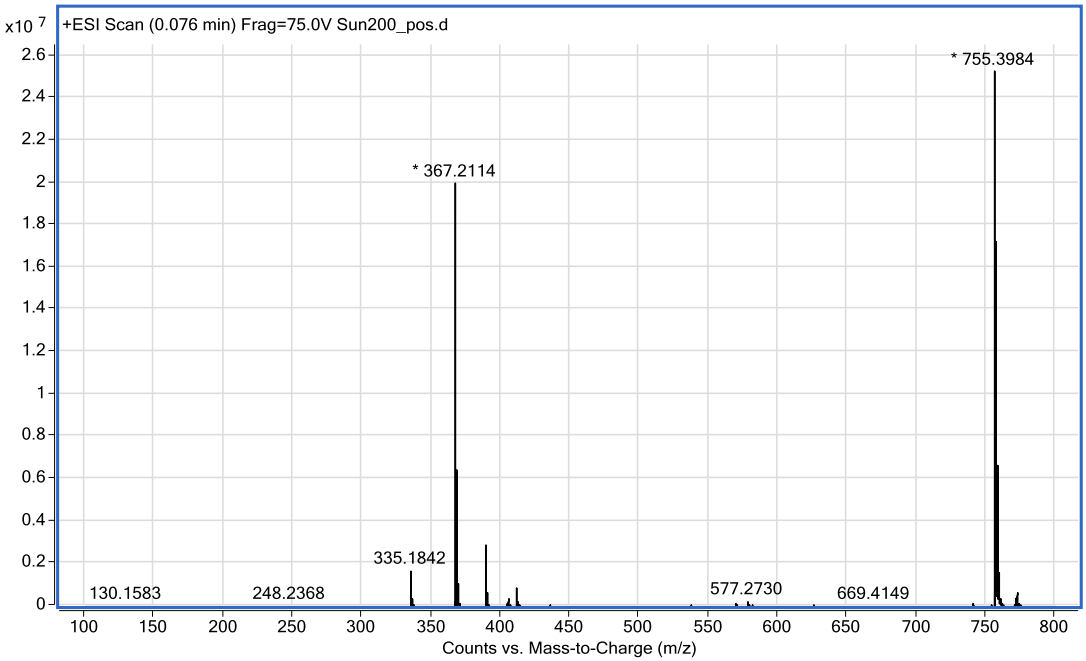
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.694	2303744	907685	99.648	99.525
2	7.979	8142	4330	0.352	0.475
Total		2311886	912015	100.000	100.000

PeakTable

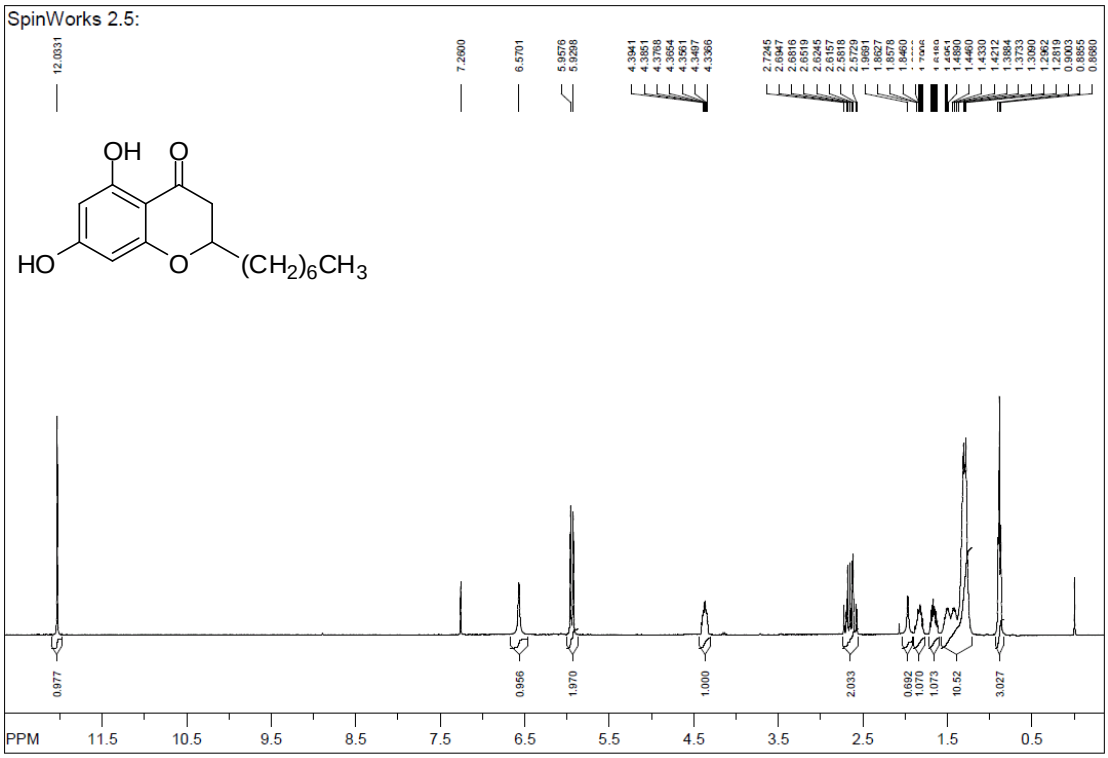
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.157	35921	13839	0.414	0.386
2	7.695	8571758	3542445	98.784	98.718
3	7.978	69571	32168	0.802	0.896
Total		8677249	3588452	100.000	100.000

HRMS of **5e**


x10 7
+ESI Scan (0.076 min) Frag=75.0V Sun200_pos.d
* 755.3984
* 367.2114
335.1842
130.1583
248.2368
577.2730
669.4149
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **5f**



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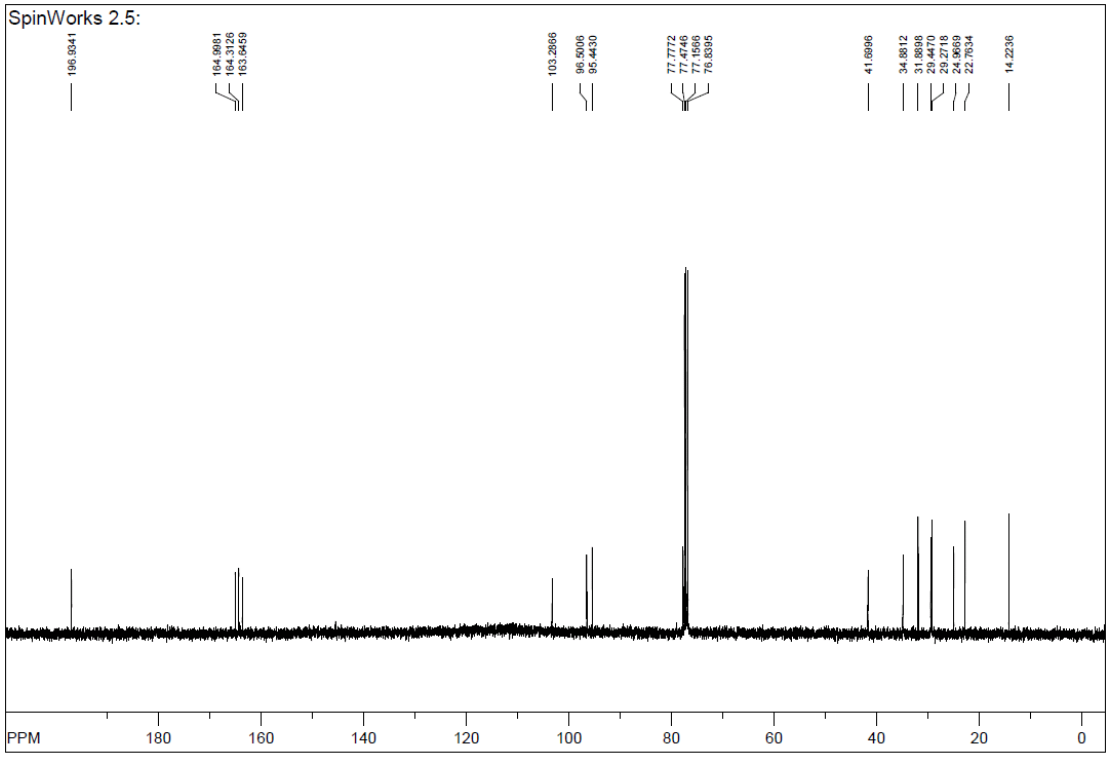
time domain size: 65536 points
width: 8012.82 Hz = 20.025463 ppm = 0.122266 Hz/pt
number of scans: 2

freq. of 0 ppm: 400.130010 MHz
processed size: 32768 complex points
LB: 0.300 GB: 0.0000
Hz/cm: 208.161 ppm/cm: 0.52023



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-80\20\fid expt: <zgpg30>
transmitter freq.: 100.622769 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.896840 ppm = 0.366798 Hz/pt
number of scans: 646

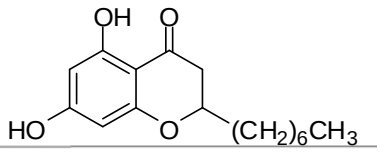
freq. of 0 ppm: 100.612755 MHz
processed size: 32768 complex points
LB: 1.000 GB: 0.0000
Hz/cm: 862.283 ppm/cm: 8.56946

HPLC profile of **5f**

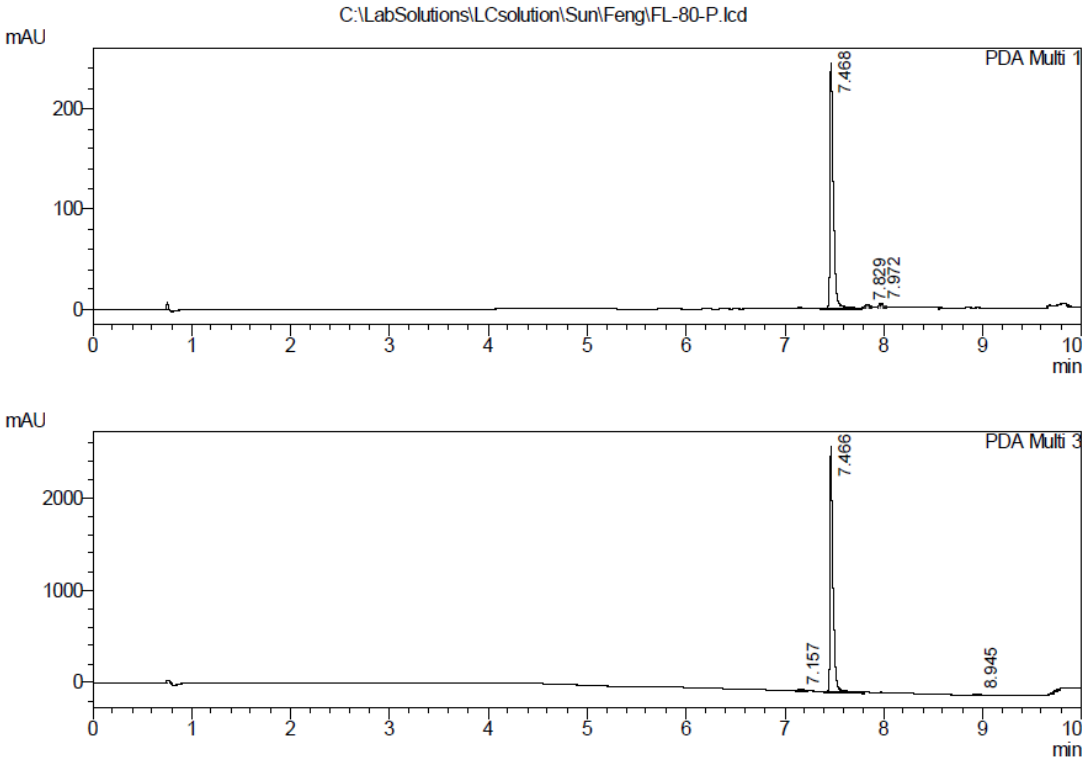
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\Feng\FL-80-P.lcd

Sample Name	: FL-80-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 4 uL
Data File Name	: FL-80-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 12/2/2011 10:45:41 AM



<Chromatogram>



1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

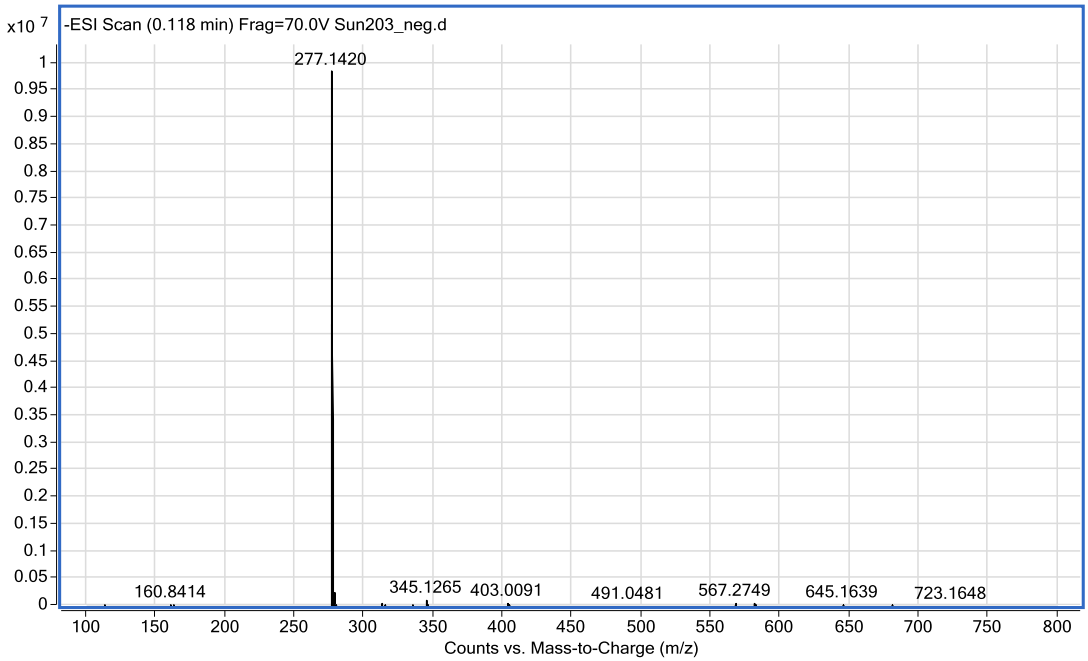
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.468	619604	244071	98.567	98.104
2	7.829	2811	1628	0.447	0.654
3	7.972	6196	3089	0.986	1.241
Total		628610	248788	100.000	100.000

PeakTable

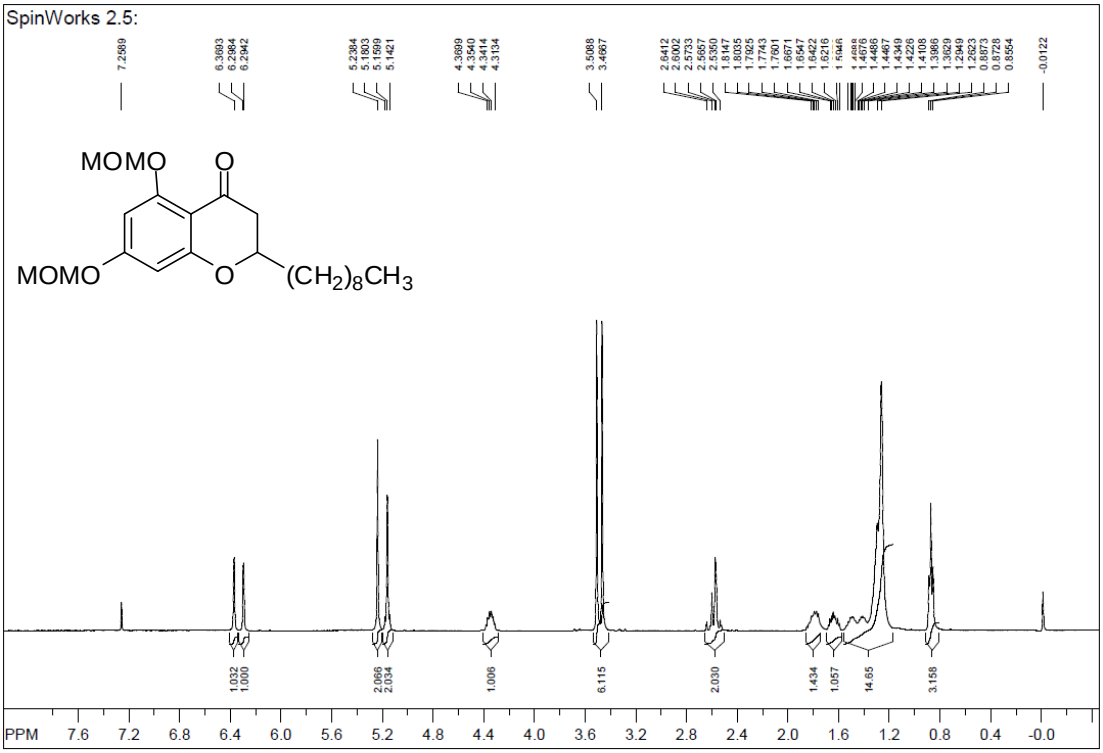
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.157	51083	16629	0.864	0.620
2	7.466	5840037	2658065	98.771	99.045
3	8.945	21566	9013	0.365	0.336
Total		5912686	2683707	100.000	100.000

HRMS of **5f**


x10 7
-ESI Scan (0.118 min) Frag=70.0V Sun203_neg.d
277.1420
160.8414
345.1265
403.0091
491.0481
567.2749
645.1639
723.1648
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **5g**



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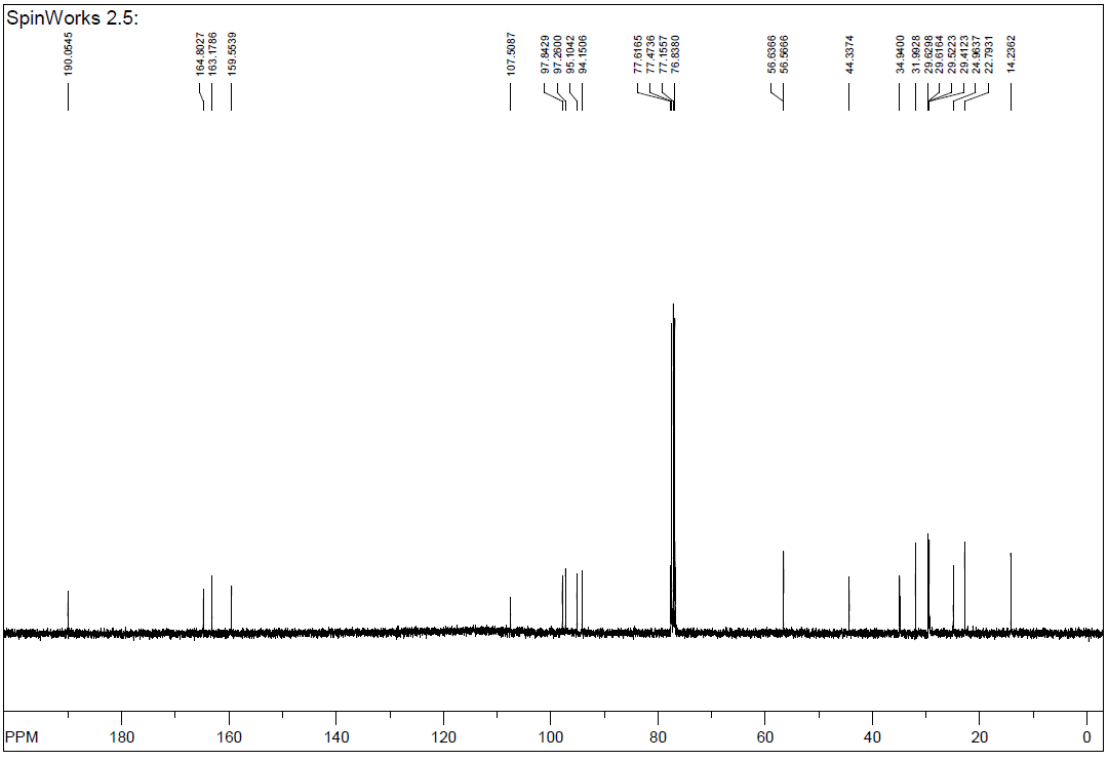
time domain size: 65536 points
width: 8012.82 Hz = 20.025463 ppm = 0.122266 Hz/pt
number of scans: 2

freq. of 0 ppm: 400.130010 MHz
processed size: 32768 complex points
LB: 0.300 GB: 0.0000
Hz/cm: 138.314 ppm/cm: 0.34567



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-78\20\fid expt: <zgpg30>
transmitter freq.: 100.622769 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.896840 ppm = 0.366798 Hz/pt
number of scans: 880

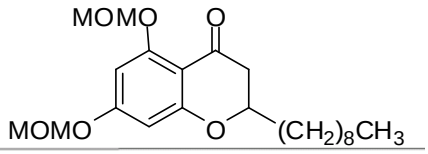
freq. of 0 ppm: 100.612756 MHz
processed size: 32768 complex points
LB: 1.000 GB: 0.0000
Hz/cm: 825.062 ppm/cm: 8.19956

HPLC profile of **5g**

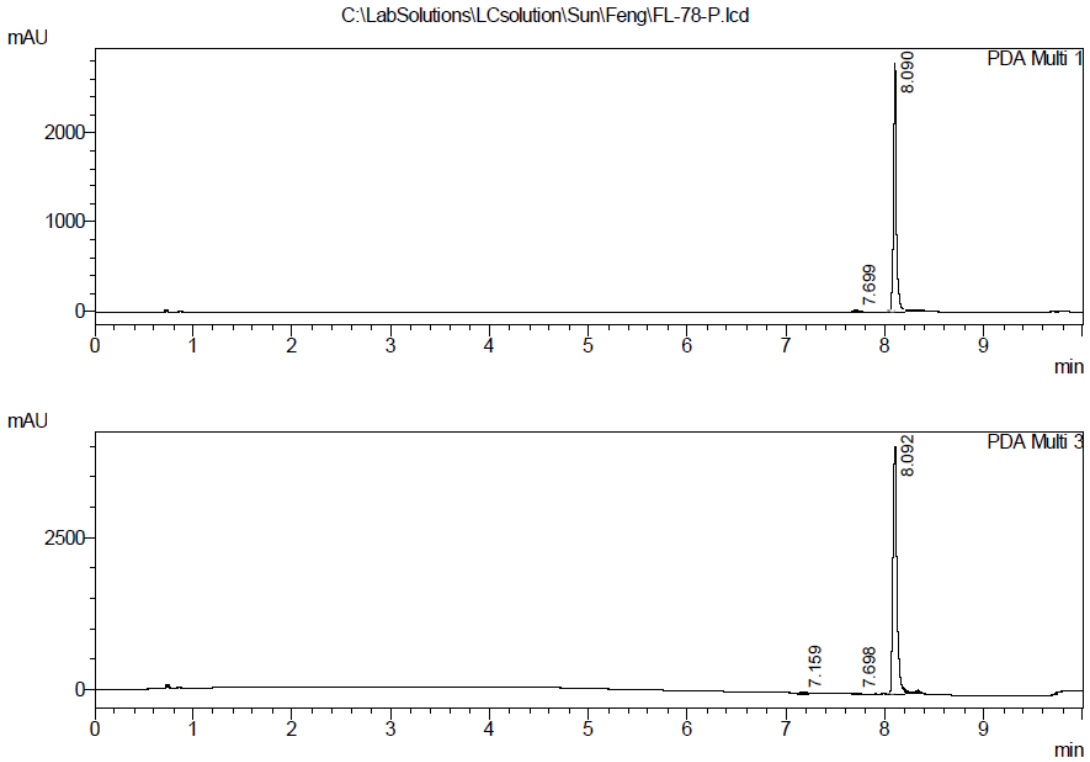
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\Feng\FL-78-P.lcd

Sample Name	: FL-78-P
Tray#	: 1
Vail #	: 93
Injection Volume	: 4 uL
Data File Name	: FL-78-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	: Batch 1.lcb
Data Acquired	: 11/30/2011 2:53:38 PM



<Chromatogram>



1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

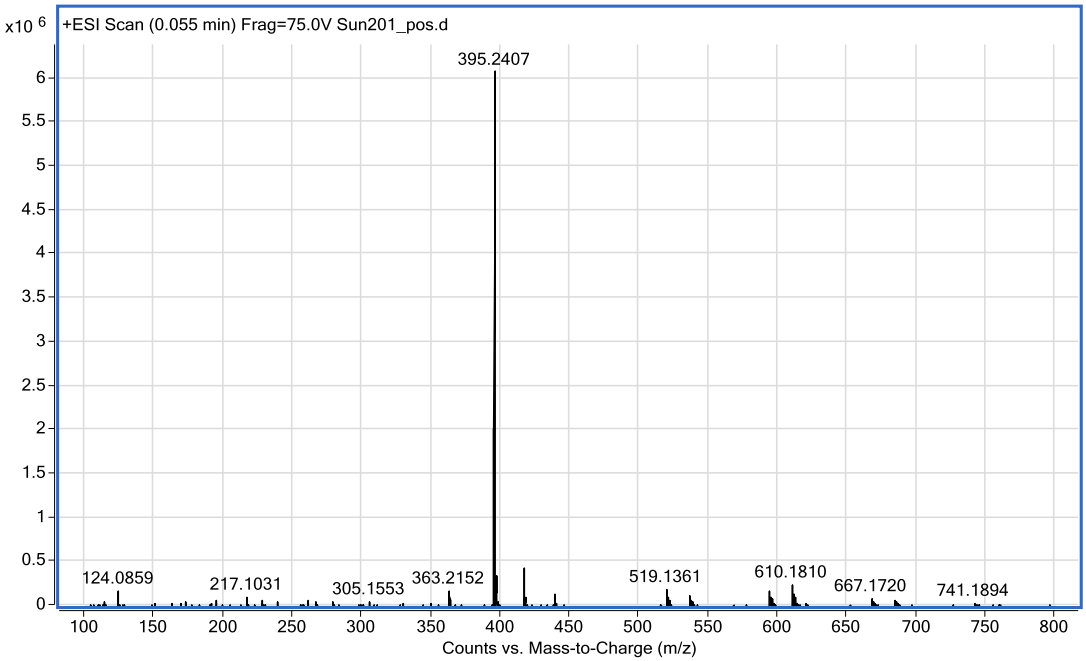
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.699	8243	3340	0.127	0.124
2	8.090	6457119	2688295	99.873	99.876
Total		6465361	2691635	100.000	100.000

PeakTable

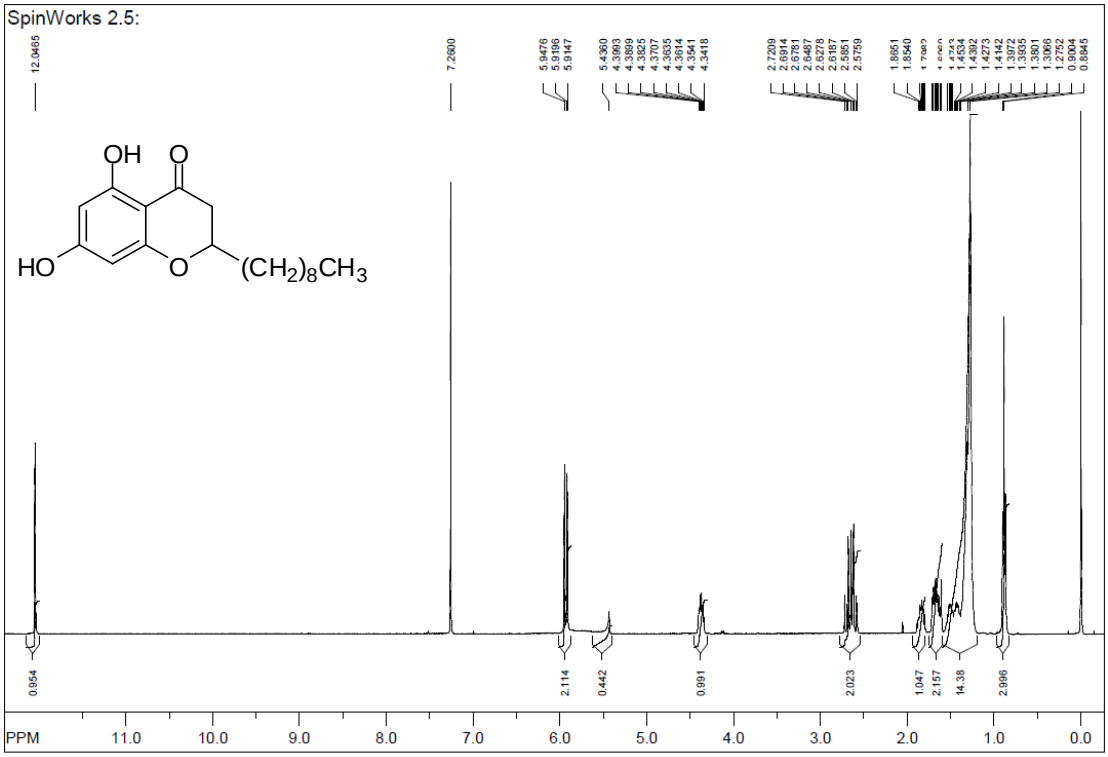
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.159	42200	15023	0.308	0.368
2	7.698	23589	10964	0.172	0.268
3	8.092	13620056	4060111	99.519	99.364
Total		13685845	4086098	100.000	100.000

HRMS of **5g**


x10 6
+ESI Scan (0.055 min) Frag=75.0V Sun201_pos.d
395.2407
124.0859
217.1031
305.1553
363.2152
519.1361
610.1810
667.1720
741.1894
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **5h**



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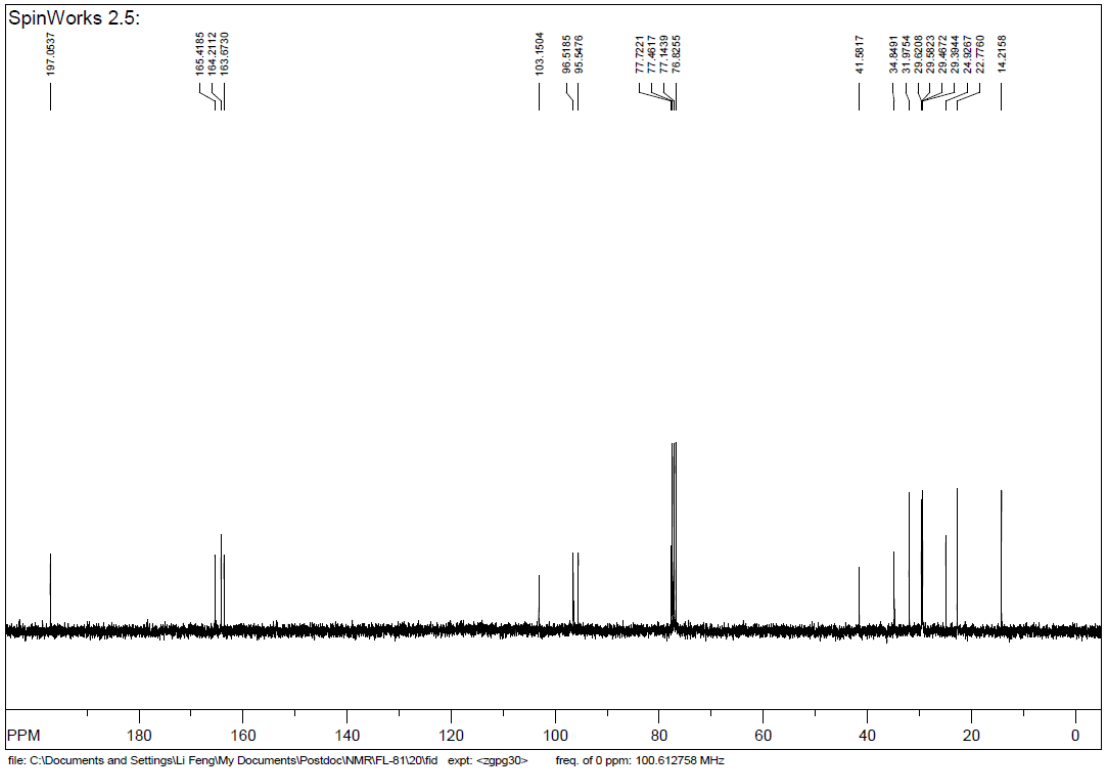
transmitter freq.: 400.131600 MHz
time domain size: 65536 points
width: 8012.82 Hz = 20.025463 ppm = 0.122266 Hz/pt
number of scans: 16

freq. of 0 ppm: 400.130010 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 202.647 ppm/cm: 0.50645



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-81\20\fid expt: <zgpg30>
transmitter freq.: 100.622769 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.896840 ppm = 0.366798 Hz/pt
number of scans: 131

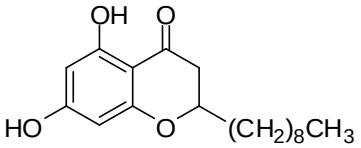
freq. of 0 ppm: 100.612758 MHz
processed size: 32768 complex points
LB: 1.000 GB: 0.0000
Hz/cm: 847.119 ppm/cm: 8.41876

HPLC profile of **5h**

==== Shimadzu LCsolution Analysis Report ====

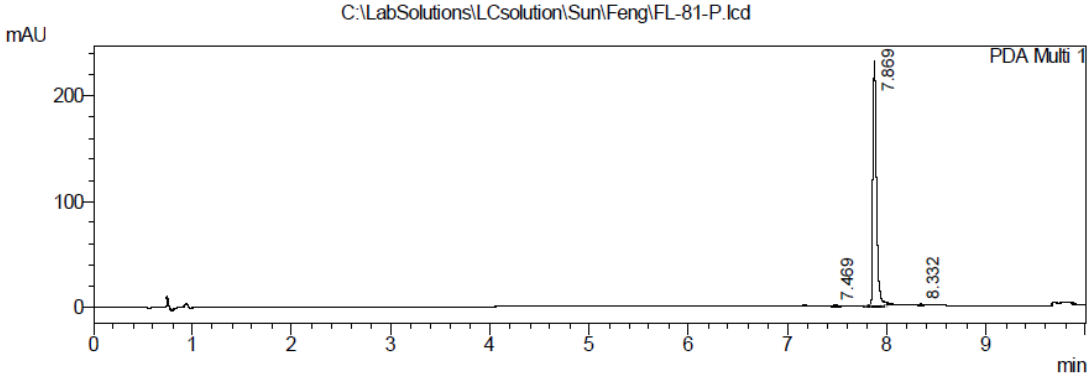
C:\LabSolutions\LCsolution\Sun\Feng\FL-81-P.lcd

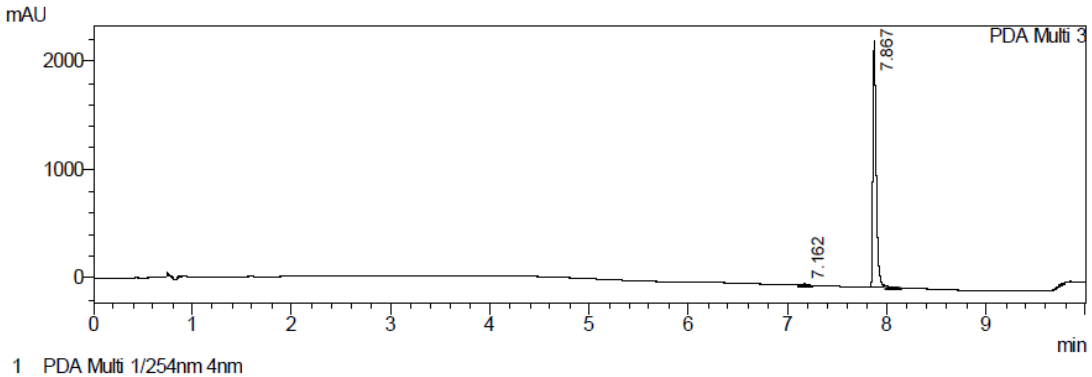
Sample Name	: FL-81-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 5 uL
Data File Name	: FL-81-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 12/2/2011 10:56:35 AM



<Chromatogram>

C:\LabSolutions\LCsolution\Sun\Feng\FL-81-P.lcd





1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

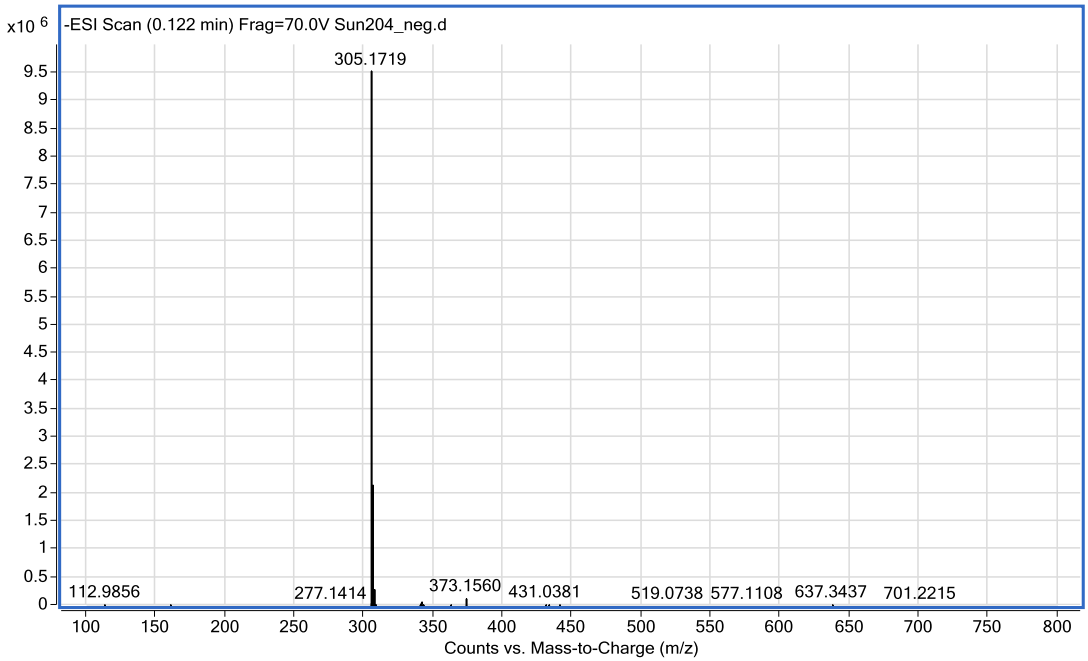
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.469	870	460	0.147	0.198
2	7.869	591105	231011	99.712	99.605
3	8.332	836	456	0.141	0.196
Total		592812	231927	100.000	100.000

PeakTable

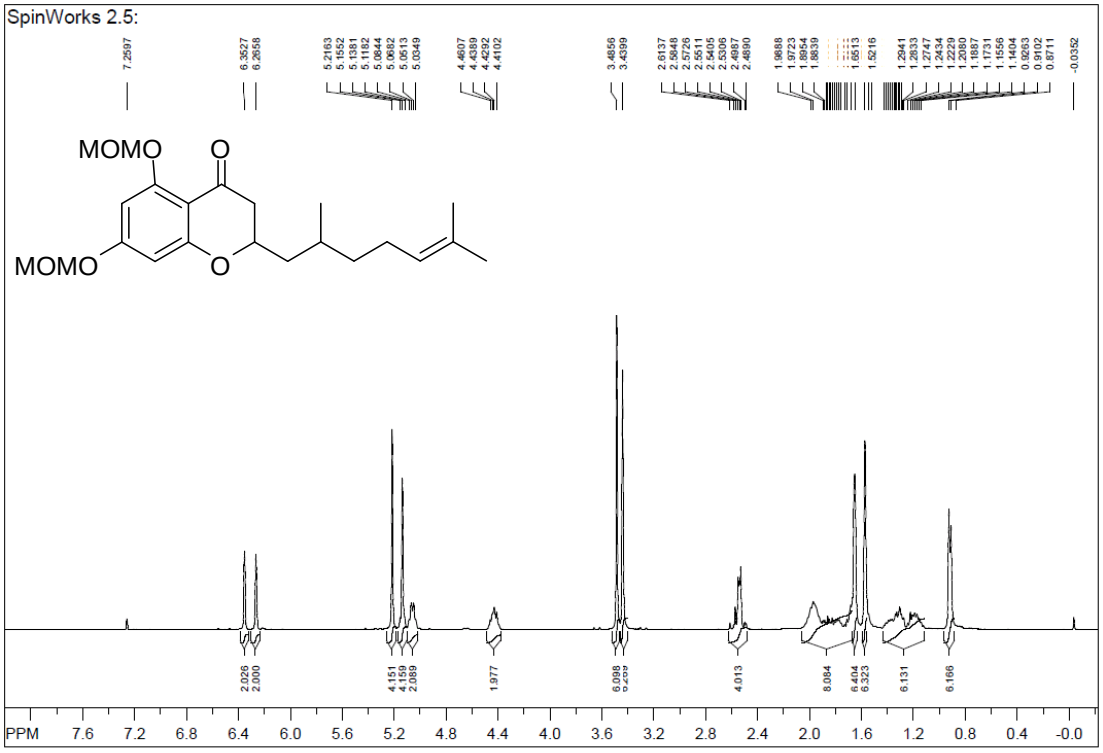
PDA Ch3 220nm 4nm

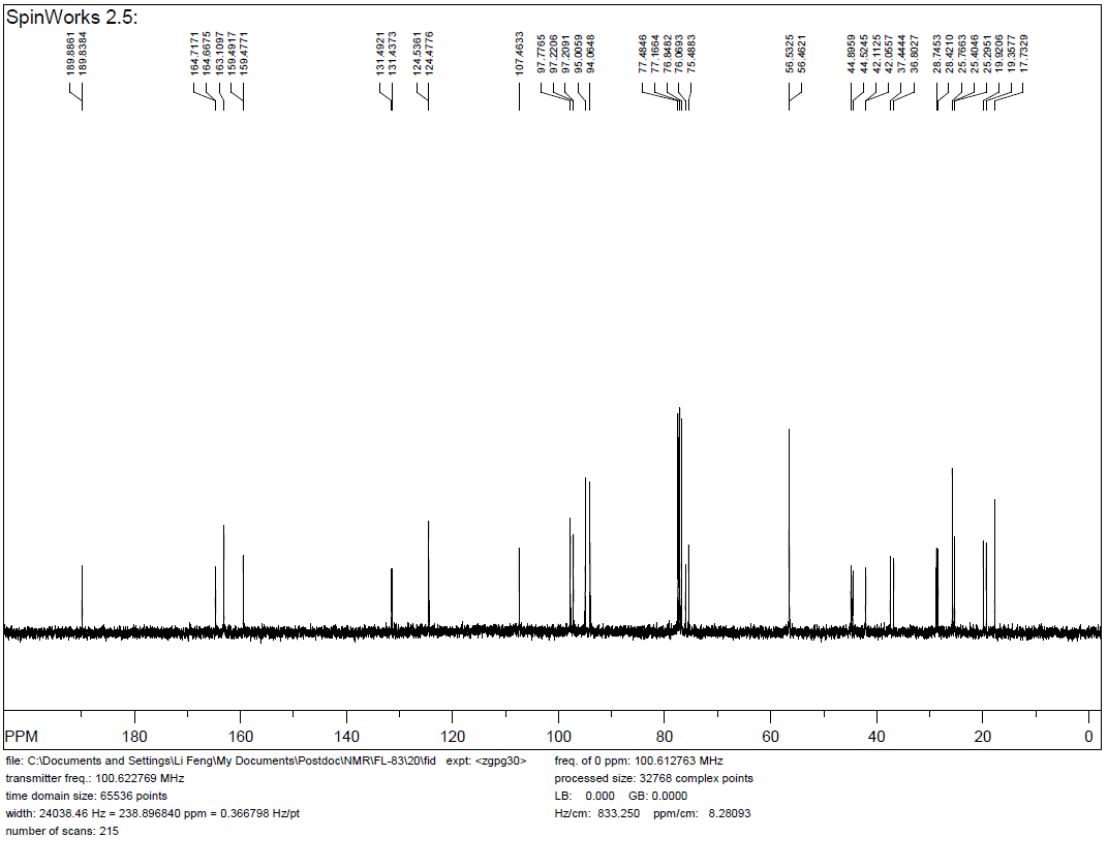
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.162	40146	12883	0.769	0.563
2	7.867	5177113	2276495	99.231	99.437
Total		5217260	2289378	100.000	100.000

HRMS of **5h**


x10 6
-ESI Scan (0.122 min) Frag=70.0V Sun204_neg.d
305.1719
112.9856
277.1414
373.1560
431.0381
519.0738
577.1108
637.3437
701.2215
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **5i**



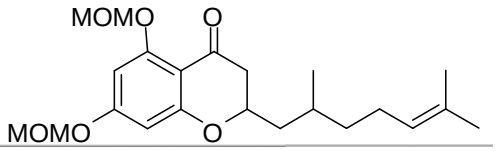


HPLC profile of **5i**

==== Shimadzu LCsolution Analysis Report ====

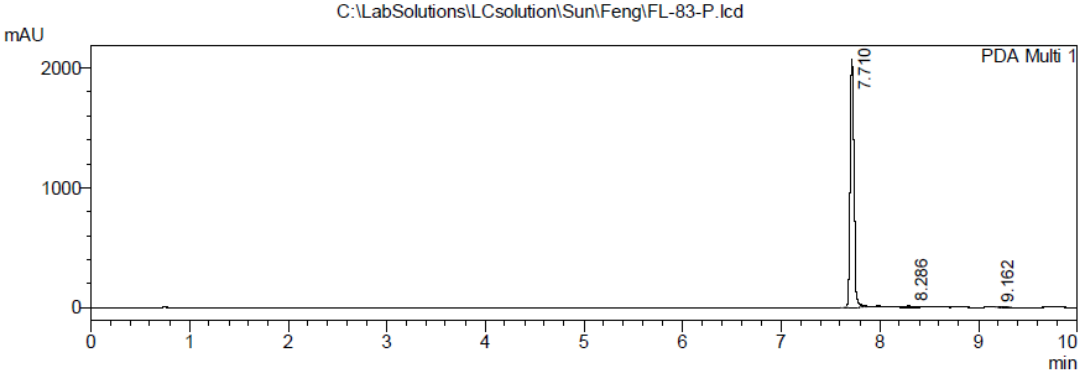
C:\LabSolutions\LCsolution\Sun\Feng\FL-83-P.lcd

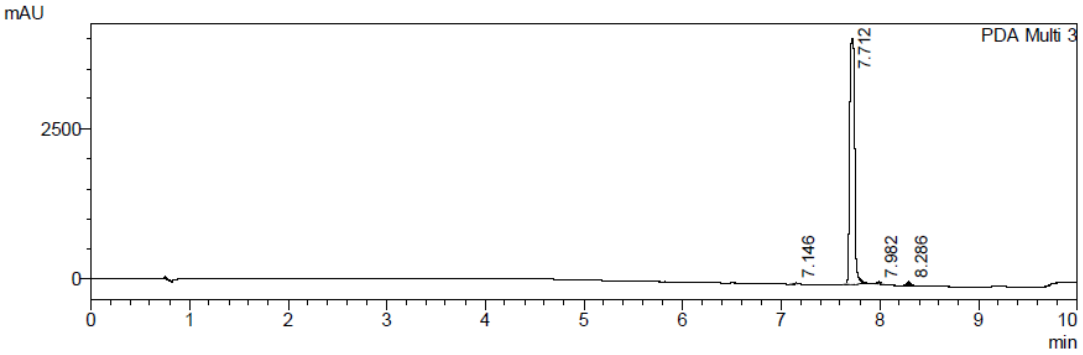
Sample Name	: FL-83-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 5 uL
Data File Name	: FL-83-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 12/7/2011 10:49:54 AM



<Chromatogram>

C:\LabSolutions\LCsolution\Sun\Feng\FL-83-P.lcd





1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

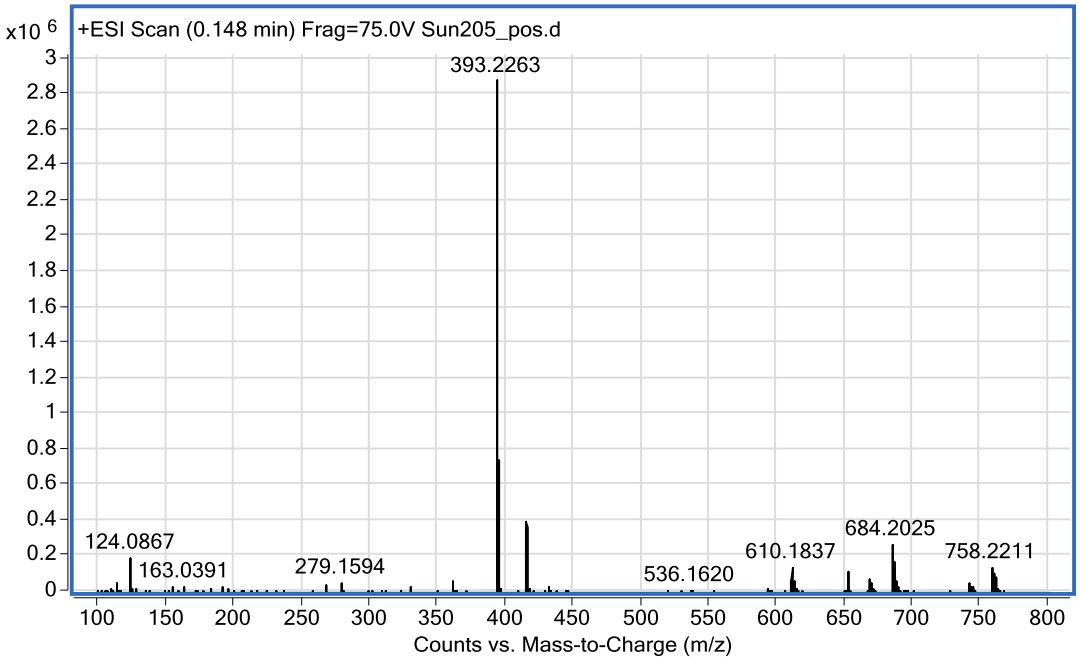
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.710	5177360	2051541	98.828	99.109
2	8.286	29363	14193	0.560	0.686
3	9.162	32026	4258	0.611	0.206
Total		5238749	2069992	100.000	100.000

PeakTable

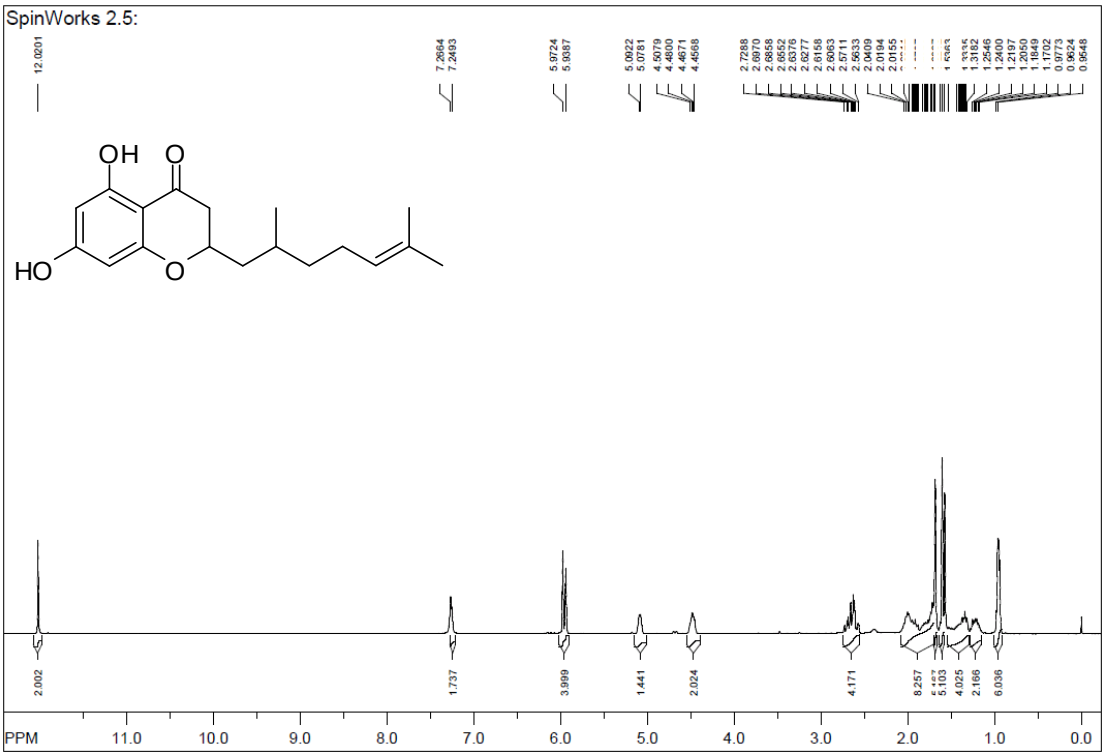
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.146	38588	14873	0.277	0.354
2	7.712	13685217	4091946	98.413	97.530
3	7.982	50242	27839	0.361	0.664
4	8.286	131891	60909	0.948	1.452
Total		13905938	4195567	100.000	100.000

HRMS of **5i**


x10 6
+ESI Scan (0.148 min) Frag=75.0V Sun205_pos.d
393.2263
124.0867
163.0391
279.1594
536.1620
610.1837
684.2025
758.2211
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **5j**



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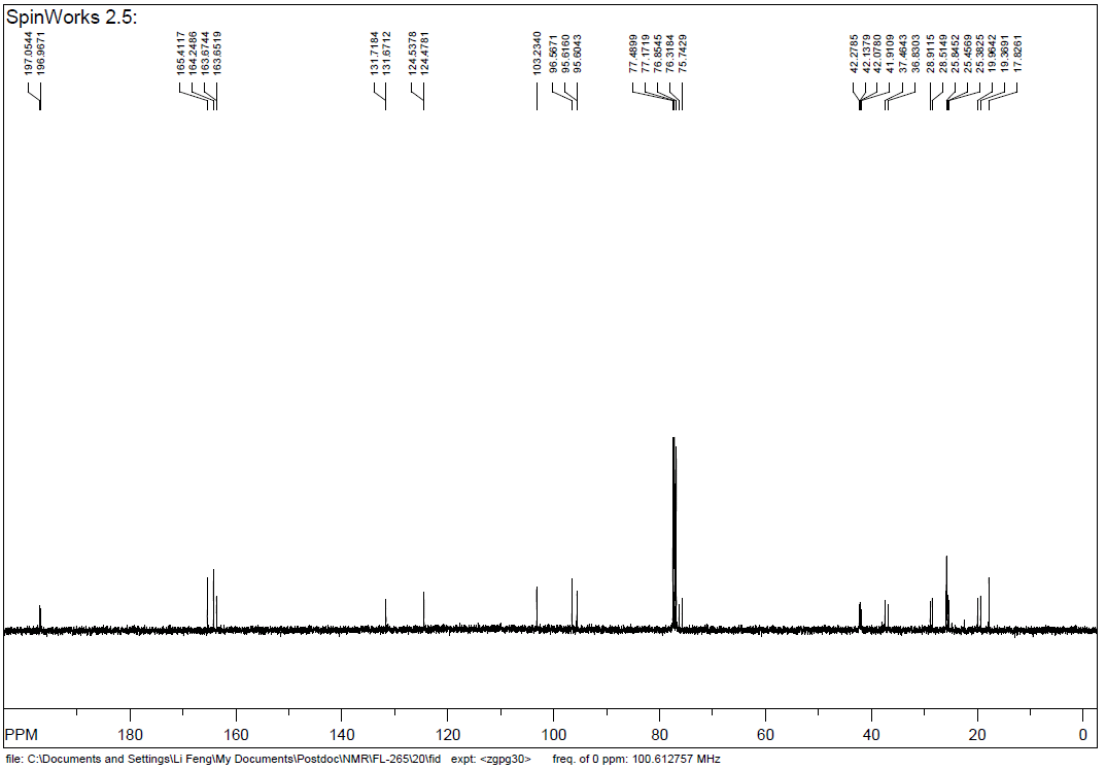
number of scans: 1
freq. of 0 ppm: 400.130007 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 202.417 ppm/cm: 0.50588



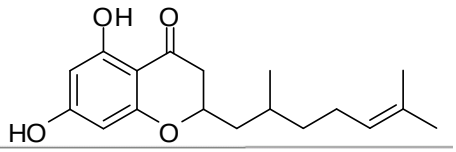
file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-265\20\fid expt: <zgpg30>
transmitter freq.: 100.622769 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.896840 ppm = 0.366798 Hz/pt
number of scans: 271
freq. of 0 ppm: 100.612757 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 831.266 ppm/cm: 8.26121

HPLC profile of **5j**

==== Shimadzu LCsolution Analysis Report ====

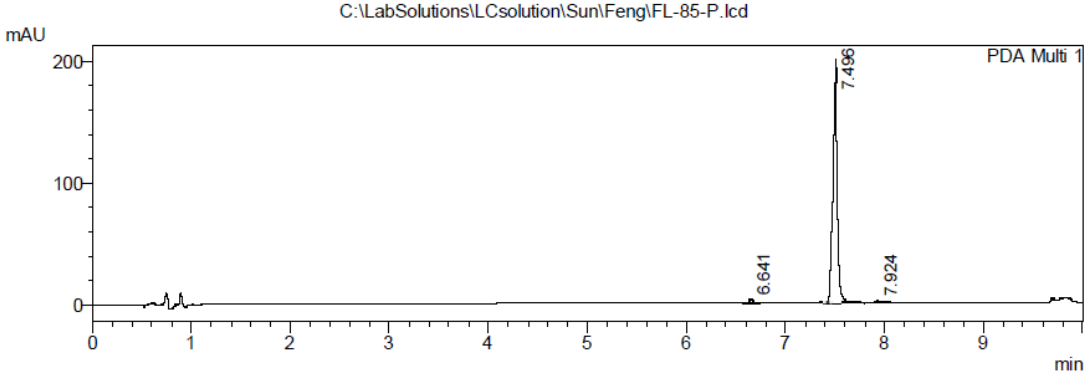
C:\LabSolutions\LCsolution\Sun\Feng\FL-85-P.lcd

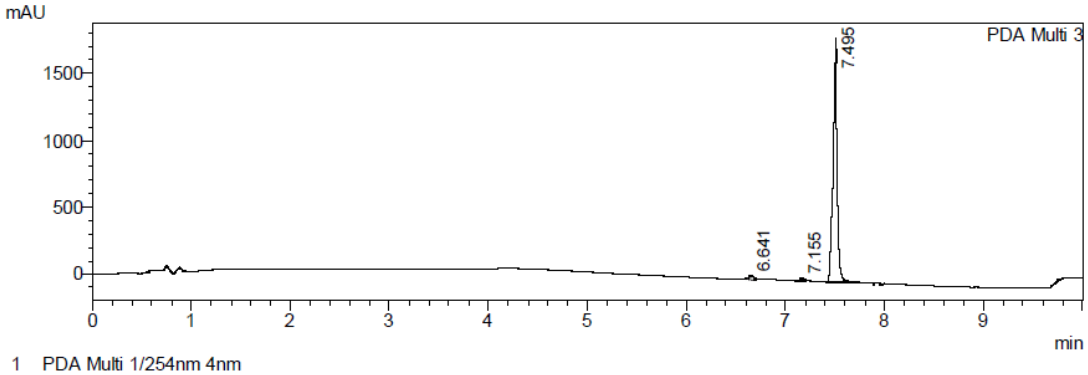
Sample Name	: FL-85-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 5 uL
Data File Name	: FL-85-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 12/7/2011 2:51:50 PM



<Chromatogram>

C:\LabSolutions\LCsolution\Sun\Feng\FL-85-P.lcd





1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

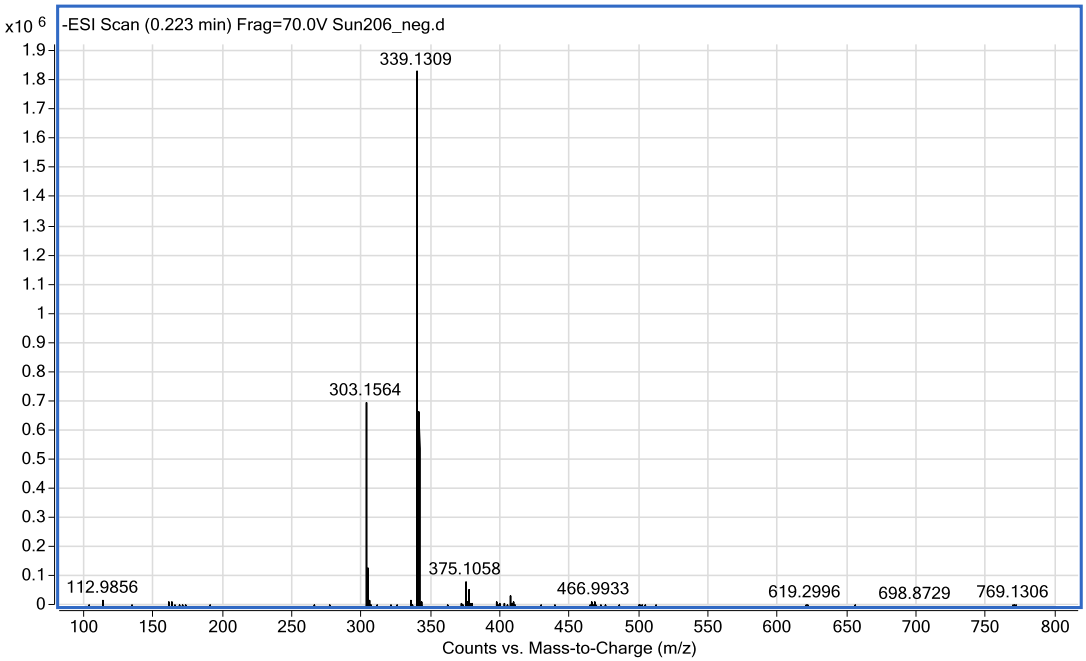
Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.641	7702	2986	1.179	1.504
2	7.496	643188	194752	98.433	98.084
3	7.924	2538	817	0.388	0.412
Total		653428	198556	100.000	100.000

PeakTable

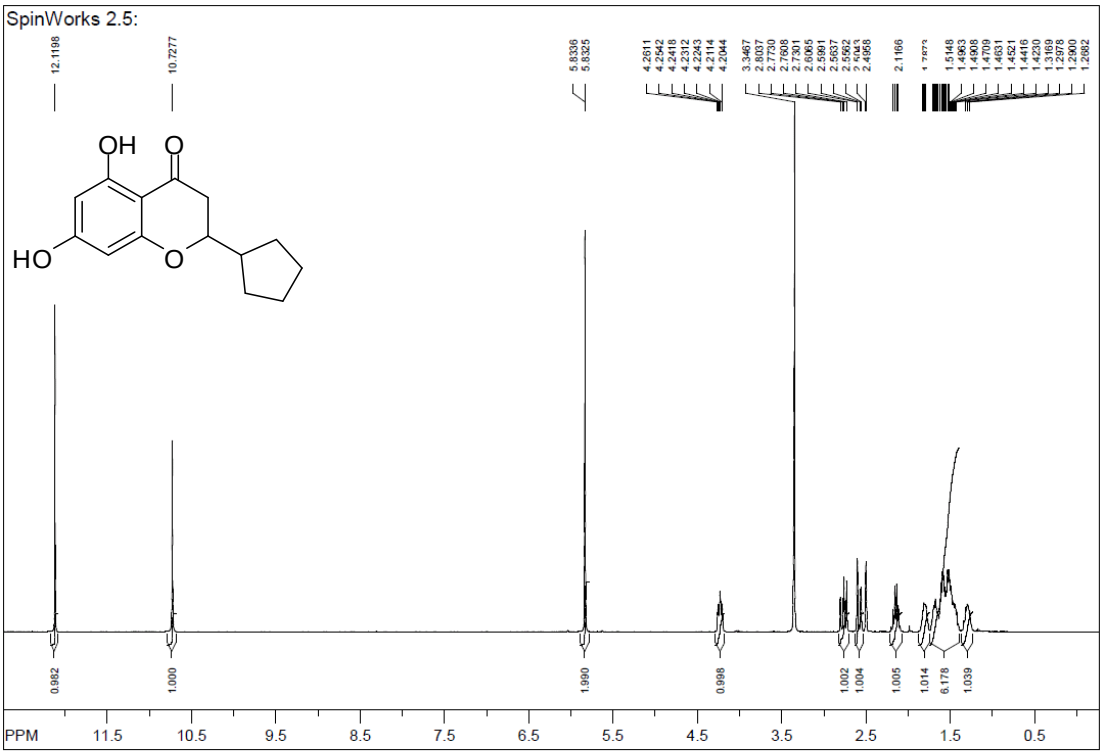
PDA Ch3 220nm 4nm

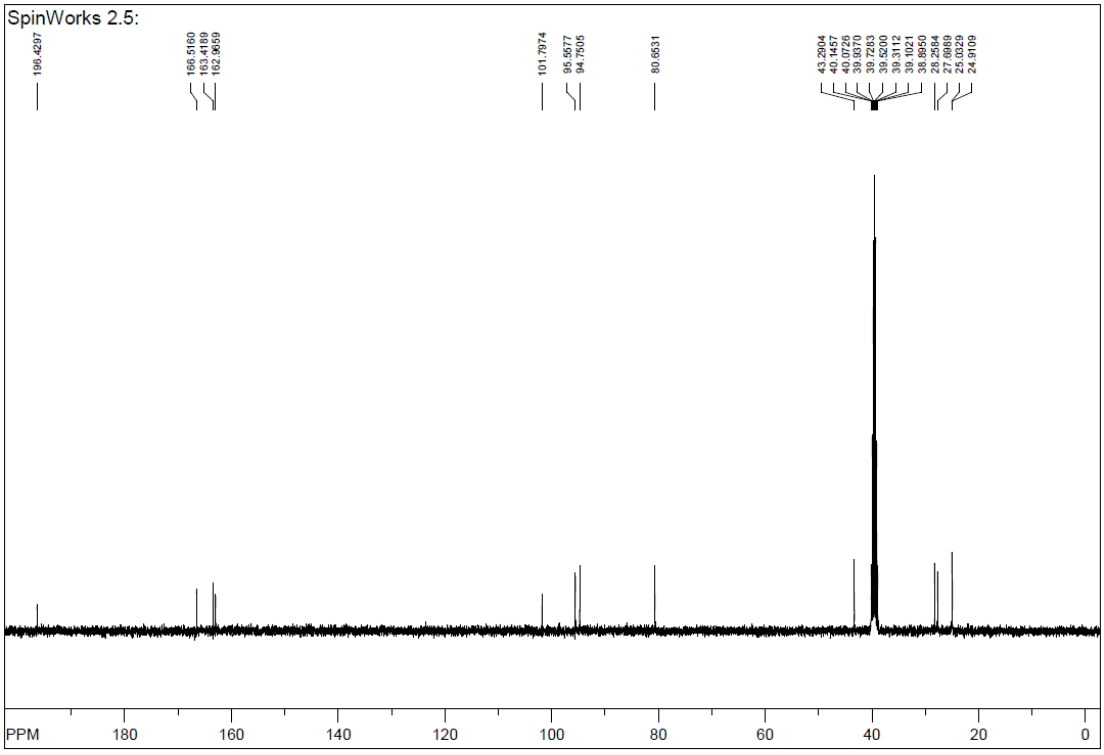
Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.641	55796	24046	0.985	1.294
2	7.155	34633	14115	0.612	0.760
3	7.495	5571532	1820010	98.403	97.946
Total		5661961	1858172	100.000	100.000

HRMS of **5j**


x10 6
-ESI Scan (0.223 min) Frag=70.0V Sun206_neg.d
339.1309
303.1564
375.1058
112.9856
466.9933
619.2996
698.8729
769.1306
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **5k**



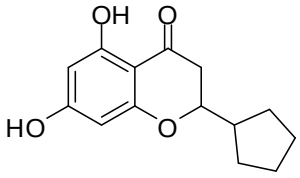


HPLC profile of **5k**

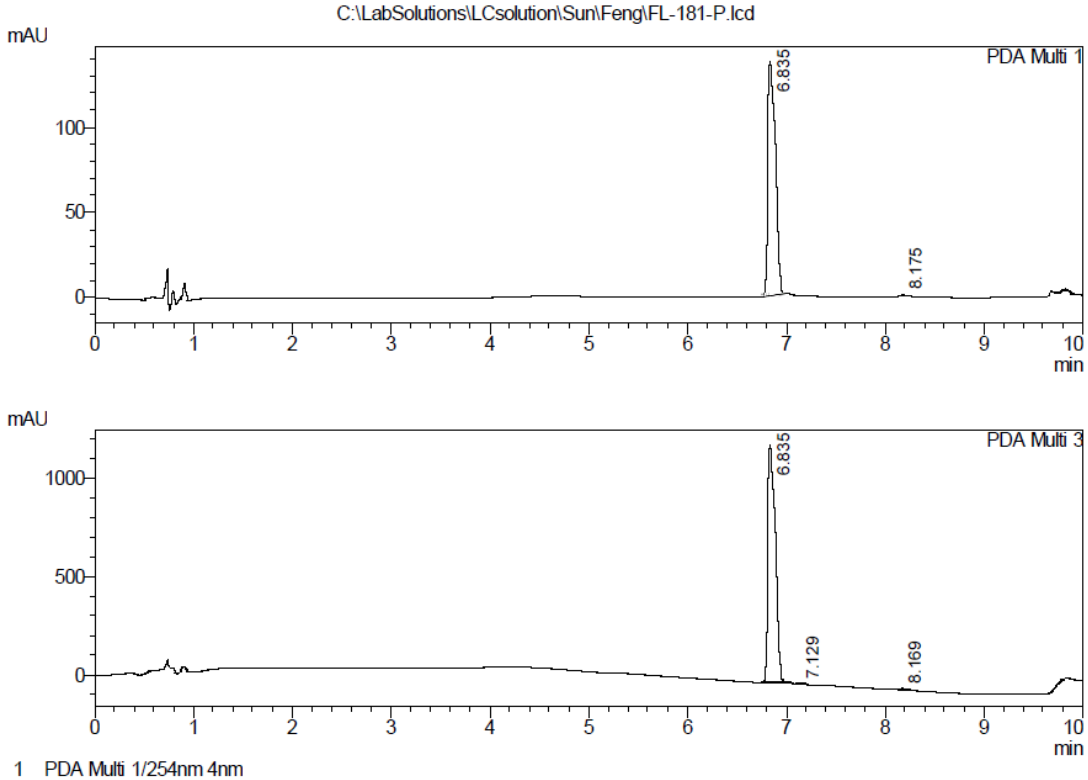
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\Feng\FL-181-P.lcd

Sample Name	: FL-181-P
Tray#	: 1
Vail #	: 95
Injection Volume	: 10 uL
Data File Name	: FL-181-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	: Batch 1.lcb
Data Acquired	: 3/8/2012 1:06:10 PM



<Chromatogram>



1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

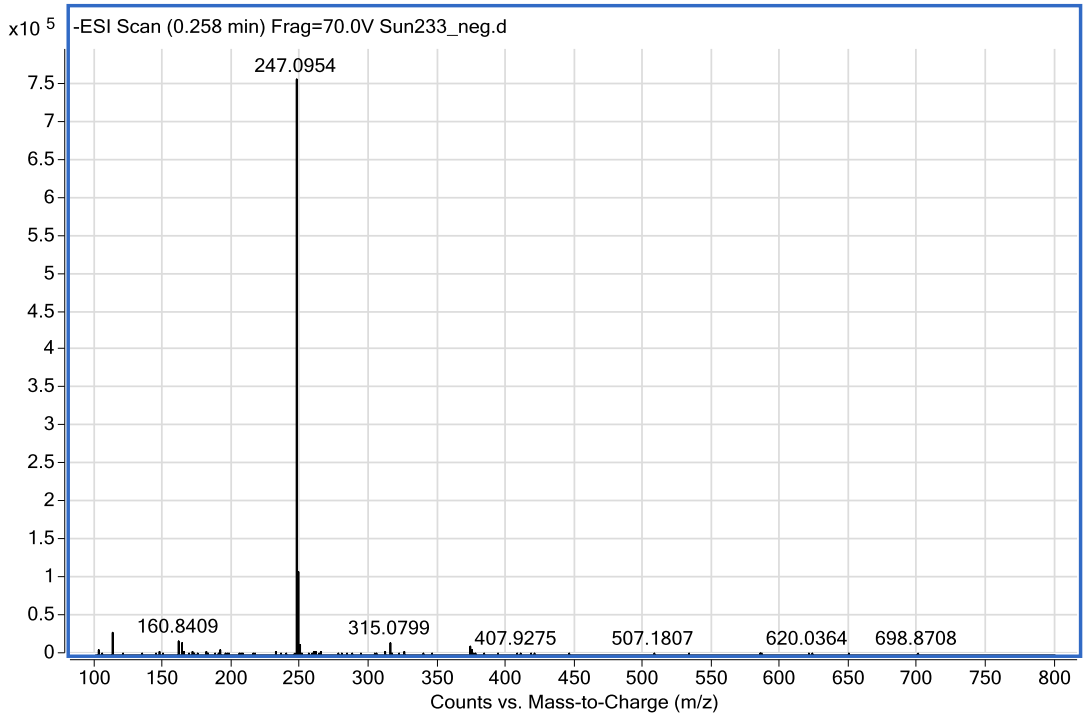
Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.835	734422	137028	99.611	99.520
2	8.175	2867	660	0.389	0.480
Total		737288	137688	100.000	100.000

PeakTable

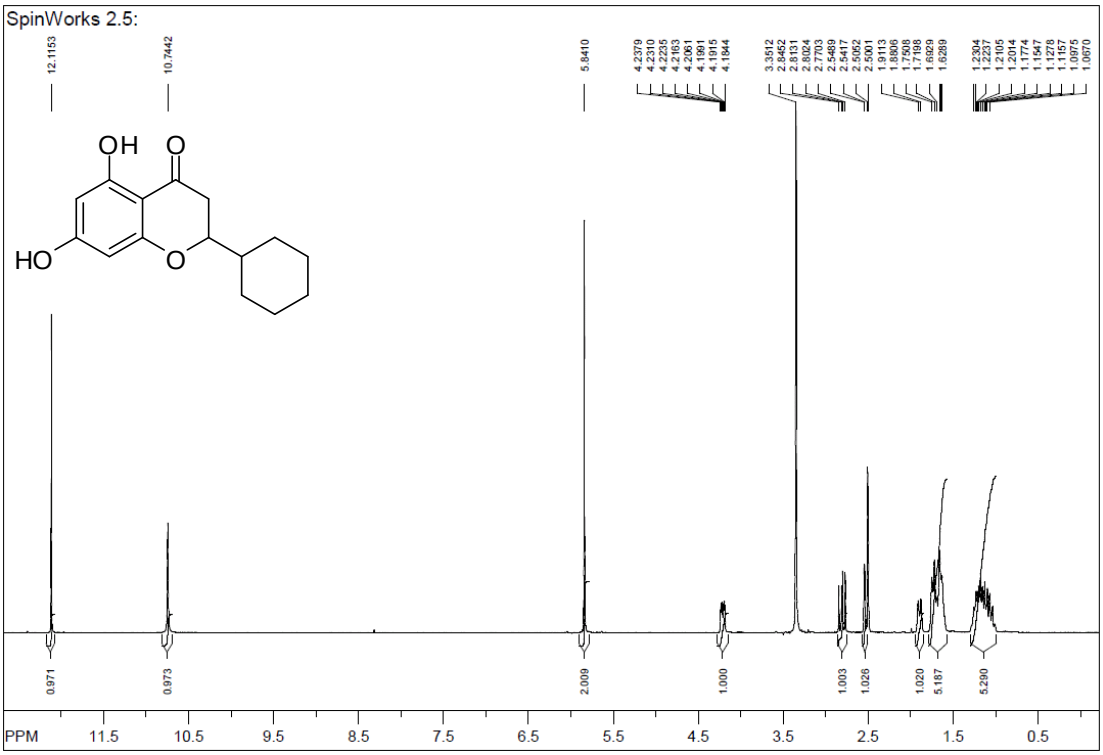
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.835	6409188	1205931	99.598	99.430
2	7.129	8049	2243	0.125	0.185
3	8.169	17836	4674	0.277	0.385
Total		6435073	1212848	100.000	100.000

HRMS of **5k**

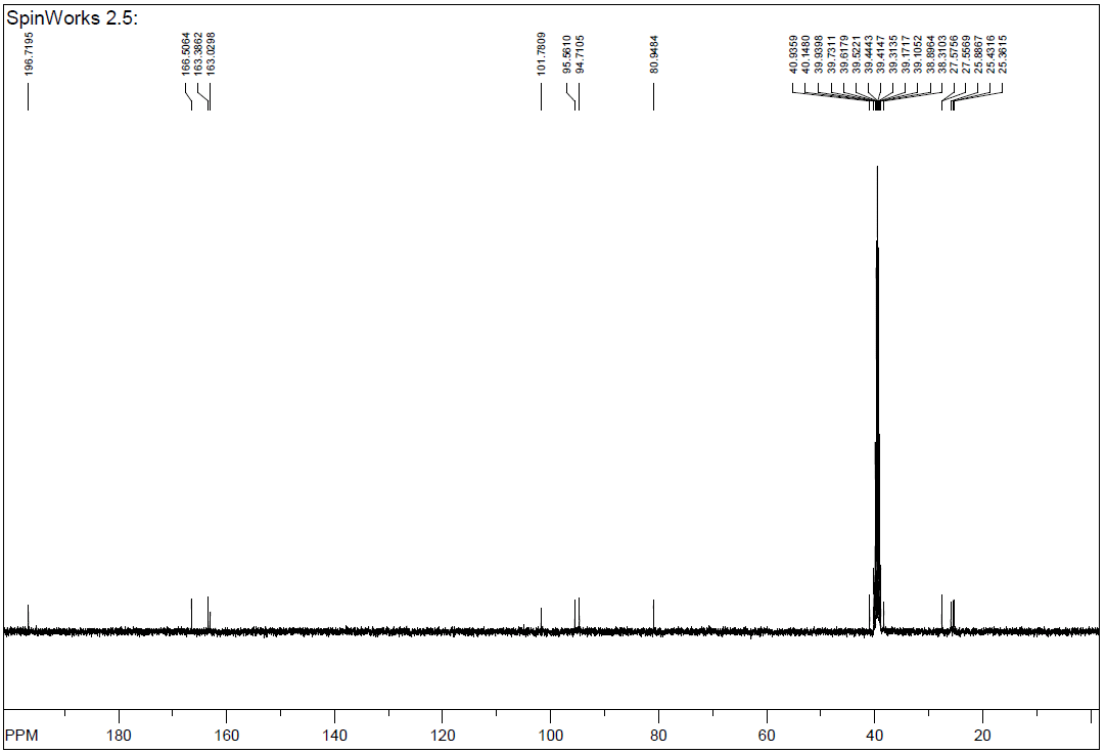

x10 5
-ESI Scan (0.258 min) Frag=70.0V Sun233_neg.d
247.0954
160.8409
315.0799
407.9275
507.1807
620.0364
698.8708
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **5l**



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-177\1\fid expt: <zg30>
transmitter freq.: 400.131600 MHz
time domain size: 65536 points
width: 8012.82 Hz = 20.025463 ppm = 0.122266 Hz/pt
number of scans: 8

freq. of 0 ppm: 400.130001 MHz
processed size: 32768 complex points
LB: 0.300 GB: 0.0000
Hz/cm: 206.323 ppm/cm: 0.51564



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-177\20\fid expt: <zgpg30>
transmitter freq.: 100.622769 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.896840 ppm = 0.366798 Hz/pt
number of scans: 1634

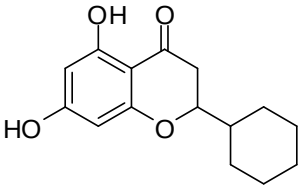
freq. of 0 ppm: 100.612817 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 816.101 ppm/cm: 8.11050

HPLC profile of **5l**

==== Shimadzu LCsolution Analysis Report ====

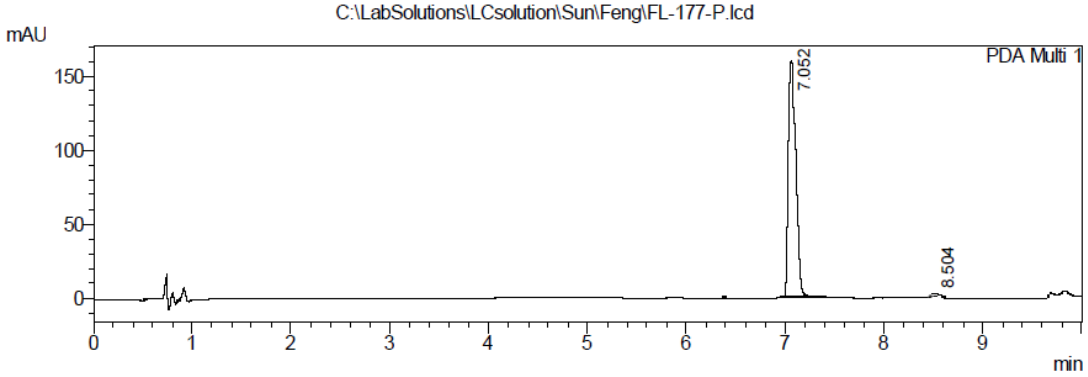
C:\LabSolutions\LCsolution\Sun\Feng\FL-177-P.lcd

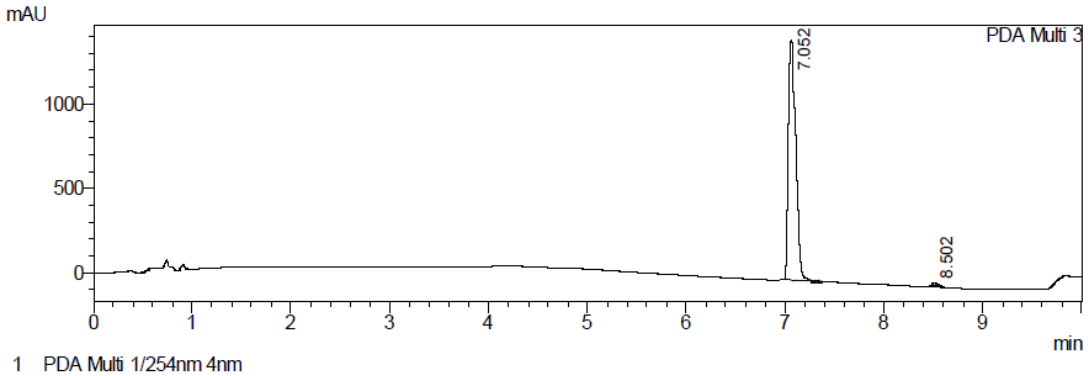
Sample Name	: FL-177-P
Tray#	: 1
Vail #	: 94
Injection Volume	: 10 uL
Data File Name	: FL-177-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	: Batch 1.lcb
Data Acquired	: 3/8/2012 12:55:44 PM



<Chromatogram>

C:\LabSolutions\LCsolution\Sun\Feng\FL-177-P.lcd





1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

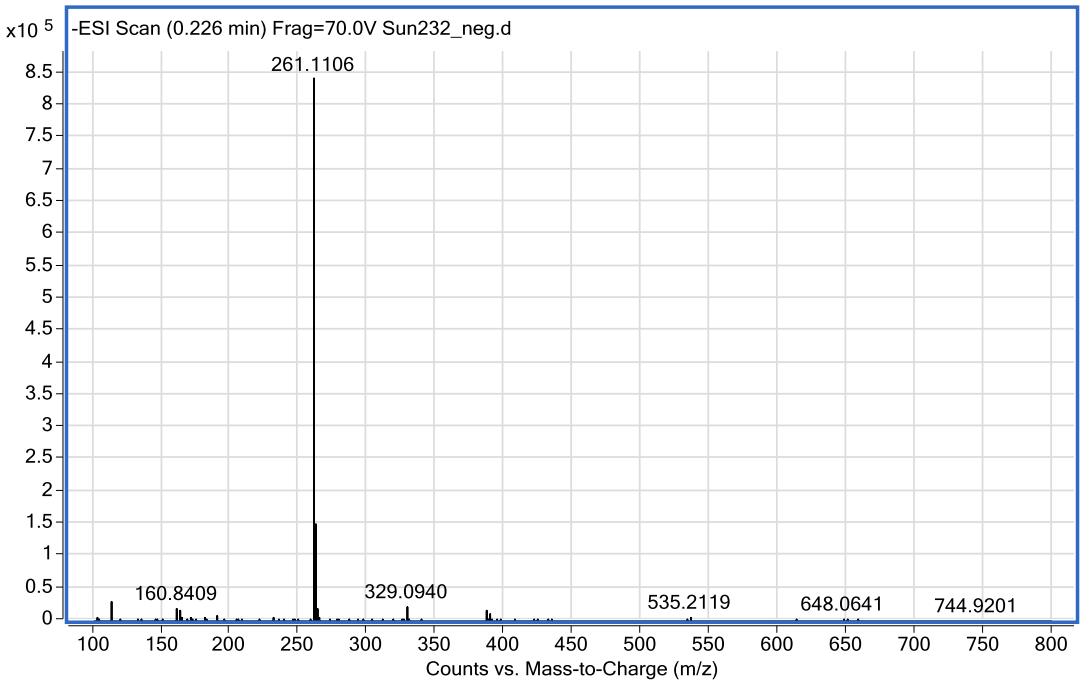
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.052	882200	159818	99.113	98.788
2	8.504	7891	1961	0.887	1.212
Total		890092	161780	100.000	100.000

PeakTable

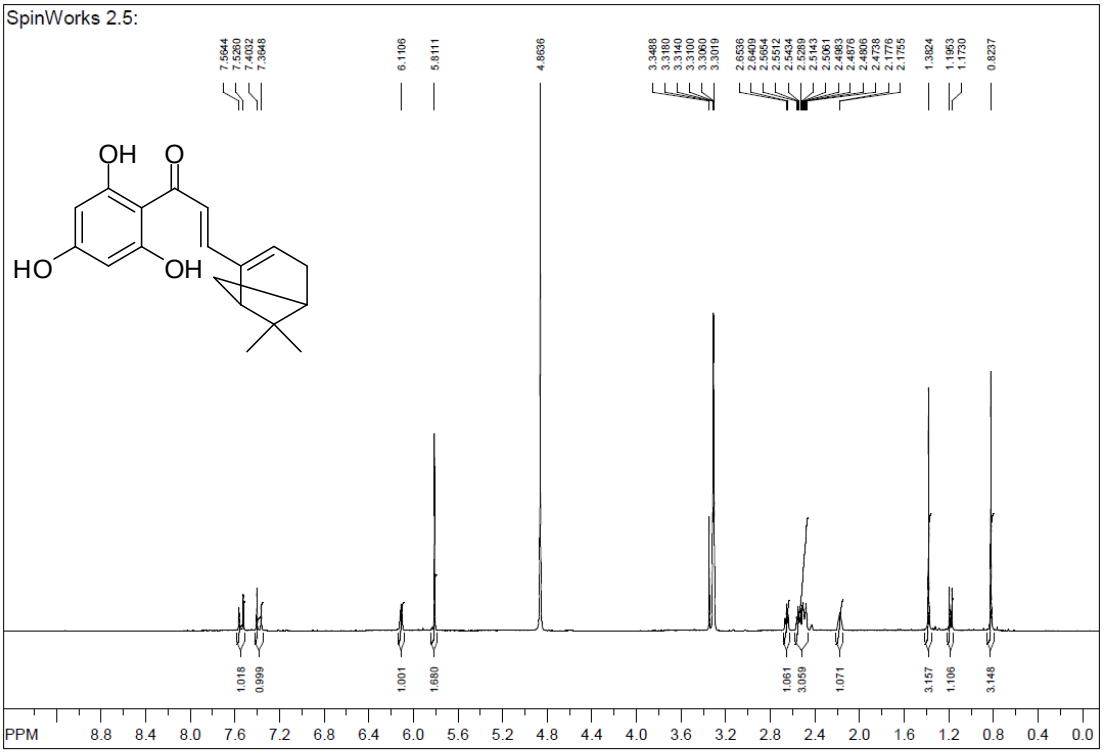
PDA Ch3 220nm 4nm

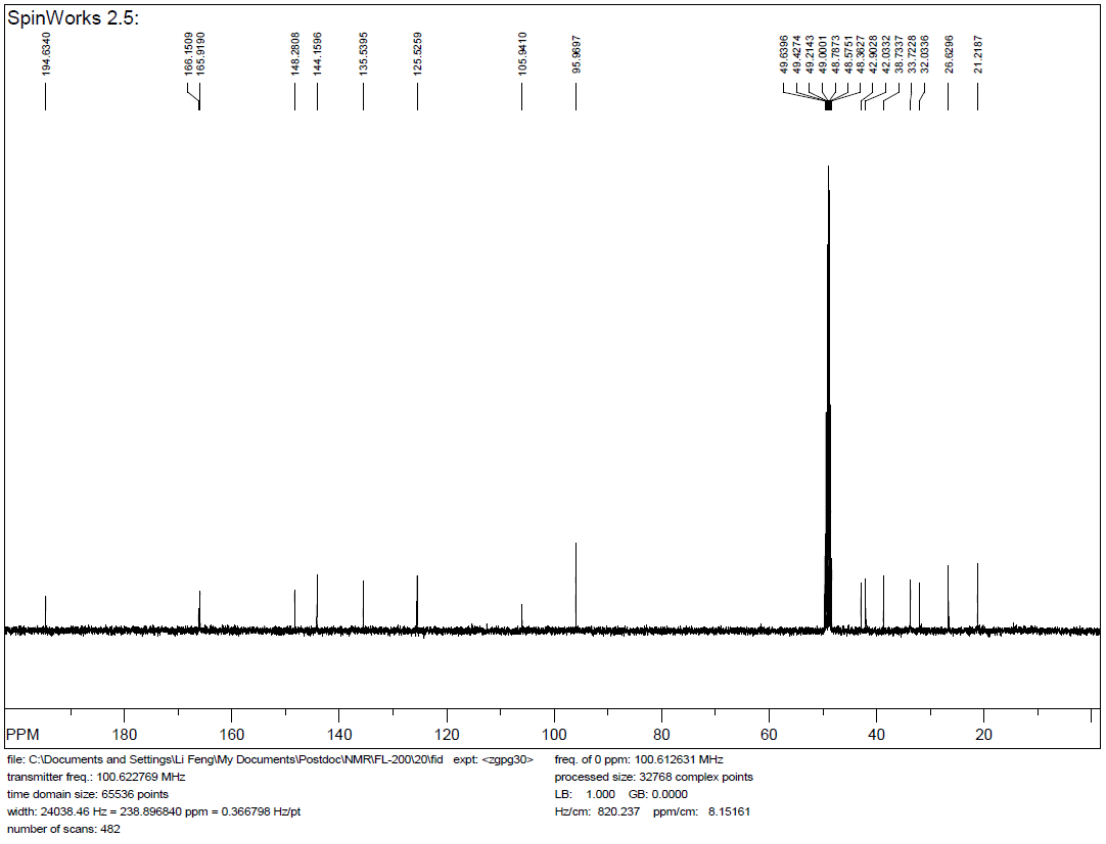
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.052	7707663	1424117	99.503	99.211
2	8.502	38510	11322	0.497	0.789
Total		7746173	1435439	100.000	100.000

HRMS of **5l**


x10 5
-ESI Scan (0.226 min) Frag=70.0V Sun232_neg.d
261.1106
160.8409
329.0940
535.2119
648.0641
744.9201
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **5m**



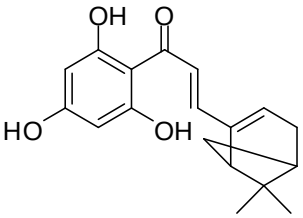


HPLC profile of **5m**

==== Shimadzu LCsolution Analysis Report ====

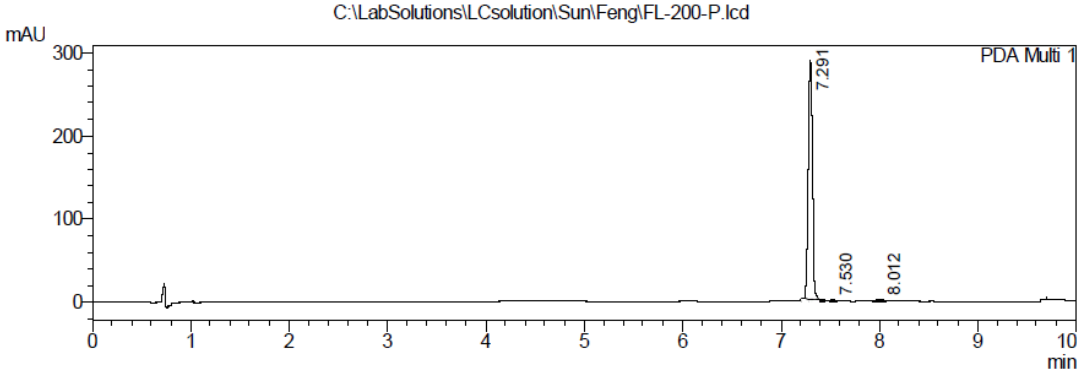
C:\LabSolutions\LCsolution\Sun\Feng\FL-200-P.lcd

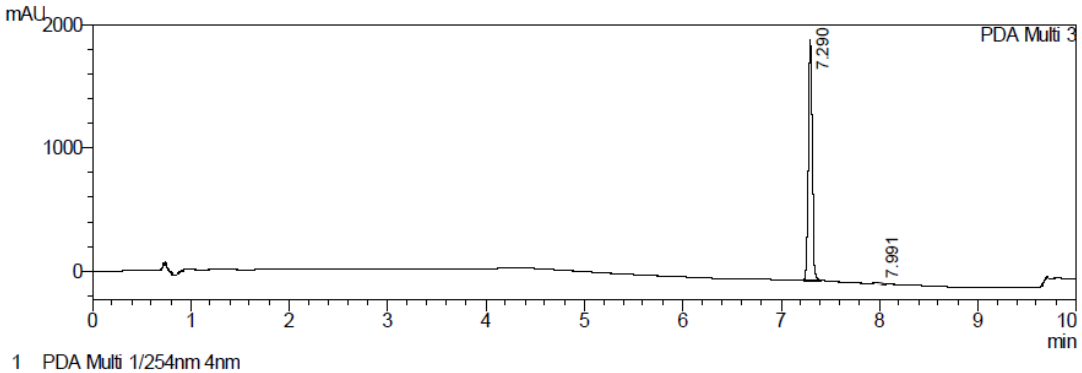
Sample Name	: FL-200-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 10 uL
Data File Name	: FL-200-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 3/29/2012 11:02:13 AM



<Chromatogram>

C:\LabSolutions\LCsolution\Sun\Feng\FL-200-P.lcd





1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

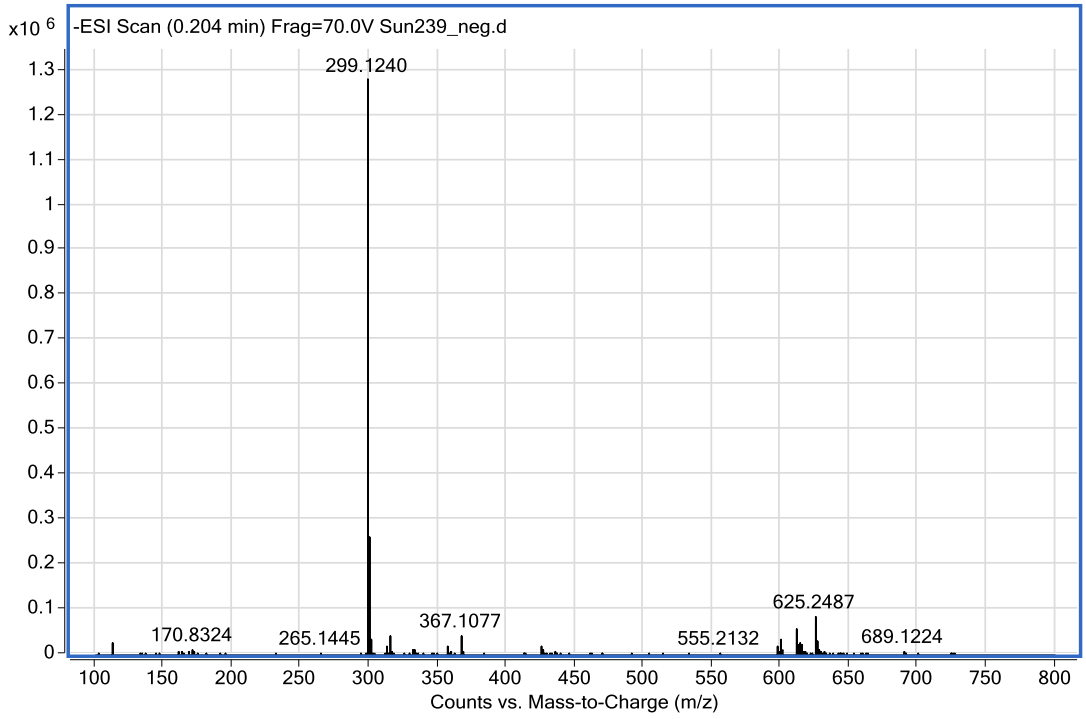
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.291	809367	286197	99.567	99.672
2	7.530	744	343	0.092	0.119
3	8.012	2773	600	0.341	0.209
Total		812885	287140	100.000	100.000

PeakTable

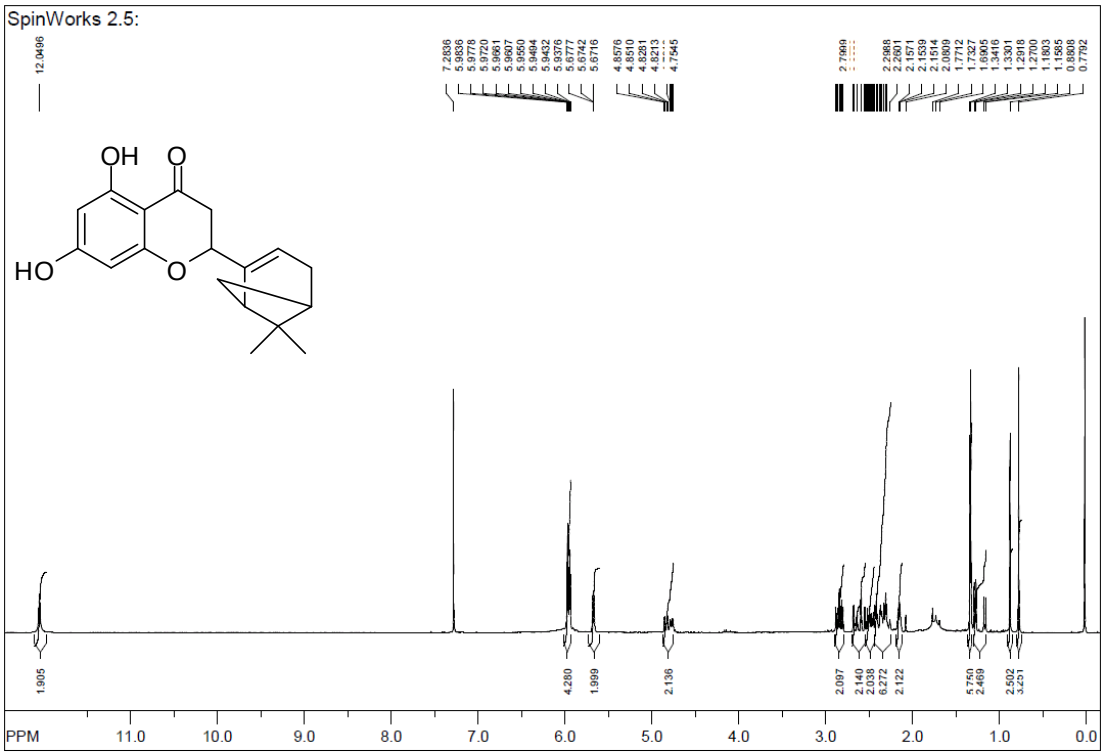
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.290	4984261	1958548	99.909	99.960
2	7.991	4561	792	0.091	0.040
Total		4988822	1959340	100.000	100.000

HRMS of **5m**

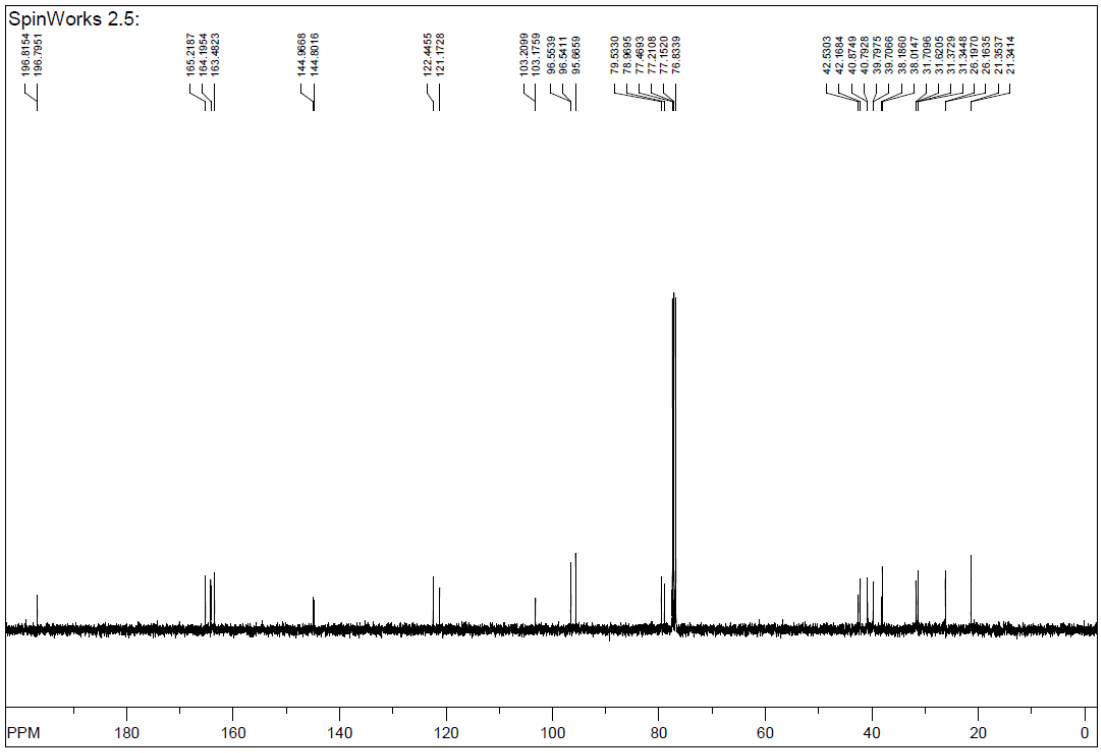

x10 6
-ESI Scan (0.204 min) Frag=70.0V Sun239_neg.d
299.1240
170.8324
265.1445
367.1077
555.2132
625.2487
689.1224
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **5n**



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-199\3\fid expt: <zg30>
transmitter freq.: 400.131600 MHz
time domain size: 65536 points
width: 8012.82 Hz = 20.025463 ppm = 0.122266 Hz/pt
number of scans: 16

freq. of 0 ppm: 400.130000 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 201.728 ppm/cm: 0.50415



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-199\20\fid expt: <zgpg30>
transmitter freq.: 100.622769 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.896840 ppm = 0.366798 Hz/pt
number of scans: 738

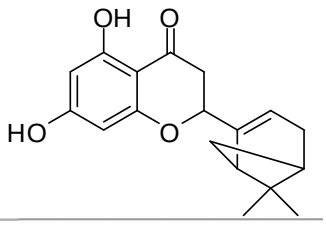
freq. of 0 ppm: 100.612756 MHz
processed size: 32768 complex points
LB: 1.000 GB: 0.0000
Hz/cm: 825.062 ppm/cm: 8.19956

HPLC profile of **5n**

==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\Feng\FL-199-P.lcd

Sample Name	: FL-199-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 9 uL
Data File Name	: FL-199-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 3/28/2012 3:14:23 PM



<Chromatogram>

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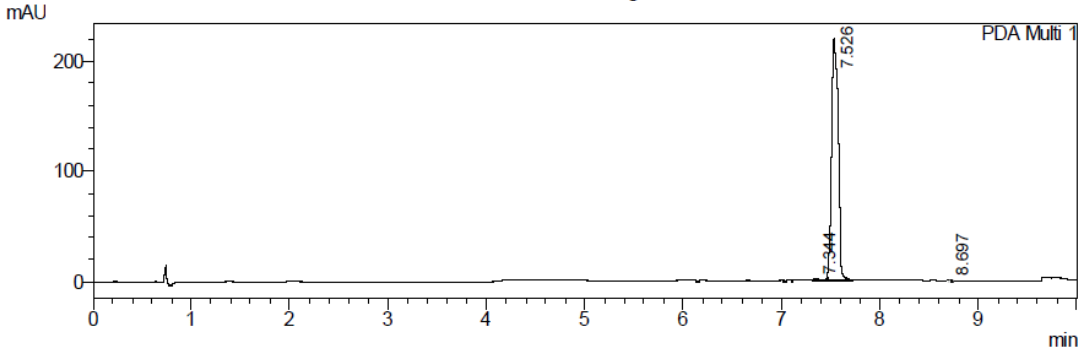
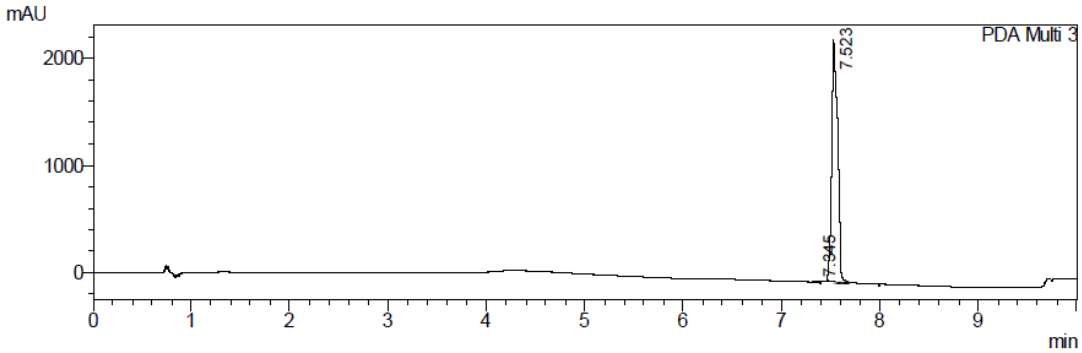




1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

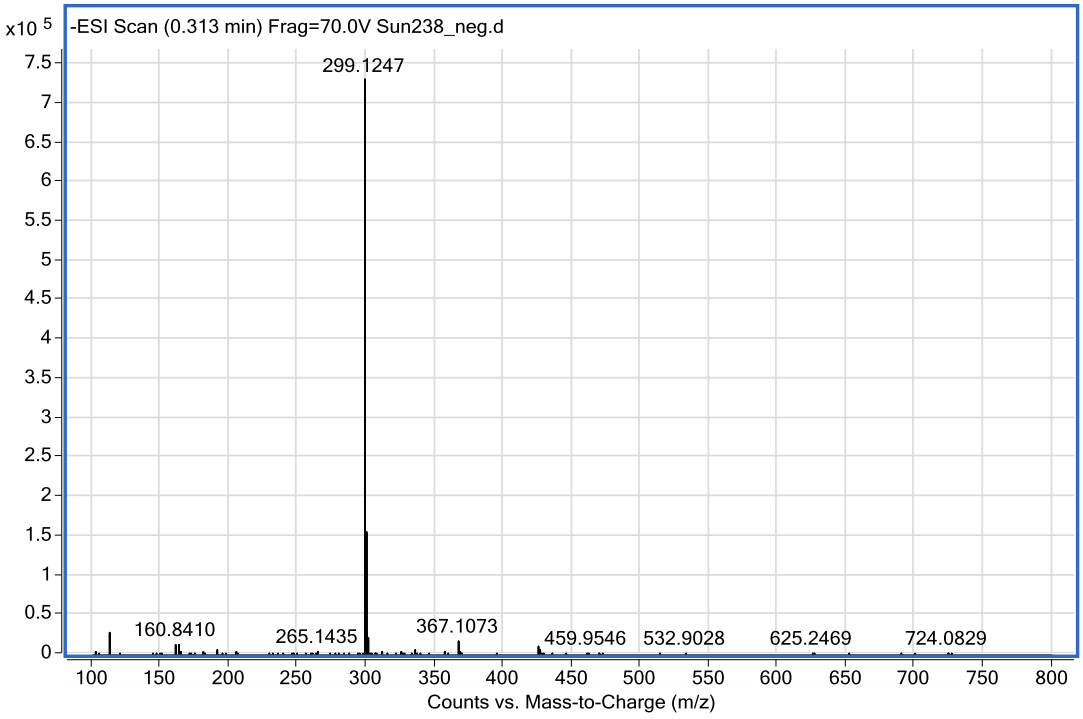
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.344	2154	1001	0.222	0.456
2	7.526	966316	218349	99.706	99.397
3	8.697	694	325	0.072	0.148
Total		969164	219674	100.000	100.000

PeakTable

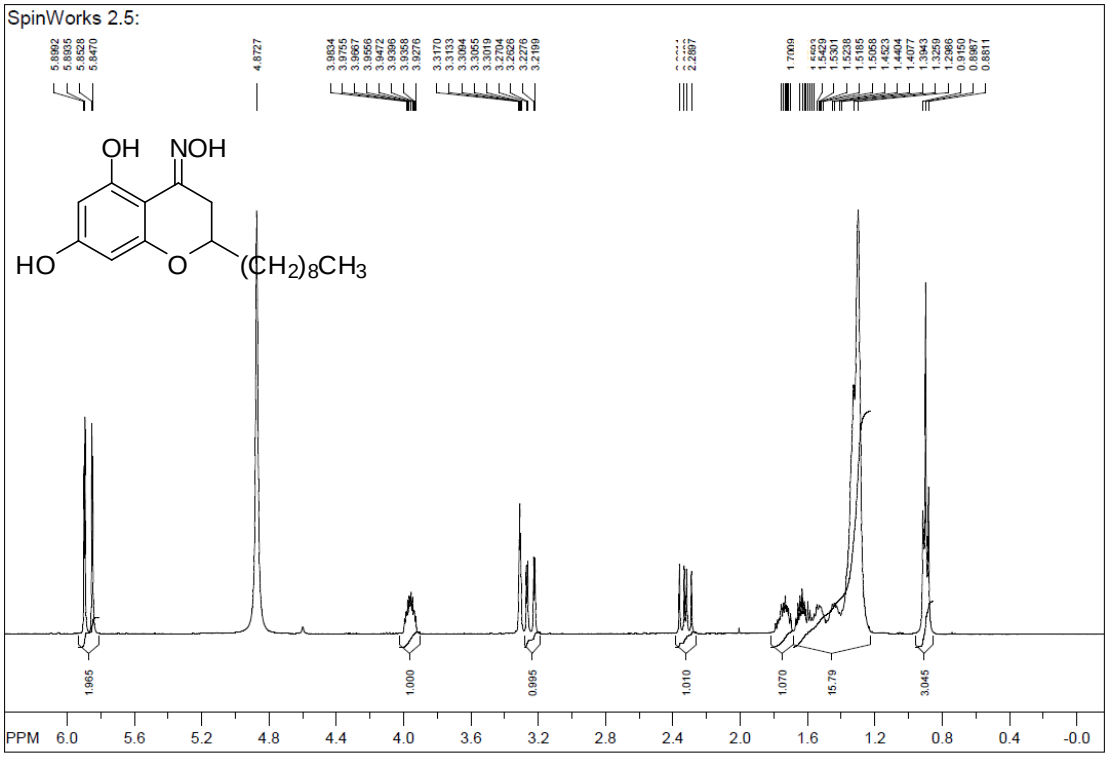
PDA Ch3 220nm 4nm

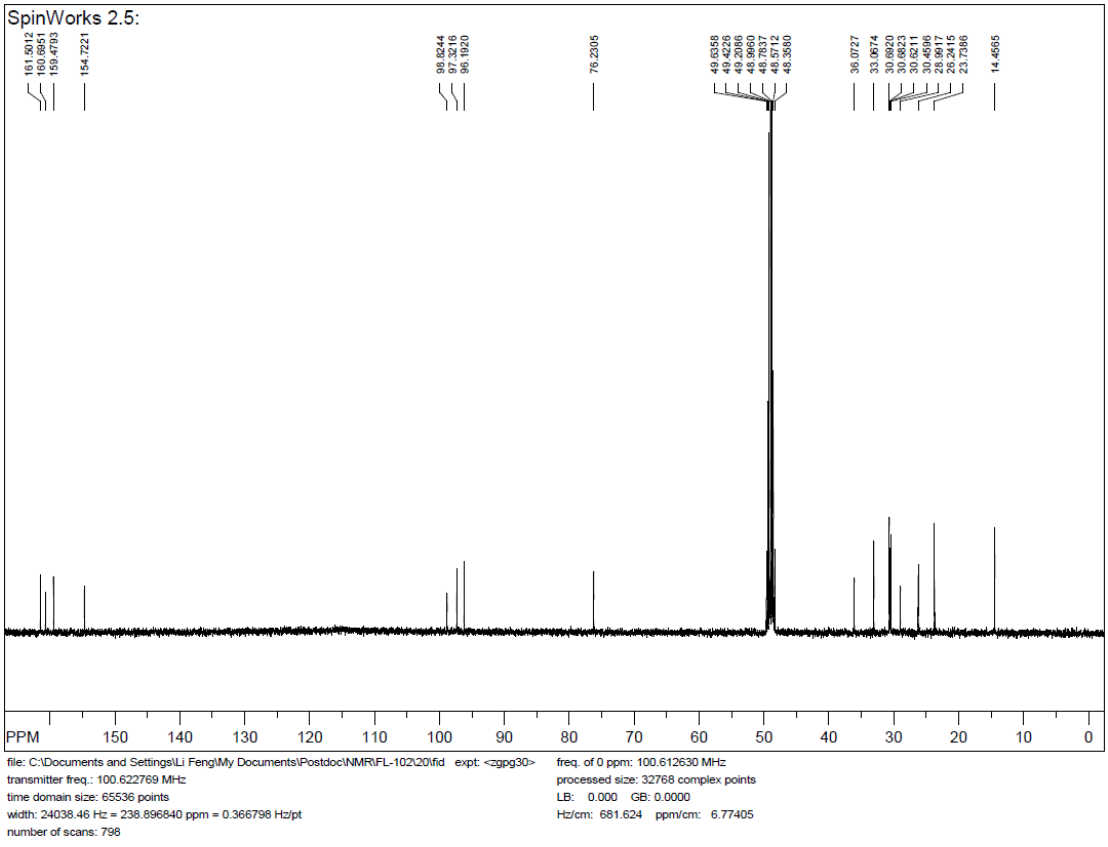
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.345	10566	6652	0.118	0.292
2	7.523	8925430	2273584	99.882	99.708
Total		8935996	2280236	100.000	100.000

HRMS of **5n**


x10 5
-ESI Scan (0.313 min) Frag=70.0V Sun238_neg.d
299.1247
160.8410
265.1435
367.1073
459.9546
532.9028
625.2469
724.0829
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **6a**



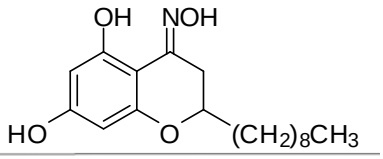


HPLC profile of **6a**

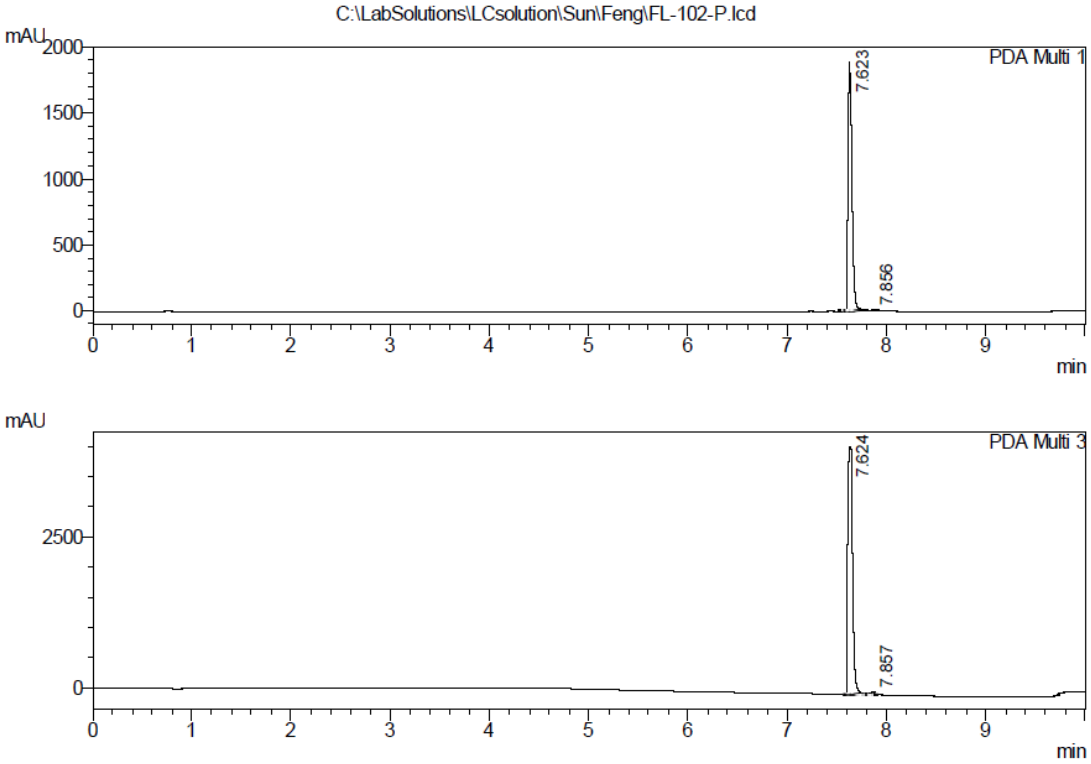
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\Feng\FL-102-P.lcd

Sample Name	: FL-102-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 12 uL
Data File Name	: FL-102-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 12/30/2011 4:20:21 PM



<Chromatogram>



1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

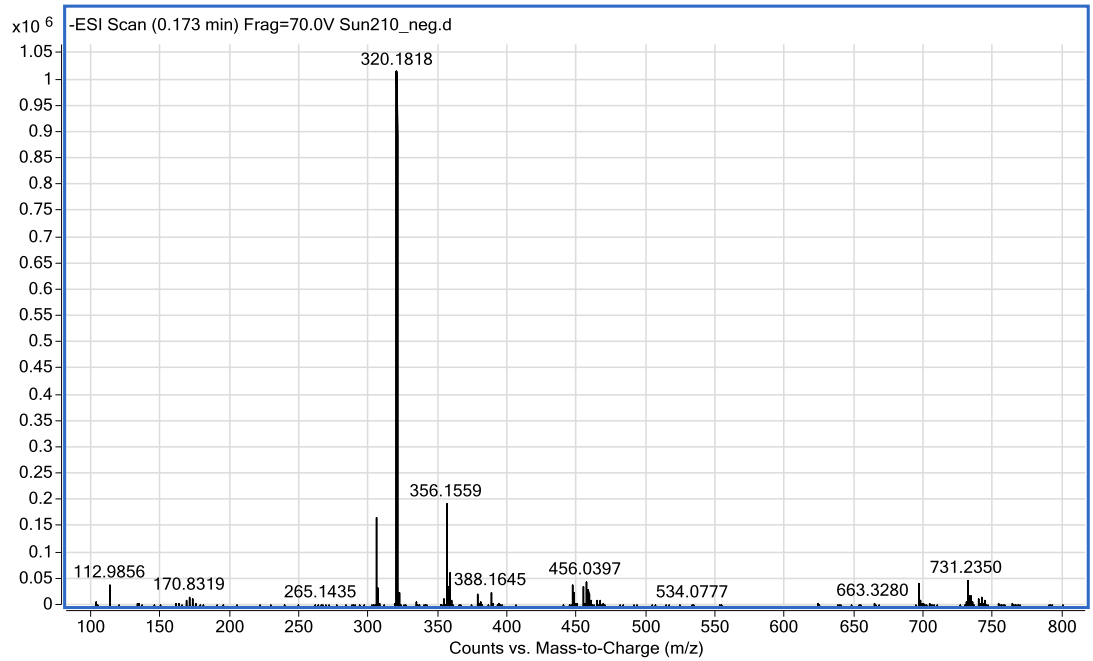
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.623	4657903	1824926	99.953	99.911
2	7.856	2208	1623	0.047	0.089
Total		4660110	1826549	100.000	100.000

PeakTable

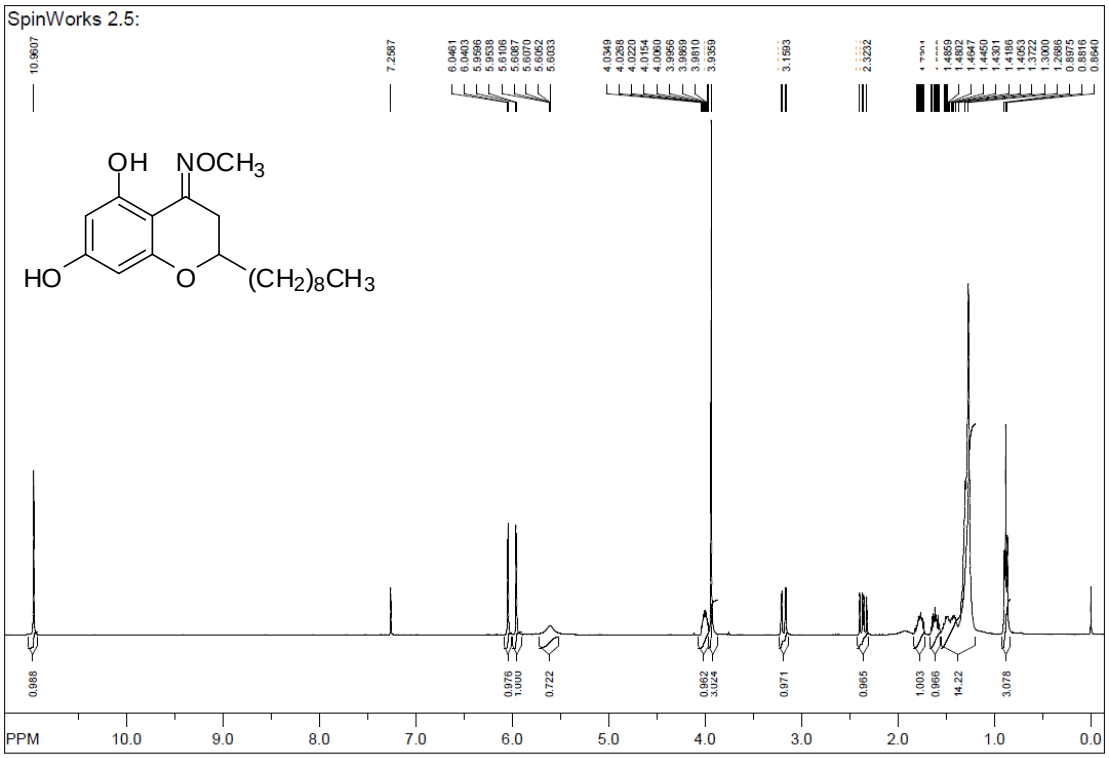
PDA Ch3 220nm 4nm

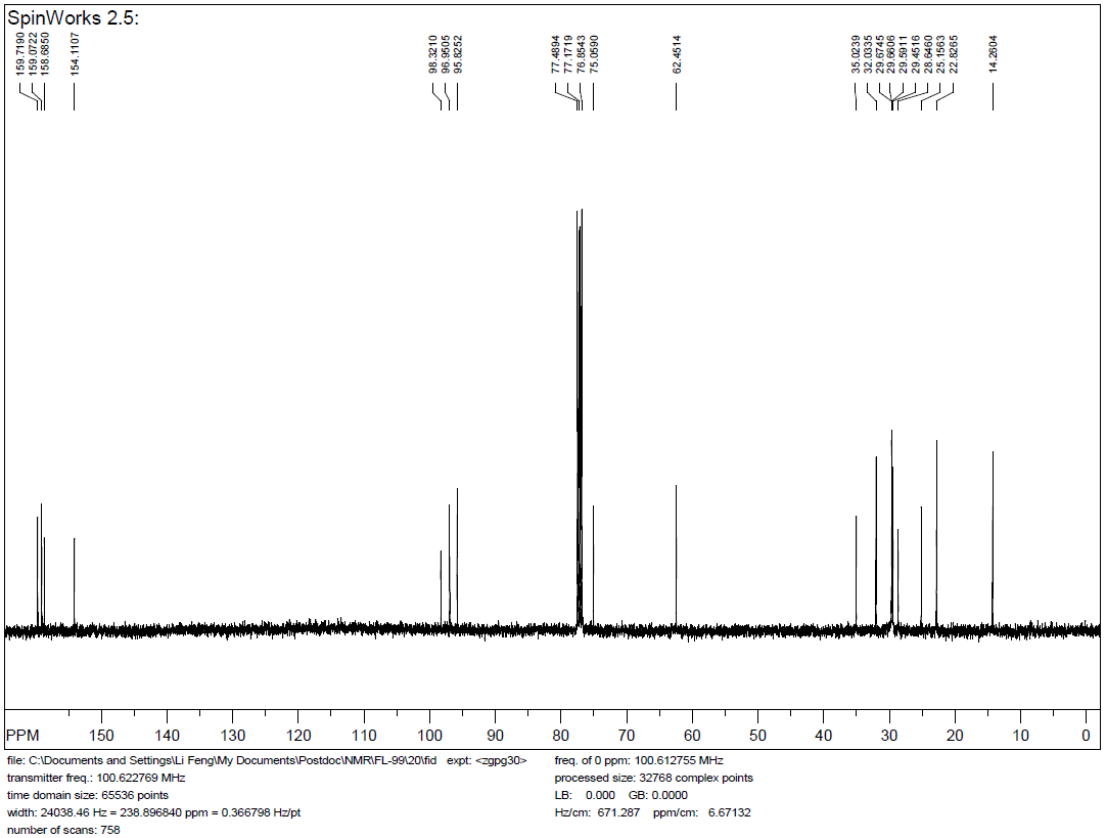
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.624	12626929	4093039	99.515	99.252
2	7.857	61508	30850	0.485	0.748
Total		12688437	4123889	100.000	100.000

HRMS of **6a**


x10 6
-ESI Scan (0.173 min) Frag=70.0V Sun210_neg.d
320.1818
356.1559
112.9856
170.8319
265.1435
388.1645
456.0397
534.0777
663.3280
731.2350
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **6b**



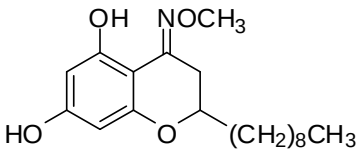


HPLC profile of **6b**

==== Shimadzu LCsolution Analysis Report ====

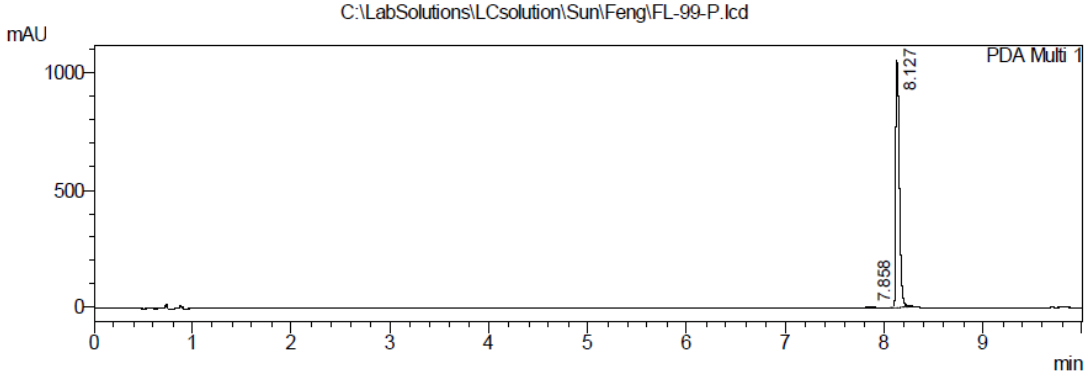
C:\LabSolutions\LCsolution\Sun\Feng\FL-99-P.lcd

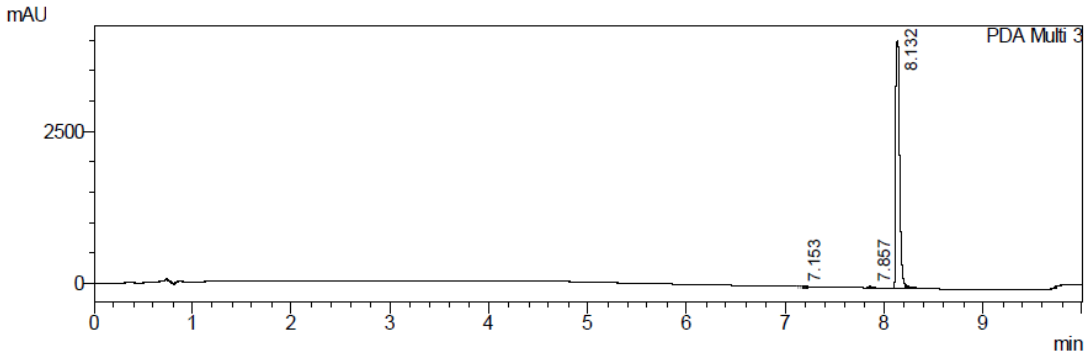
Sample Name	: FL-99-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 6 uL
Data File Name	: FL-99-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 12/22/2011 11:06:10 AM



<Chromatogram>

C:\LabSolutions\LCsolution\Sun\Feng\FL-99-P.lcd





1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

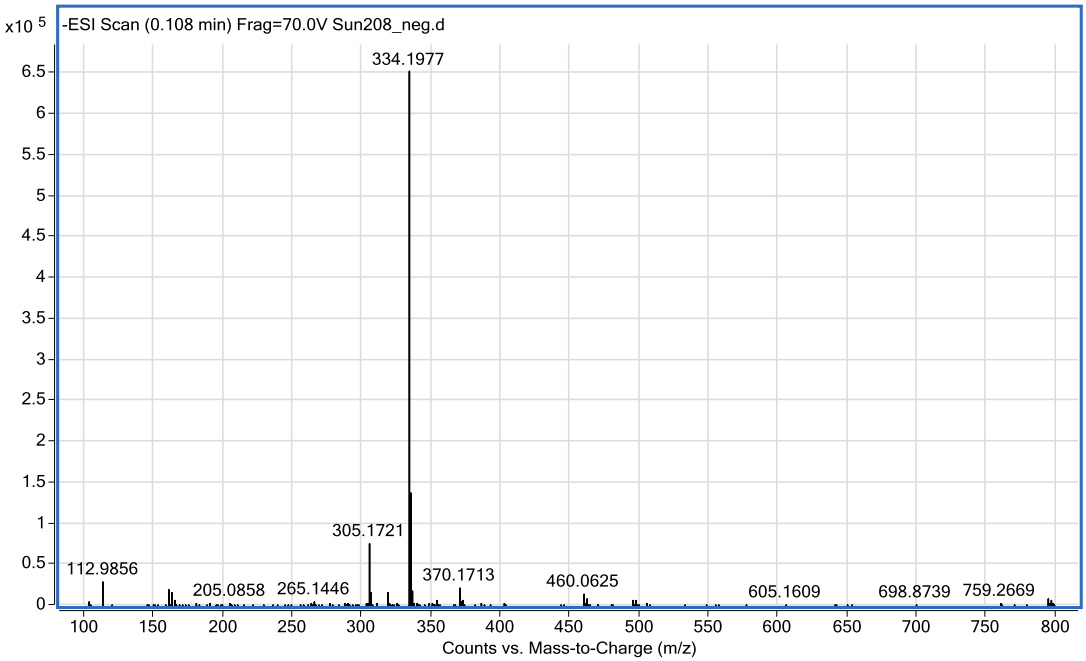
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.858	5670	2701	0.219	0.264
2	8.127	2580357	1022083	99.781	99.736
Total		2586028	1024784	100.000	100.000

PeakTable

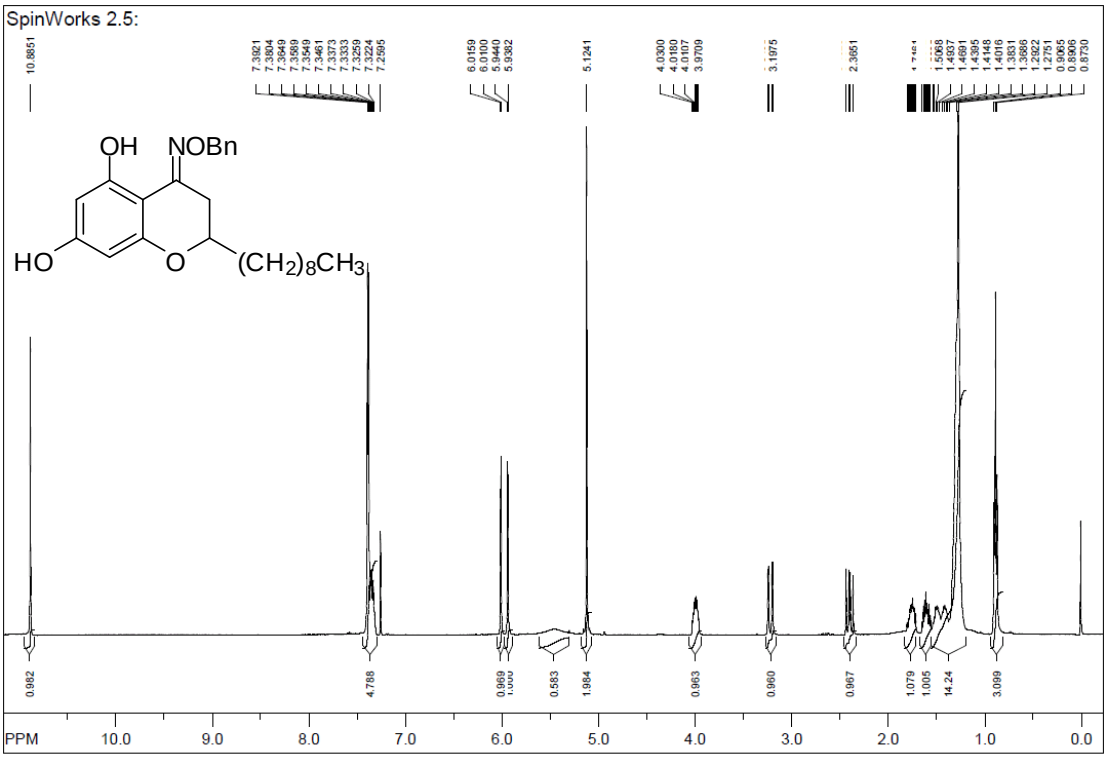
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.153	41434	14363	0.378	0.350
2	7.857	51559	22962	0.470	0.559
3	8.132	10868510	4070346	99.152	99.091
Total		10961502	4107671	100.000	100.000

HRMS of **6b**

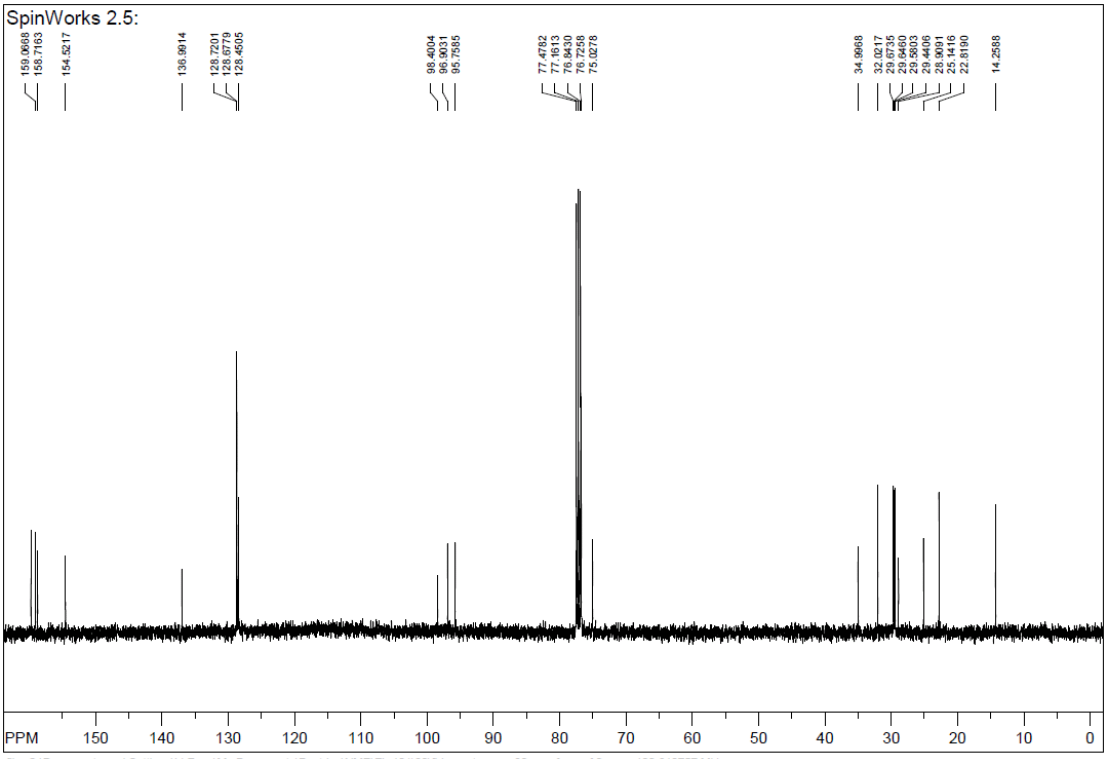

-ESI Scan (0.108 min) Frag=70.0V Sun208_neg.d
x10 5
334.1977
305.1721
112.9856
205.0858
265.1446
370.1713
460.0625
605.1609
698.8739
759.2669
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **6c**



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-101\1\1\fid expt: <zg30>
transmitter freq.: 400.131600 MHz
time domain size: 65536 points
width: 8012.82 Hz = 20.025463 ppm = 0.122266 Hz/pt
number of scans: 5

freq. of 0 ppm: 400.130010 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 182.198 ppm/cm: 0.45535



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-101\20\fid expt: <zgpg30>
transmitter freq.: 100.622769 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.896840 ppm = 0.366798 Hz/pt
number of scans: 465

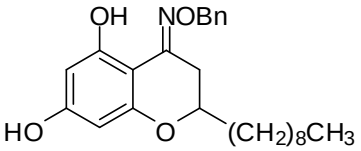
freq. of 0 ppm: 100.612757 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 667.152 ppm/cm: 6.63023

HPLC profile of **6c**

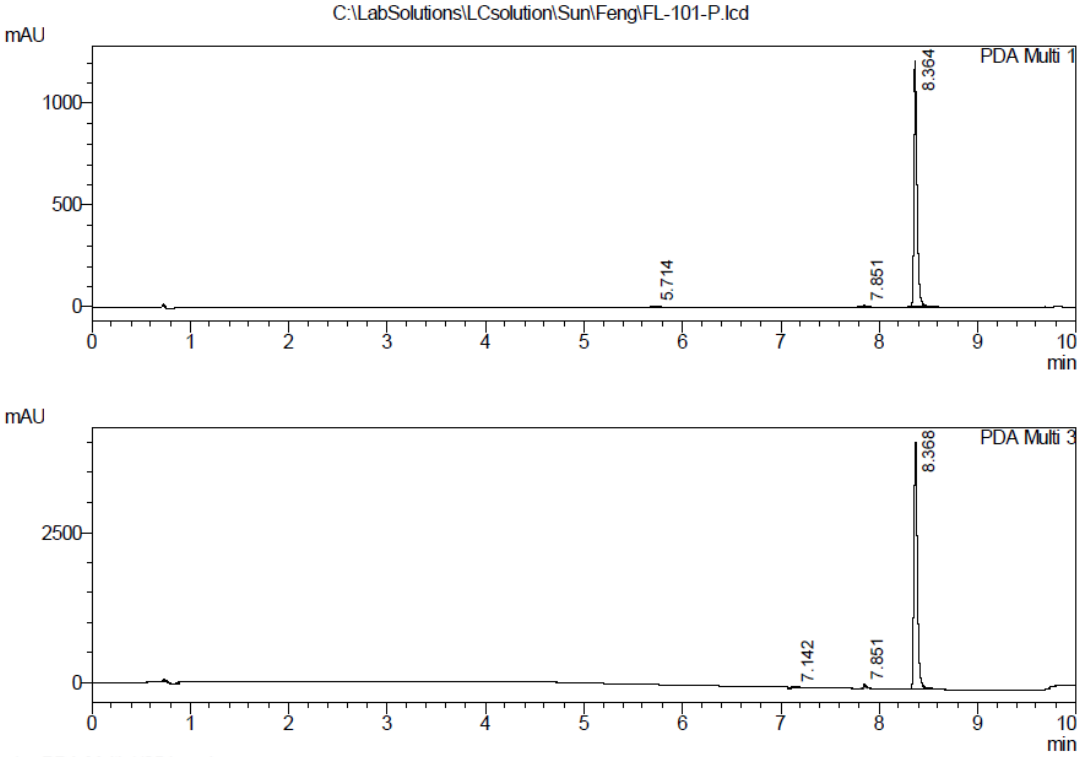
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\Feng\FL-101-P.lcd

Sample Name	: FL-101-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 12 uL
Data File Name	: FL-101-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 12/27/2011 11:44:01 AM



<Chromatogram>



1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

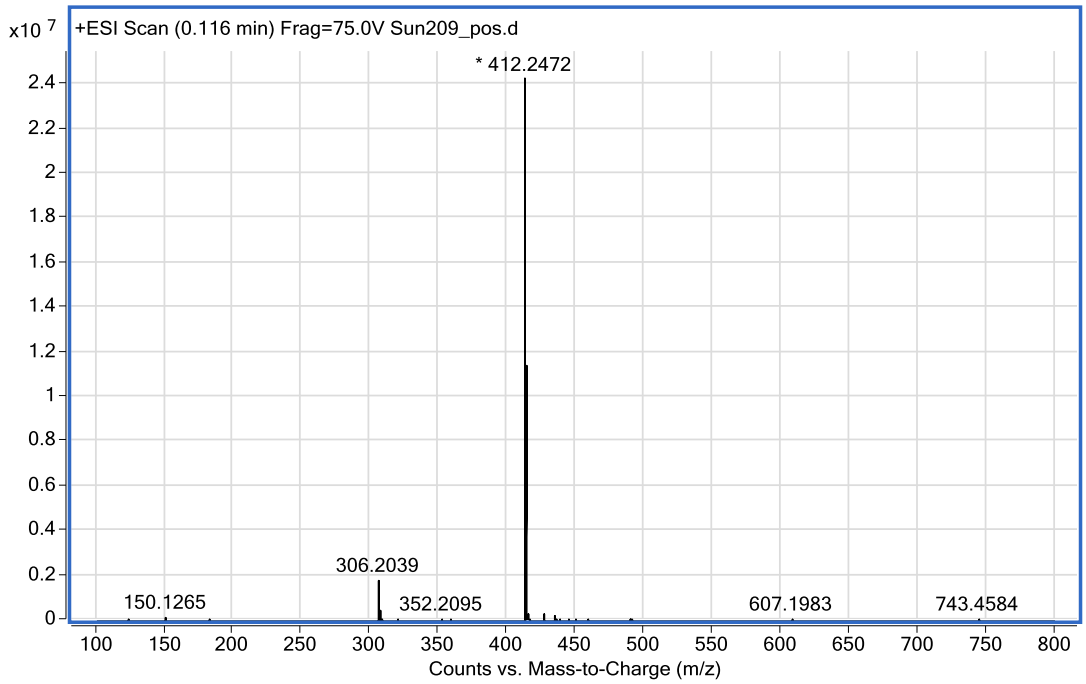
Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.714	9931	3362	0.333	0.276
2	7.851	18236	8254	0.611	0.678
3	8.364	2957732	1206365	99.057	99.046
Total		2985898	1217982	100.000	100.000

PeakTable

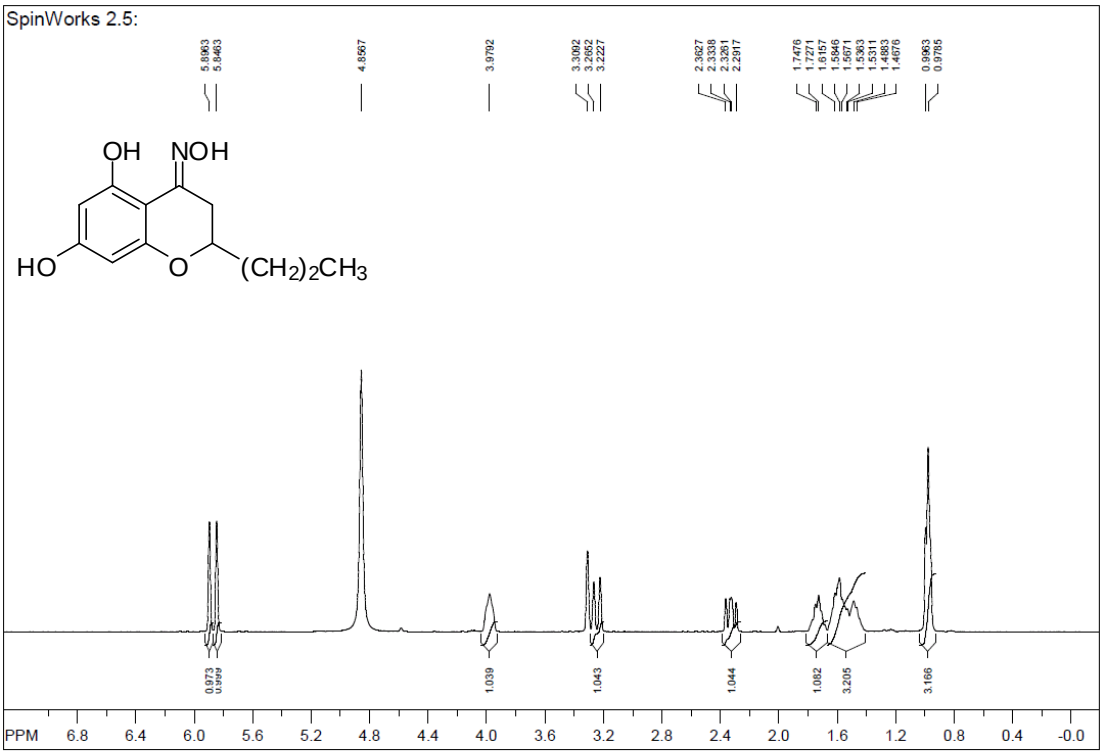
PDA Ch3 220nm 4nm

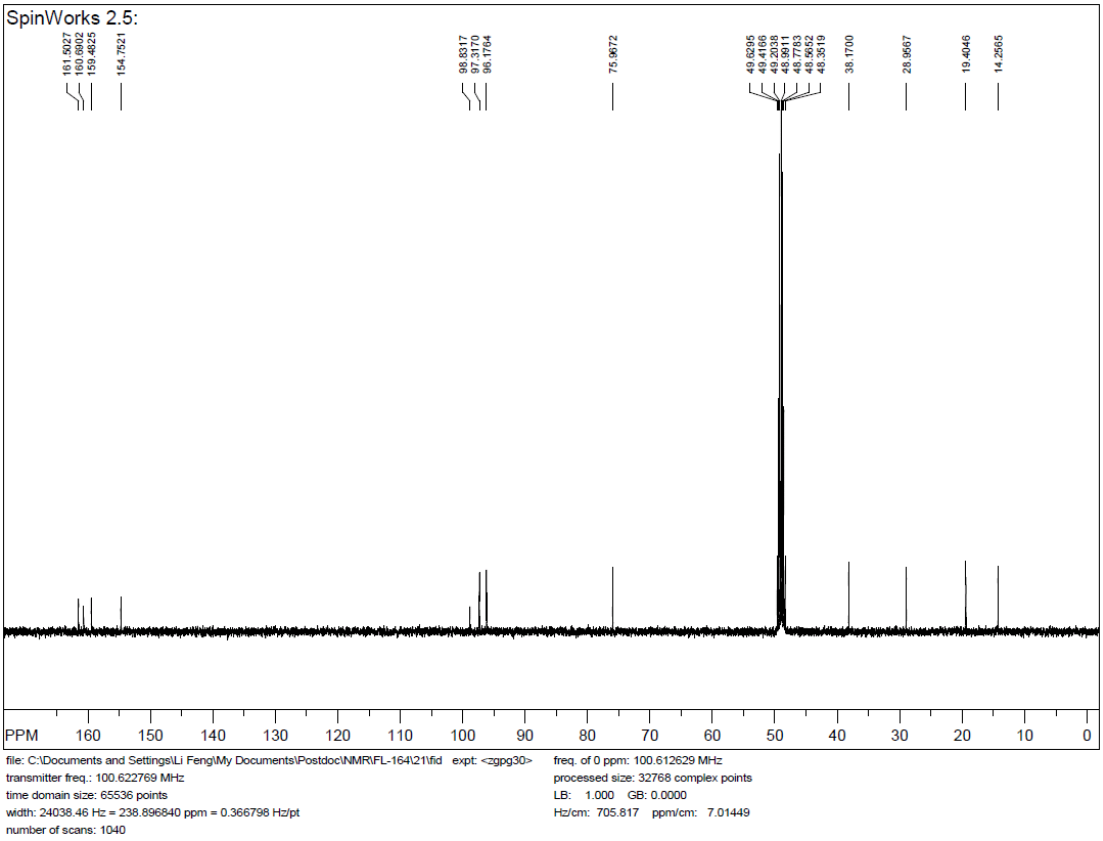
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.142	15147	6815	0.129	0.164
2	7.851	142973	63995	1.214	1.537
3	8.368	11615362	4093380	98.657	98.300
Total		11773482	4164191	100.000	100.000

HRMS of **6c**


x10 7
+ESI Scan (0.116 min) Frag=75.0V Sun209_pos.d
* 412.2472
306.2039
150.1265
352.2095
607.1983
743.4584
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **6d**



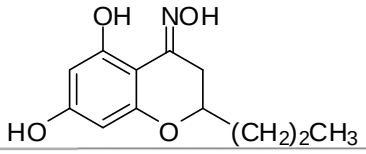


HPLC profile of **6d**

==== Shimadzu LCsolution Analysis Report ====

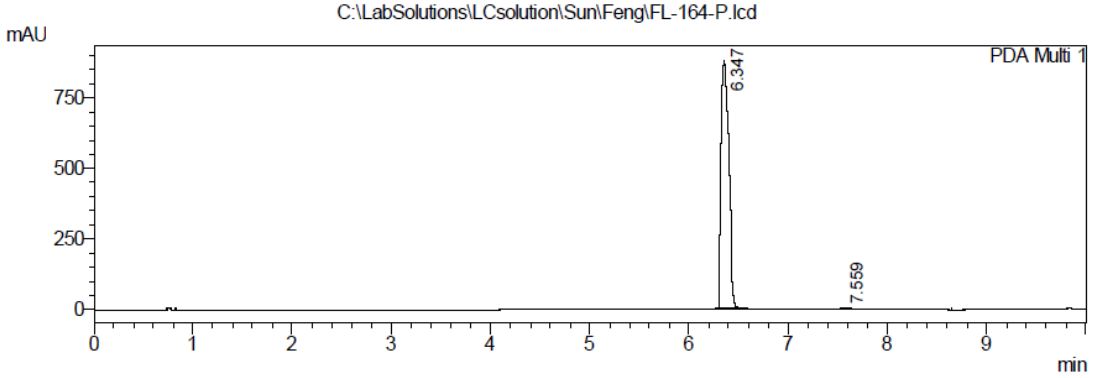
C:\LabSolutions\LCsolution\Sun\Feng\FL-164-P.lcd

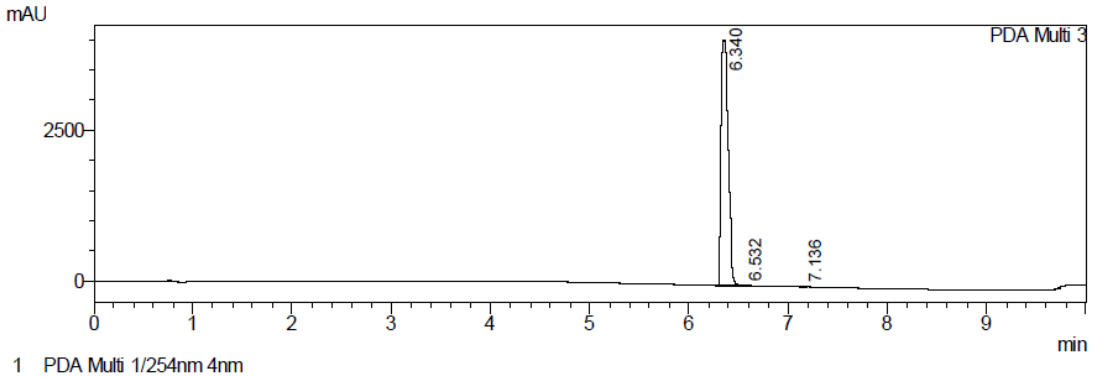
Sample Name	: FL-164-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 10 uL
Data File Name	: FL-164-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	: Batch 1.lcb
Data Acquired	: 3/8/2012 12:24:24 PM



<Chromatogram>

C:\LabSolutions\LCsolution\Sun\Feng\FL-164-P.lcd





1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

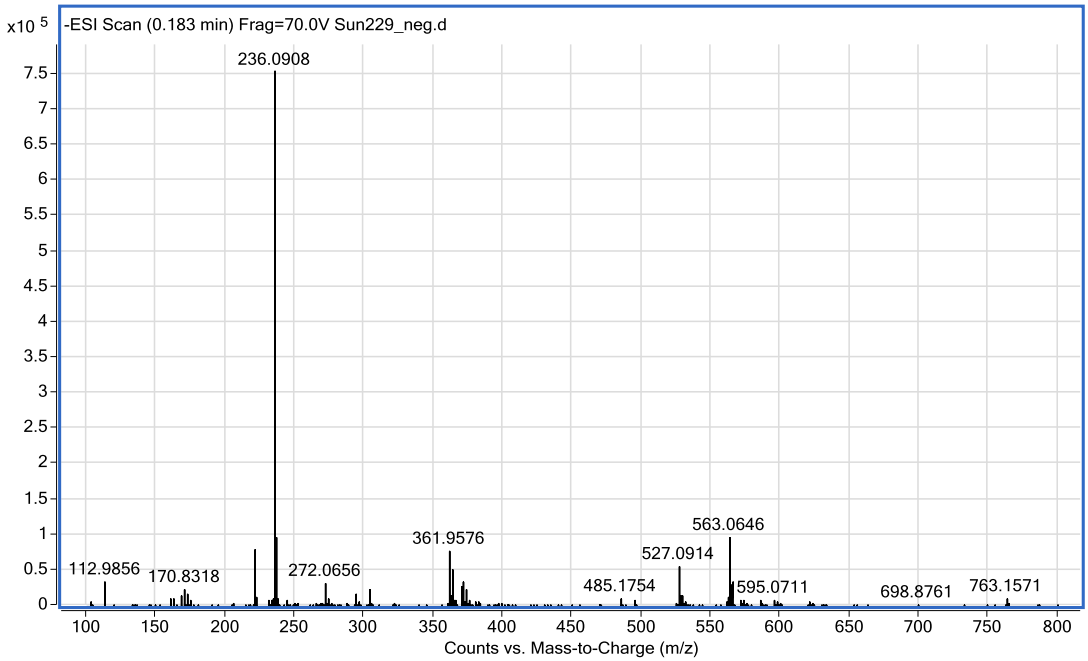
Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.347	4577805	882105	99.924	99.893
2	7.559	3477	943	0.076	0.107
Total		4581282	883048	100.000	100.000

PeakTable

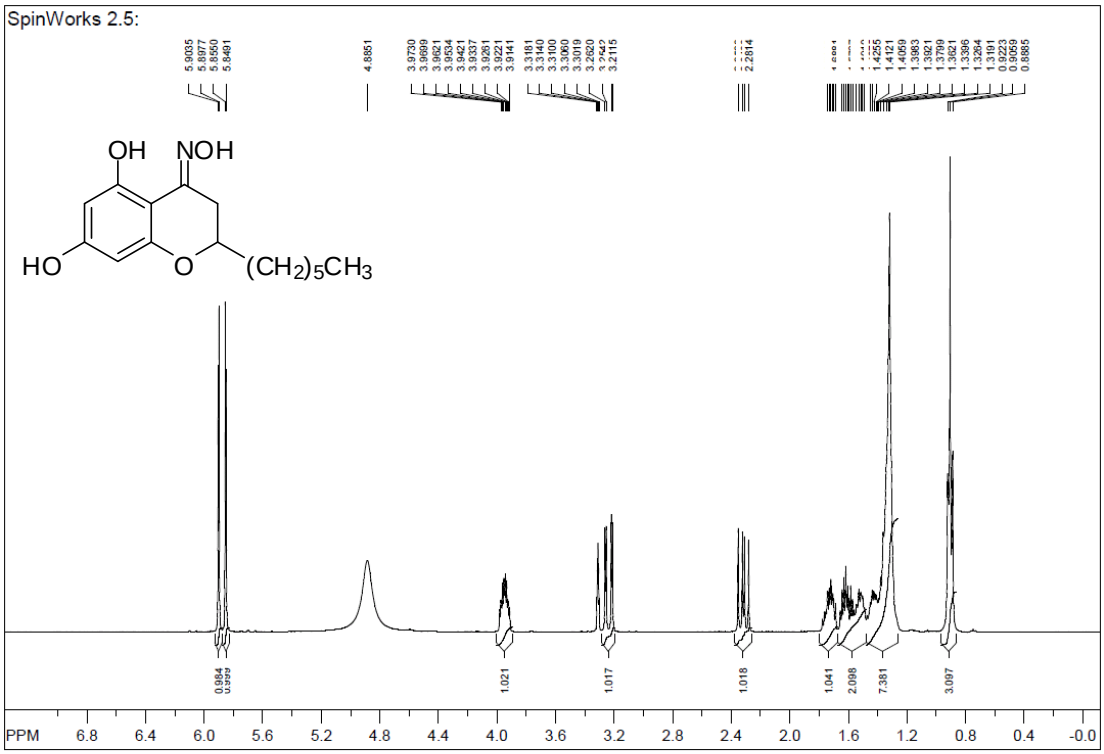
PDA Ch3 220nm 4nm

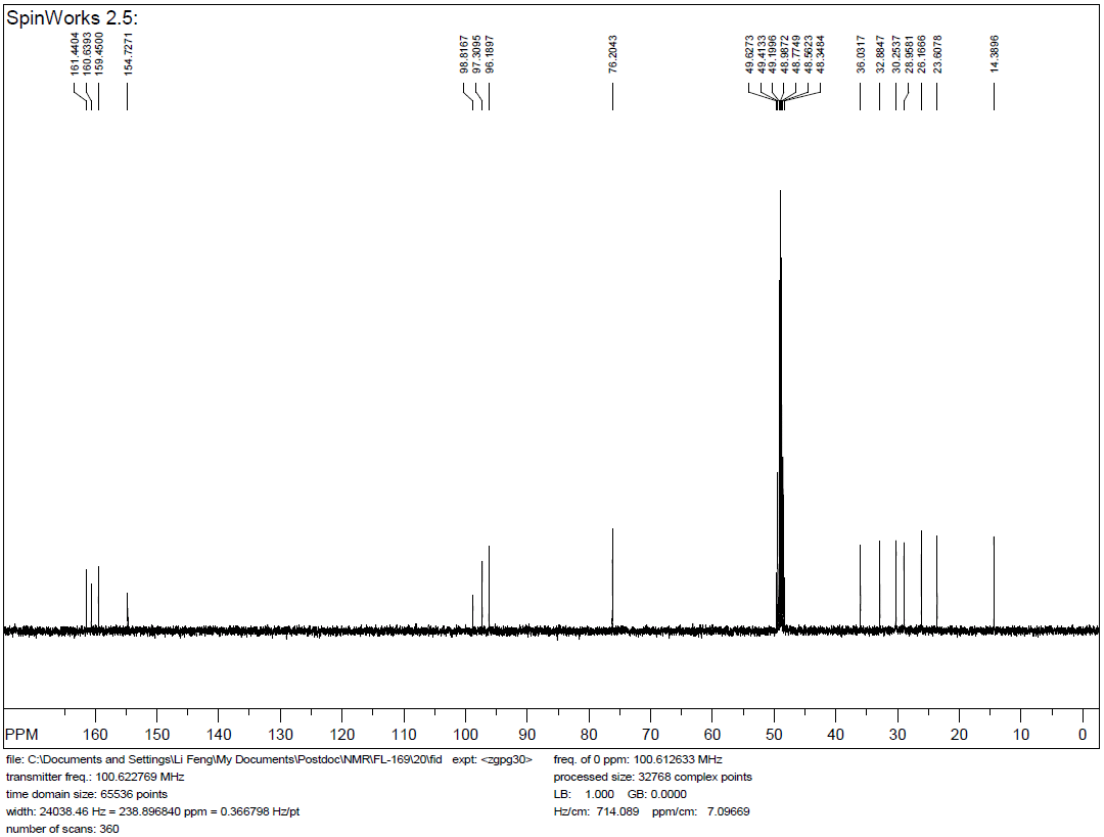
Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.340	19049401	4058134	99.960	99.955
2	6.532	4522	617	0.024	0.015
3	7.136	3117	1195	0.016	0.029
Total		19057041	4059946	100.000	100.000

HRMS of **6d**


x10 5
-ESI Scan (0.183 min) Frag=70.0V Sun229_neg.d
236.0908
112.9856
170.8318
272.0656
361.9576
485.1754
527.0914
563.0646
595.0711
698.8761
763.1571
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **6e**



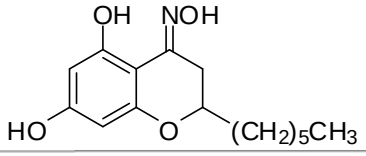


HPLC profile of **6e**

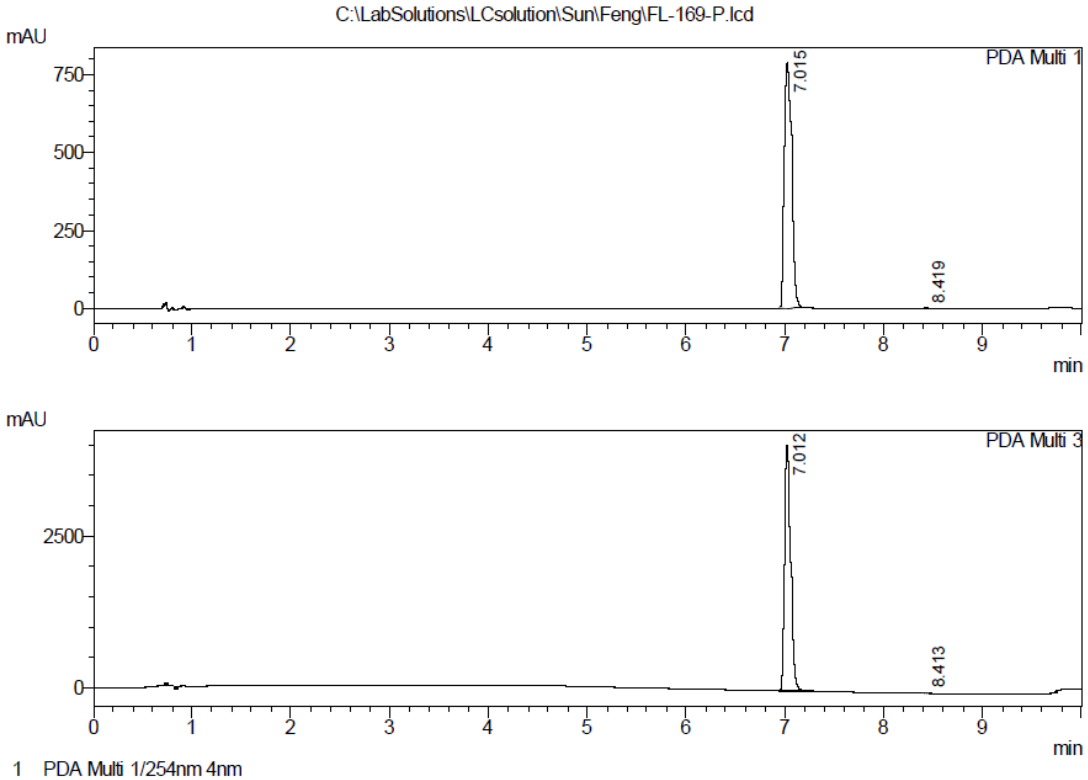
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\Feng\FL-169-P.lcd

Sample Name	: FL-169-P
Tray#	: 1
Vail #	: 93
Injection Volume	: 10 uL
Data File Name	: FL-169-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	: Batch 1.lcb
Data Acquired	: 3/8/2012 12:45:17 PM



<Chromatogram>



1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

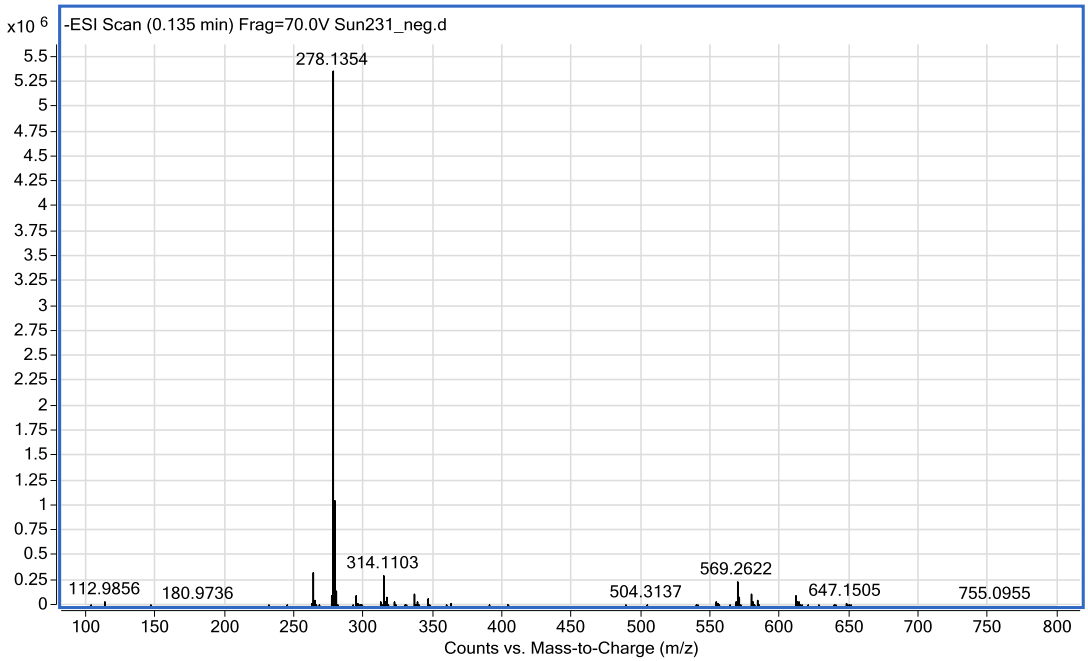
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.015	4095196	784863	99.776	99.768
2	8.419	9180	1824	0.224	0.232
Total		4104377	786687	100.000	100.000

PeakTable

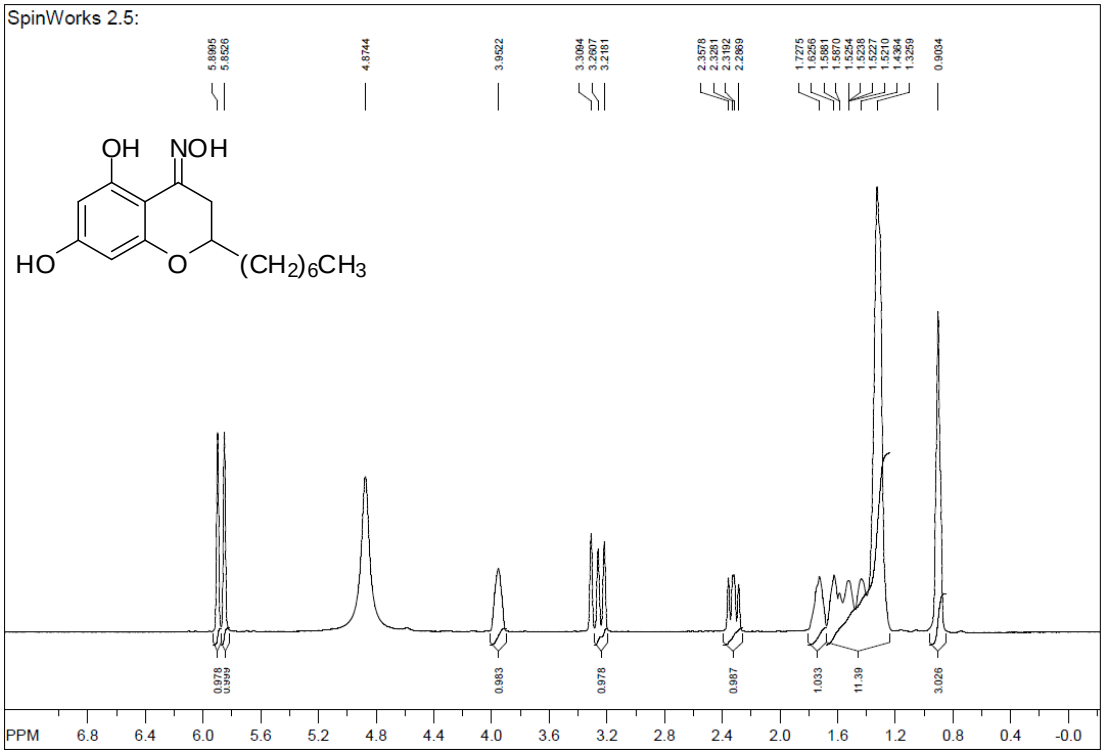
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.012	16956366	4040211	99.959	99.954
2	8.413	7015	1878	0.041	0.046
Total		16963381	4042089	100.000	100.000

HRMS of **6e**

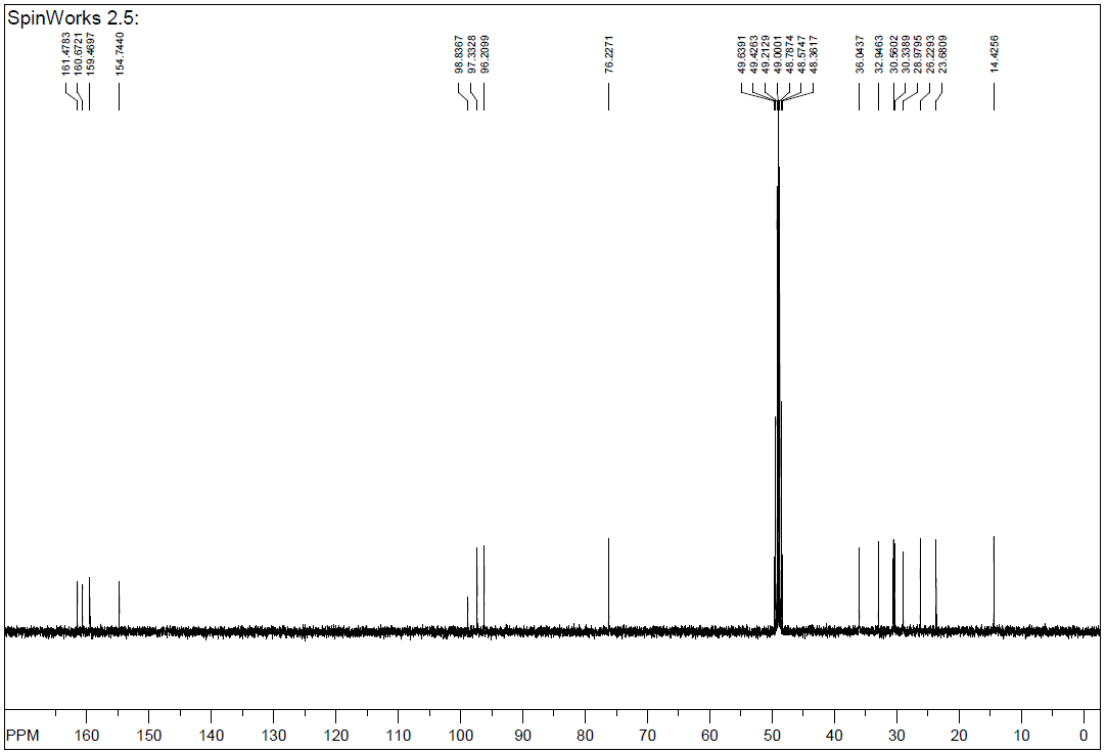

x10 6
-ESI Scan (0.135 min) Frag=70.0V Sun231_neg.d
278.1354
314.1103
569.2622
112.9856
180.9736
504.3137
647.1505
755.0955
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **6f**



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-165\1\fid expt: <zg30>
transmitter freq.: 400.131600 MHz
time domain size: 65536 points
width: 8012.82 Hz = 20.025463 ppm = 0.122266 Hz/pt
number of scans: 4

freq. of 0 ppm: 400.130008 MHz
processed size: 32768 complex points
LB: 0.300 GB: 0.0000
Hz/cm: 121.542 ppm/cm: 0.30376



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-165\20\fid expt: <zgpg30>
transmitter freq.: 100.622769 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.896840 ppm = 0.366798 Hz/pt
number of scans: 674

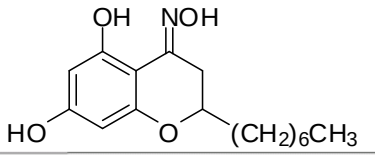
freq. of 0 ppm: 100.612631 MHz
processed size: 32768 complex points
LB: 1.000 GB: 0.0000
Hz/cm: 707.196 ppm/cm: 7.02819

HPLC profile of **6f**

==== Shimadzu LCsolution Analysis Report ====

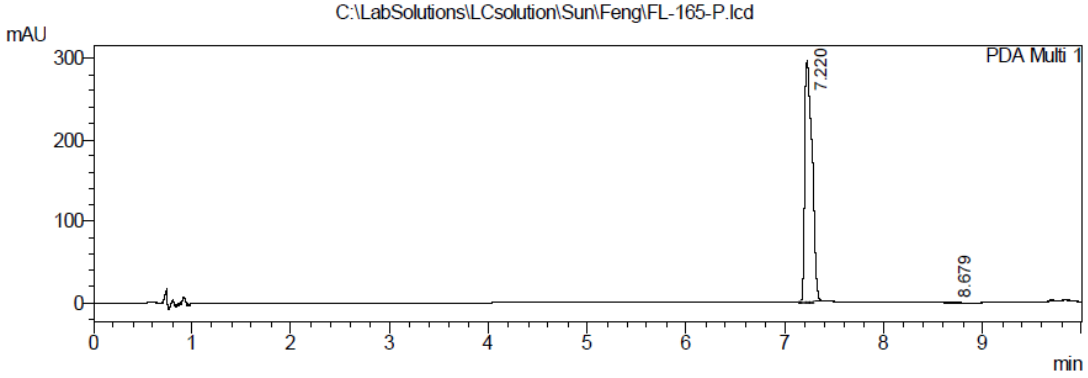
C:\LabSolutions\LCsolution\Sun\Feng\FL-165-P.lcd

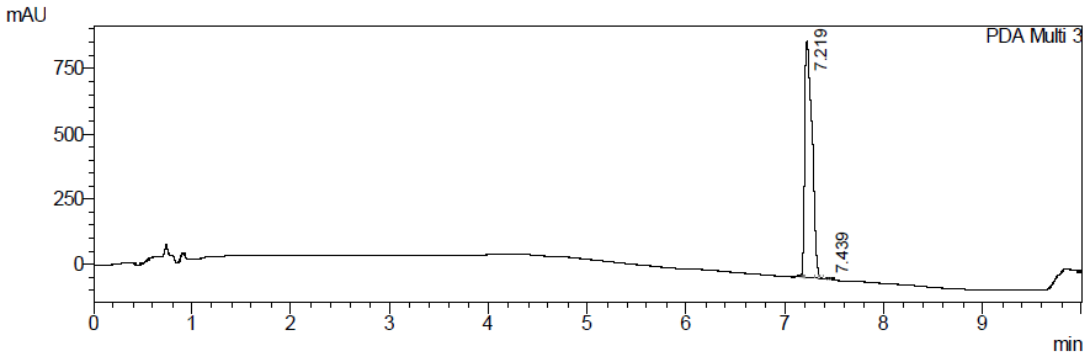
Sample Name	: FL-165-P
Tray#	: 1
Vail #	: 92
Injection Volume	: 10 uL
Data File Name	: FL-165-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	: Batch 1.lcb
Data Acquired	: 3/8/2012 12:34:51 PM



<Chromatogram>

C:\LabSolutions\LCsolution\Sun\Feng\FL-165-P.lcd





1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

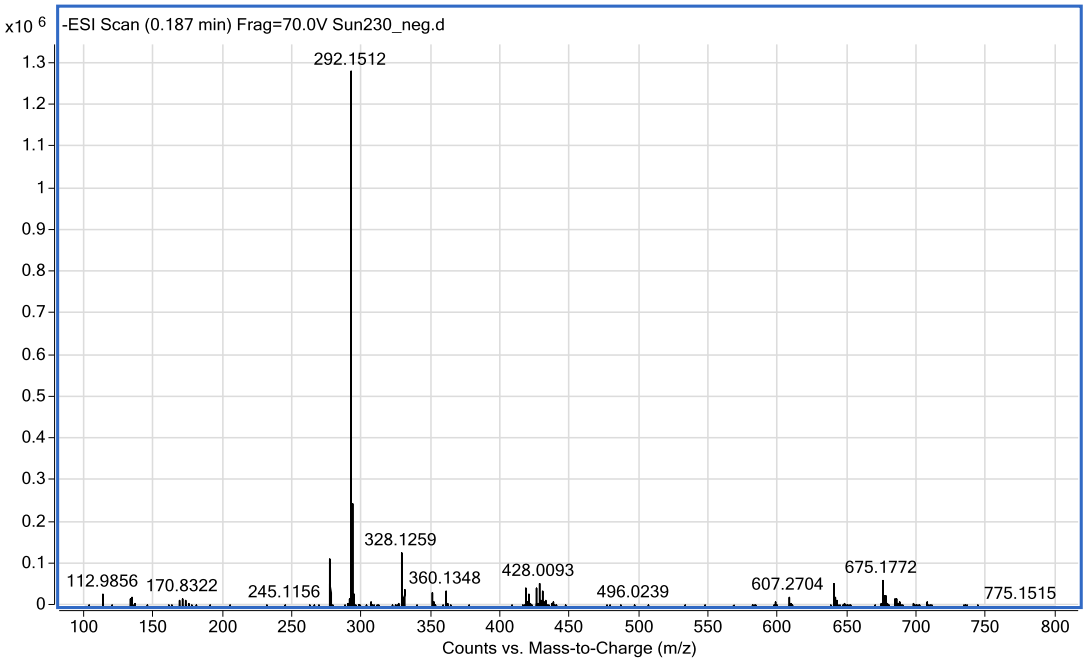
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.220	1543111	295890	99.859	99.845
2	8.679	2184	461	0.141	0.155
Total		1545295	296350	100.000	100.000

PeakTable

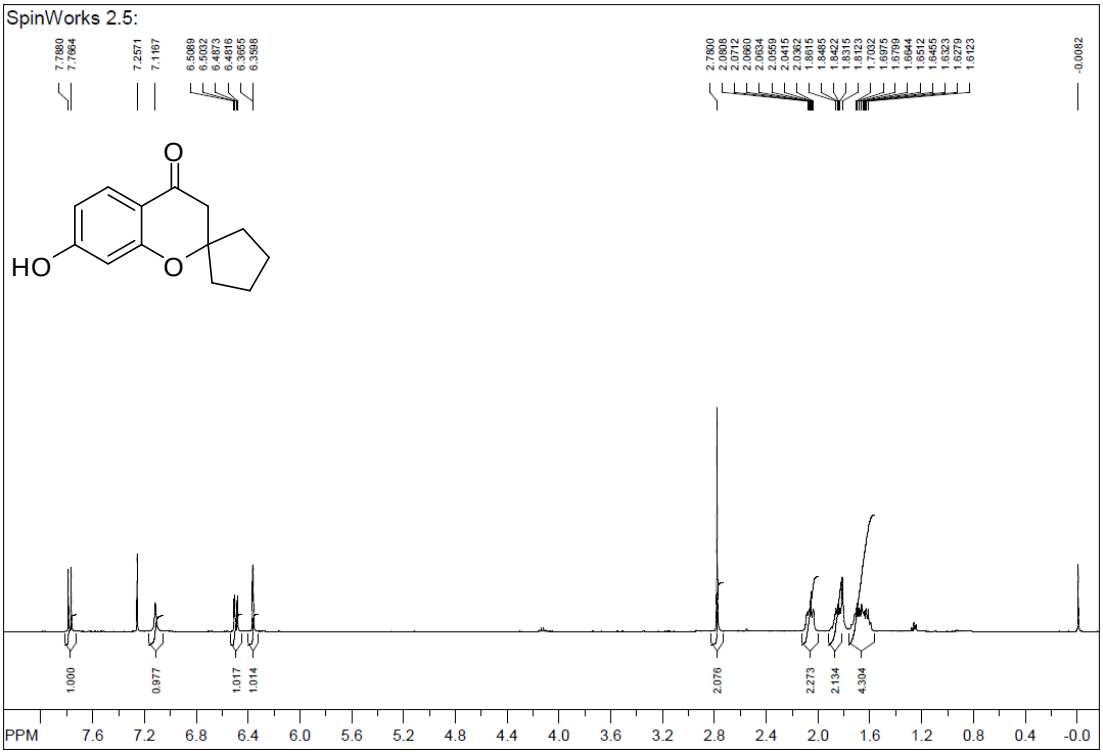
PDA Ch3 220nm 4nm

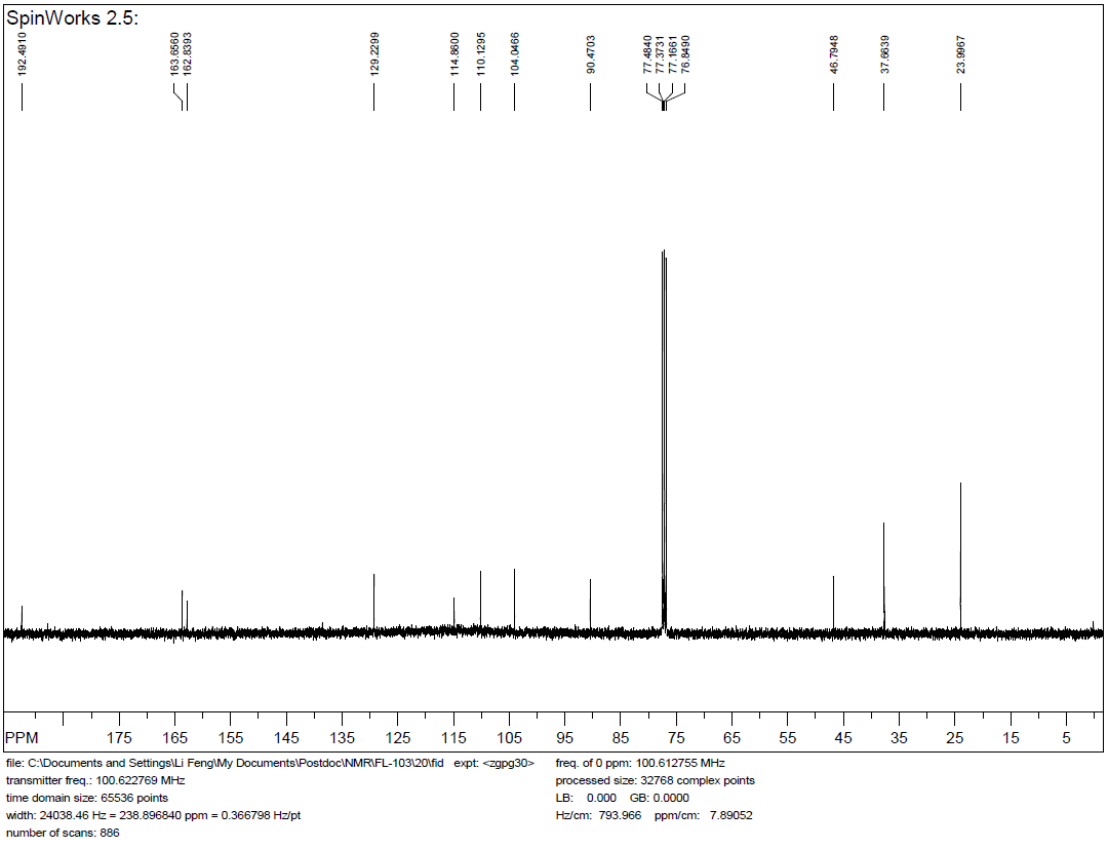
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.219	4647097	900043	99.848	99.770
2	7.439	7077	2079	0.152	0.230
Total		4654174	902122	100.000	100.000

HRMS of **6f**


x10 6
-ESI Scan (0.187 min) Frag=70.0V Sun230_neg.d
292.1512
328.1259
112.9856
170.8322
245.1156
360.1348
428.0093
496.0239
607.2704
675.1772
775.1515
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **7a**



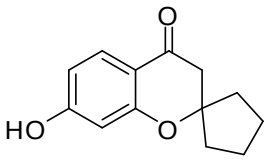


HPLC profile of **7a**

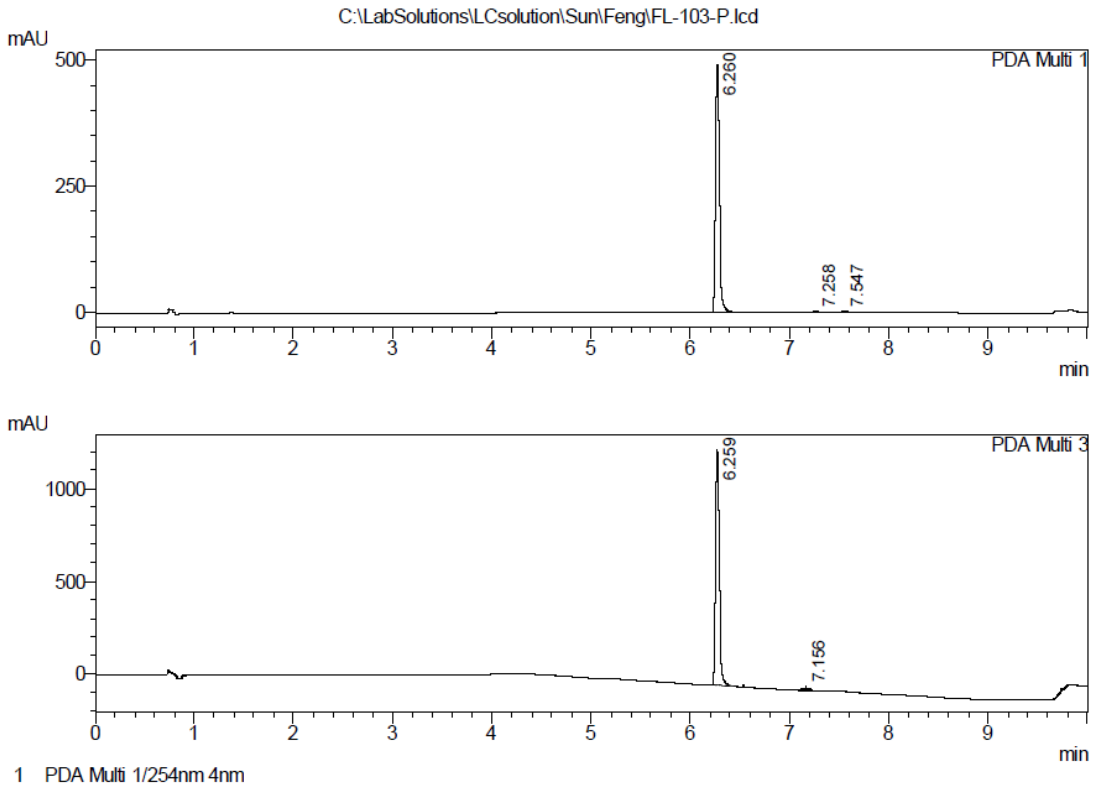
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\Feng\FL-103-P.lcd

Sample Name	: FL-103-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 10 uL
Data File Name	: FL-103-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 12/30/2011 12:34:18 PM



<Chromatogram>



1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

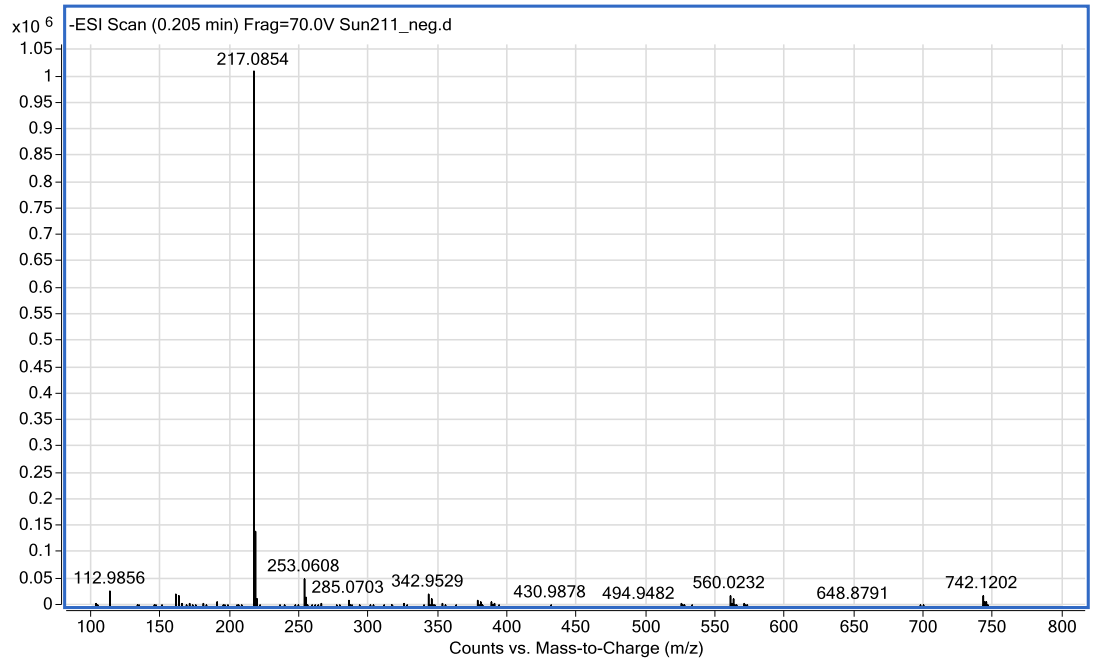
Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.260	1282041	490535	99.066	98.940
2	7.258	6268	2927	0.484	0.590
3	7.547	5823	2327	0.450	0.469
Total		1294132	495790	100.000	100.000

PeakTable

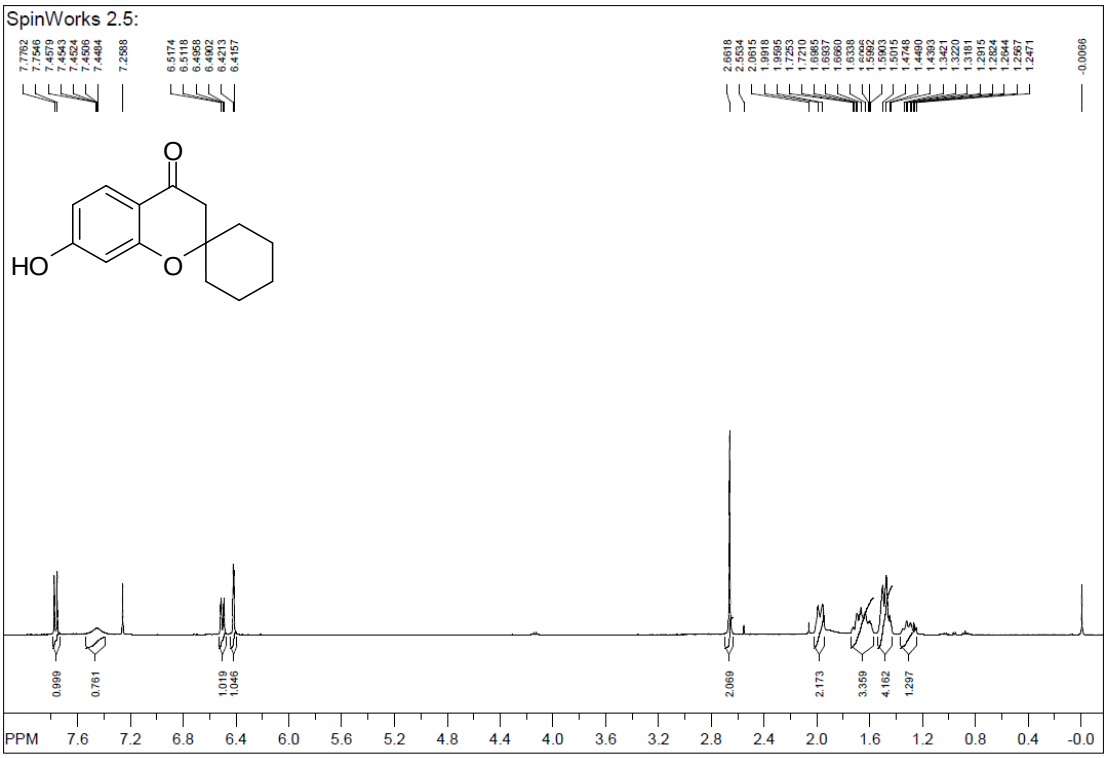
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.259	3187173	1271963	98.659	98.951
2	7.156	43331	13486	1.341	1.049
Total		3230504	1285449	100.000	100.000

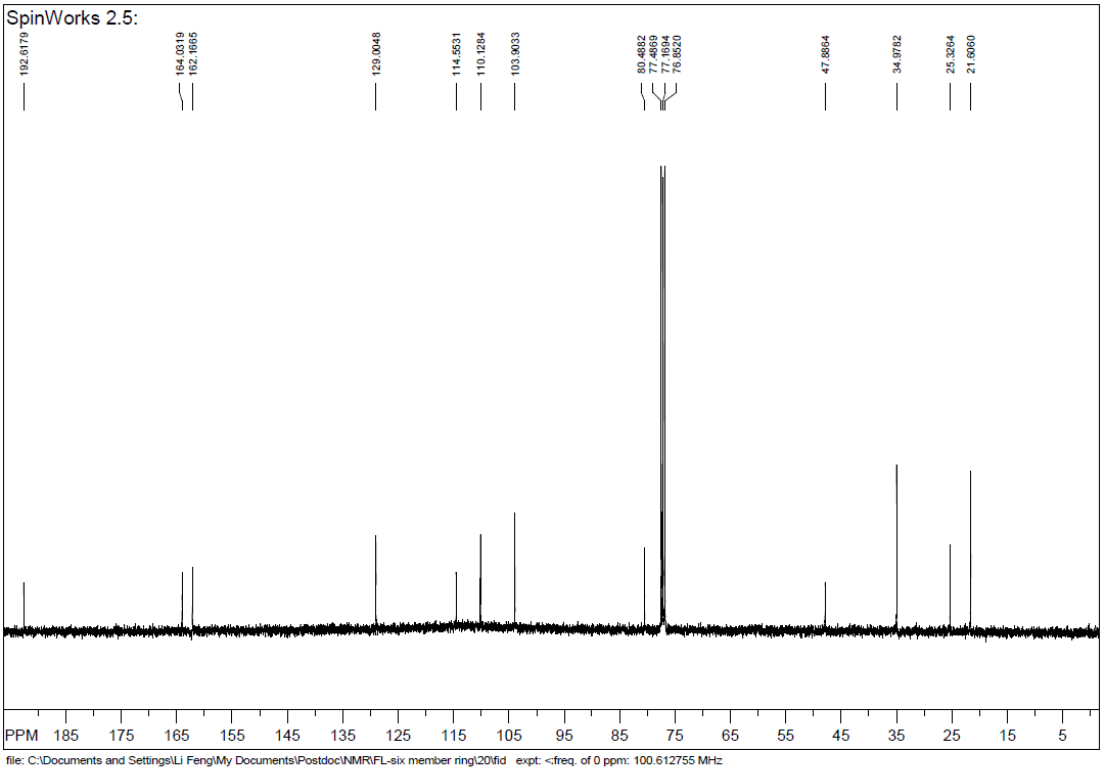
HRMS of **7a**


x10 6
-ESI Scan (0.205 min) Frag=70.0V Sun211_neg.d
217.0854
253.0608
285.0703
342.9529
112.9856
430.9878
494.9482
560.0232
648.8791
742.1202
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **7b**



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-six member ring\1\fid expt: <z;freq. of 0 ppm: 400.130010 MHz
transmitter freq.: 400.131600 MHz processed size: 32768 complex points
time domain size: 65536 points LB: 0.000 GB: 0.0000
width: 8012.82 Hz = 20.025463 ppm = 0.122266 Hz/pt Hz/cm: 133.260 ppm/cm: 0.33304
number of scans: 3



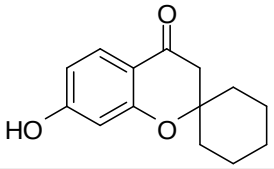
file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-six member ring\20\fid expt: <;freq. of 0 ppm: 100.612755 MHz
transmitter freq.: 100.622769 MHz processed size: 32768 complex points
time domain size: 65536 points LB: 0.000 GB: 0.0000
width: 24038.46 Hz = 238.896840 ppm = 0.366798 Hz/pt Hz/cm: 796.033 ppm/cm: 7.91106
number of scans: 1470

HPLC profile of **7b**

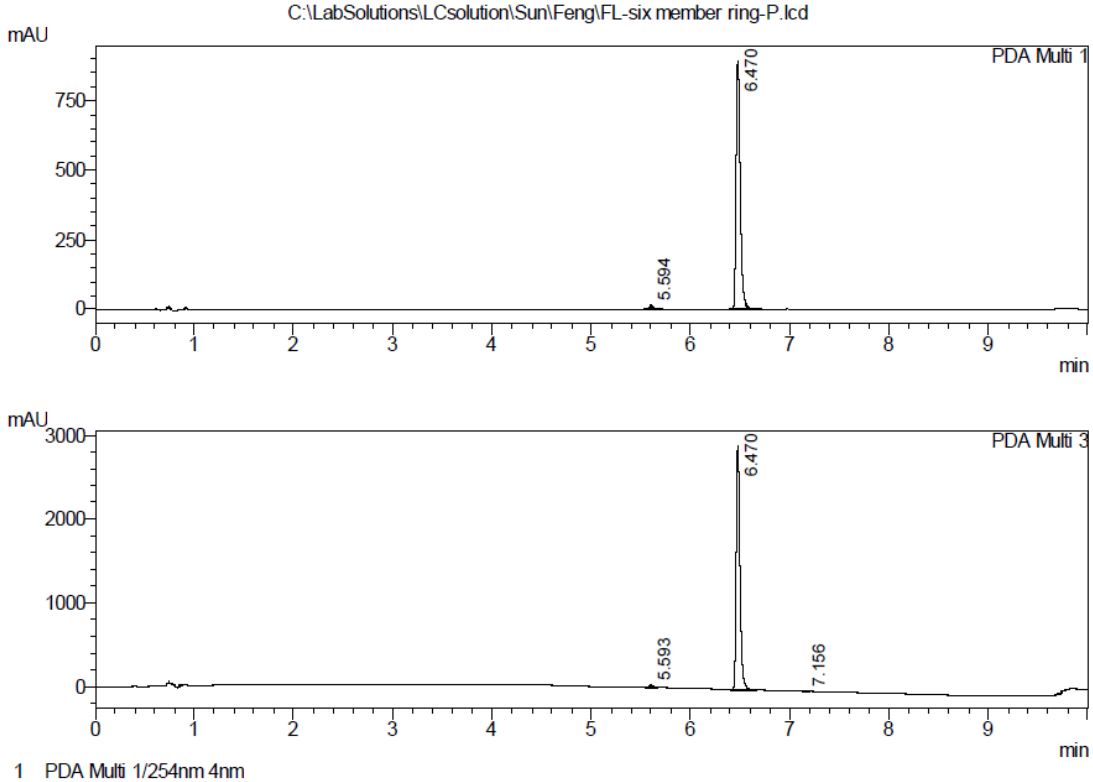
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\Feng\FL-six member ring-P.lcd

Sample Name	: FL-six member ring-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 8 uL
Data File Name	: FL-six member ring-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 1/4/2012 11:20:49 AM



<Chromatogram>



1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

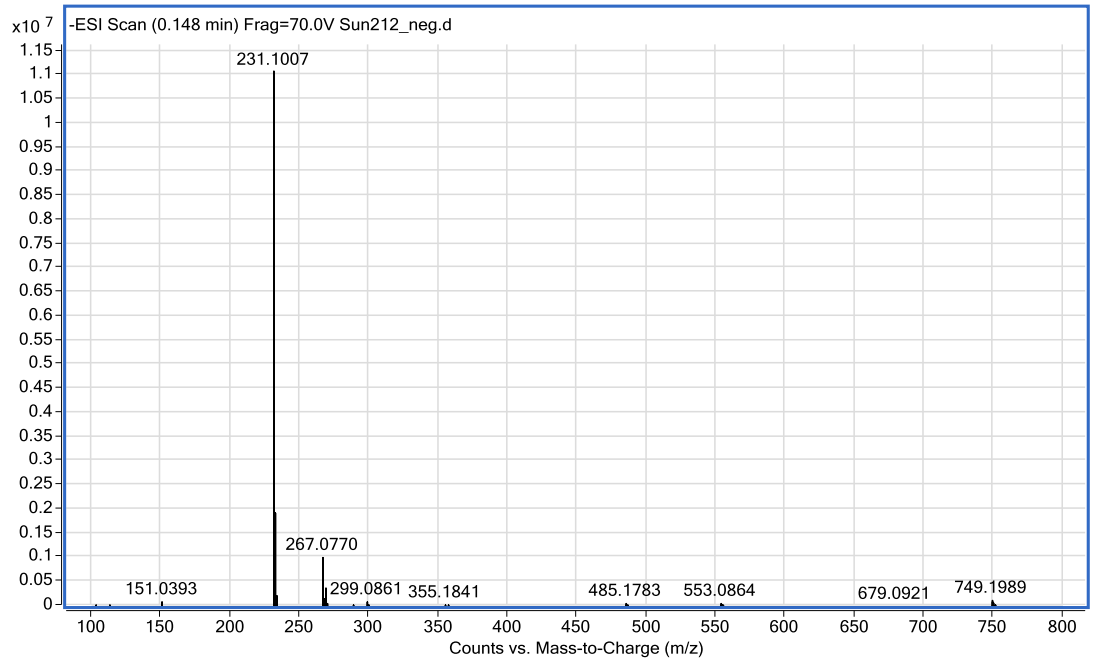
Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.594	41671	15246	1.777	1.710
2	6.470	2303034	876593	98.223	98.290
Total		2344705	891839	100.000	100.000

PeakTable

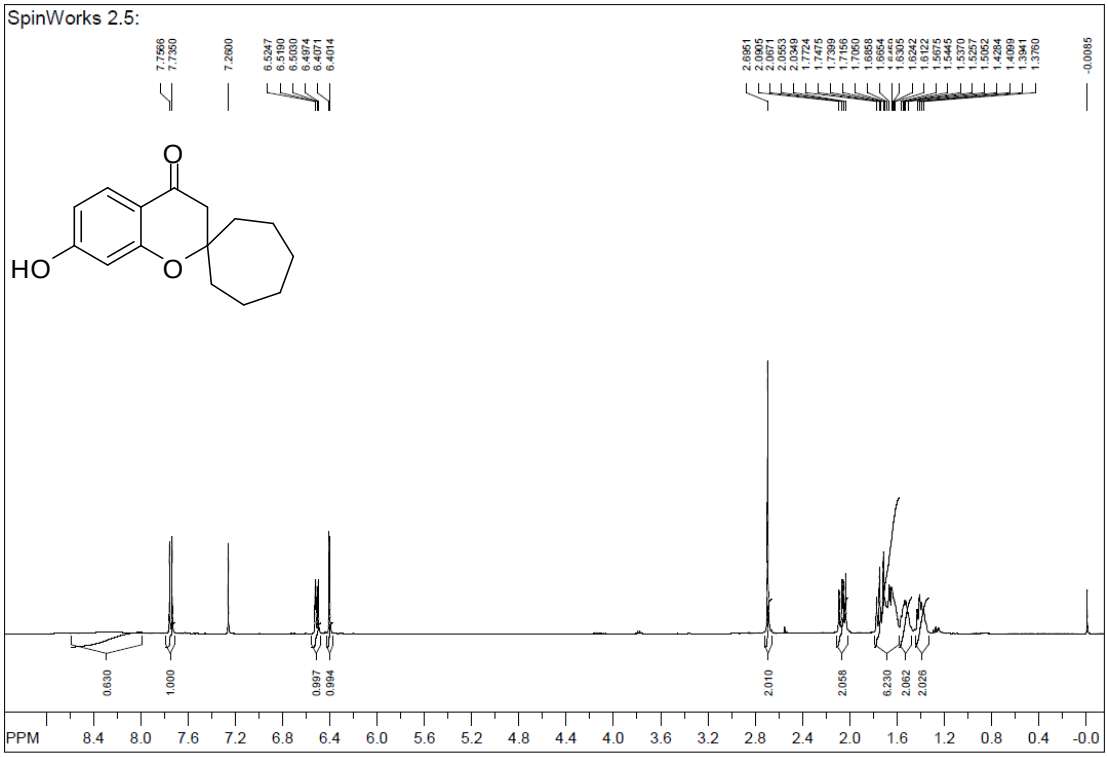
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.593	64580	25820	0.949	0.876
2	6.470	6722305	2914502	98.752	98.841
3	7.156	20377	8359	0.299	0.283
Total		6807262	2948681	100.000	100.000

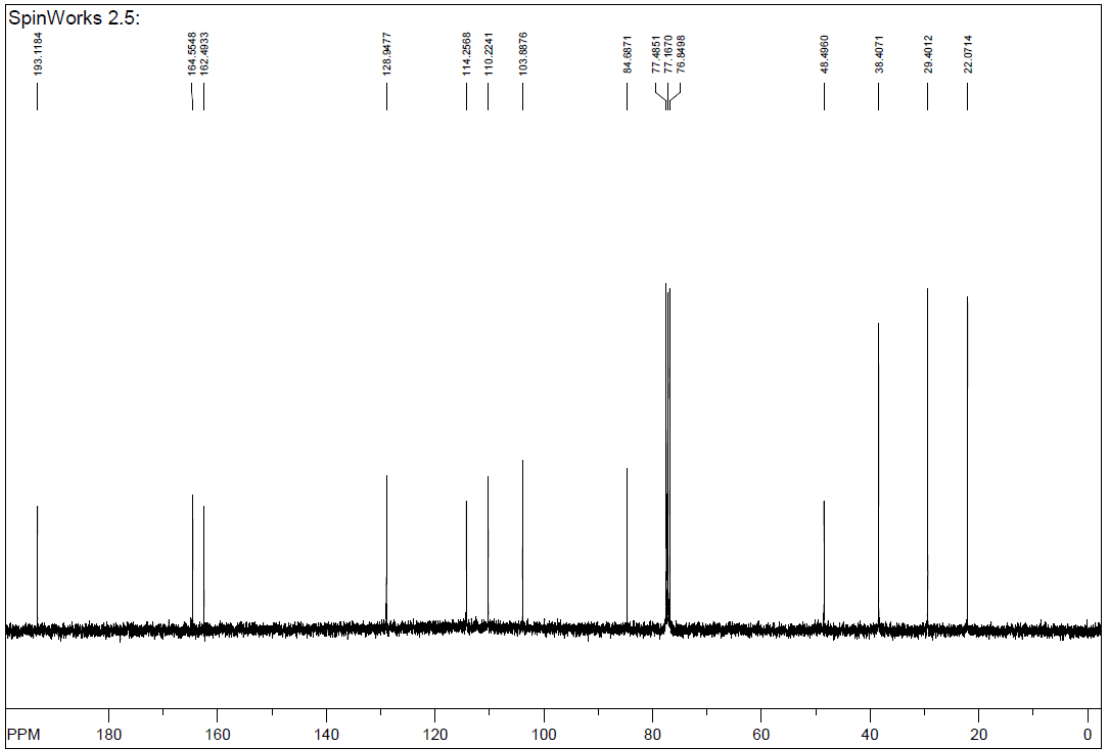
HRMS of **7b**


-ESI Scan (0.148 min) Frag=70.0V Sun212_neg.d
x10 7
231.1007
267.0770
151.0393
299.0861
355.1841
485.1783
553.0864
679.0921
749.1989
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **7c**



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-seven member ring\1\fid expt: freq. of 0 ppm: 400.130009 MHz
transmitter freq.: 400.131600 MHz processed size: 32768 complex points
time domain size: 65536 points LB: 0.000 GB: 0.0000
width: 8012.82 Hz = 20.025463 ppm = 0.122266 Hz/pt Hz/cm: 148.883 ppm/cm: 0.37209
number of scans: 4



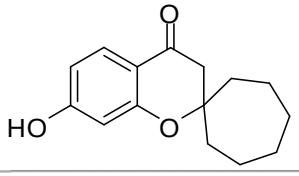
file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-seven member ring\20\fid exp: freq. of 0 ppm: 100.612757 MHz
transmitter freq.: 100.622769 MHz processed size: 32768 complex points
time domain size: 65536 points LB: 0.000 GB: 0.0000
width: 24038.46 Hz = 238.896840 ppm = 0.366798 Hz/pt Hz/cm: 810.507 ppm/cm: 8.05490
number of scans: 460

HPLC profile of **7c**

==== Shimadzu LCsolution Analysis Report ====

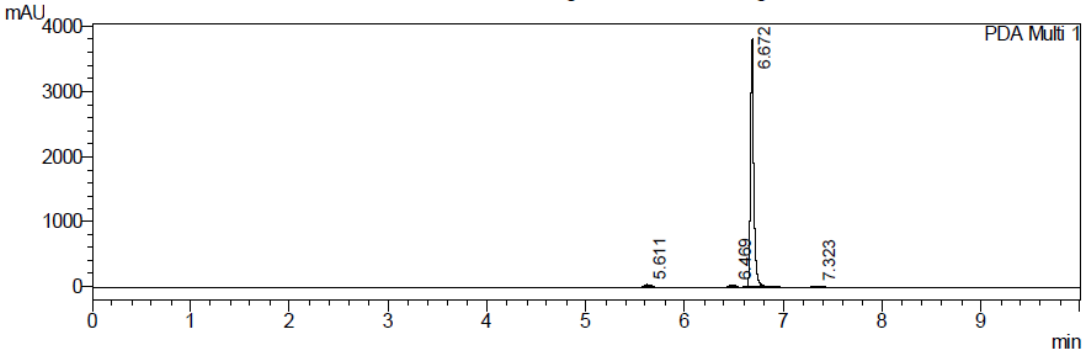
C:\LabSolutions\LCsolution\Sun\Feng\FL-seven member ring-P.lcd

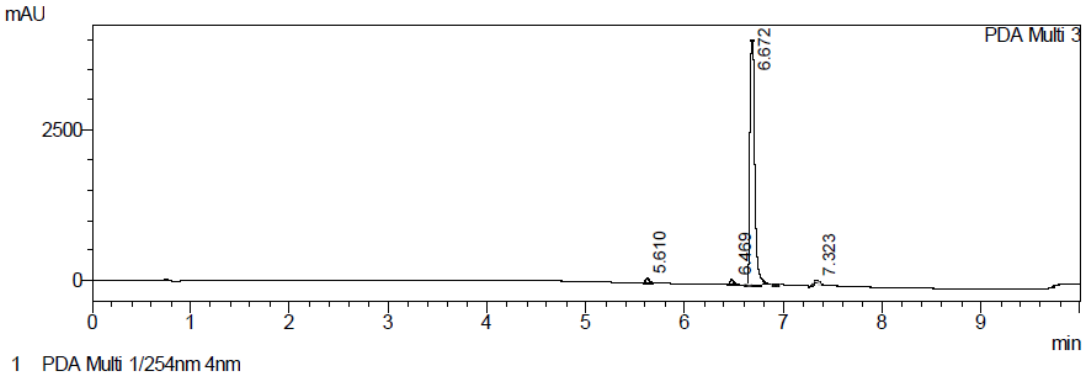
Sample Name	: FL-seven member ring-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 10 uL
Data File Name	: FL-seven member ring-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 1/3/2012 5:00:52 PM



<Chromatogram>

C:\LabSolutions\LCsolution\Sun\Feng\FL-seven member ring-P.lcd





1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

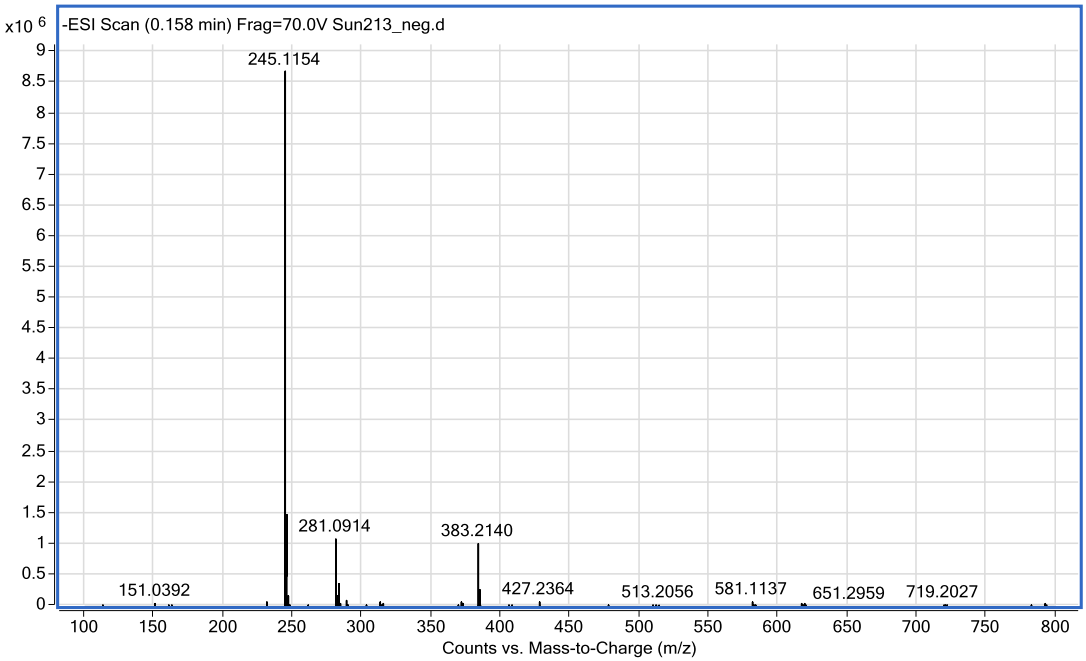
Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.611	110221	41408	1.076	1.098
2	6.469	81938	34438	0.800	0.913
3	6.672	9978682	3675941	97.415	97.503
4	7.323	72684	18284	0.710	0.485
Total		10243525	3770071	100.000	100.000

PeakTable

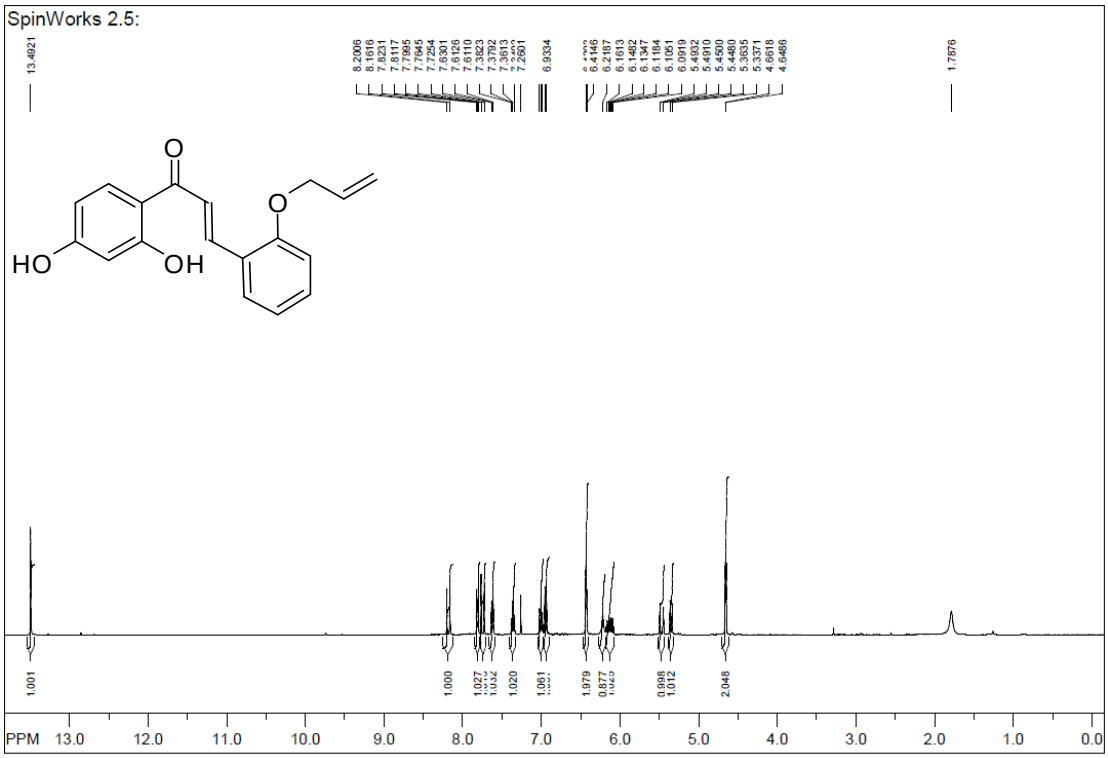
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.610	170952	69024	1.080	1.620
2	6.469	192009	80053	1.214	1.878
3	6.672	15346457	4064527	96.990	95.368
4	7.323	113315	48326	0.716	1.134
Total		15822733	4261930	100.000	100.000

HRMS of **7c**

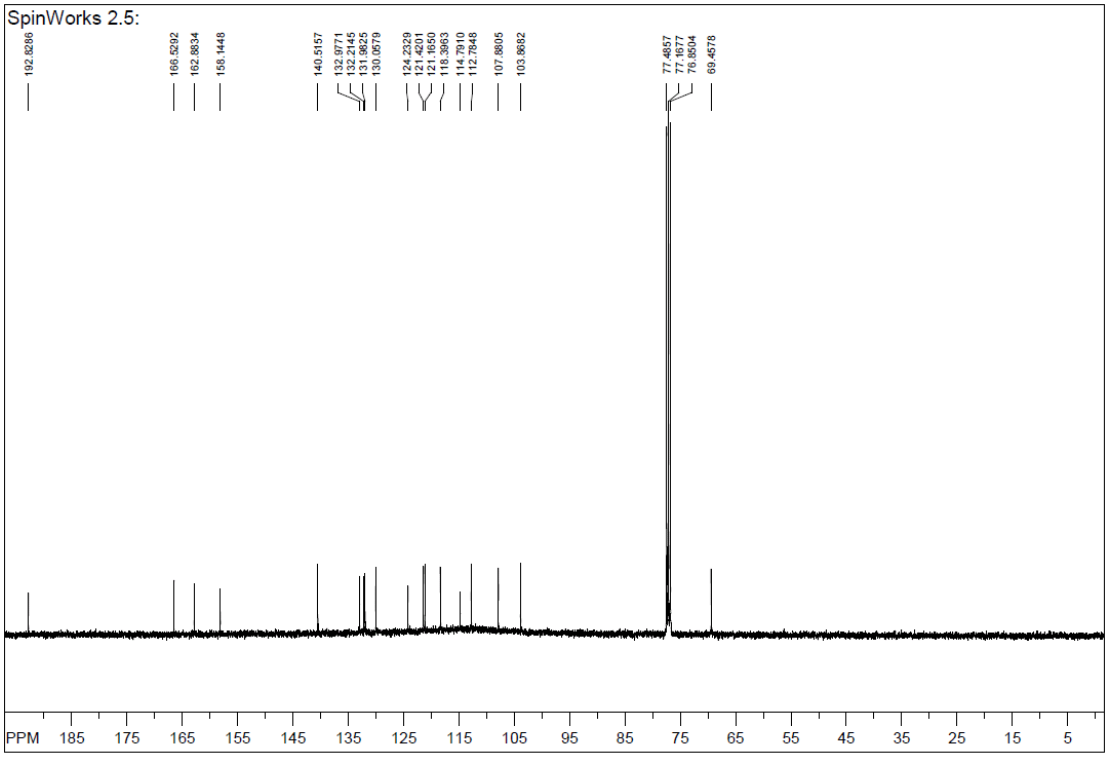

x10 6
-ESI Scan (0.158 min) Frag=70.0V Sun213_neg.d
245.1154
281.0914
383.2140
151.0392
427.2364
513.2056
581.1137
651.2959
719.2027
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **8a**



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-16\1\fid expt: <zg30>
transmitter freq.: 400.131600 MHz
time domain size: 65536 points
width: 10000.00 Hz = 24.991778 ppm = 0.152588 Hz/pt
number of scans: 16

freq. of 0 ppm: 400.130009 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 223.656 ppm/cm: 0.55896



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-16\21\fid expt: <zgpg30>
transmitter freq.: 100.622769 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.896840 ppm = 0.366798 Hz/pt
number of scans: 3000

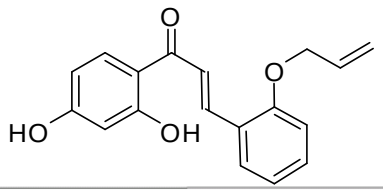
freq. of 0 ppm: 100.612753 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 799.479 ppm/cm: 7.94531

HPLC profile of **8a**

==== Shimadzu LCsolution Analysis Report ====

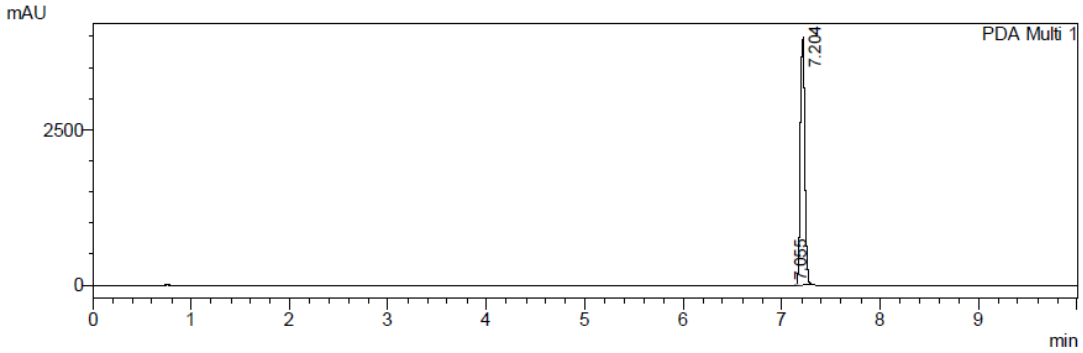
C:\LabSolutions\LCsolution\Sun\Feng\FL-16-P.lcd

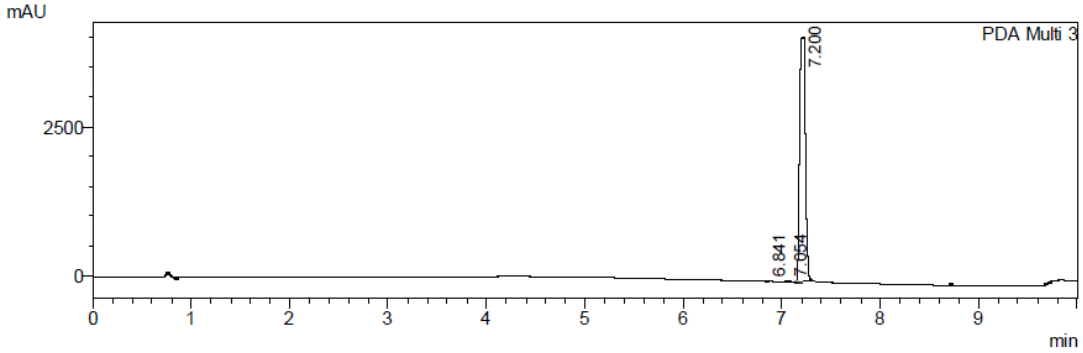
Sample Name	: FL-16-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 10 uL
Data File Name	: FL-16-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 7/27/2012 11:14:15 AM



<Chromatogram>

C:\LabSolutions\LCsolution\Sun\Feng\FL-16-P.lcd





1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

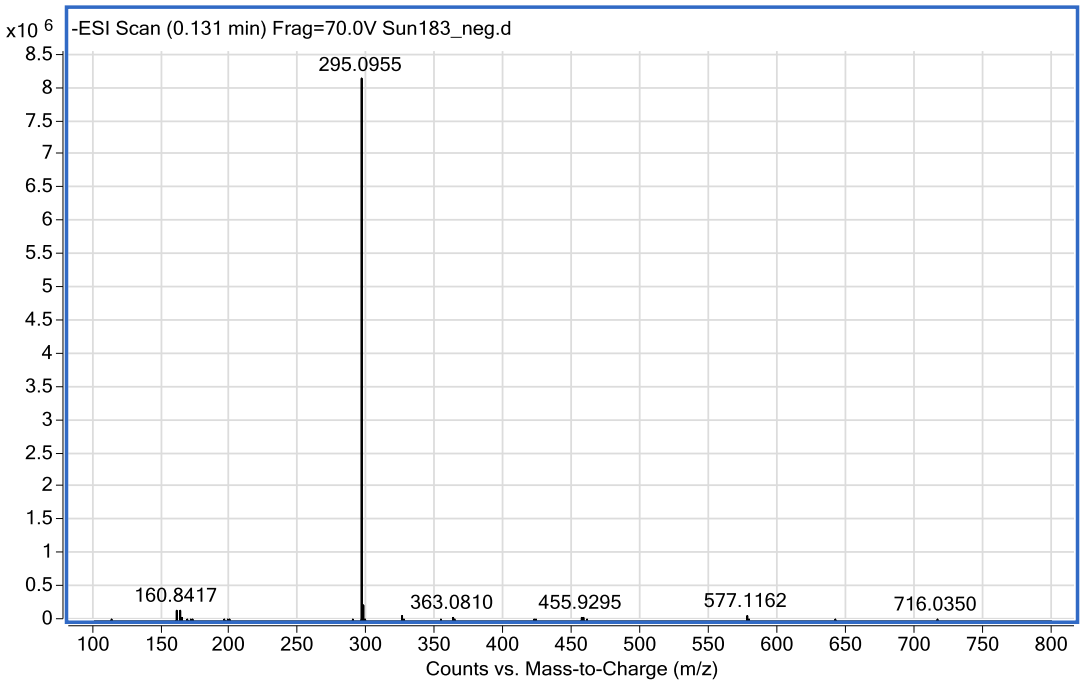
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.055	1525	1353	0.013	0.034
2	7.204	11375325	3961397	99.987	99.966
Total		11376849	3962750	100.000	100.000

PeakTable

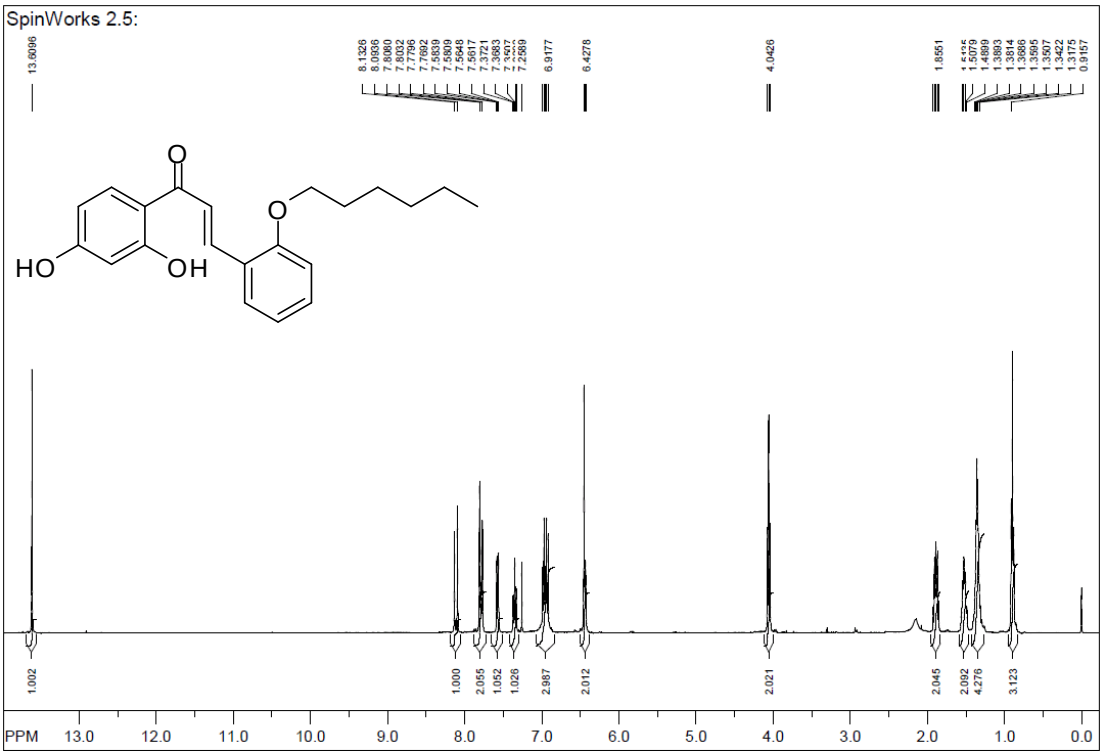
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.841	6312	5295	0.042	0.129
2	7.054	10553	8050	0.069	0.196
3	7.200	15178952	4093726	99.889	99.675
Total		15195817	4107071	100.000	100.000

HRMS of **8a**

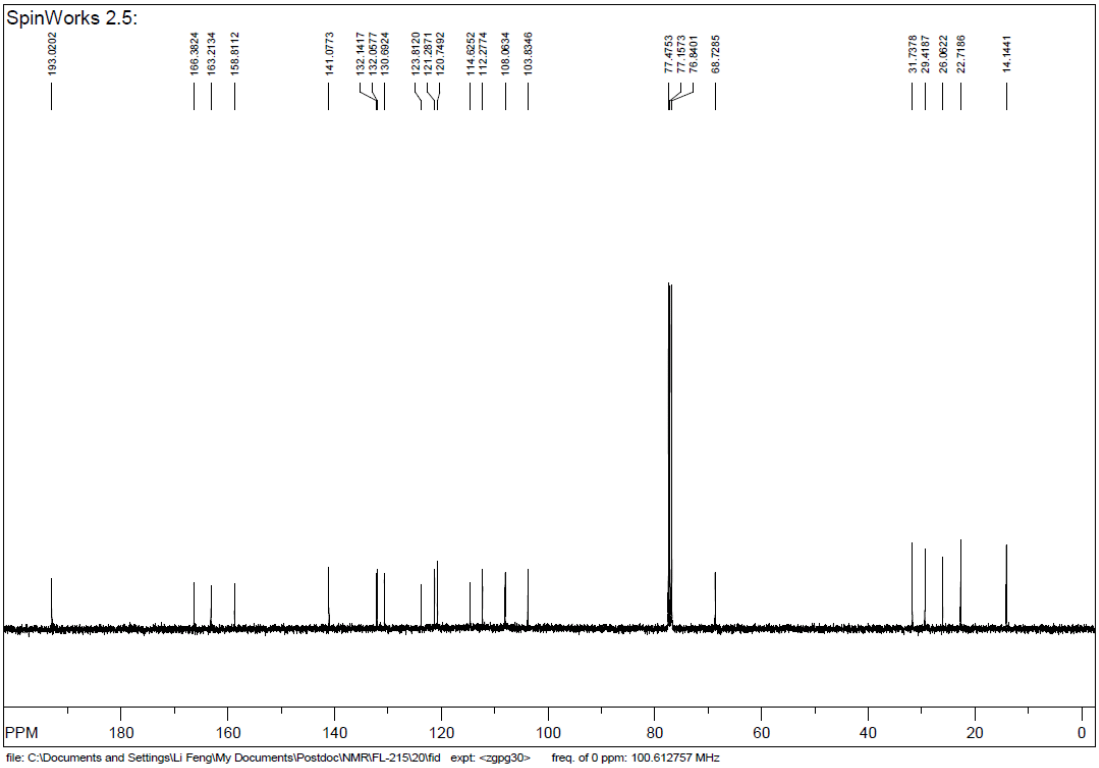

-ESI Scan (0.131 min) Frag=70.0V Sun183_neg.d
x10 6
295.0955
160.8417
363.0810
455.9295
577.1162
716.0350
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **8b**



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-215\1\fid expt: <zg30>
transmitter freq.: 400.131600 MHz
time domain size: 65536 points
width: 8012.82 Hz = 20.025463 ppm = 0.122266 Hz/pt
number of scans: 6

freq. of 0 ppm: 400.130009 MHz
processed size: 32768 complex points
LB: 0.300 GB: 0.0000
Hz/cm: 227.231 ppm/cm: 0.56789



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-215\20\fid expt: <zgpg30>
transmitter freq.: 100.622769 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.896840 ppm = 0.366798 Hz/pt
number of scans: 844

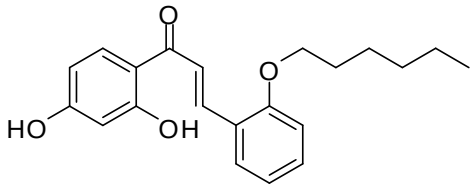
freq. of 0 ppm: 100.612757 MHz
processed size: 32768 complex points
LB: 1.000 GB: 0.0000
Hz/cm: 822.994 ppm/cm: 8.17901

HPLC profile of **8b**

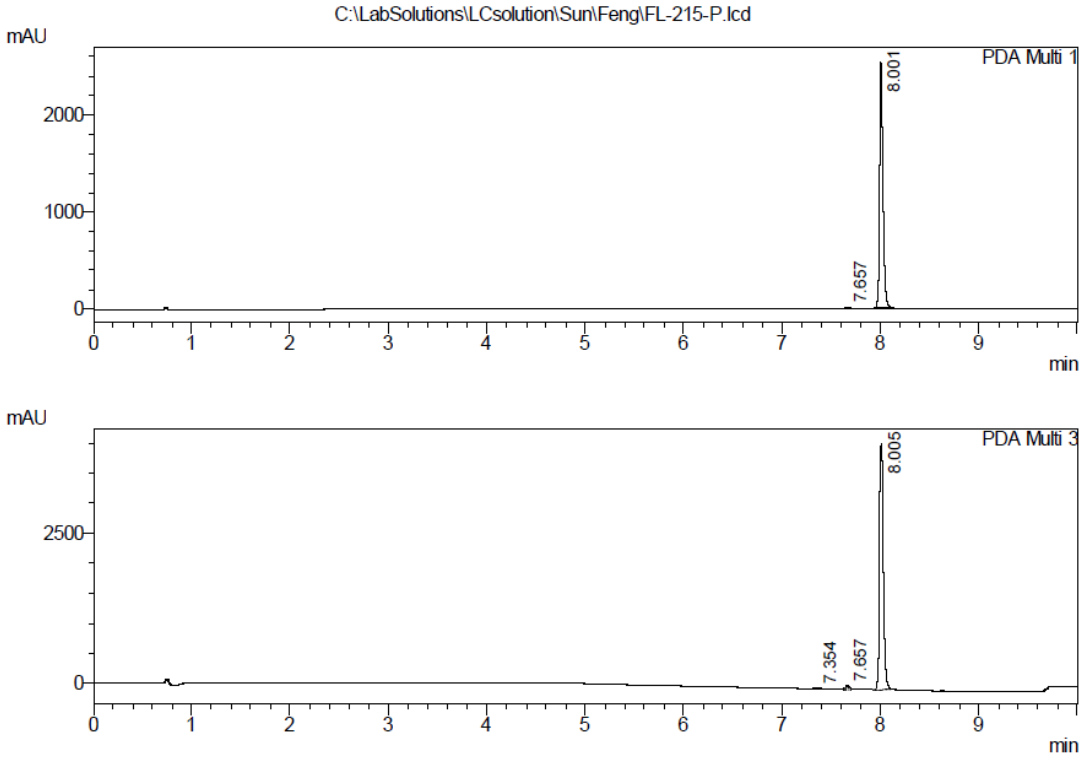
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\Feng\FL-215-P.lcd

Sample Name	: FL-215-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 8 uL
Data File Name	: FL-215-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 4/18/2012 3:10:19 PM



<Chromatogram>



1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

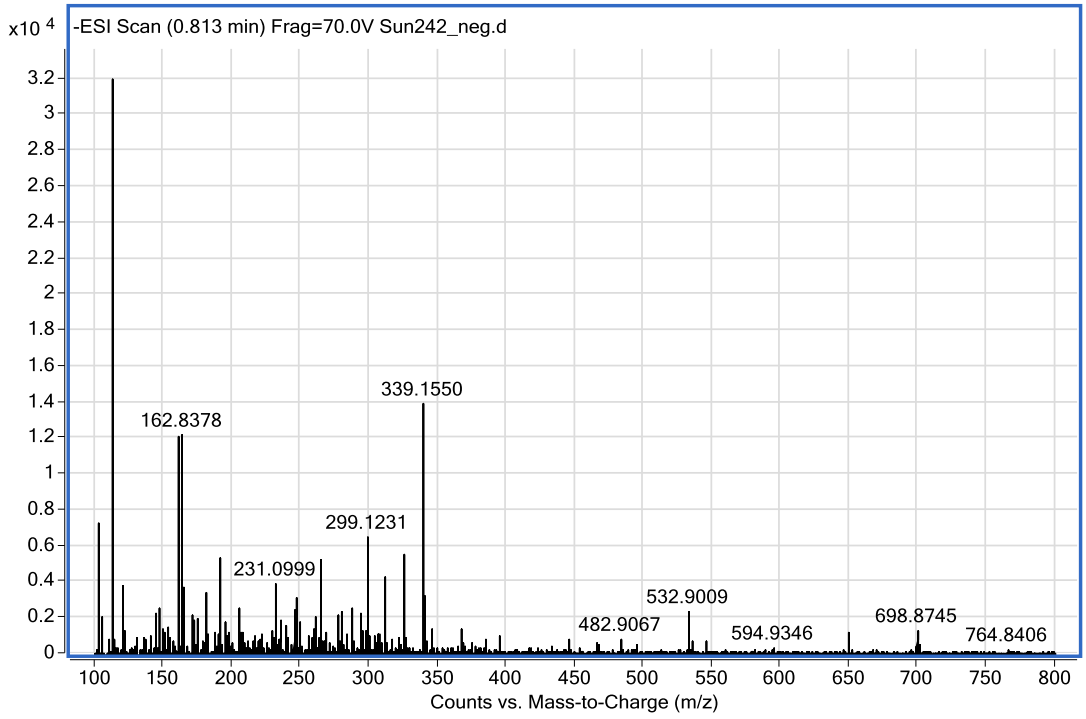
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.657	23687	12103	0.387	0.499
2	8.001	6101539	2415172	99.613	99.501
Total		6125226	2427275	100.000	100.000

PeakTable

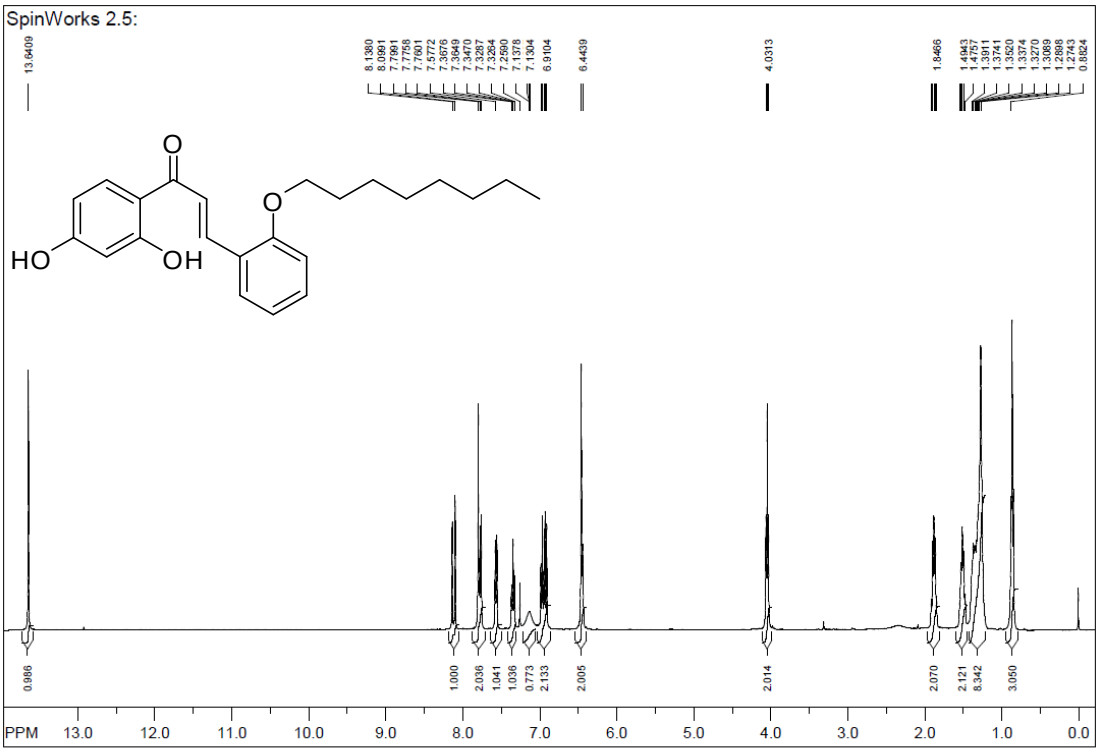
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.354	25073	10662	0.212	0.256
2	7.657	109800	50556	0.930	1.216
3	8.005	11673867	4096151	98.858	98.527
Total		11808740	4157369	100.000	100.000

HRMS of **8b**

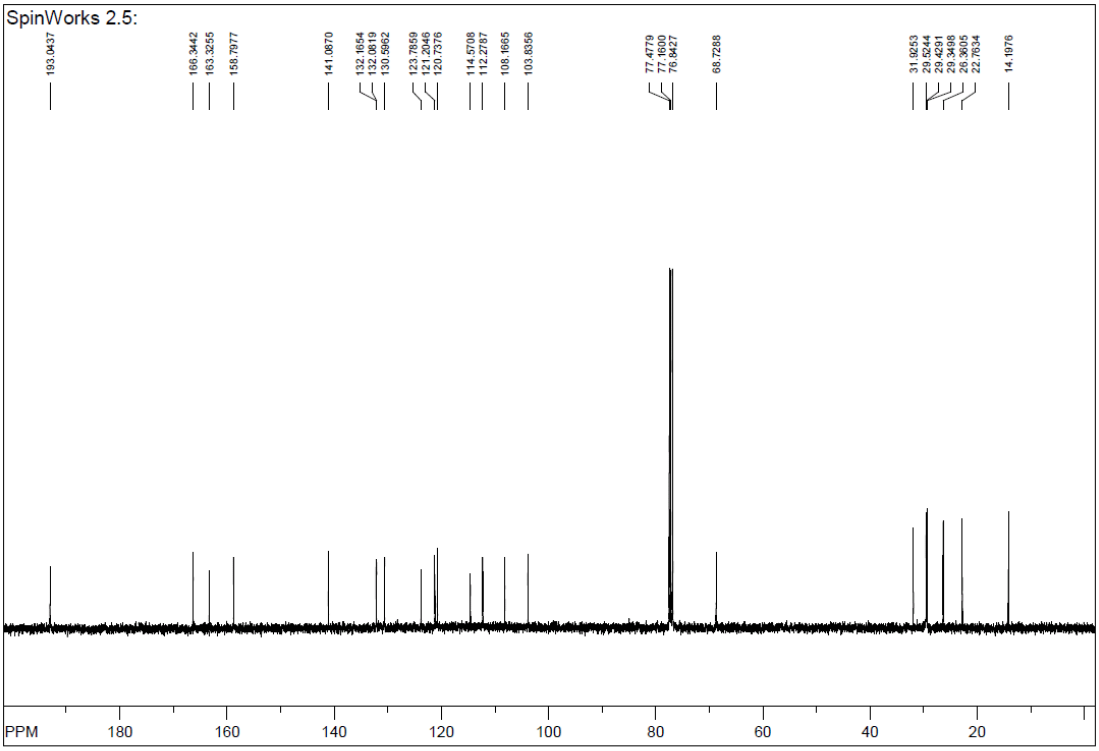

x10 4
-ESI Scan (0.813 min) Frag=70.0V Sun242_neg.d
3.2
3
2.8
2.6
2.4
2.2
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
339.1550
162.8378
299.1231
231.0999
532.9009
482.9067
594.9346
698.8745
764.8406
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **8c**



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-209\1\fid expt: <zg30>
transmitter freq.: 400.131600 MHz
time domain size: 65536 points
width: 8012.82 Hz = 20.025463 ppm = 0.122266 Hz/pt
number of scans: 4

freq. of 0 ppm: 400.130009 MHz
processed size: 32768 complex points
LB: 0.300 GB: 0.0000
Hz/cm: 226.771 ppm/cm: 0.56674



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-209\20\fid expt: <zgpg30>
transmitter freq.: 100.622769 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.896840 ppm = 0.366798 Hz/pt
number of scans: 484

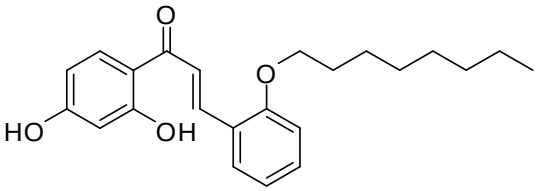
freq. of 0 ppm: 100.612758 MHz
processed size: 32768 complex points
LB: 1.000 GB: 0.0000
Hz/cm: 819.548 ppm/cm: 8.14476

HPLC profile of **8c**

==== Shimadzu LCsolution Analysis Report ====

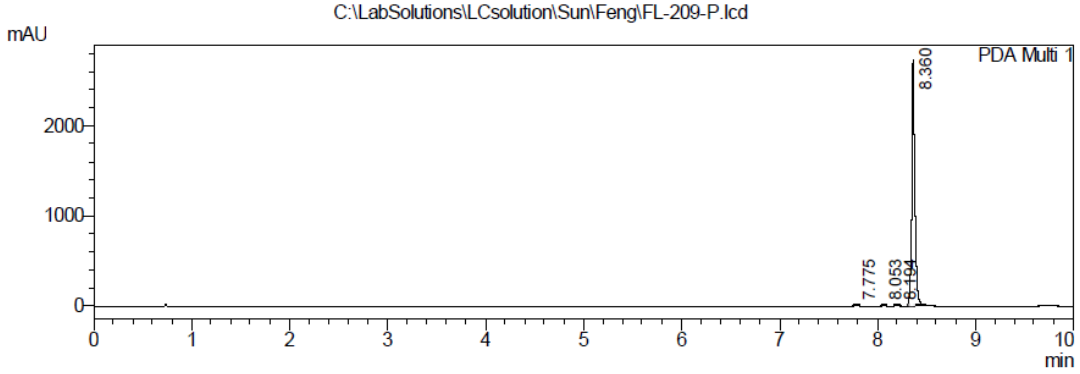
C:\LabSolutions\LCsolution\Sun\Feng\FL-209-P.lcd

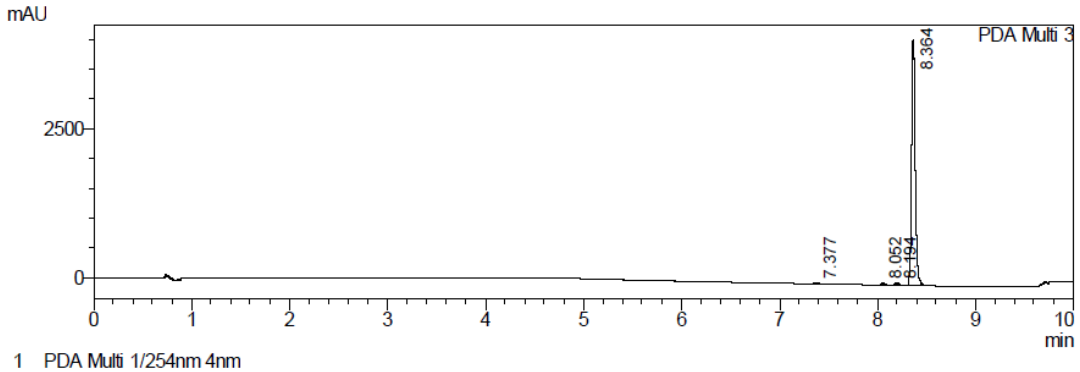
Sample Name	: FL-209-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 10 uL
Data File Name	: FL-209-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 4/12/2012 12:23:11 PM



<Chromatogram>

C:\LabSolutions\LCsolution\Sun\Feng\FL-209-P.lcd





1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

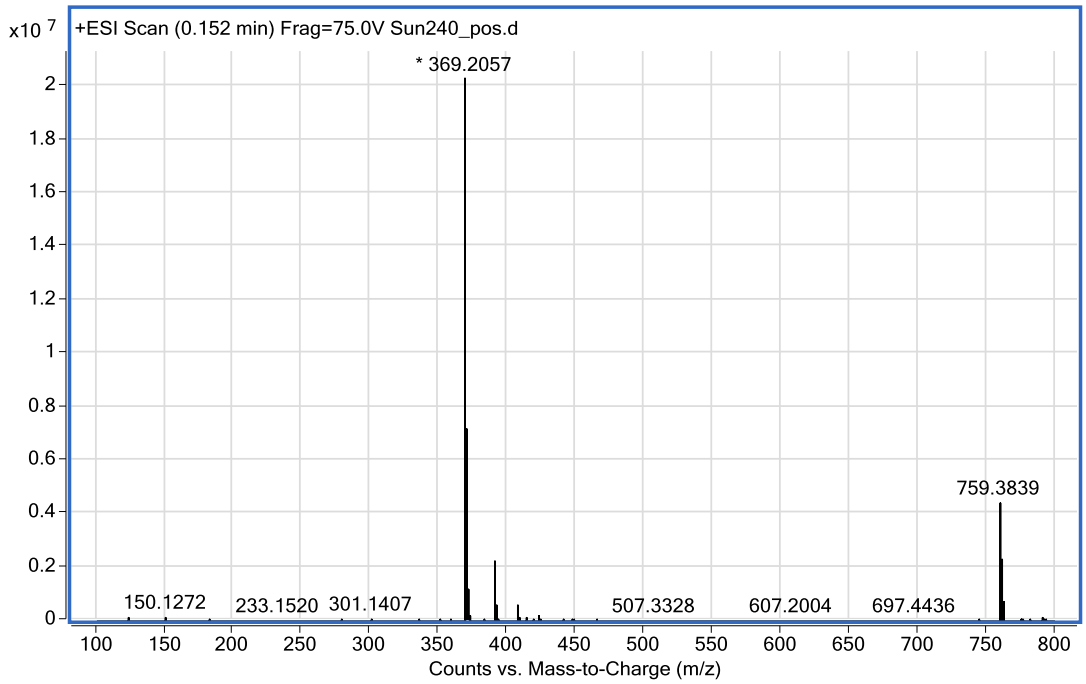
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.775	12512	6297	0.192	0.242
2	8.053	6266	4474	0.096	0.172
3	8.194	11235	6670	0.172	0.256
4	8.360	6490778	2587108	99.540	99.330
Total		6520790	2604549	100.000	100.000

PeakTable

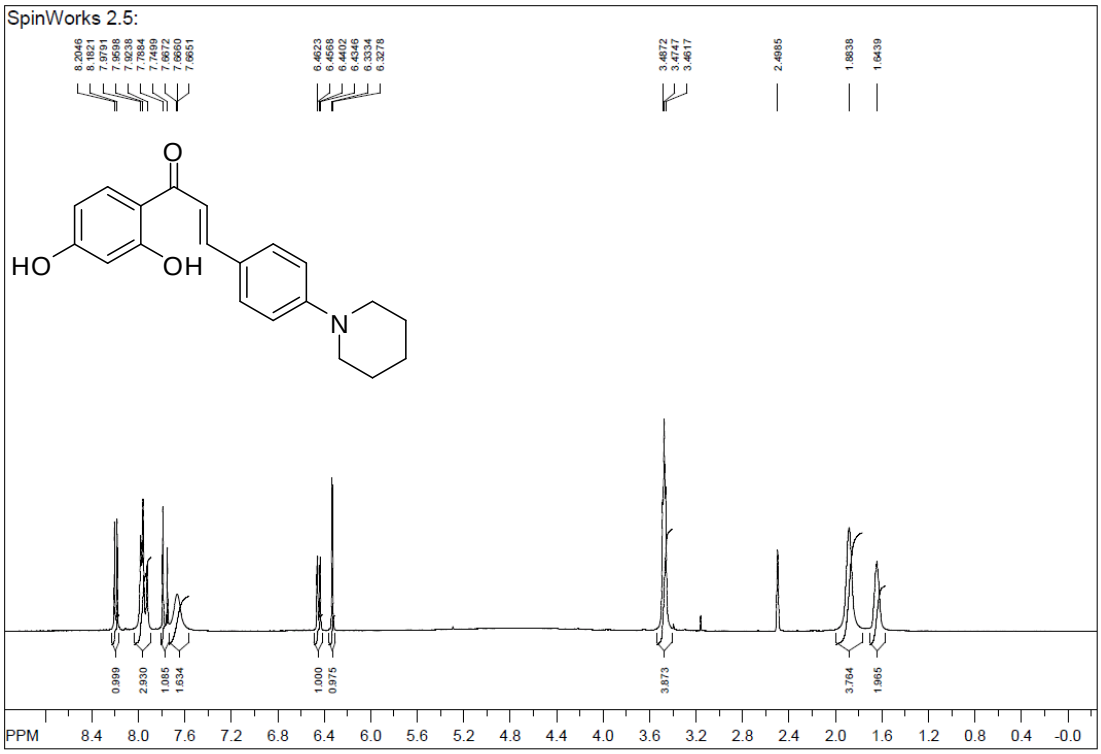
PDA Ch3 220nm 4nm

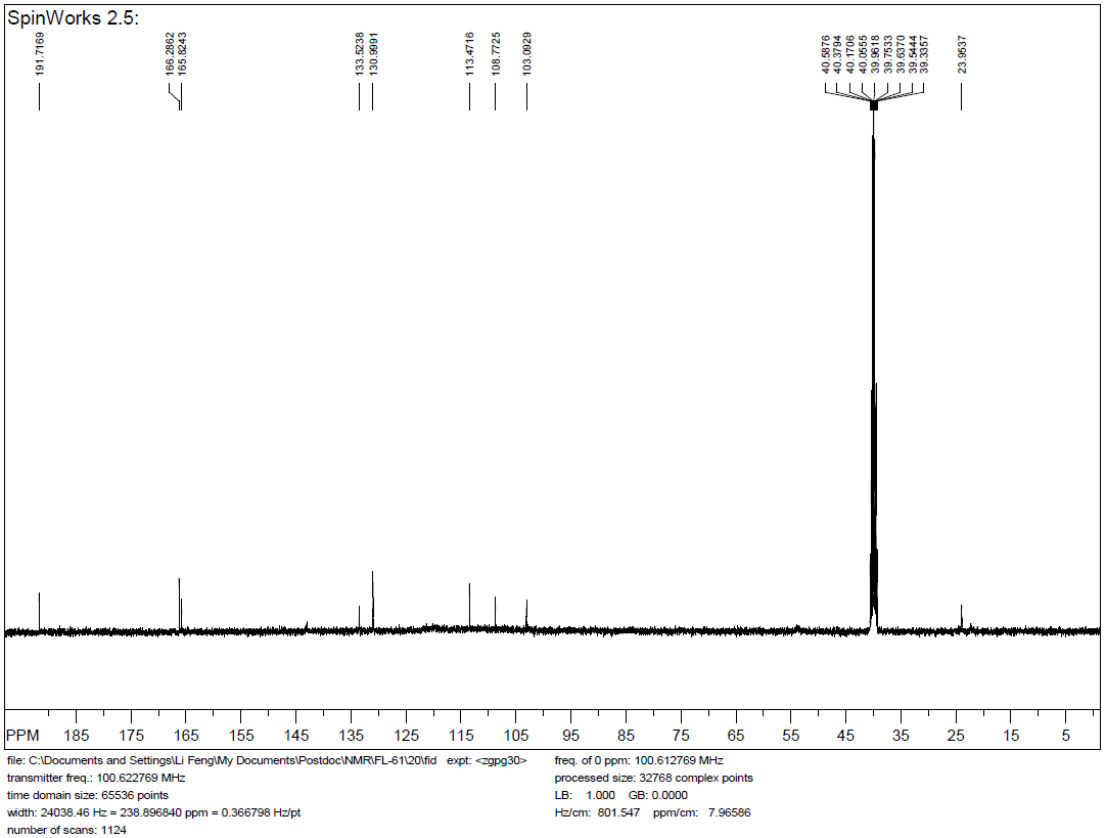
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.377	7083	4676	0.059	0.113
2	8.052	23508	16003	0.196	0.386
3	8.194	43361	25503	0.361	0.614
4	8.364	11943340	4104825	99.385	98.887
Total		12017292	4151008	100.000	100.000

HRMS of **8c**


x10 7
+ESI Scan (0.152 min) Frag=75.0V Sun240_pos.d
* 369.2057
759.3839
150.1272
233.1520
301.1407
507.3328
607.2004
697.4436
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **8d**

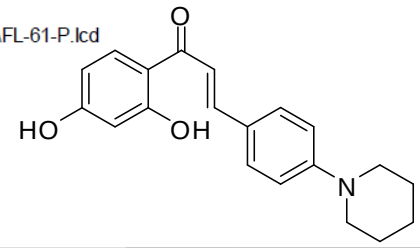




HPLC profile of **8d**

==== Shimadzu LCsolution Analysis Report ====

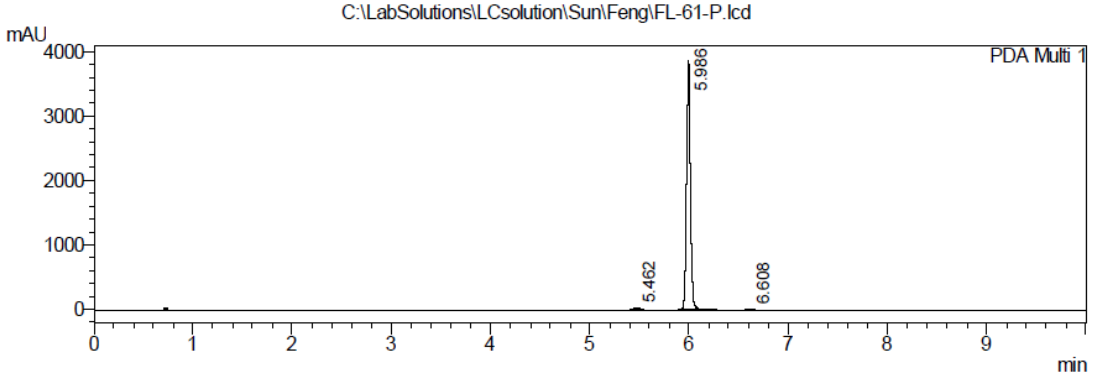
C:\LabSolutions\LCsolution\Sun\Feng\FL-61-P.lcd

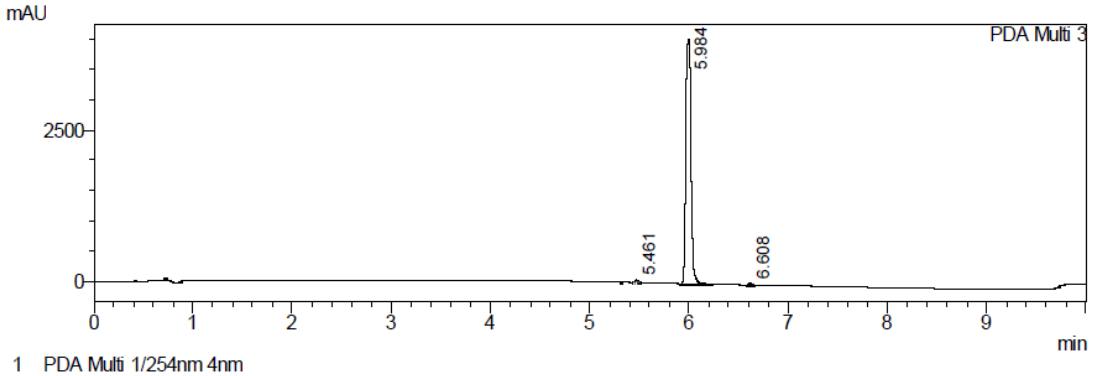


Sample Name	: FL-61-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 12 uL
Data File Name	: FL-61-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 12/28/2011 3:01:36 PM

<Chromatogram>

C:\LabSolutions\LCsolution\Sun\Feng\FL-61-P.lcd





1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

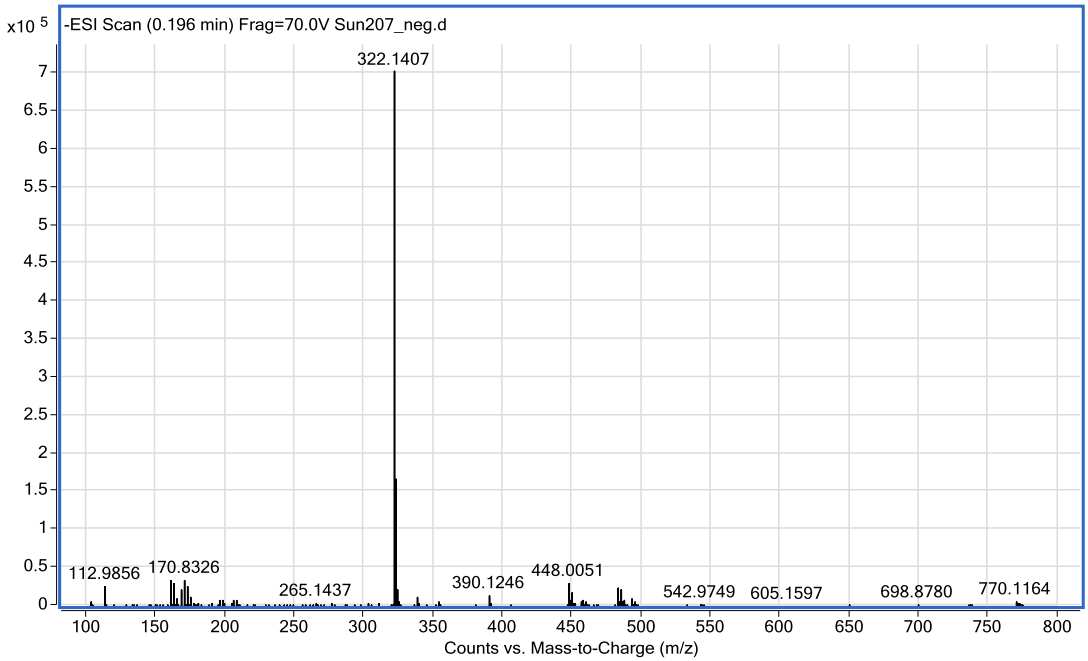
Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.462	60587	24274	0.638	0.626
2	5.986	9395389	3837779	98.970	98.957
3	6.608	37199	16161	0.392	0.417
Total		9493174	3878214	100.000	100.000

PeakTable

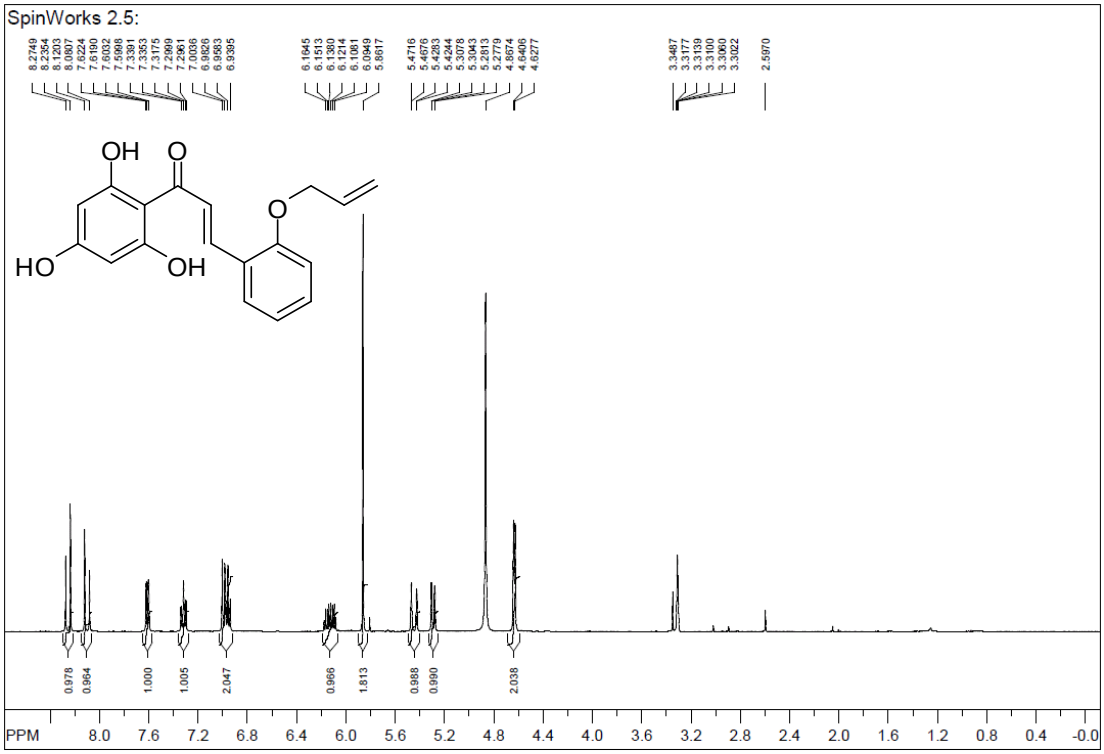
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.461	93383	41668	0.688	1.016
2	5.984	13417081	4029253	98.813	98.234
3	6.608	67839	30754	0.500	0.750
Total		13578303	4101675	100.000	100.000

HRMS of **8d**

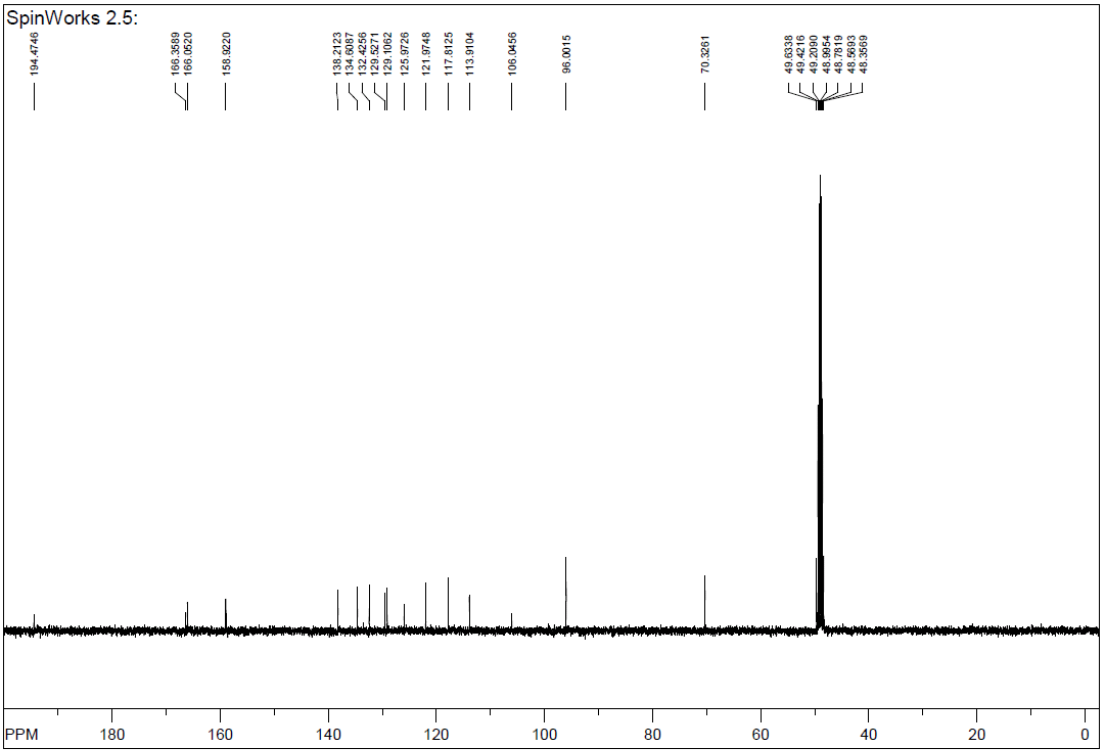

-ESI Scan (0.196 min) Frag=70.0V Sun207_neg.d
x10 5
322.1407
112.9856
170.8326
265.1437
390.1246
448.0051
542.9749
605.1597
698.8780
770.1164
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **8e**



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-190\4\fid expt: <zg30>
transmitter freq.: 400.131600 MHz
time domain size: 65536 points
width: 8012.82 Hz = 20.025463 ppm = 0.122266 Hz/pt
number of scans: 6

freq. of 0 ppm: 400.130007 MHz
processed size: 32768 complex points
LB: 0.300 GB: 0.0000
Hz/cm: 142.220 ppm/cm: 0.35543



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-190\20\fid expt: <zgpg30>
transmitter freq.: 100.622769 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.896840 ppm = 0.366798 Hz/pt
number of scans: 997

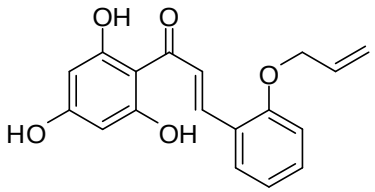
freq. of 0 ppm: 100.612629 MHz
processed size: 32768 complex points
LB: 1.000 GB: 0.0000
Hz/cm: 815.412 ppm/cm: 8.10365

HPLC profile of **8e**

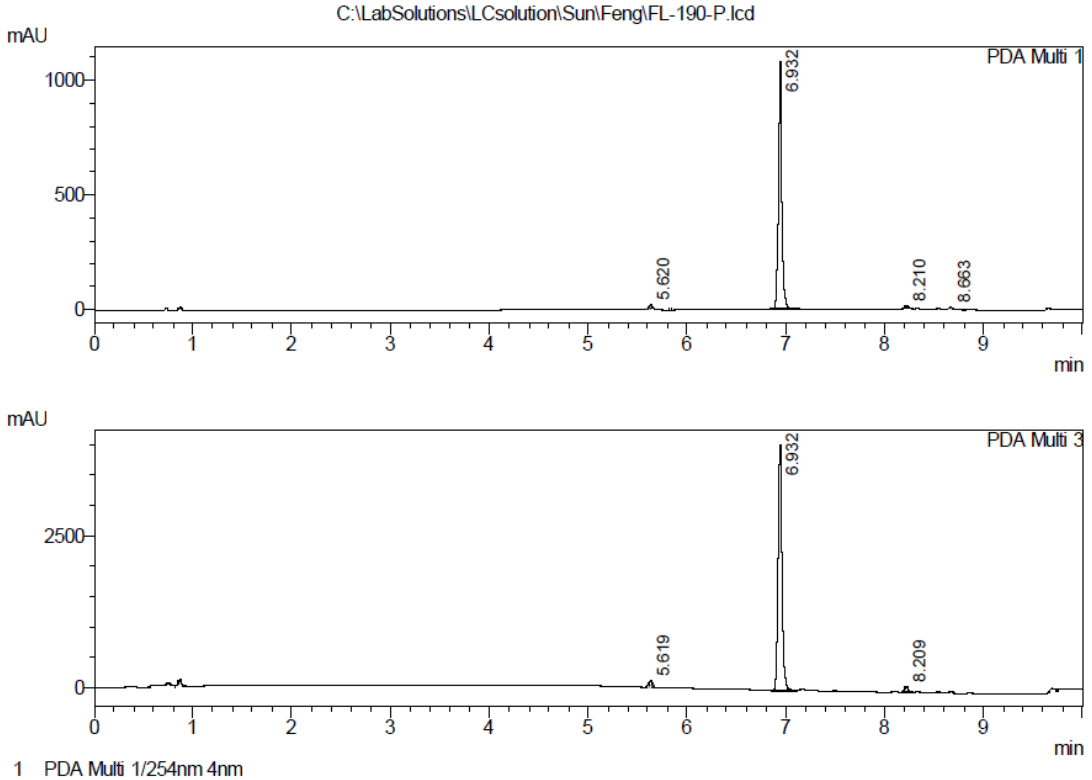
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\Feng\FL-190-P.lcd

Sample Name	: FL-190-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 2 uL
Data File Name	: FL-190-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 3/19/2012 3:34:00 PM



<Chromatogram>



1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

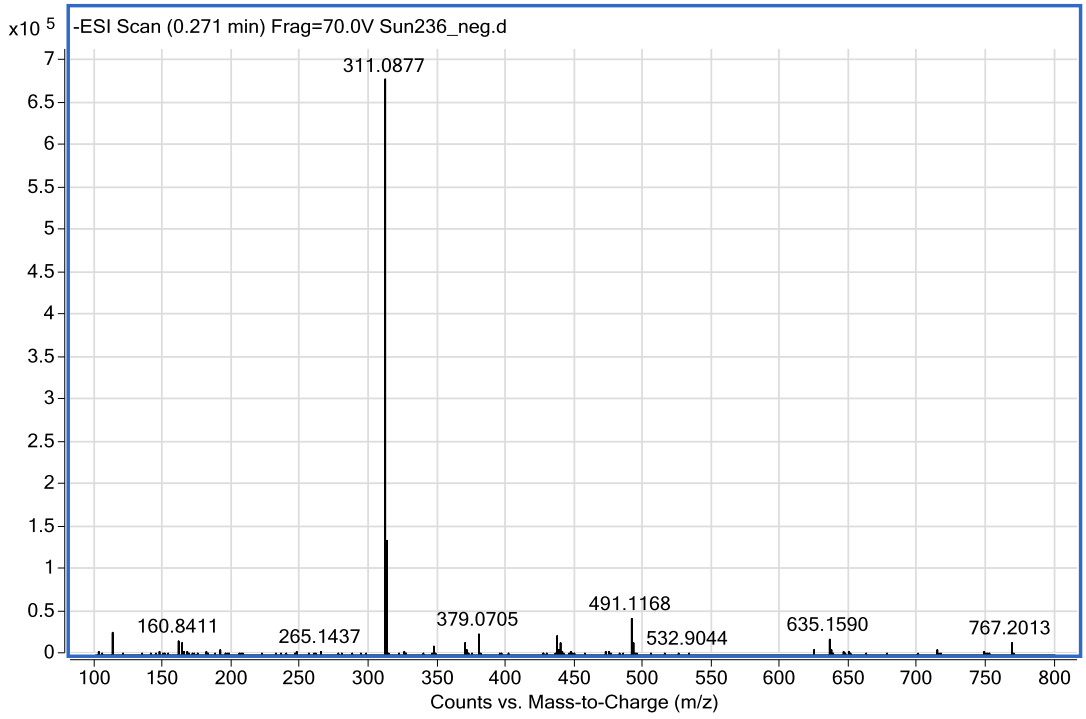
Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.620	31164	15706	1.031	1.409
2	6.932	2948049	1079579	97.496	96.826
3	8.210	31180	12760	1.031	1.144
4	8.663	13375	6923	0.442	0.621
Total		3023769	1114968	100.000	100.000

PeakTable

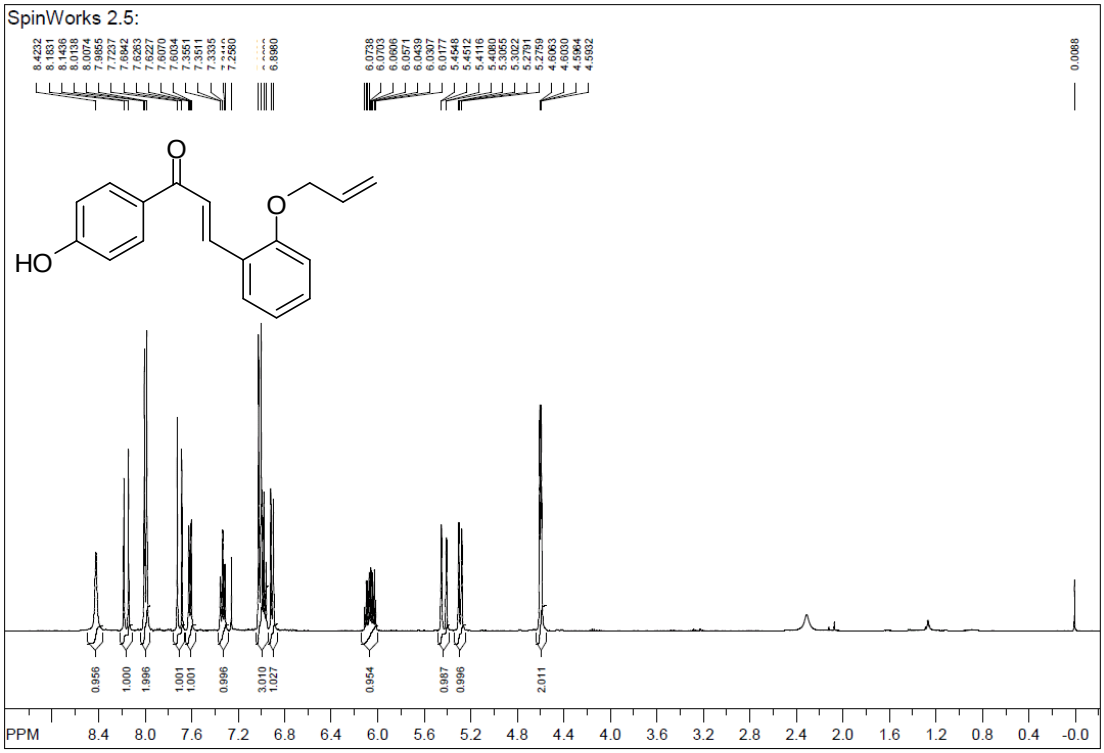
PDA Ch3 220nm 4nm

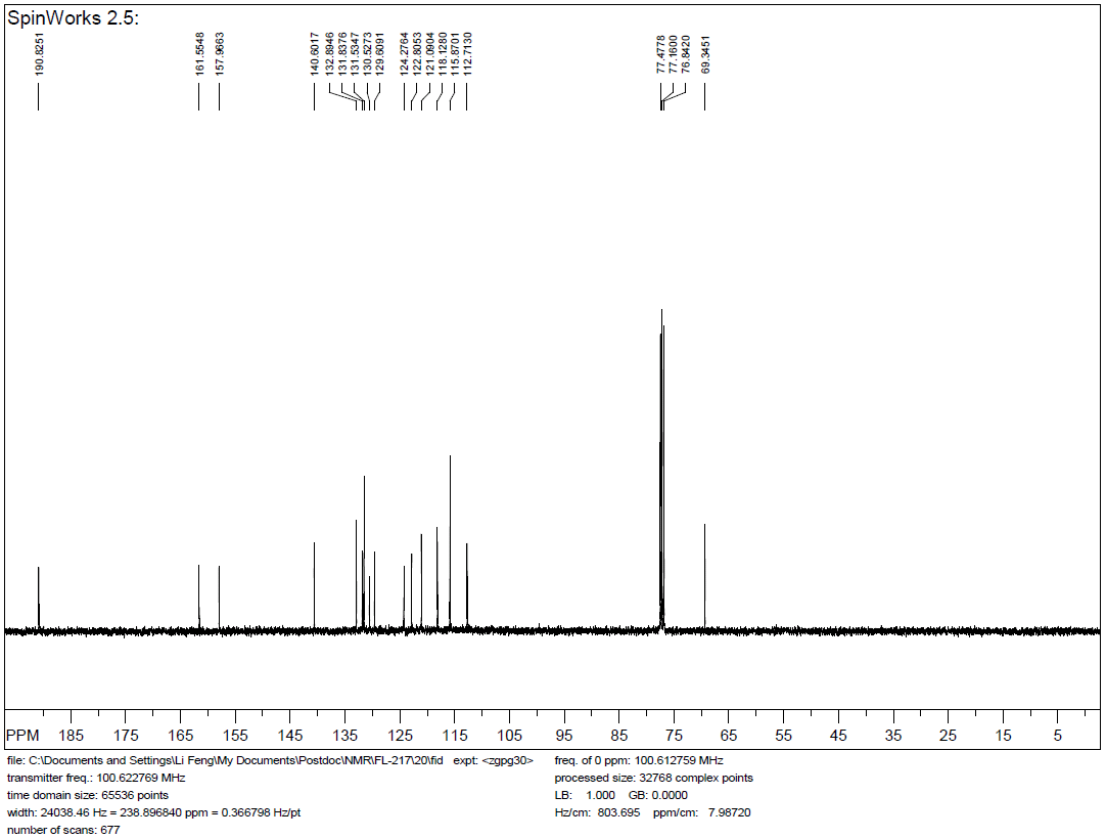
Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.619	181512	85313	1.335	2.029
2	6.932	13214180	4034852	97.216	95.977
3	8.209	196851	83802	1.448	1.993
Total		13592543	4203966	100.000	100.000

HRMS of **8e**


x10 5
-ESI Scan (0.271 min) Frag=70.0V Sun236_neg.d
311.0877
160.8411
265.1437
379.0705
491.1168
532.9044
635.1590
767.2013
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **8f**



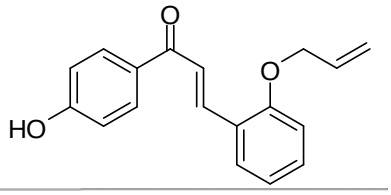


HPLC profile of **8f**

==== Shimadzu LCsolution Analysis Report ====

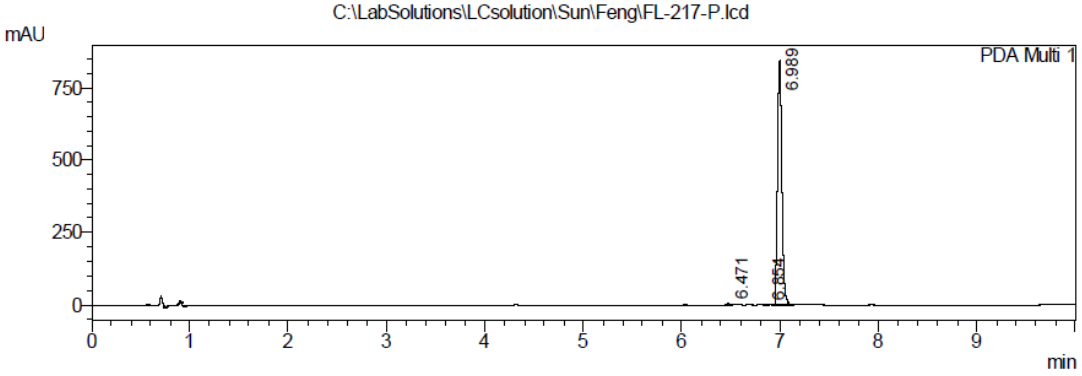
C:\LabSolutions\LCsolution\Sun\Feng\FL-217-P.lcd

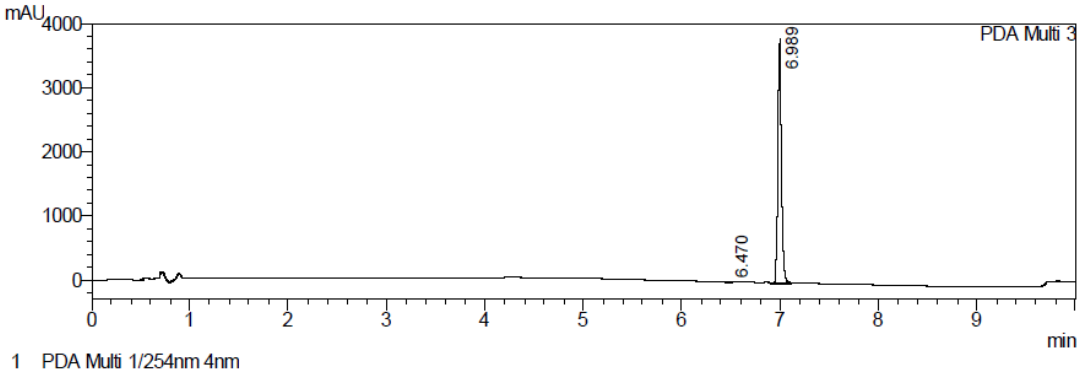
Sample Name	: FL-217-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 10 uL
Data File Name	: FL-217-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 4/23/2012 11:54:07 AM



<Chromatogram>

C:\LabSolutions\LCsolution\Sun\Feng\FL-217-P.lcd





1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

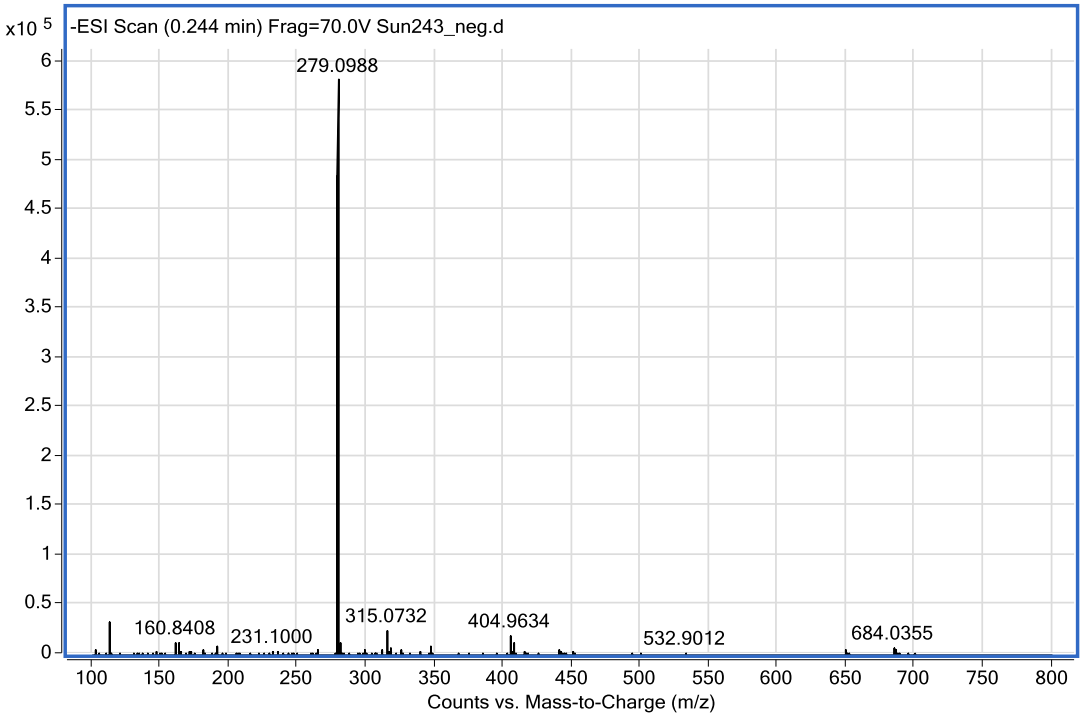
Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.471	5761	2977	0.247	0.353
2	6.854	3541	1929	0.152	0.229
3	6.989	2318329	838671	99.600	99.418
Total		2327630	843577	100.000	100.000

PeakTable

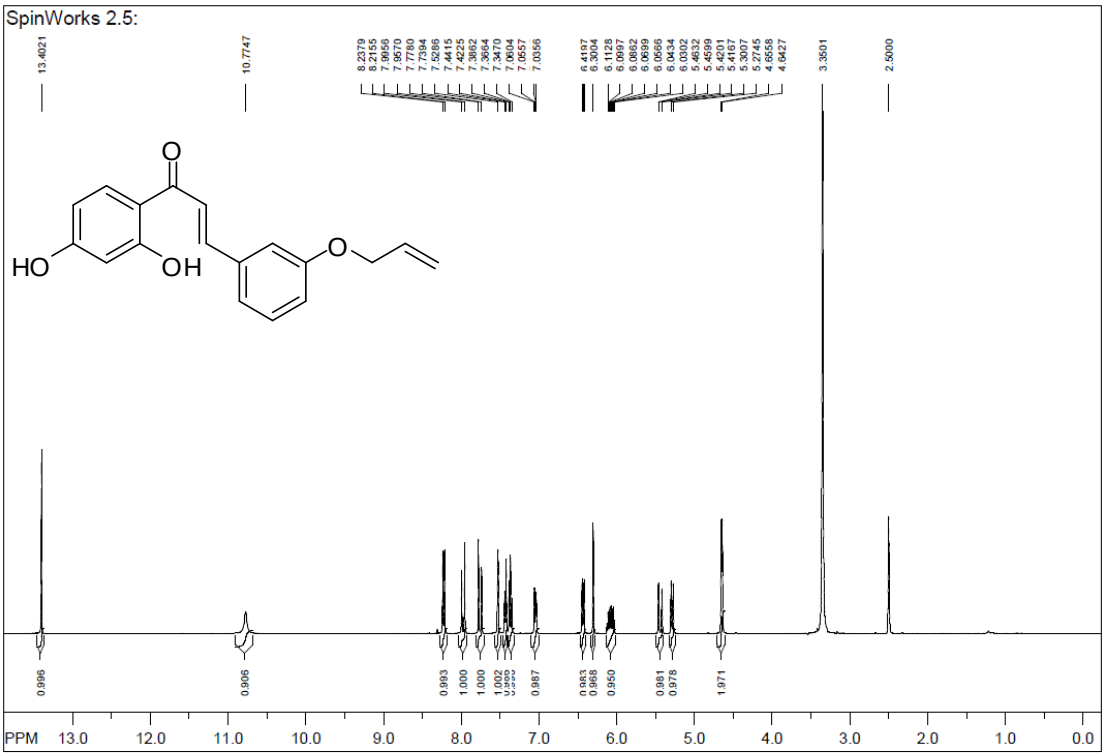
PDA Ch3 220nm 4nm

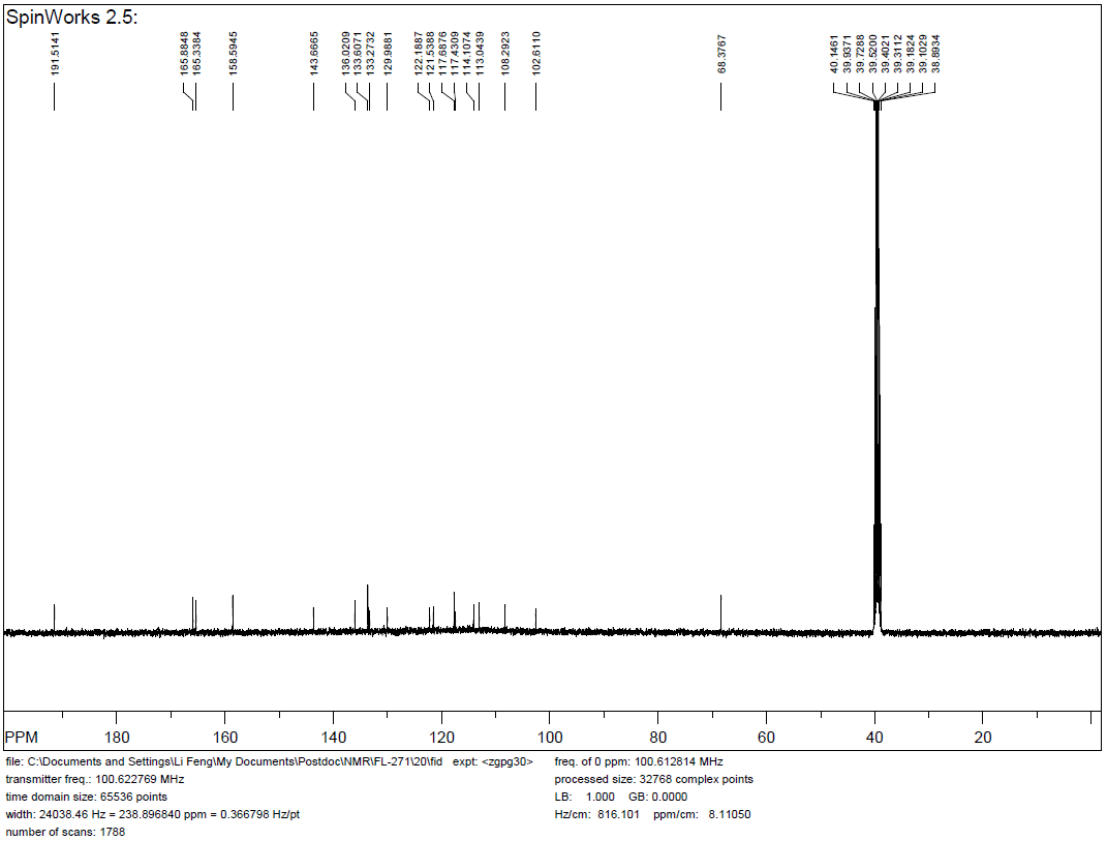
Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.470	16347	7261	0.197	0.190
2	6.989	8271827	3805815	99.803	99.810
Total		8288174	3813077	100.000	100.000

HRMS of **8f**


x10 5
-ESI Scan (0.244 min) Frag=70.0V Sun243_neg.d
279.0988
160.8408
231.1000
315.0732
404.9634
532.9012
684.0355
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **8g**



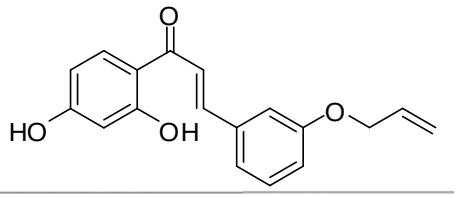


HPLC profile of **8g**

==== Shimadzu LCsolution Analysis Report ====

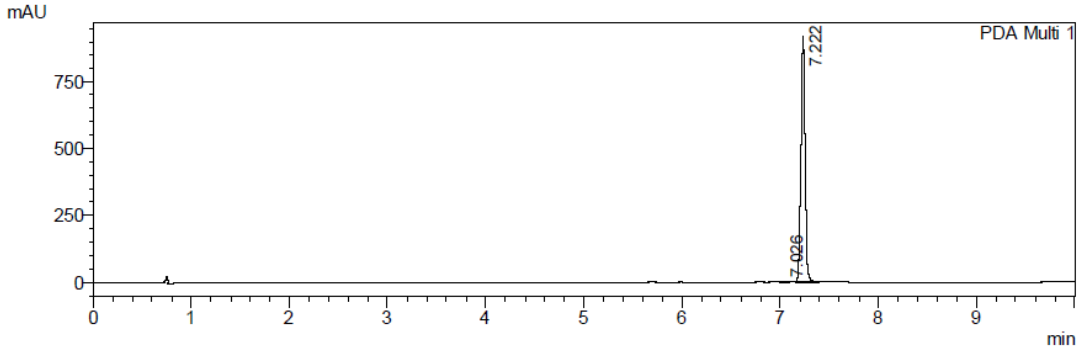
C:\LabSolutions\LCsolution\Sun\Feng\FL-271-P.lcd

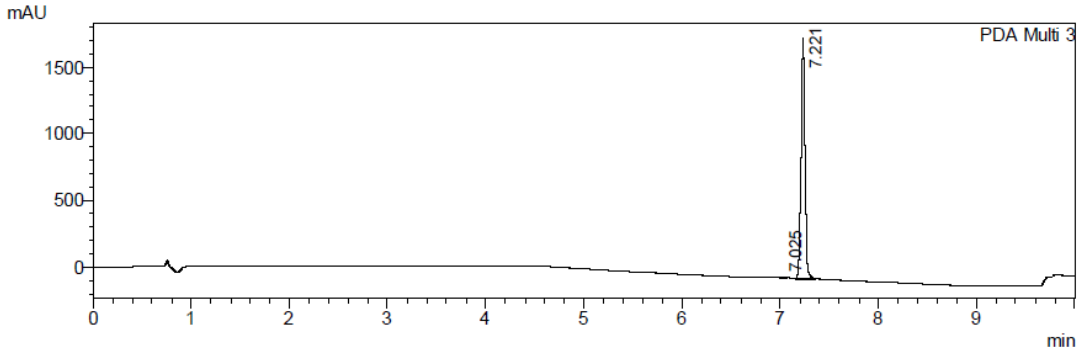
Sample Name	: FL-271-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 12 uL
Data File Name	: FL-271-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 6/28/2012 4:36:48 PM



<Chromatogram>

C:\LabSolutions\LCsolution\Sun\Feng\FL-271-P.lcd





1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

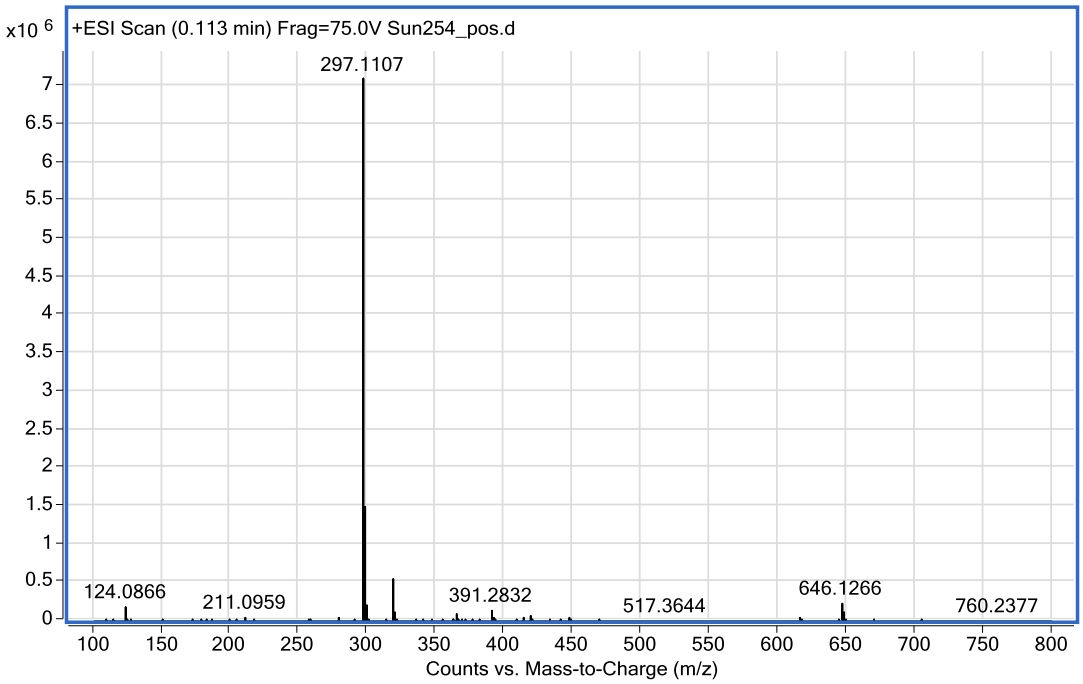
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.026	7865	3240	0.309	0.357
2	7.222	2535579	904548	99.691	99.643
Total		2543444	907788	100.000	100.000

PeakTable

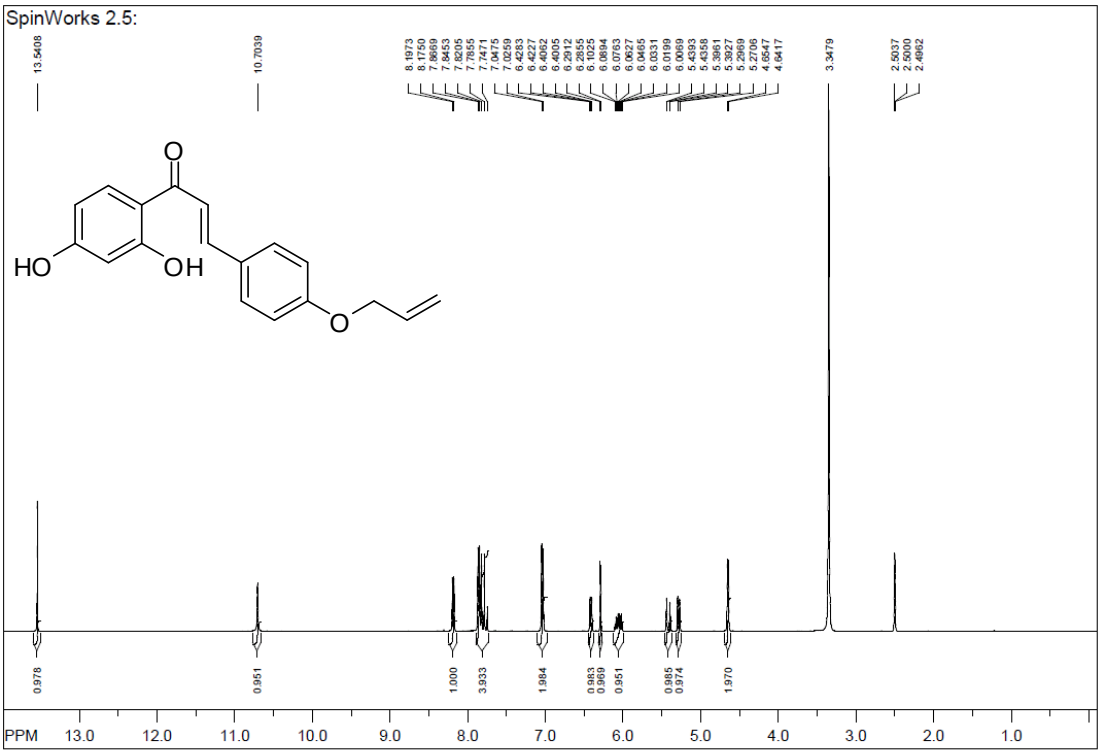
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.025	18998	9982	0.404	0.551
2	7.221	4684871	1800059	99.596	99.449
Total		4703869	1810040	100.000	100.000

HRMS of **8g**


x10 6
+ESI Scan (0.113 min) Frag=75.0V Sun254_pos.d
297.1107
124.0866
211.0959
391.2832
517.3644
646.1266
760.2377
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **8h**



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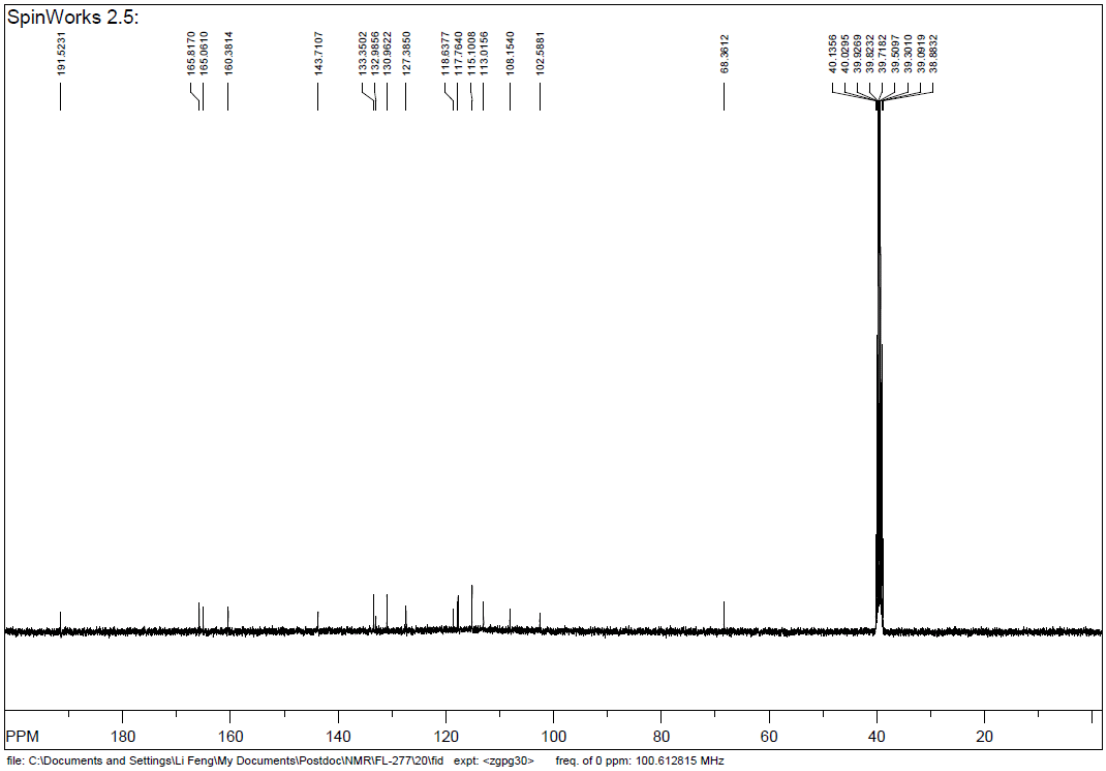
transmitter freq.: 400.131600 MHz
time domain size: 65536 points
width: 8012.82 Hz = 20.025463 ppm = 0.122266 Hz/pt
number of scans: 6

freq. of 0 ppm: 400.130003 MHz
processed size: 32768 complex points
LB: 0.300 GB: 0.0000
Hz/cm: 225.393 ppm/cm: 0.56330



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-277\20\fid expt: <zgpg30>
transmitter freq.: 100.622769 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.896840 ppm = 0.366798 Hz/pt
number of scans: 1141

freq. of 0 ppm: 100.612815 MHz
processed size: 32768 complex points
LB: 1.000 GB: 0.0000
Hz/cm: 820.237 ppm/cm: 8.15161

HPLC profile of **8h**

==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\Feng\FL-277-P.lcd

Sample Name	: FL-277-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 20 uL
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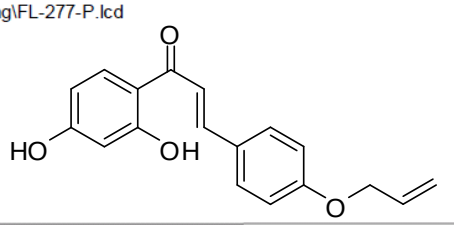
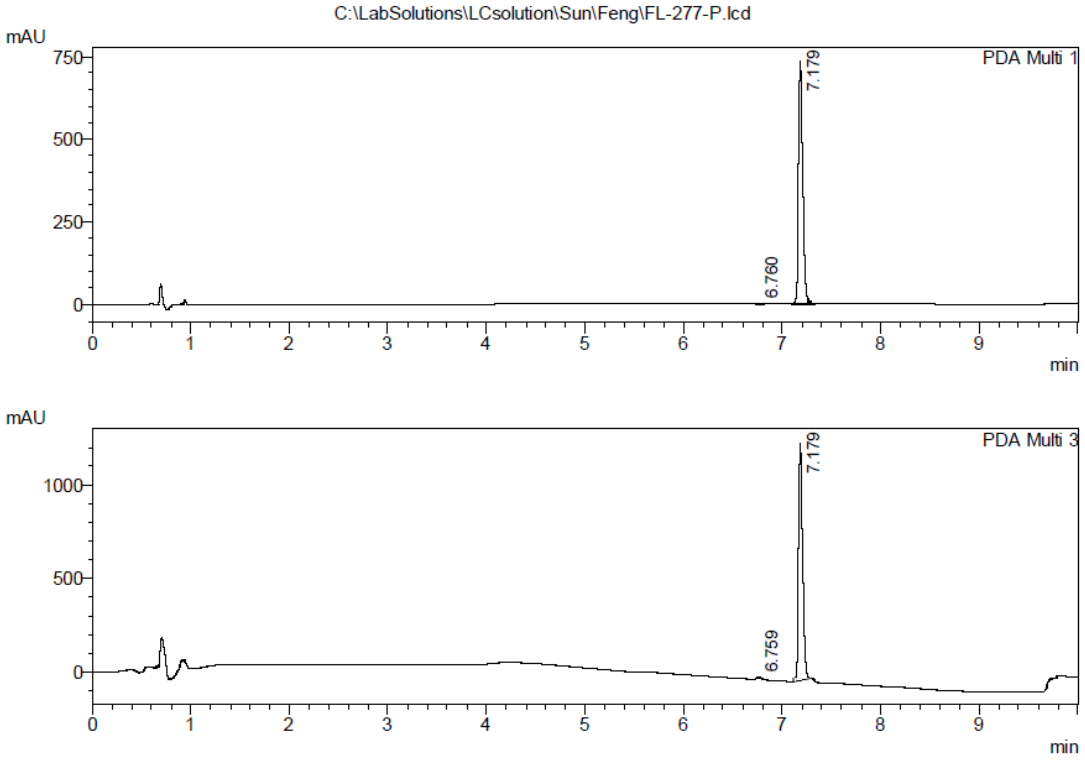
Method File Name	: SDQ gradient.lcm
Batch File Name	:
Data Acquired	: 7/5/2012 1:33:34 PM



<Chromatogram>



1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

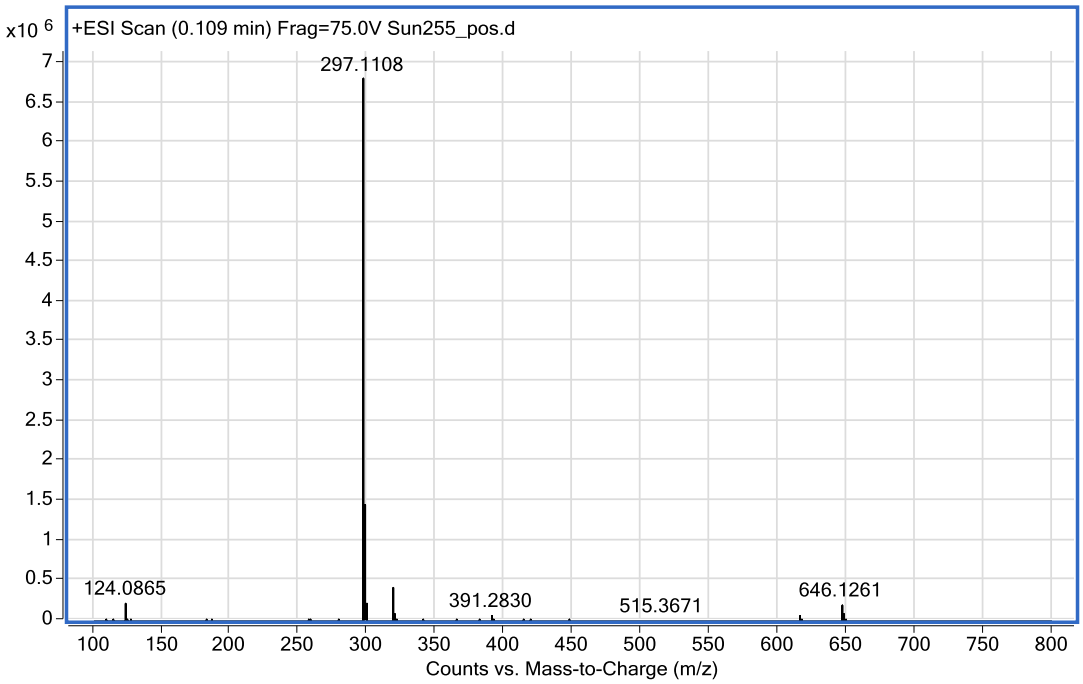
Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.760	5369	2472	0.246	0.338
2	7.179	2178745	729324	99.754	99.662
Total		2184114	731797	100.000	100.000

PeakTable

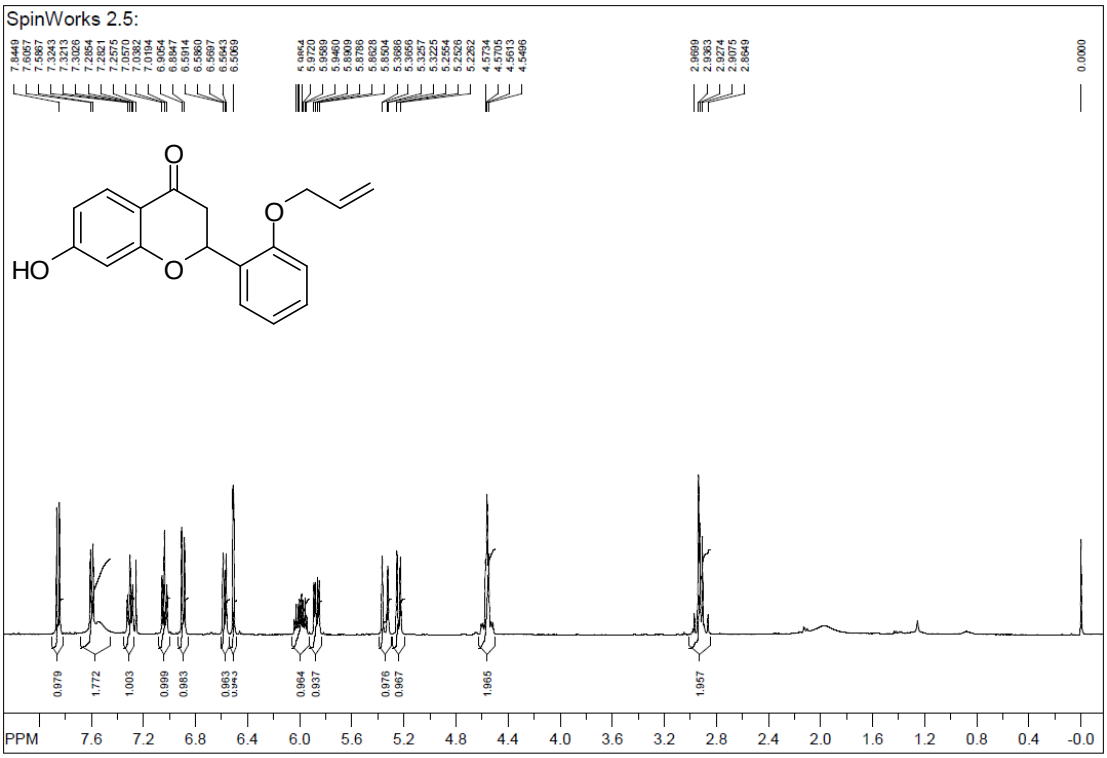
PDA Ch3 220nm 4nm

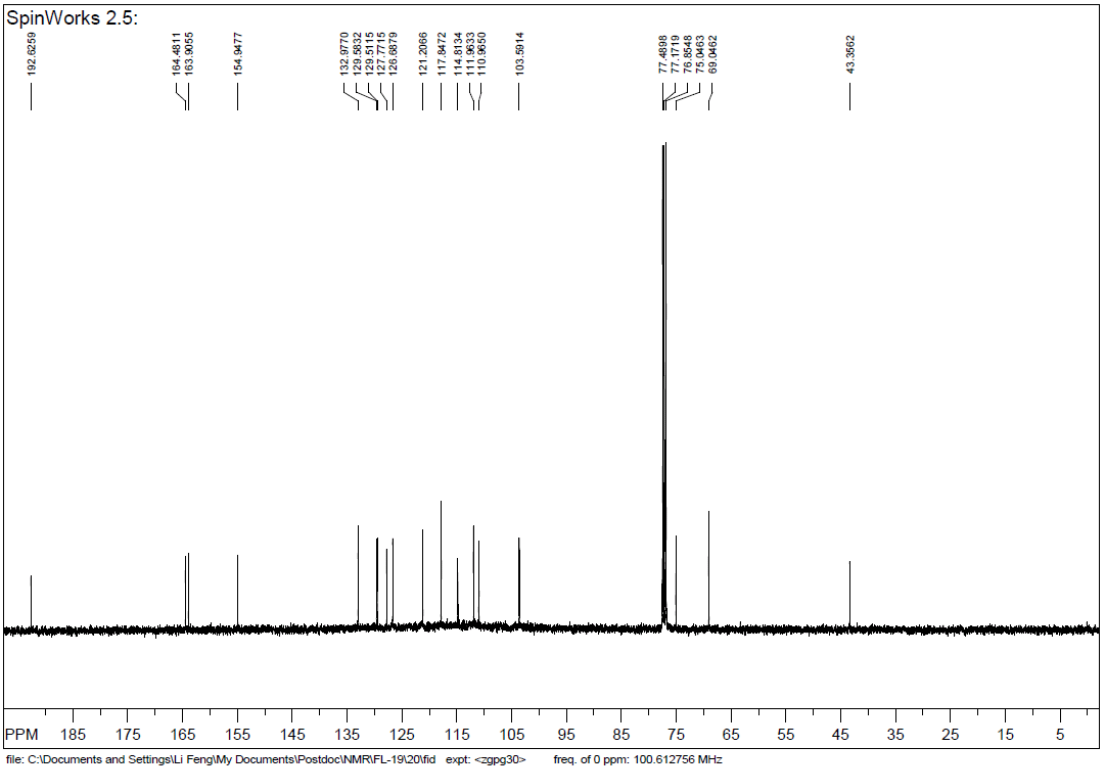
Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.759	13216	7124	0.368	0.561
2	7.179	3582399	1262708	99.632	99.439
Total		3595615	1269832	100.000	100.000

HRMS of **8h**


x10 6
+ESI Scan (0.109 min) Frag=75.0V Sun255_pos.d
297.1108
124.0865
391.2830
515.3671
646.1261
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **8i**



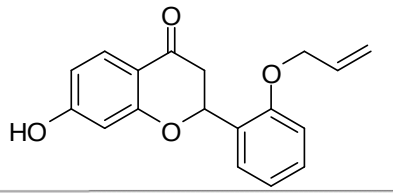


HPLC profile of **8i**

==== Shimadzu LCsolution Analysis Report ====

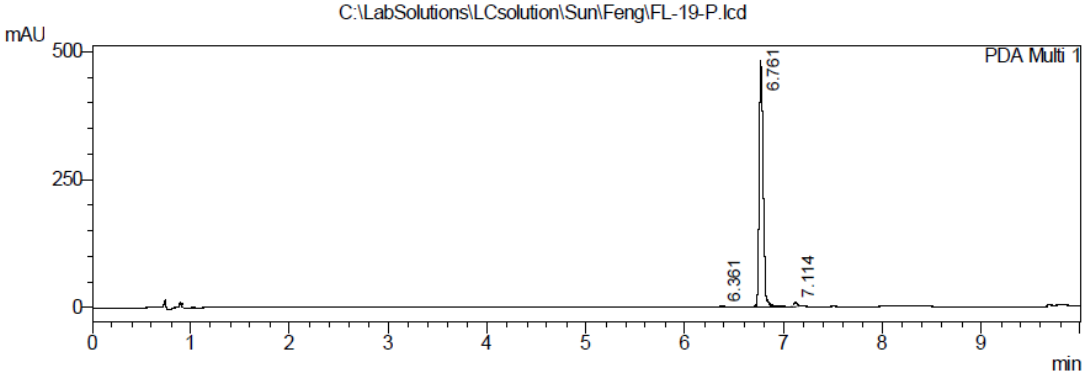
C:\LabSolutions\LCsolution\Sun\Feng\FL-19-P.lcd

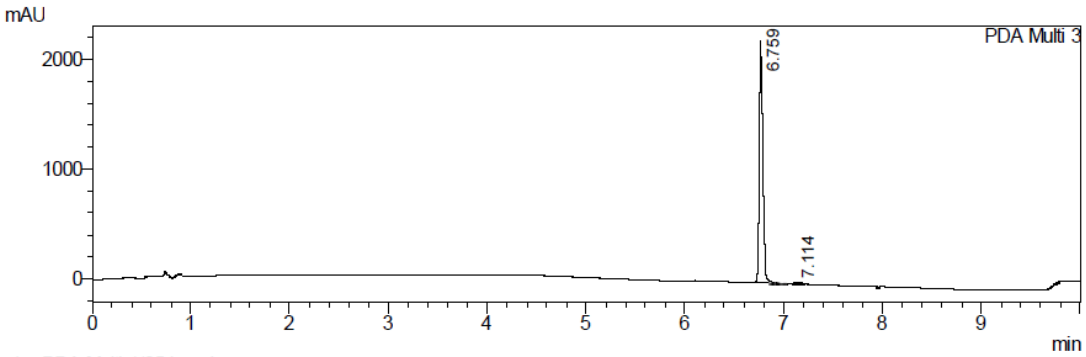
Sample Name	: FL-19-P
Tray#	: 1
Vail #	: 92
Injection Volume	: 5 uL
Data File Name	: FL-19-P.lcd
Method File Name	: SDQ gradient.lcm
Batch File Name	: Batch 1.lcb
Data Acquired	: 12/2/2011 11:30:13 AM



<Chromatogram>

C:\LabSolutions\LCsolution\Sun\Feng\FL-19-P.lcd





1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

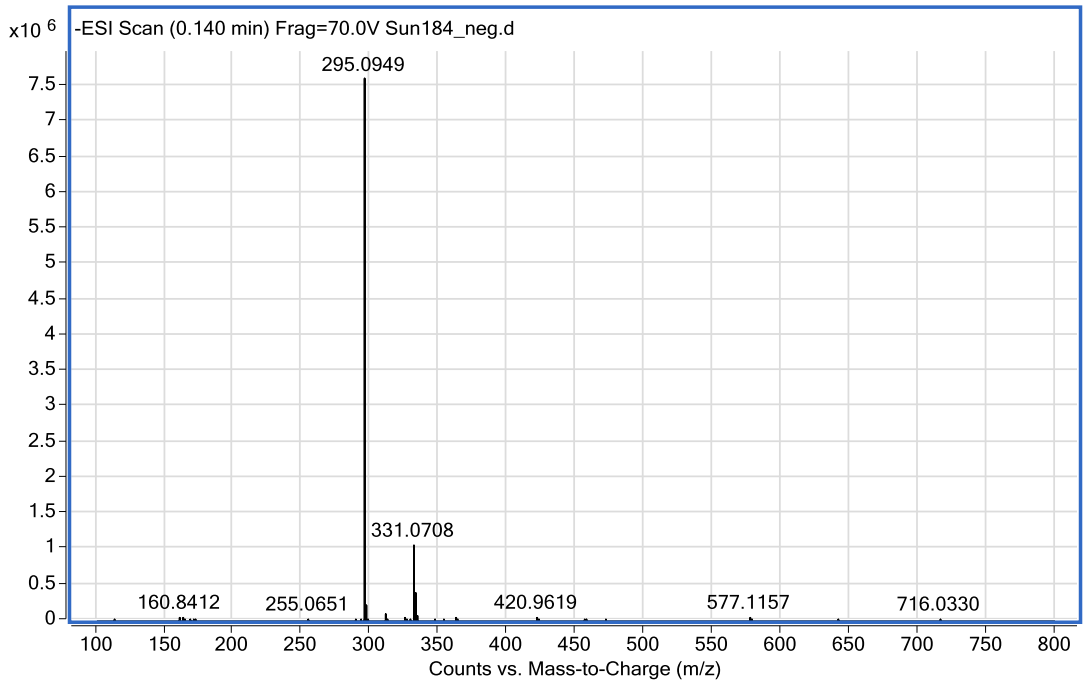
Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.361	4970	2057	0.397	0.429
2	6.761	1228161	469041	97.986	97.920
3	7.114	20276	7907	1.618	1.651
Total		1253407	479005	100.000	100.000

PeakTable

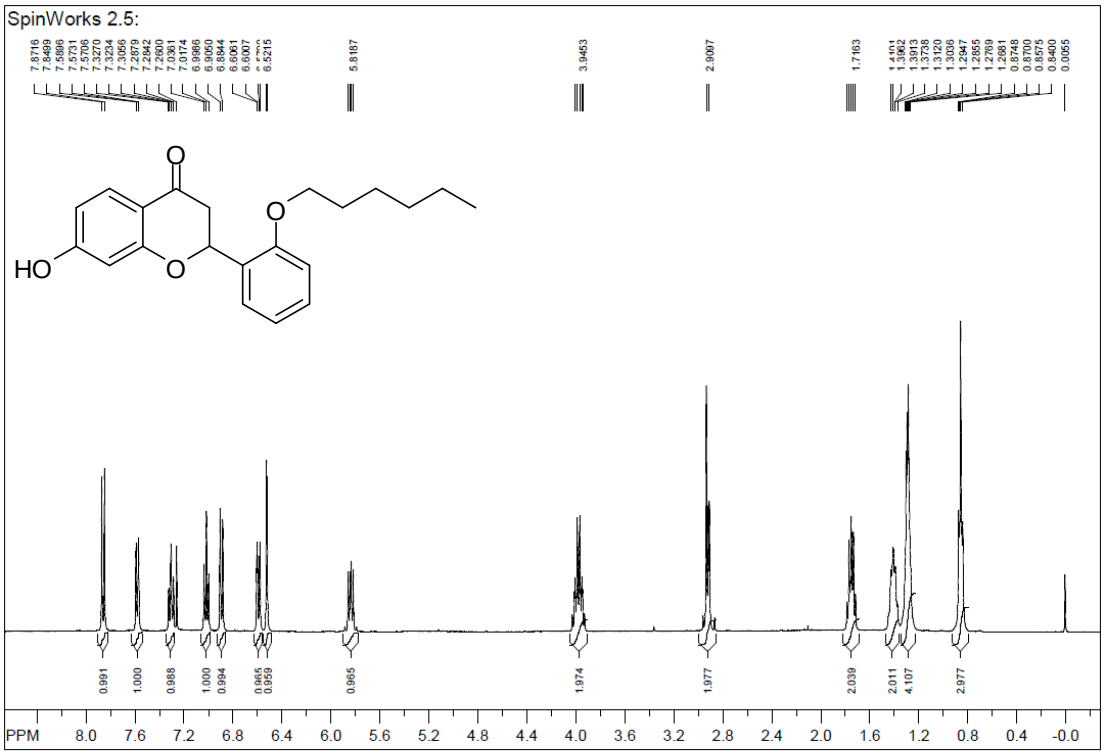
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.759	5006876	2212550	98.950	99.412
2	7.114	53148	13086	1.050	0.588
Total		5060025	2225636	100.000	100.000

HRMS of **8i**


-ESI Scan (0.140 min) Frag=70.0V Sun184_neg.d
x10 6
295.0949
331.0708
160.8412
255.0651
420.9619
577.1157
716.0330
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **8j**



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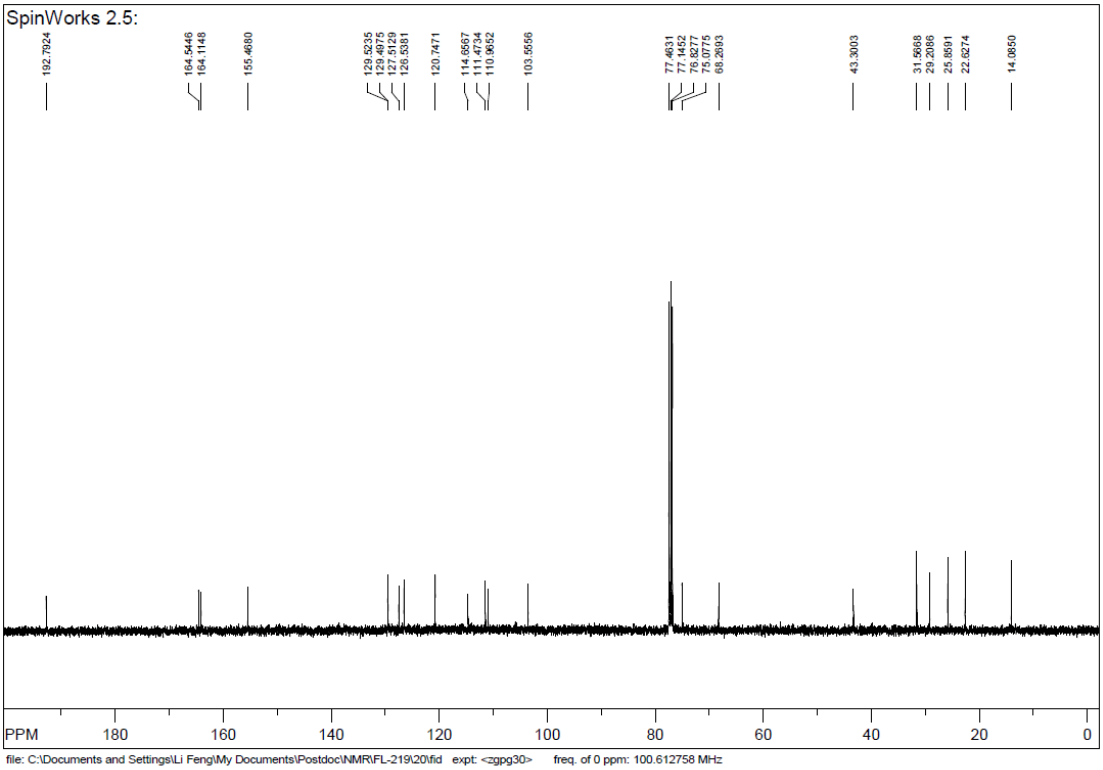
time domain size: 65536 points
width: 8012.82 Hz = 20.025463 ppm = 0.122266 Hz/pt
number of scans: 3

freq. of 0 ppm: 400.130009 MHz
processed size: 32768 complex points
LB: 0.300 GB: 0.0000
Hz/cm: 143.139 ppm/cm: 0.35773



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-219\20\fid expt: <zgpg30>
transmitter freq.: 100.622769 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.896840 ppm = 0.366798 Hz/pt
number of scans: 555

freq. of 0 ppm: 100.612758 MHz
processed size: 32768 complex points
LB: 1.000 GB: 0.0000
Hz/cm: 816.101 ppm/cm: 8.11050

HPLC profile of **8j**

==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\Feng\FL-219-P.lcd

Sample Name	: FL-219-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 10 uL
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Method File Name	: SDQ gradient.lcm
Batch File Name	:
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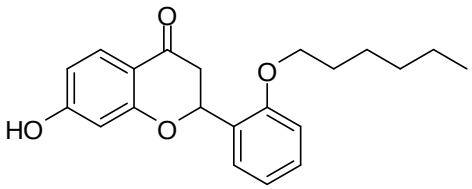

<Chromatogram>

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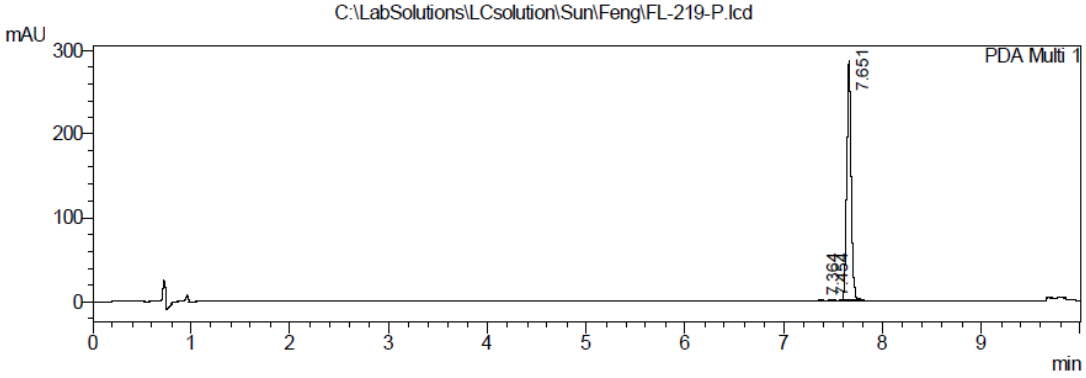

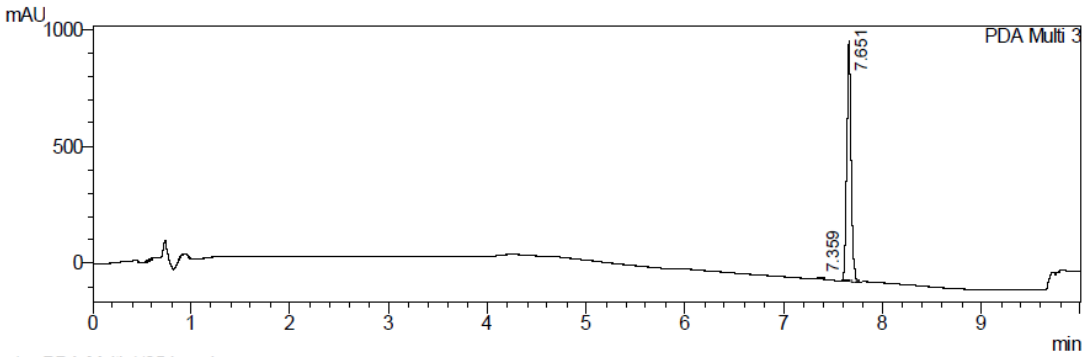

1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

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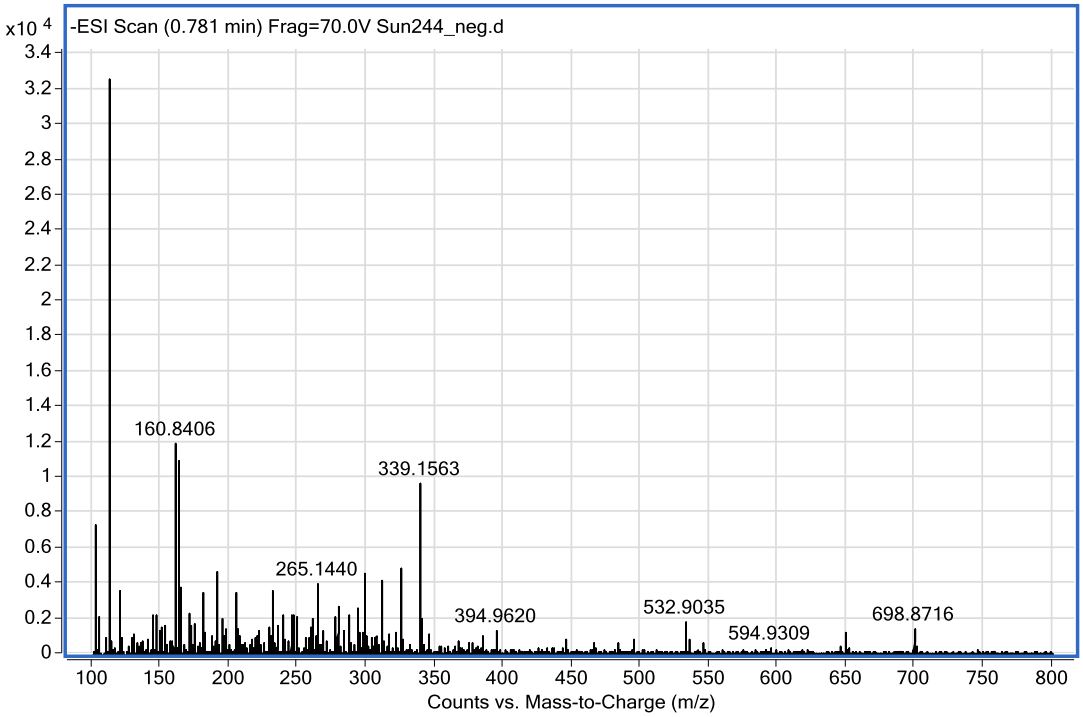
1	7.364	277	181	0.035	0.064
2	7.454	157	91	0.020	0.032
3	7.651	801228	284171	99.946	99.904
Total		801661	284443	100.000	100.000

PeakTable

PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.359	11768	5504	0.414	0.534
2	7.651	2830467	1024726	99.586	99.466
Total		2842235	1030230	100.000	100.000

HRMS of **8j**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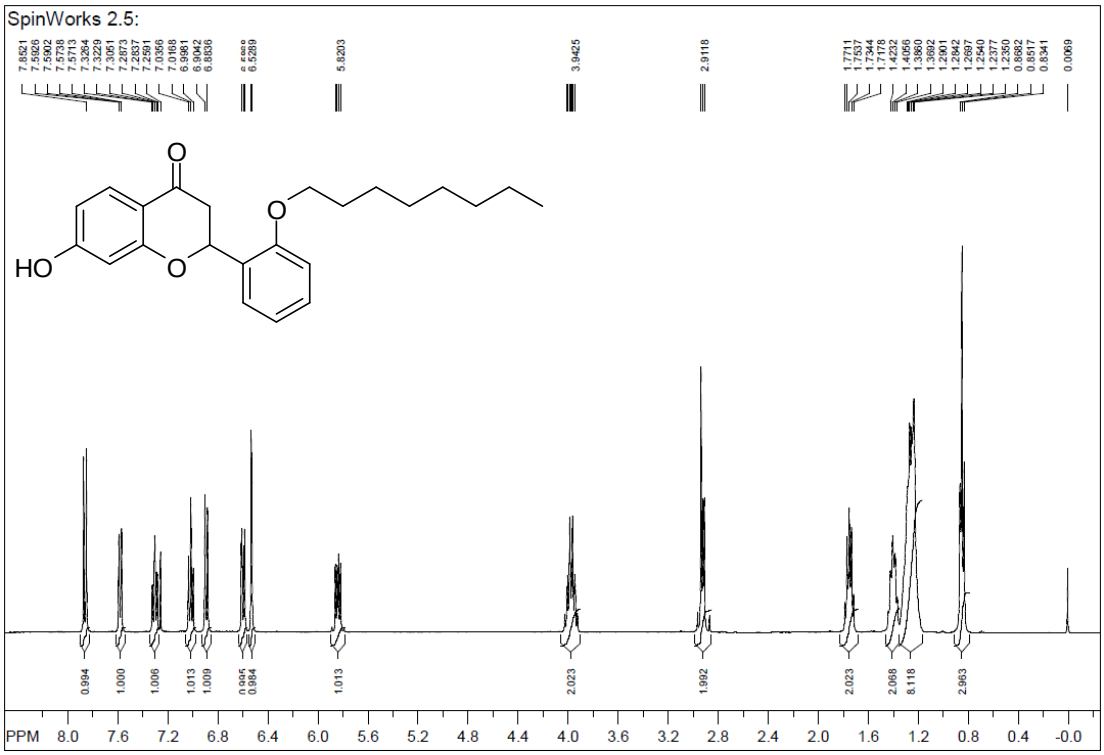
x10 4
160.8406
339.1563
265.1440
394.9620
532.9035
594.9309
698.8716
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **8k**



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number of scans: 4

freq. of 0 ppm: 400.130009 MHz
processed size: 32768 complex points
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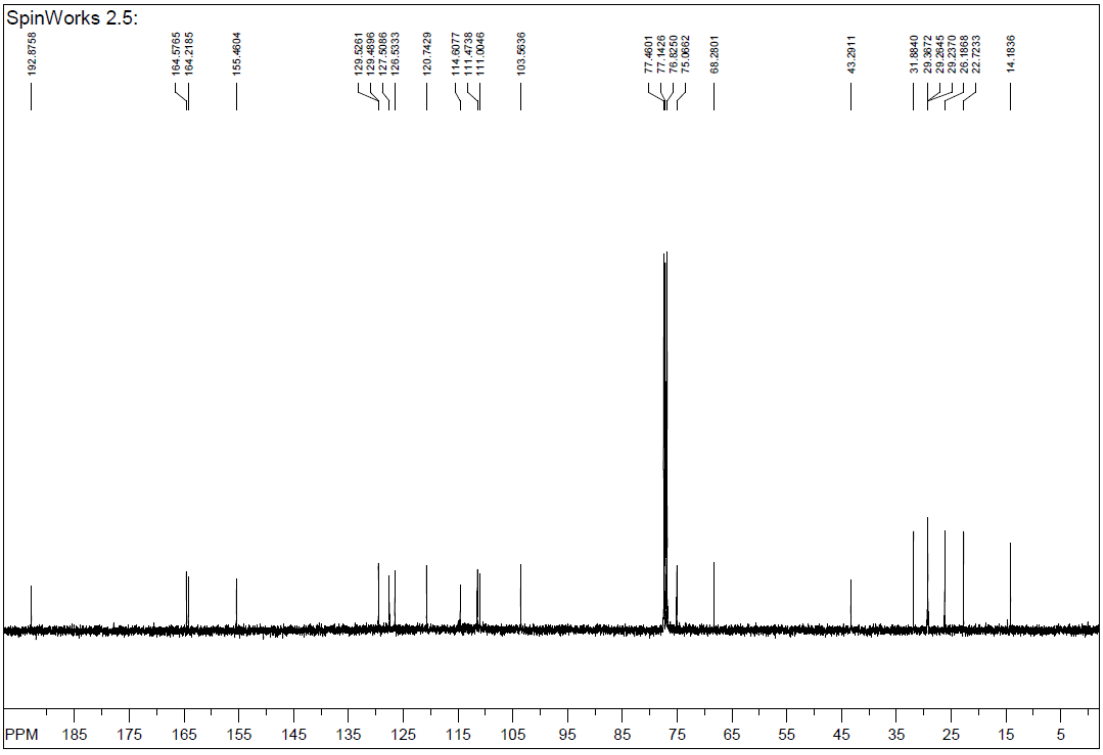
Hz/cm: 140.153 ppm/cm: 0.35027



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-213\20\fid expt: <zgpg30>
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time domain size: 65536 points
width: 24038.46 Hz = 238.896840 ppm = 0.366798 Hz/pt
number of scans: 647

freq. of 0 ppm: 100.612758 MHz
processed size: 32768 complex points
LB: 1.000 GB: 0.0000
Hz/cm: 804.384 ppm/cm: 7.99405

HPLC profile of **8k**

==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\Feng\FL-213-P.lcd

Sample Name	: FL-213-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 10 uL
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Method File Name	: SDQ gradient.lcm
Batch File Name	:
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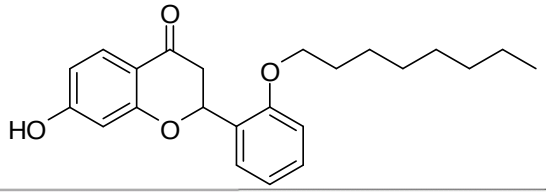

<Chromatogram>

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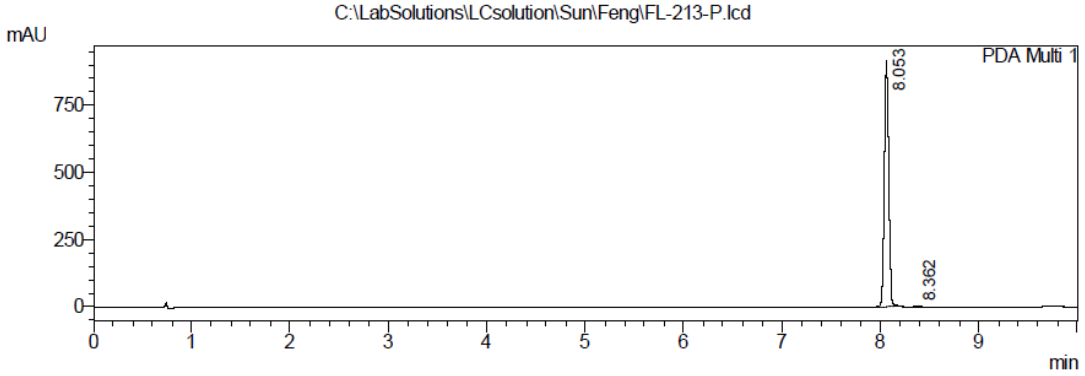
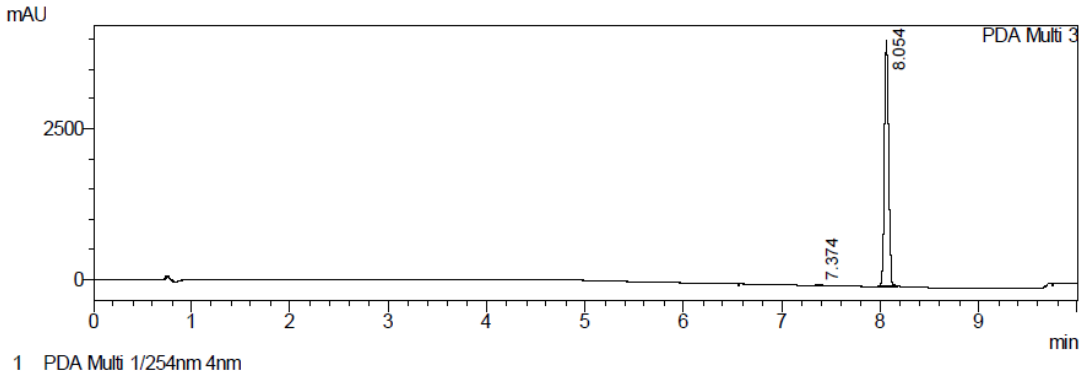




1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

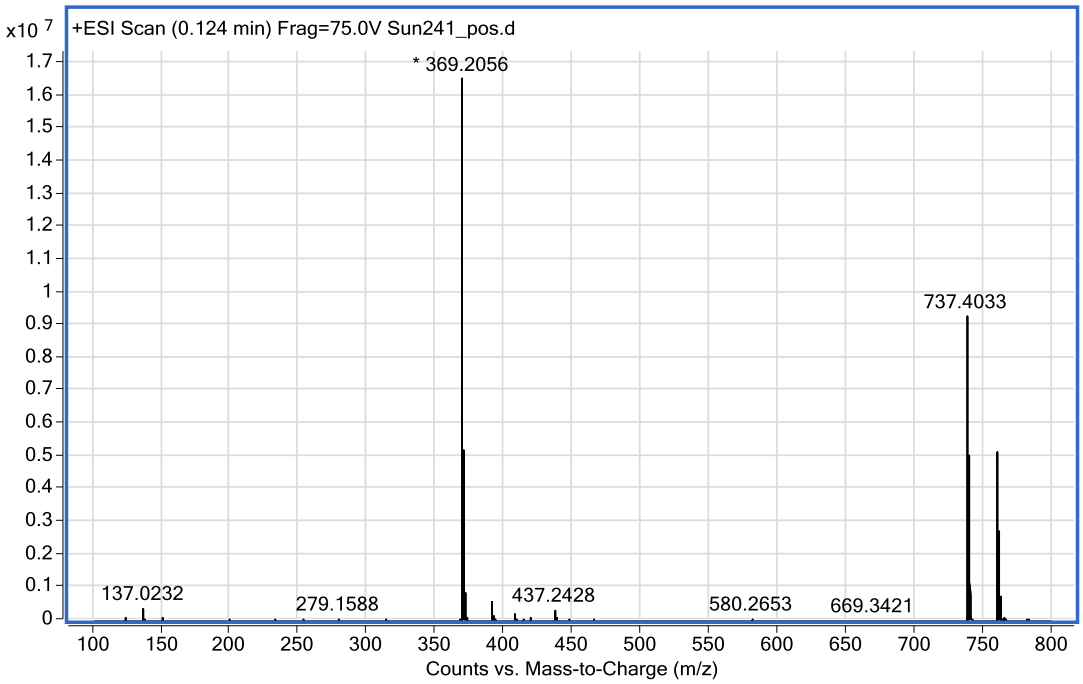
Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.053	2585666	912445	99.902	99.874
2	8.362	2537	1155	0.098	0.126
Total		2588203	913600	100.000	100.000

PeakTable

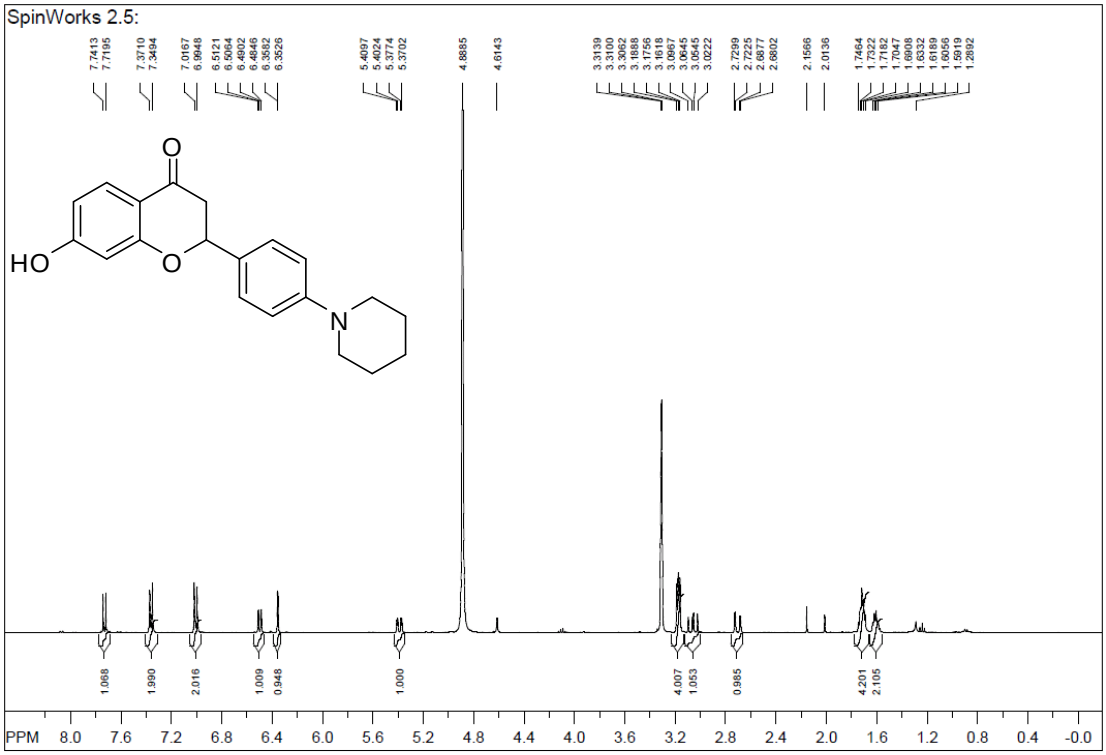
PDA Ch3 220nm 4nm

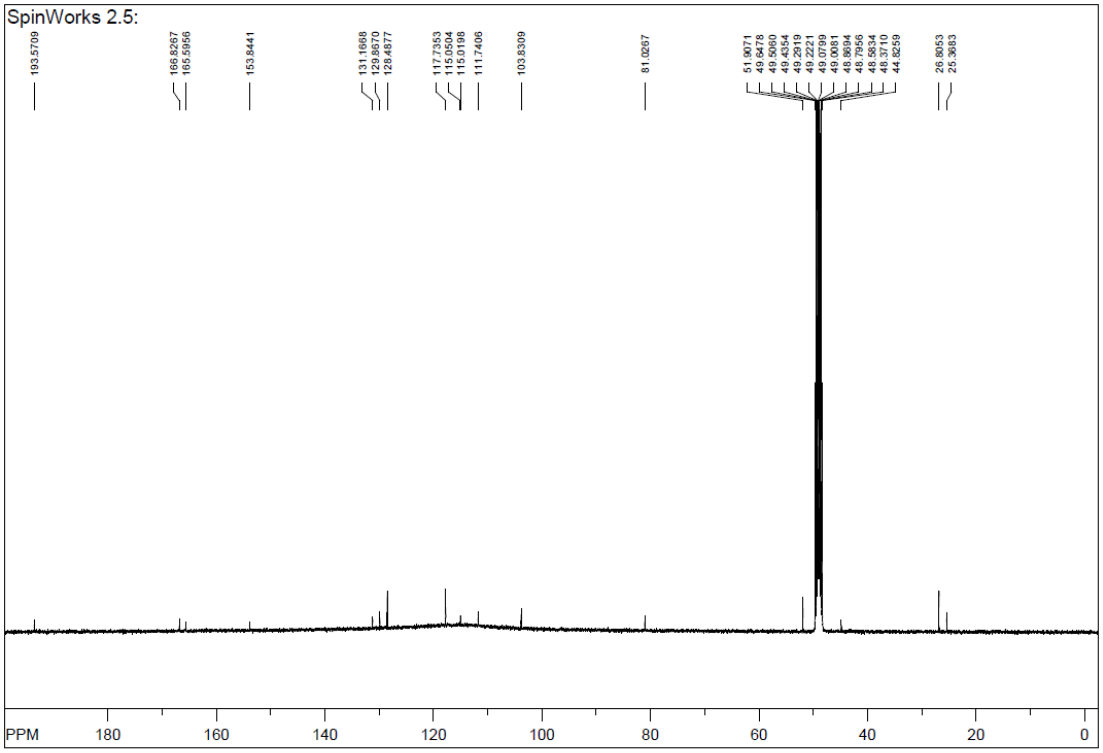
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.374	13629	7606	0.124	0.186
2	8.054	10948403	4082189	99.876	99.814
Total		10962032	4089795	100.000	100.000

HRMS of **8k**


x10 7
+ESI Scan (0.124 min) Frag=75.0V Sun241_pos.d
* 369.2056
737.4033
137.0232
279.1588
437.2428
580.2653
669.3421
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **8l**





HPLC profile of **8l**

==== Shimadzu LCsolution Analysis Report ====

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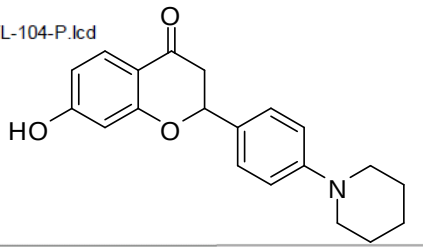

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Tray#	: 1
Vail #	: 91
Injection Volume	: 12 uL
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Method File Name	: SDQ gradient.lcm
Batch File Name	:
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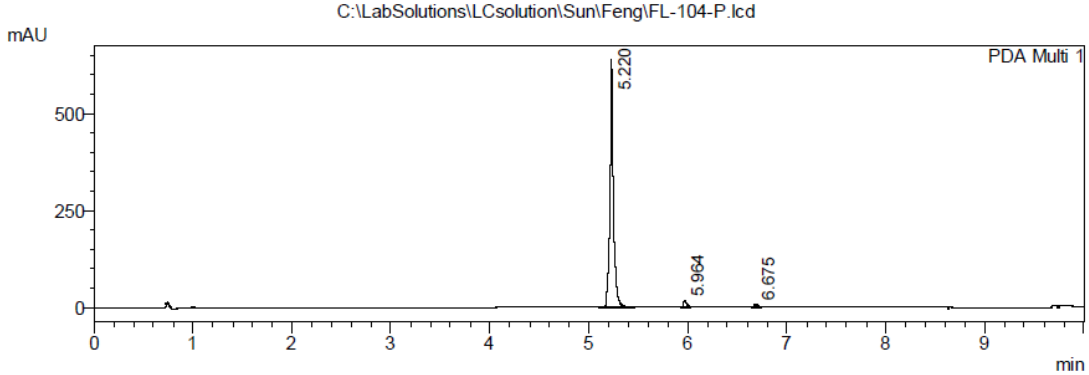
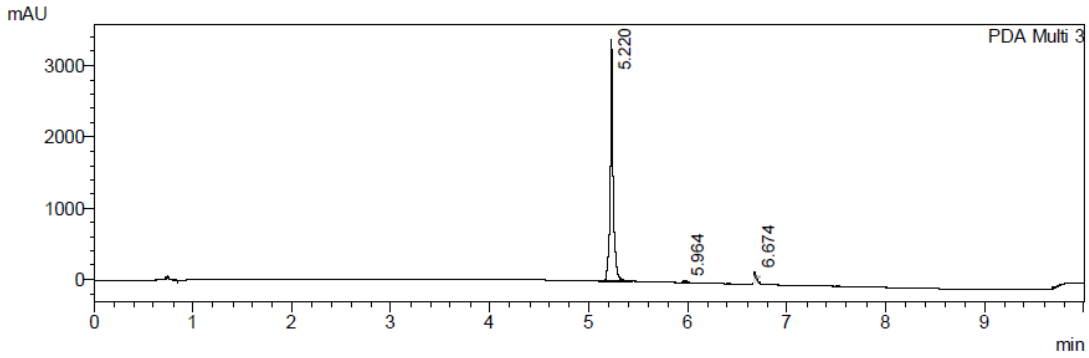




1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

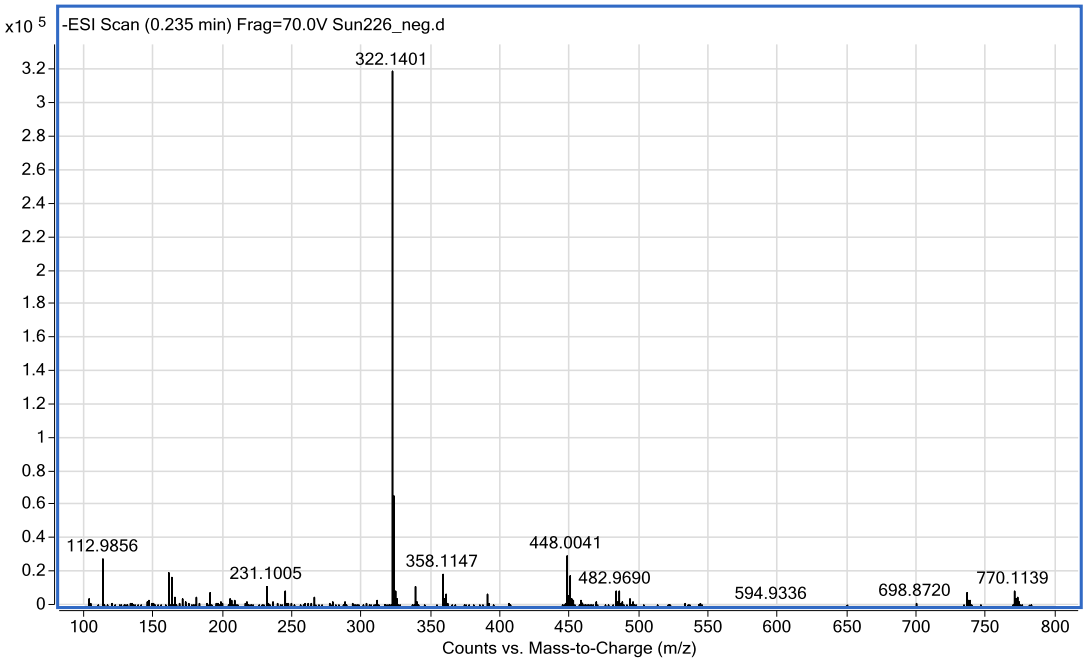
Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.220	1817452	636873	97.357	96.712
2	5.964	32317	14413	1.731	2.189
3	6.675	17026	7242	0.912	1.100
Total		1866796	658528	100.000	100.000

PeakTable

PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.220	8360664	3379359	98.652	97.696
2	5.964	19959	13573	0.236	0.392
3	6.674	94314	66114	1.113	1.911
Total		8474937	3459047	100.000	100.000

HRMS of **8l**


x10 5
-ESI Scan (0.235 min) Frag=70.0V Sun226_neg.d
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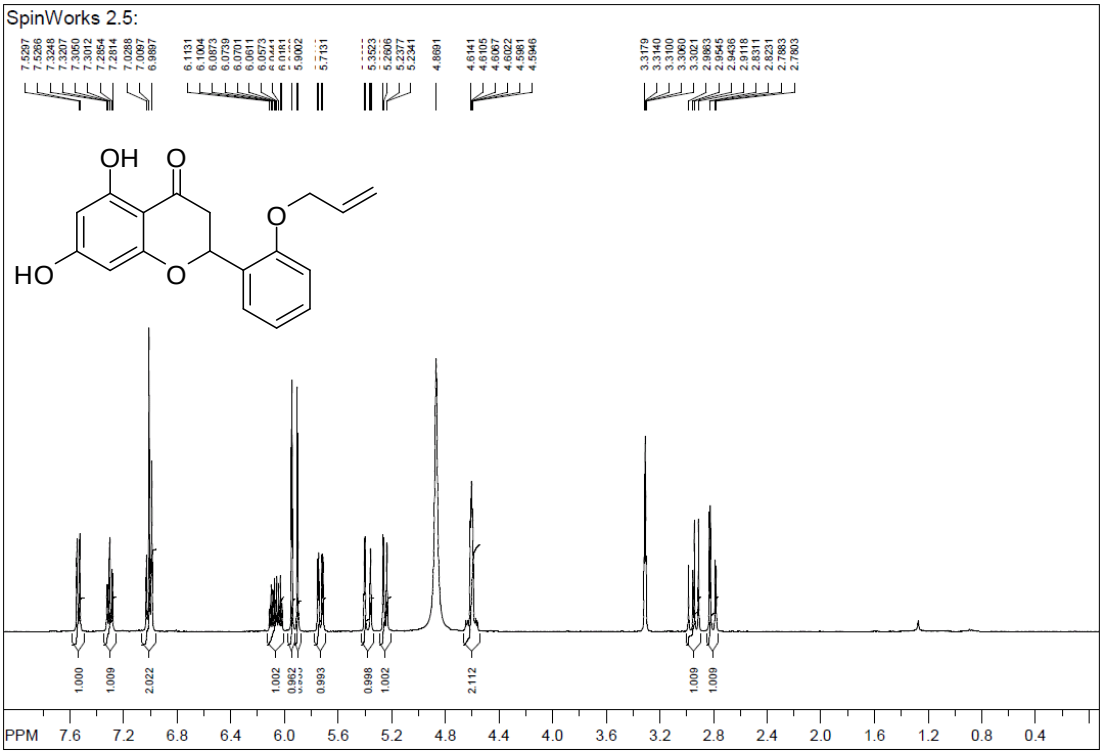
112.9856
231.1005
358.1147
448.0041
482.9690
594.9336
698.8720
770.1139
Counts vs. Mass-to-Charge (m/z)

^{1}H and ^{13}C NMR spectra of **8m**



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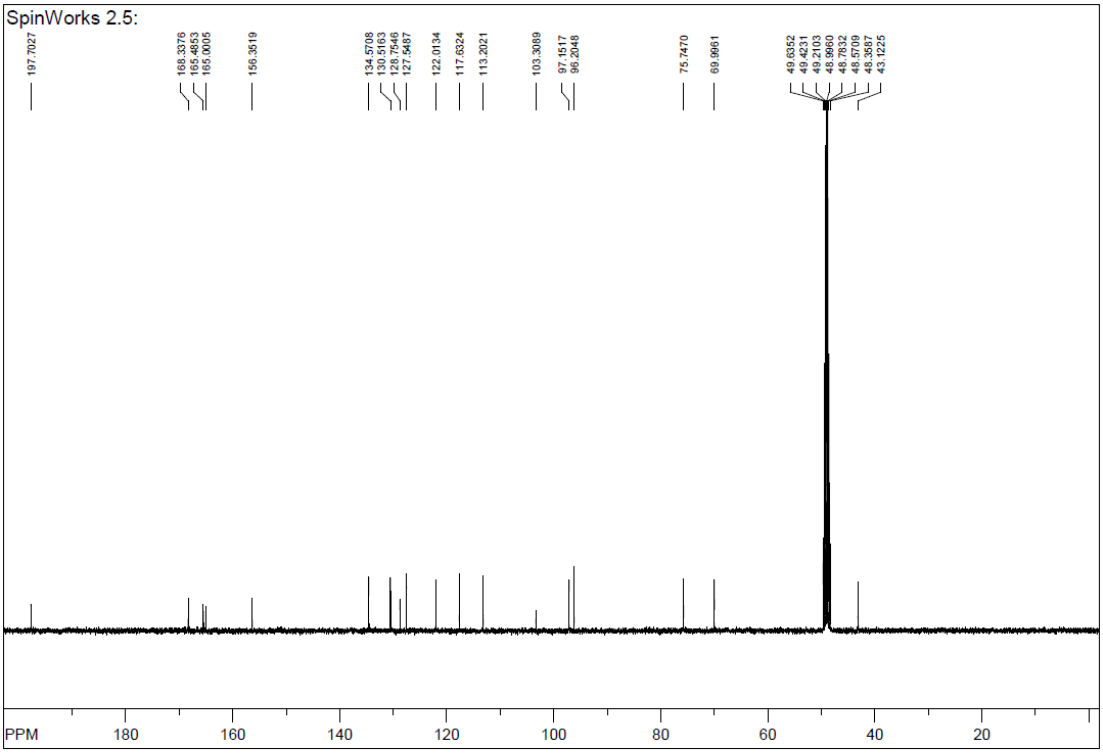
time domain size: 65536 points
width: 8012.82 Hz = 20.025463 ppm = 0.122266 Hz/pt
number of scans: 8

freq. of 0 ppm: 400.130007 MHz
processed size: 32768 complex points
LB: 0.300 GB: 0.0000
Hz/cm: 130.732 ppm/cm: 0.32672



file: C:\Documents and Settings\Li Feng\My Documents\Postdoc\NMR\FL-194\20\fid expt: <zgpg30>
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time domain size: 65536 points
width: 24038.46 Hz = 238.896840 ppm = 0.366798 Hz/pt
number of scans: 2836

freq. of 0 ppm: 100.612628 MHz
processed size: 32768 complex points
LB: 1.000 GB: 0.0000
Hz/cm: 823.683 ppm/cm: 8.18586

HPLC profile of **8m**

==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\Feng\FL-194-P.lcd

Sample Name	: FL-194-P
Tray#	: 1
Vail #	: 91
Injection Volume	: 15 uL
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Method File Name	: SDQ gradient.lcm
Batch File Name	:
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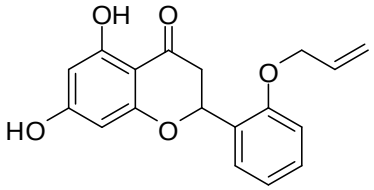

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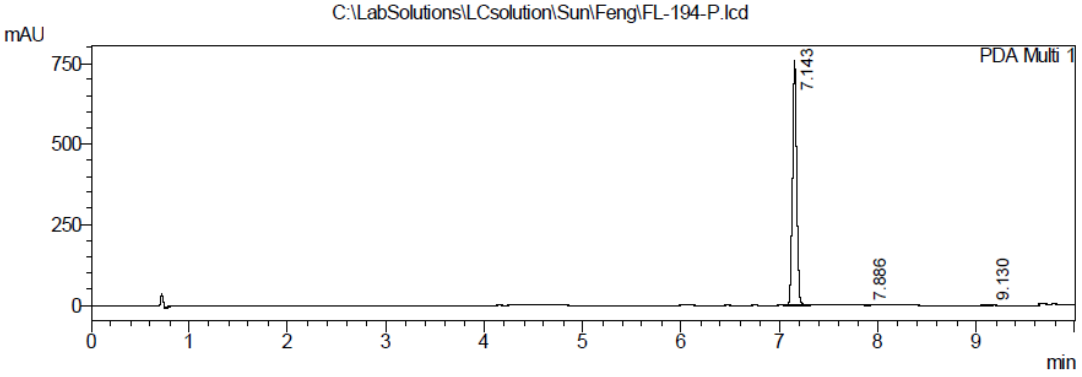
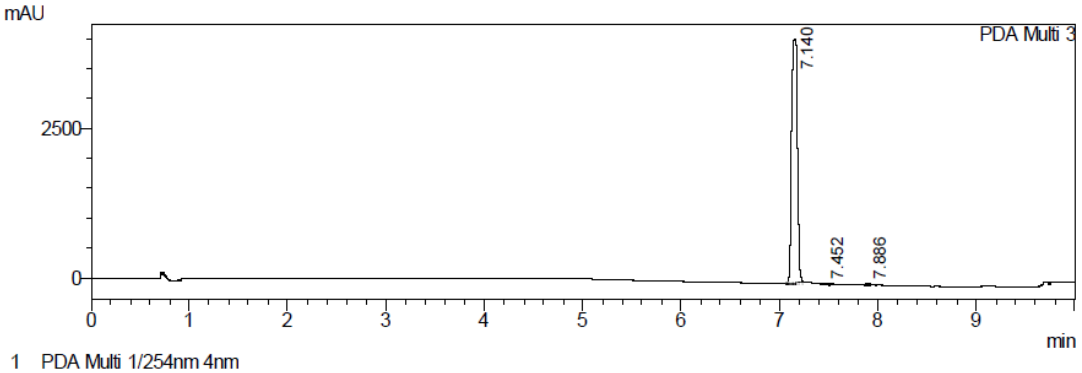




1 PDA Multi 1/254nm 4nm
2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

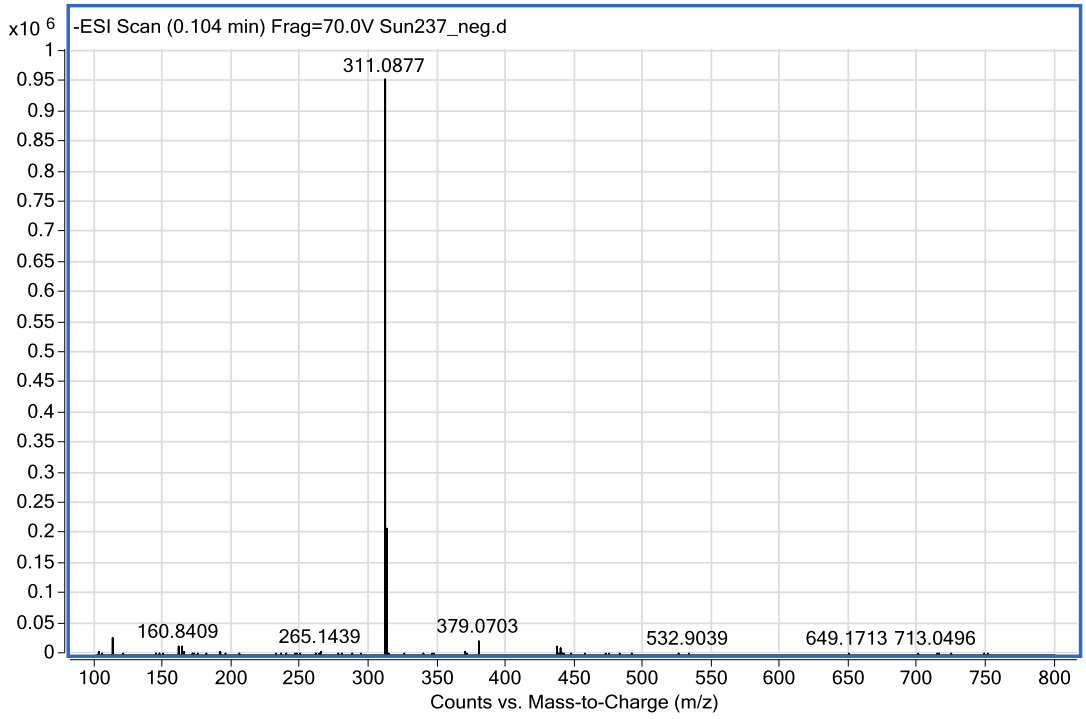
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.143	2092674	739887	99.815	99.723
2	7.886	2882	1525	0.137	0.206
3	9.130	1006	527	0.048	0.071
Total		2096561	741940	100.000	100.000

PeakTable

PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.140	15611265	4073885	99.640	99.307
2	7.452	14910	7418	0.095	0.181
3	7.886	41434	21009	0.264	0.512
Total		15667609	4102312	100.000	100.000

HRMS of **8m**


-ESI Scan (0.104 min) Frag=70.0V Sun237_neg.d
x10 6
311.0877
160.8409
265.1439
379.0703
532.9039
649.1713 713.0496
Counts vs. Mass-to-Charge (m/z)

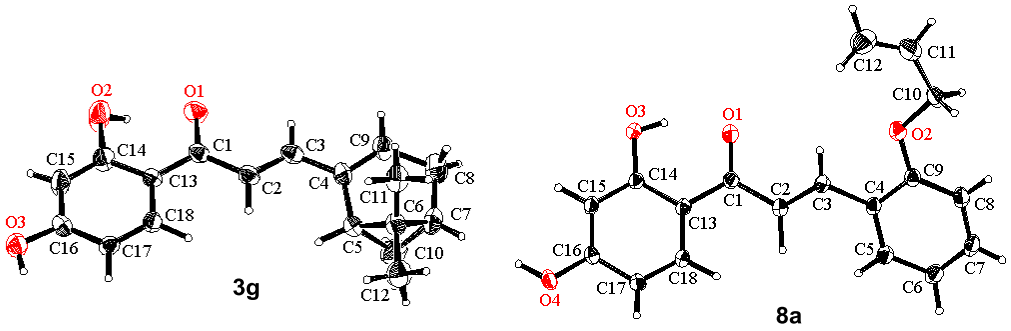
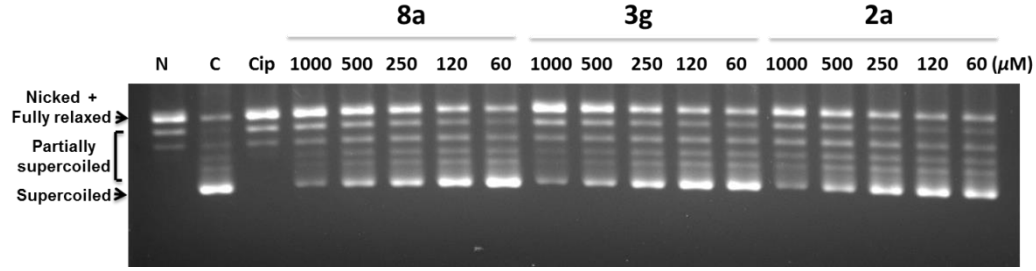


Figure S1. ORTEP views of the molecular structures of **3g** and **8a**. ORTEP drawing of **3g** showing one of the two crystallographically independent molecules in the asymmetric unit; displacement ellipsoids are drawn at the 20% probability level at 298 K. For **8a**, displacement ellipsoids are drawn at the 20% probability level at 298 K.

X-ray Crystal Structure of **3g**. A parallelepiped of **3g**, recrystallized from ethyl acetate and hexane, of approximate dimensions 0.25 × 0.25 × 0.20 mm was mounted on a glass fiber. X-ray data were collected at 298 K using a Nonius Kappa CCD diffractometer to a maximum 2θ of 60.1^{o} with monochromatic Mo Kα radiation; 8822 unique reflections were collected. The data were integrated and scaled using the HKL suit of XdisplayF, Denzo and Scalepack. Unit cell parameters were retrieved and refined on all reflections. Crystal data for **3g**: $C_{18}H_{20}O_3$, M = 284.35, monoclinic space group $P2_1$, a = 15.3222(8) Å, b = 7.3574(3) Å, c = 15.4514(7) Å, β = 114.057(3)^{o}, V = 1590.56(13) Å^3, Z = 4, ρ = 1.187 g/cm^3, μ = 0.079 mm^{-1}. The structure was solved by directed methods (SHELXD). All non-H atoms were refined anisotropically and H atoms refined isotropically with fixed B values of 5 Å^2 in the full-matrix least-squares refinement cycle on F, which converged at R = 0.0601, wR = 0.0688 and GOF = 1.146 for 2571 reflections with I > 3σ(I); a Robust-resistant weighting scheme was used in the least-squares refinements of the 379 variables. The final Fourier difference map revealed

max./min. peaks of 0.32 and -0.41 e-/Å^3 at chemically implausible positions. X-ray Crystal Structure of **8a**. A parallelepiped of **8a**, recrystallized from ethyl acetate and hexane, of approximate dimensions 0.30 × 0.30 × 0.25 mm was mounted on a glass fiber. X-ray data were collected at 298 K using a Nonius Kappa CCD diffractometer to a maximum 2θ of 63.9^o with monochromatic Mo Kα radiation; 5080 unique reflections were collected. The data were integrated and scaled using the HKL suit of XdisplayF, Denzo and Scalepack. Unit cell parameters were retrieved and refined on all reflections. Crystal data for **8a**: $C_{18}H_{16}O_4$, M = 296.32, orthorhombic space group Pbca, a = 8.0566(2) Å, b = 13.7233(4) Å, c = 27.1736(8) Å , V = 3004.40(2) Å^3, Z = 8, ρ = 1.310 g/cm^3, μ = 0.092 mm^{-1}. The structure was solved by directed methods (SHELXD). All non-H atoms were refined anisotropically and H's isotropically in the full-matrix least-squares refinement cycle on F, which converged at R = 0.0768, wR = 0.0927 and GOF = 1.008 for 1685 reflections with I > 3σ(I); a Robust-resistant weighting scheme was used in the least-squares refinements of the 254 variables. The final Fourier difference map revealed max./min. peaks of 1.21 and -0.53 e-/Å^3, indicating some disorder about the C10-C11 propylene single bond. All crystallographic calculations were performed using Crystal Structure Analysis Package (4.0), Rigaku Corporation. Crystallographic data (excluding structure factor tables) for **3g** (CCDC 1004364) and **8a** (CCDC 1004363) have been deposited with the Cambridge Crystallographic Data Centre. Copies of the data can be obtained free of charge, on application to the Director, CCDC. 12 Union Road, Cambridge CB2 1Ez (fax: +44(0)1223-336033 or e-mail: deposit@ccdc.cam.ac.uk).

A) Inhibition of *E. coli* DNA gyrase by **8a**, **3g**, and **2a**.



B) Inhibition of decatenation activity of *E. coli* topo IV by **2e** and **2a**

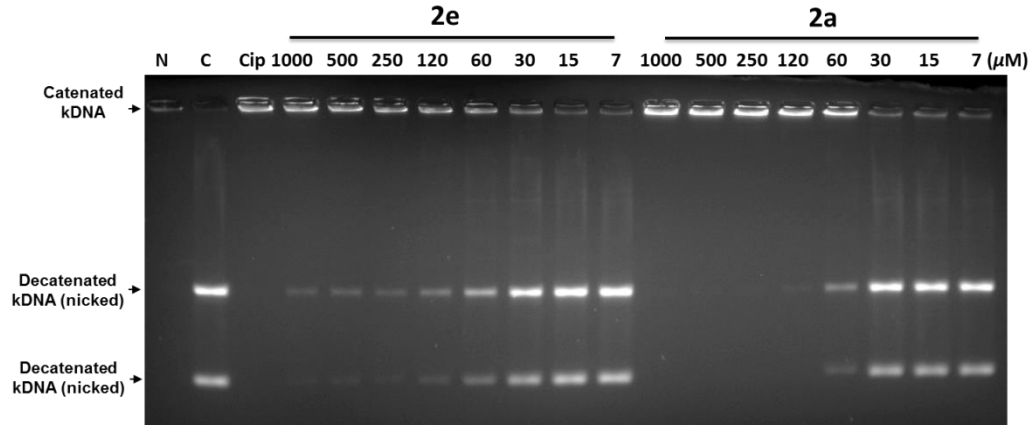


Figure S2. Inhibition against bacterial DNA gyrase and topo IV. (A) N = No enzyme added; Control (C) = DMSO; Cip = ciprofloxacin (150 μM); Enzyme = 1.25 U *E. coli* gyrase, gyrase substrate = 300 ng relaxed plasmid DNA; Incubation 37 ºC, 30 min. (B) N = No enzyme added; Control (C) = DMSO; Cip = ciprofloxacin (150 μM); Enzyme = 0.25 U *E. coli* topoisomerase IV/lane, ATP = 1 mM; catenated kinetoplast DNA = 289 ng/lane; Incubation 37 ºC, 30 min.