Electronic supplementary information (ESI)

Design, Synthesis, Antiviral Activity and SARs of 14-Amino-phenanthroindolizidines

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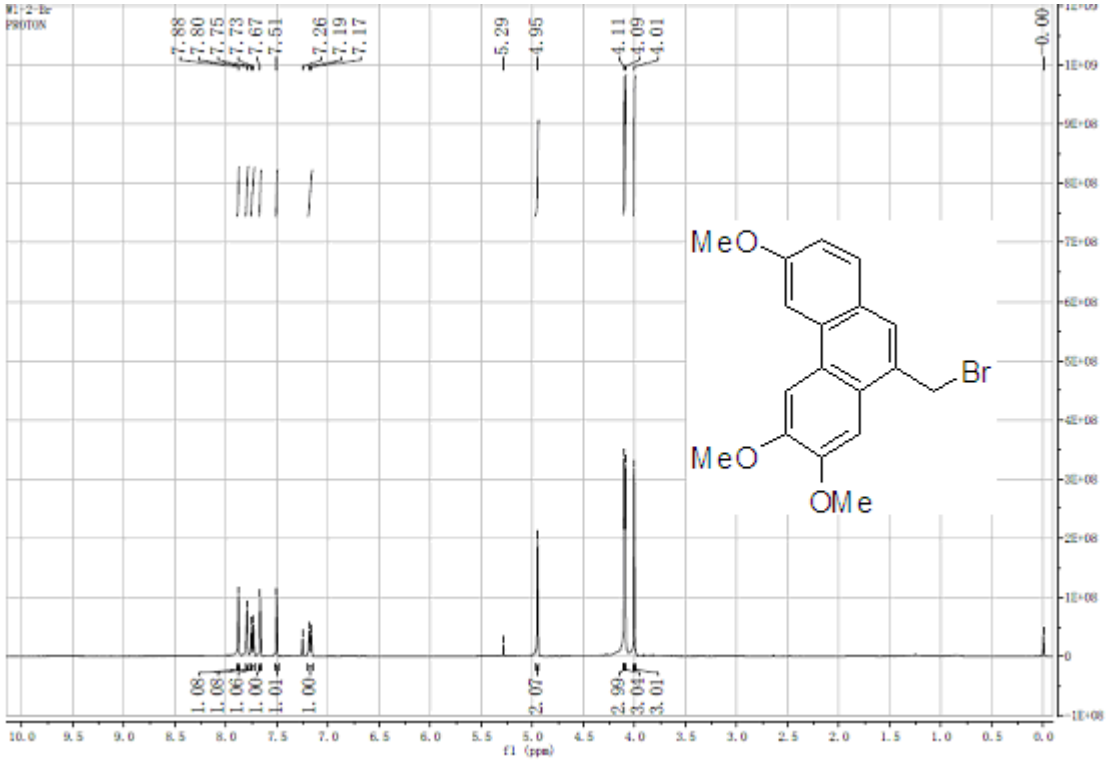
Contents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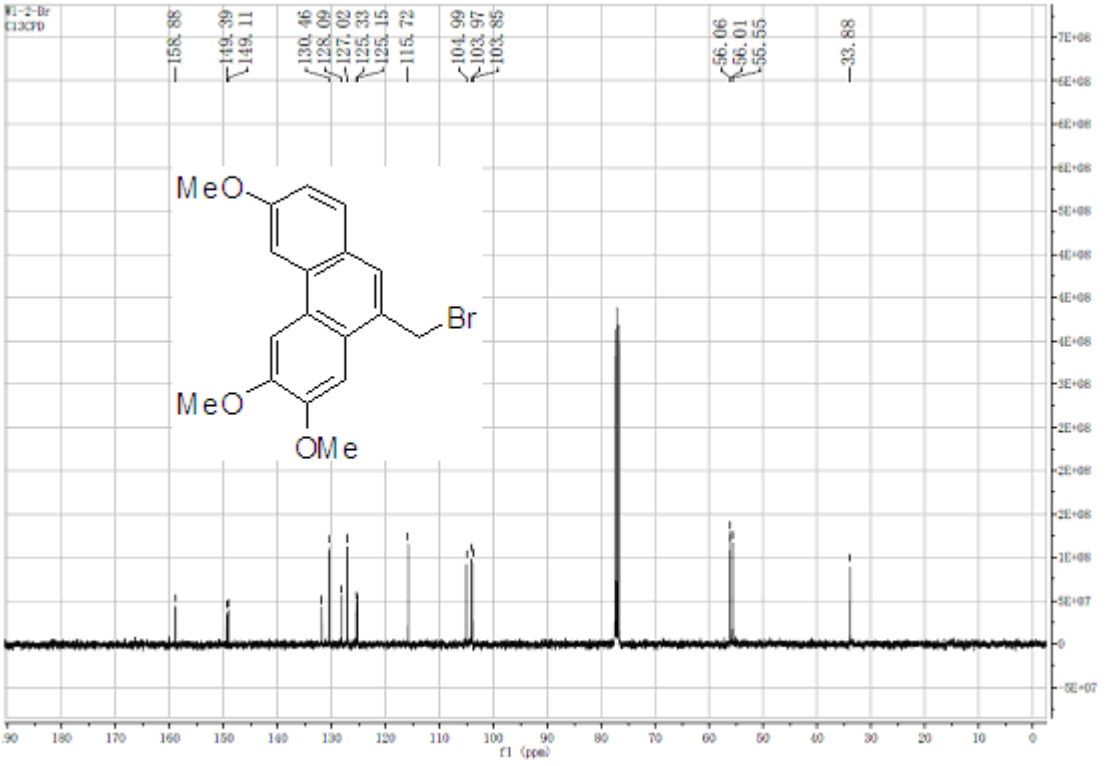
Br
MeO
OMe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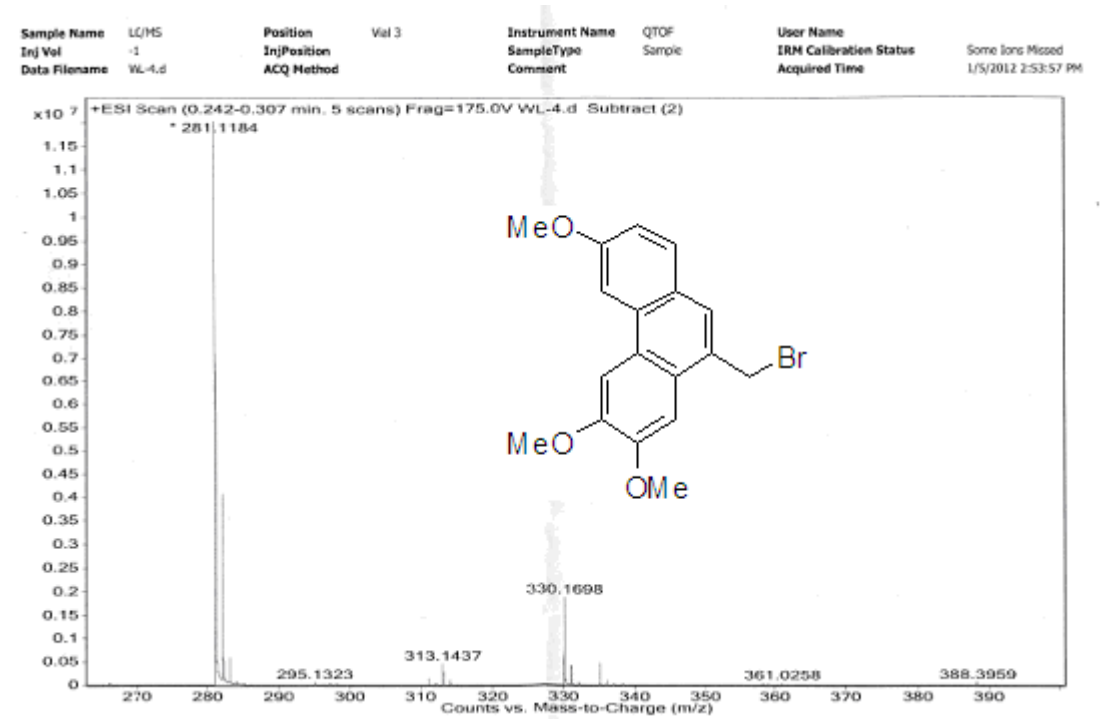
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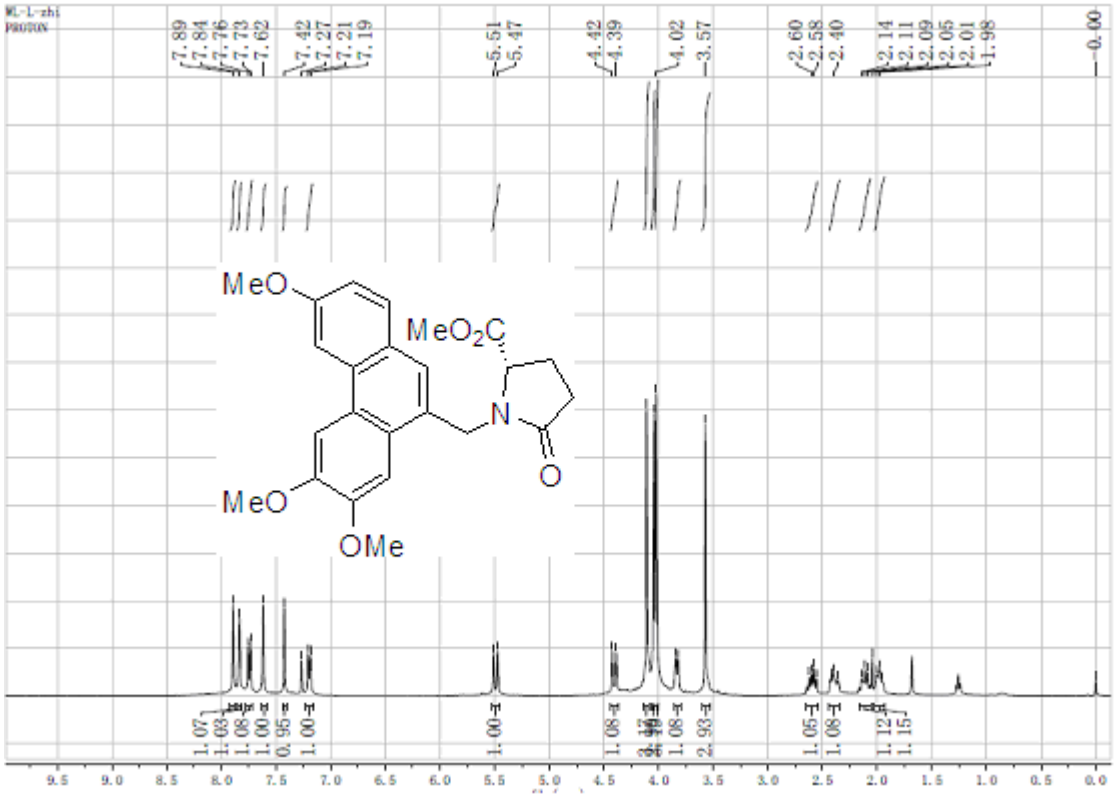
Position Vial 3
Instrument Name QTOF
User Name
Inj Vol -1
InjPosition
SampleType Sample
IRM Calibration Status Some Ions Missed
Data Filename WL-4.d
ACQ Method
Comment
Acquired Time 1/5/2012 2:53:57 PM
+ESI Scan (0.242-0.307 min, 5 scans) Frag=175.0V WL-4.d Subtract (2)
x10 7
* 281.1184
330.1698
313.1437
295.1323
361.0258
388.3959
MeO
Br
MeO
OMe
Counts vs. Mass-to-Charge (m/z)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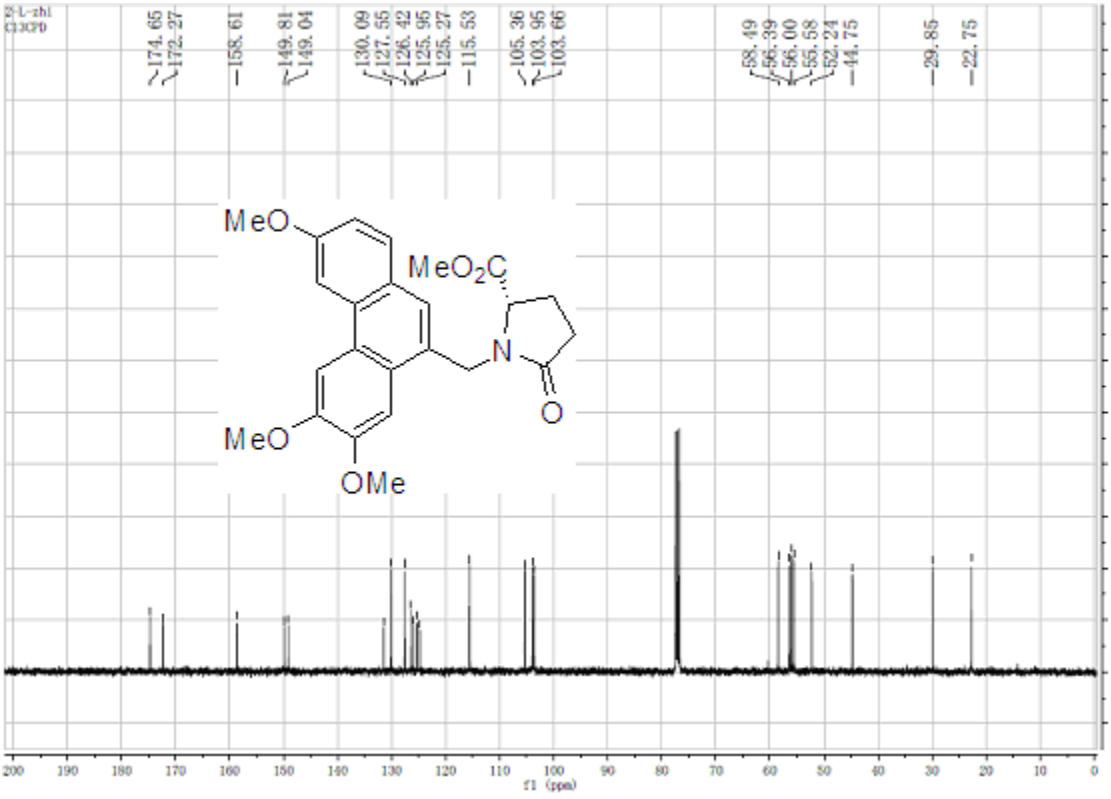
MeO2C
N
O
MeO
OMe



424.1735

Sample Name	LC/MS	**Position**	Vial 3	**Instrument Name**	QTOF	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRH Calibration Status**	Some Ions Missed
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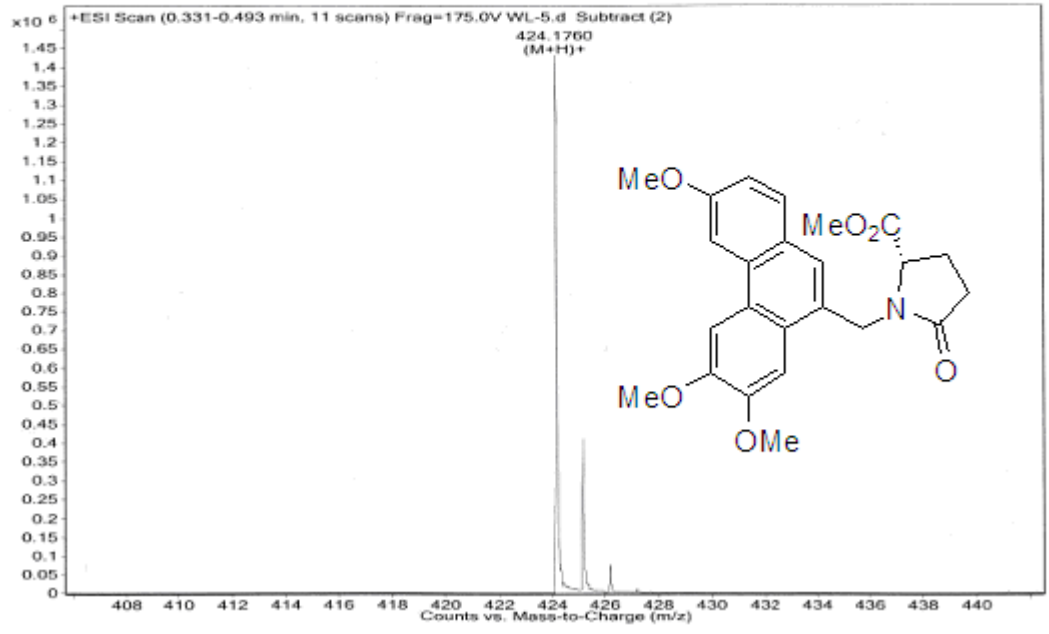

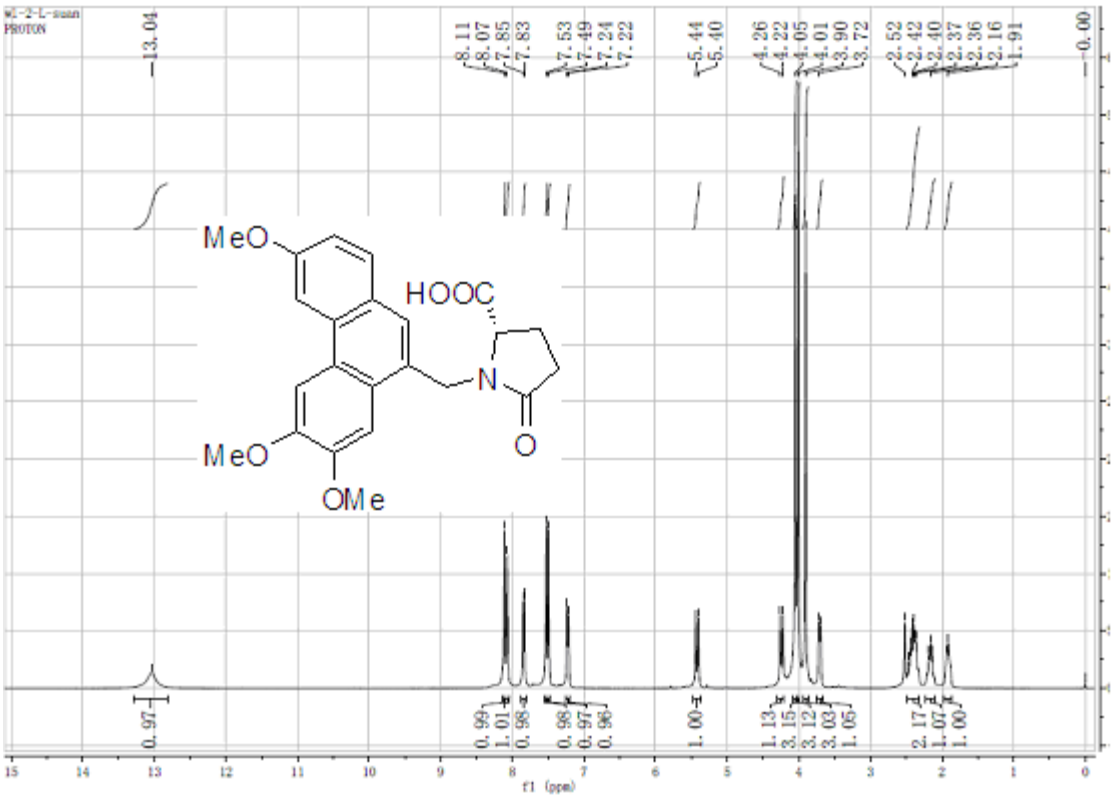
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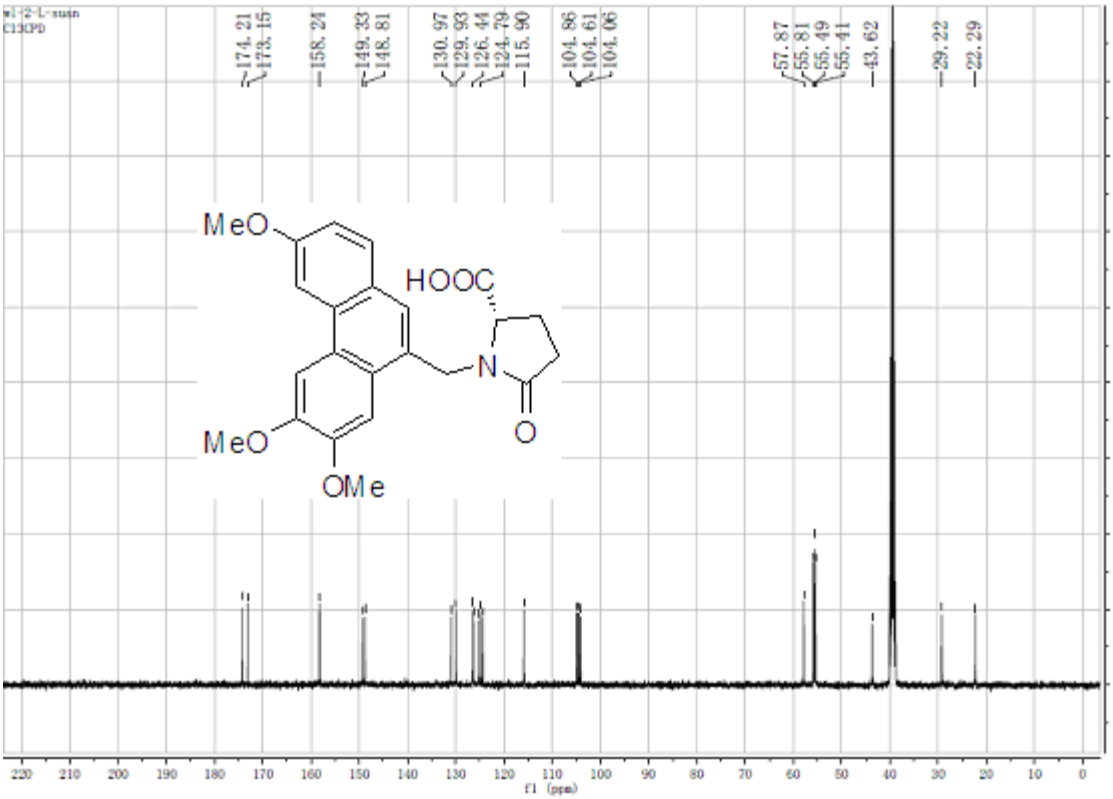
HOOC
N
O
MeO
OMe


MeO
HOOC
N
O
MeO
OMe

410.1578

Sample Name	LC/MS	**Position**	Vial 3	**Instrument Name**	QTOF	**User Name**	
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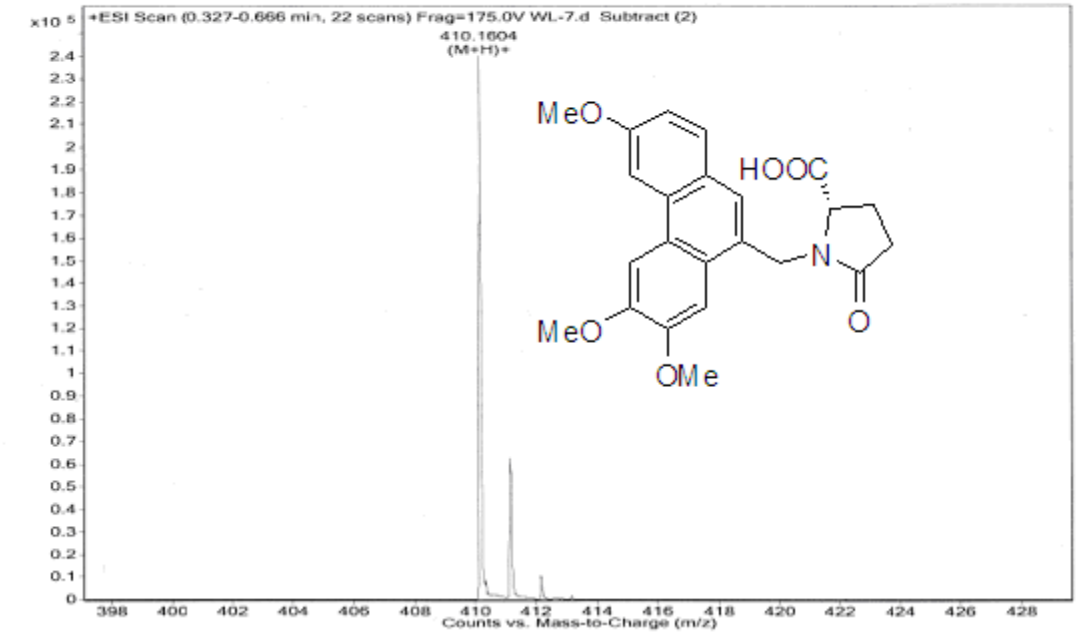

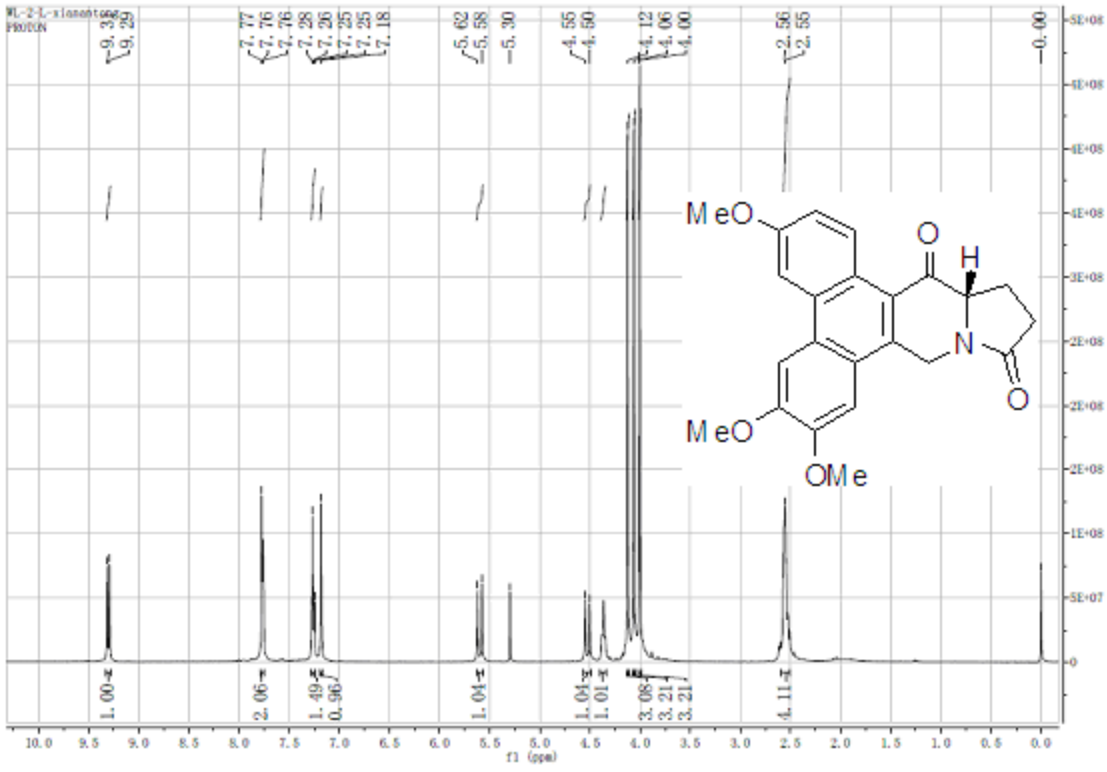

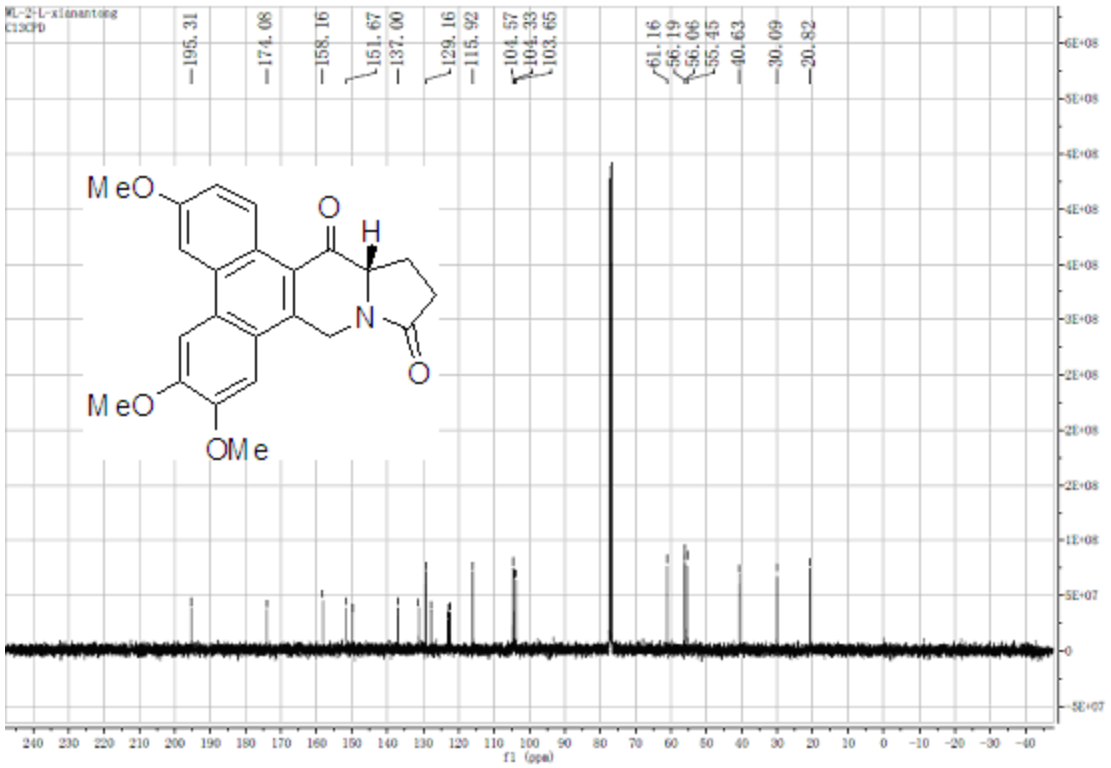

Sample Name	LC/MS	**Position**	Vial 3	**Instrument Name**	QTOF	**User Name**	
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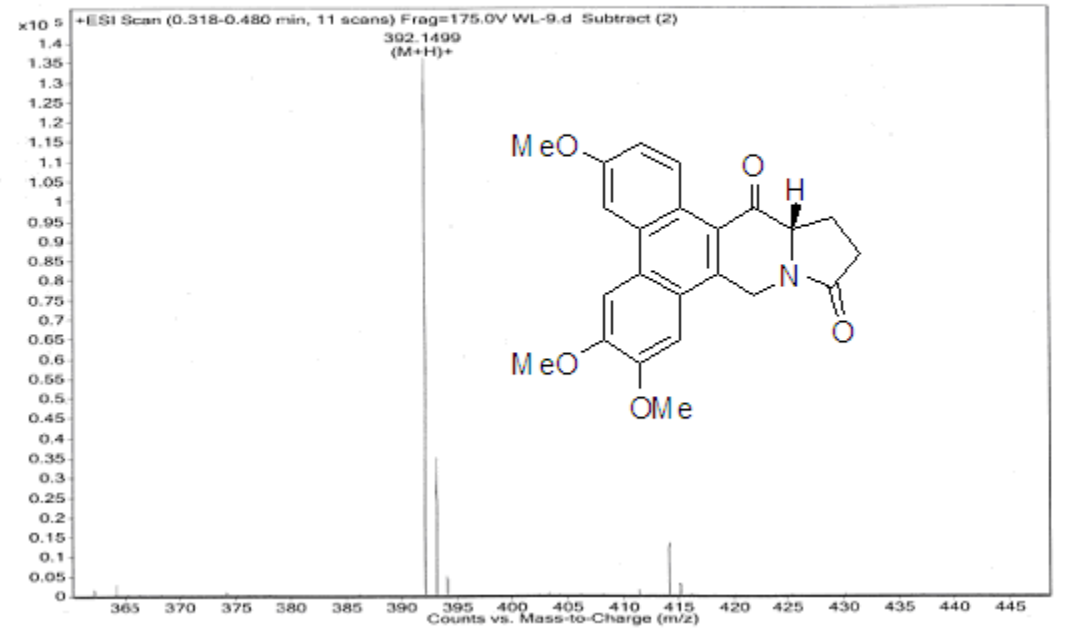

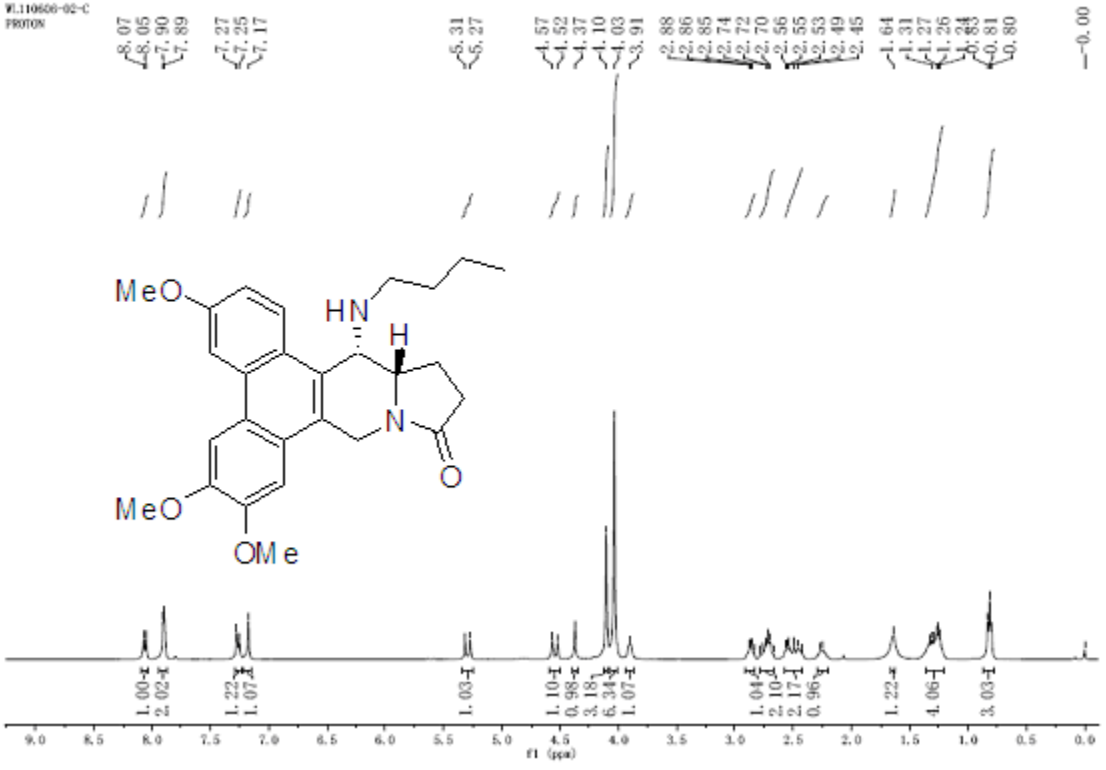
MeO
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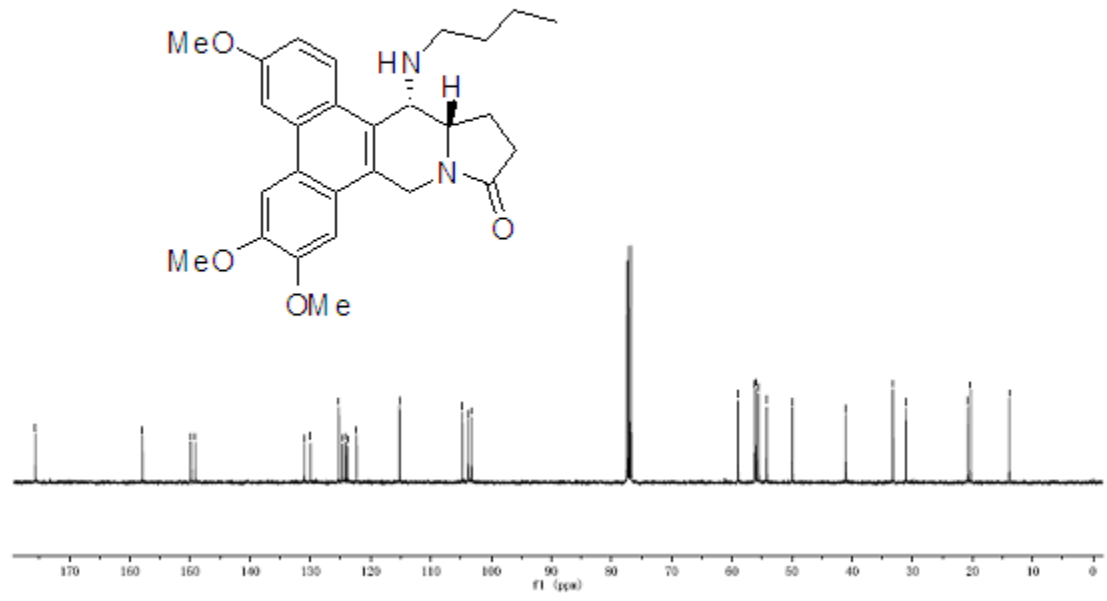
H
N
O
MeO
OMe
f1 (ppm)


MeO
HN
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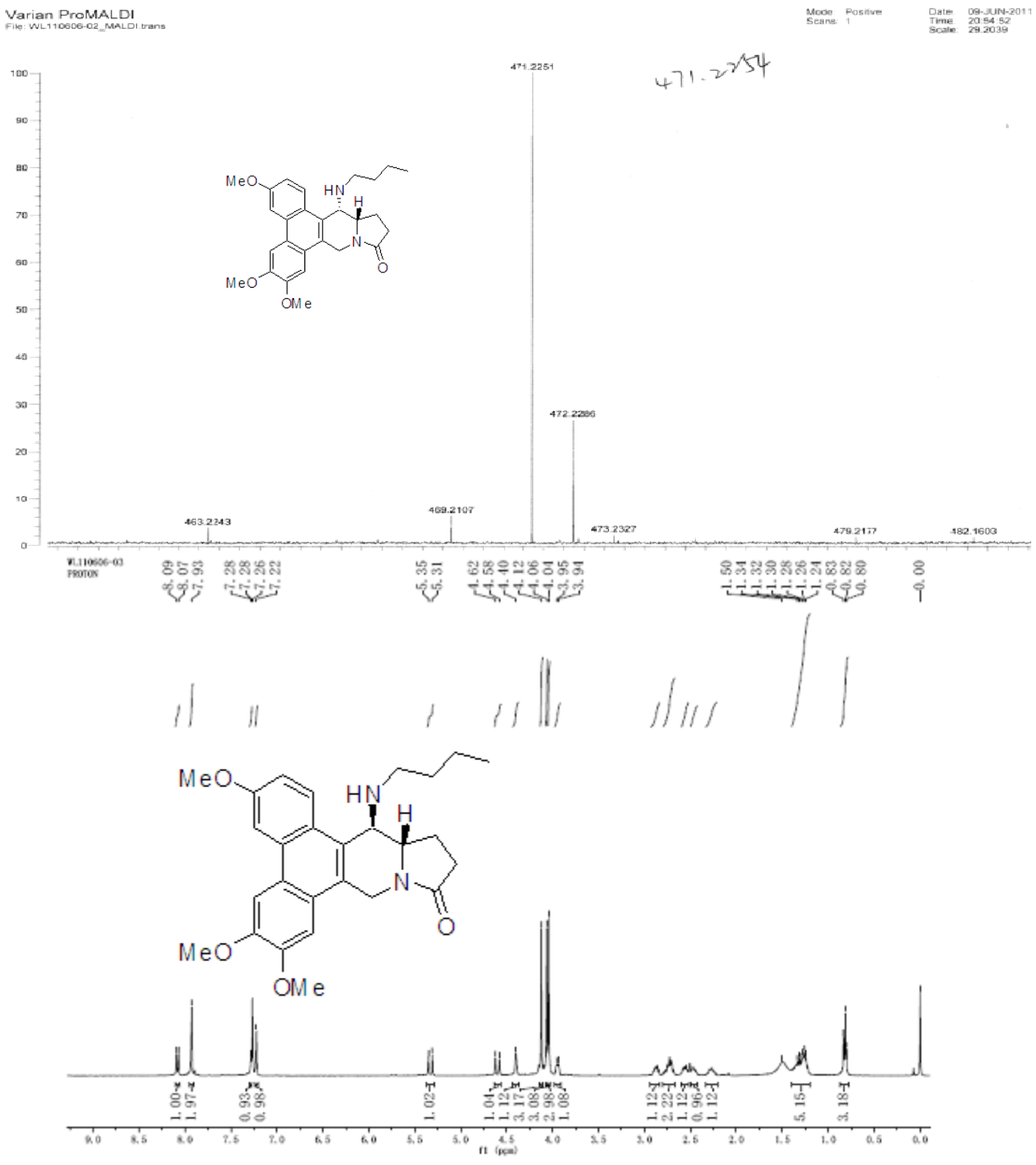
O
MeO
OMe
f1 (ppm)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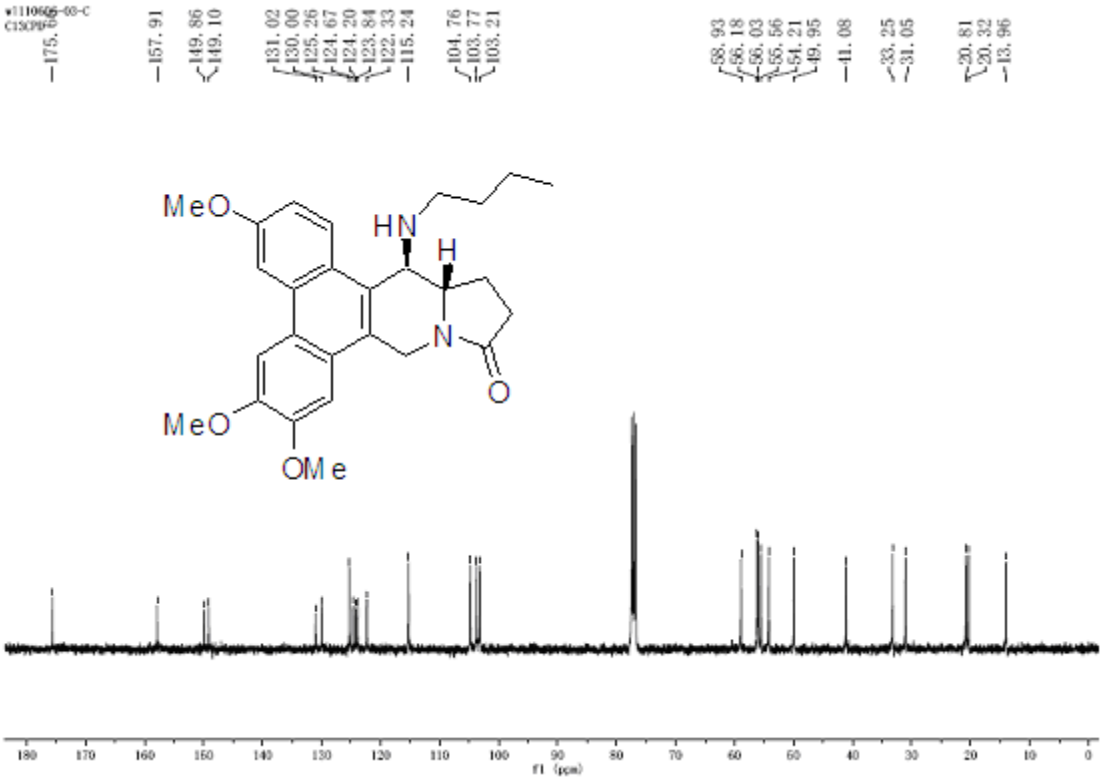
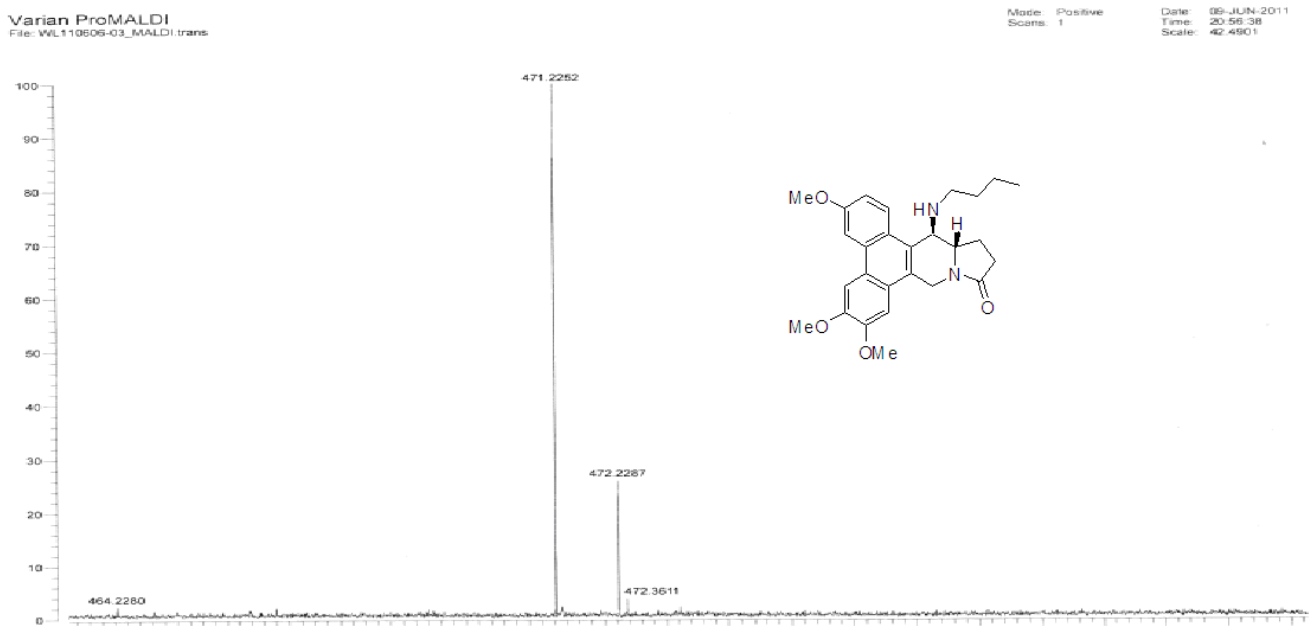
File: WL110606-02_MALDI.trans
Mode Positive
Scans: 1
Date 09-JUN-2011
Time 20:54:52
Scale: 29.2039
471.2251
472.2286
463.2243
469.2107
473.2327
479.2117
482.1603
MeO
HN
H
N
O
MeO
OMe
WL110606-03
PROTON
f1 (ppm)


175.61
157.91
149.86
149.10
131.02
130.00
125.26
124.67
124.20
123.84
122.33
115.24
104.76
103.77
103.21
68.93
66.18
66.03
55.56
54.21
49.95
41.08
33.25
31.05
20.81
20.32
13.96
MeO
HN
H
N
O
MeO
OMe
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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Mode: Positive
Scans: 1
Date: 09-JUN-2011
Time: 20:56:38
Scale: 42.4901
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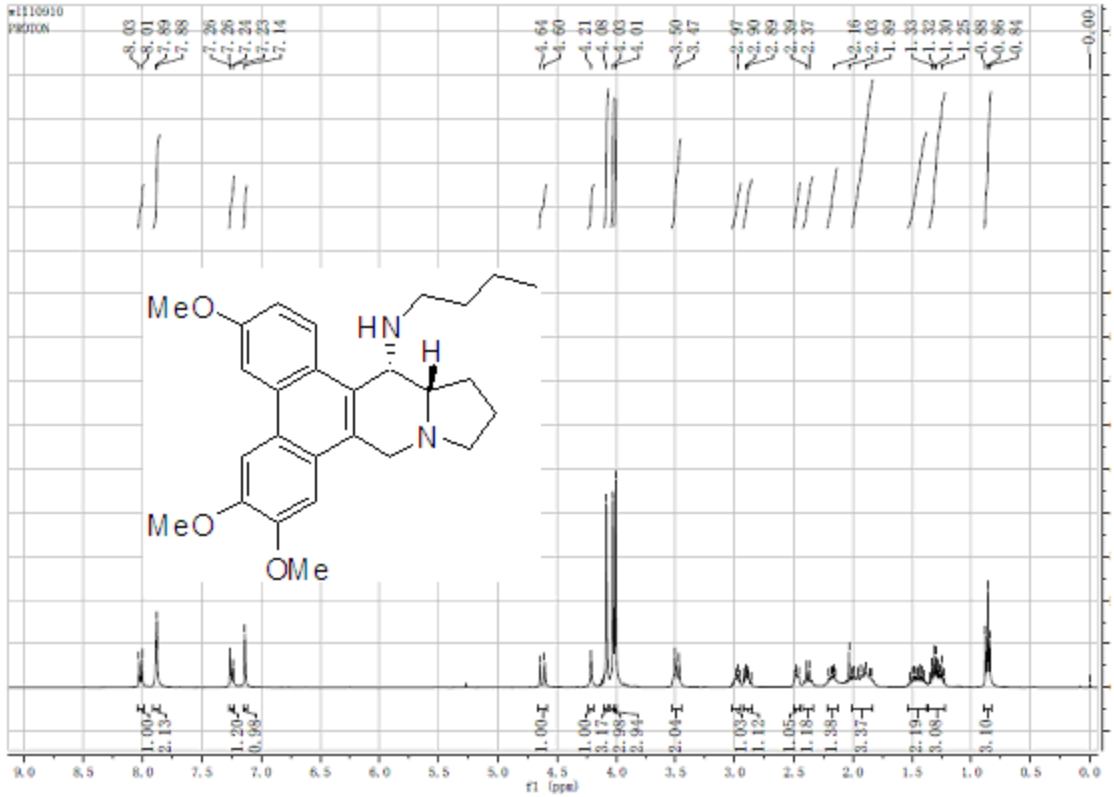
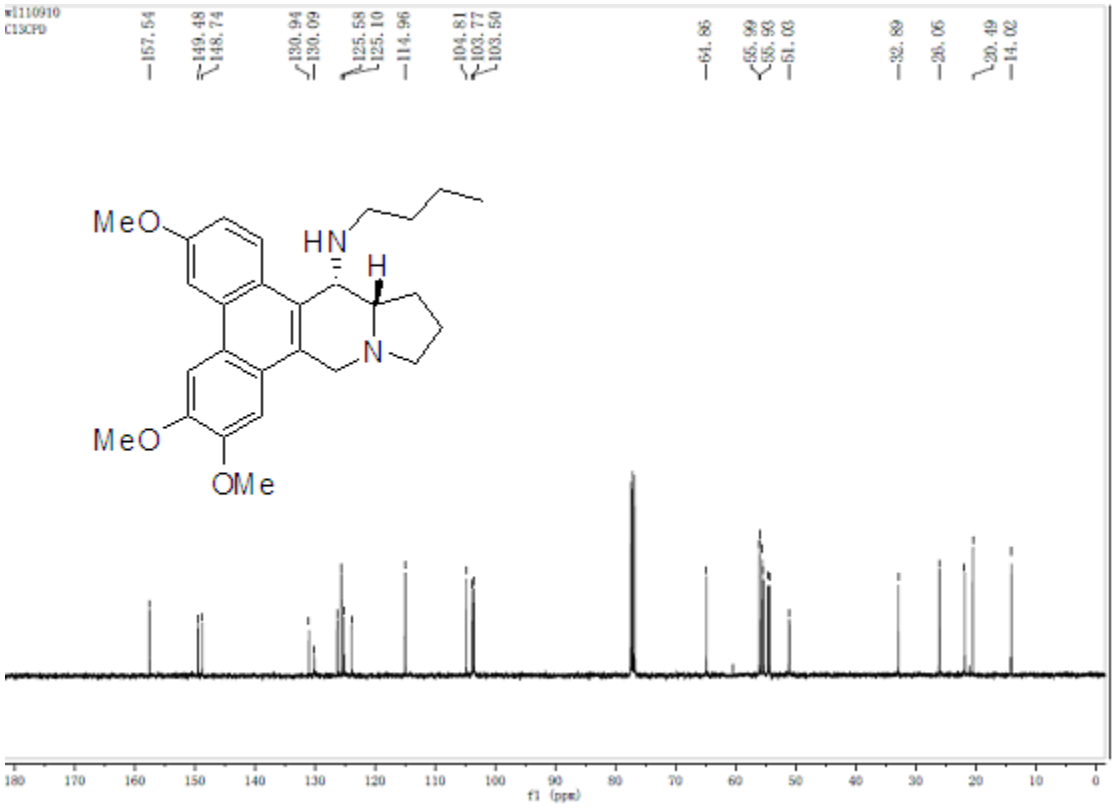
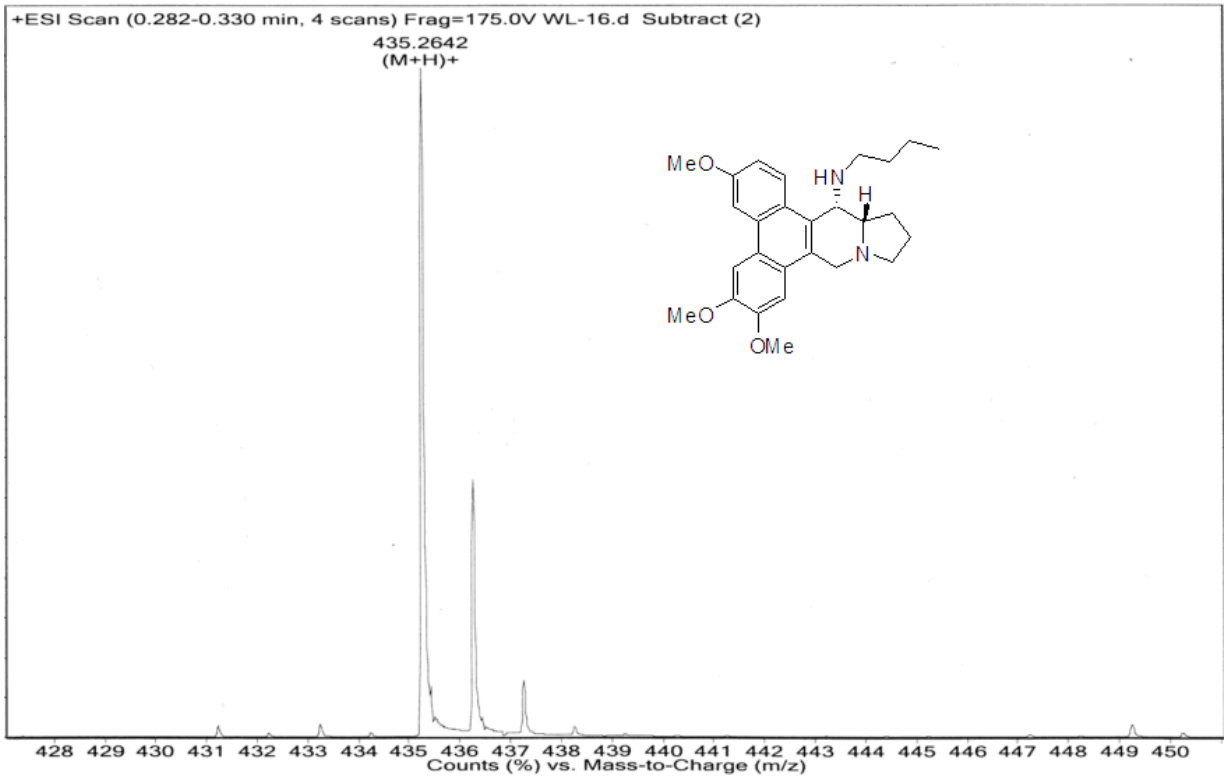
472.2287
472.3611
464.2280
MeO
HN
H
N
O
MeO
OMe


MeO
HN
H
N
MeO
OMe
f1 (ppm)


MeO
HN
H
N
MeO
OMe
f1 (ppm)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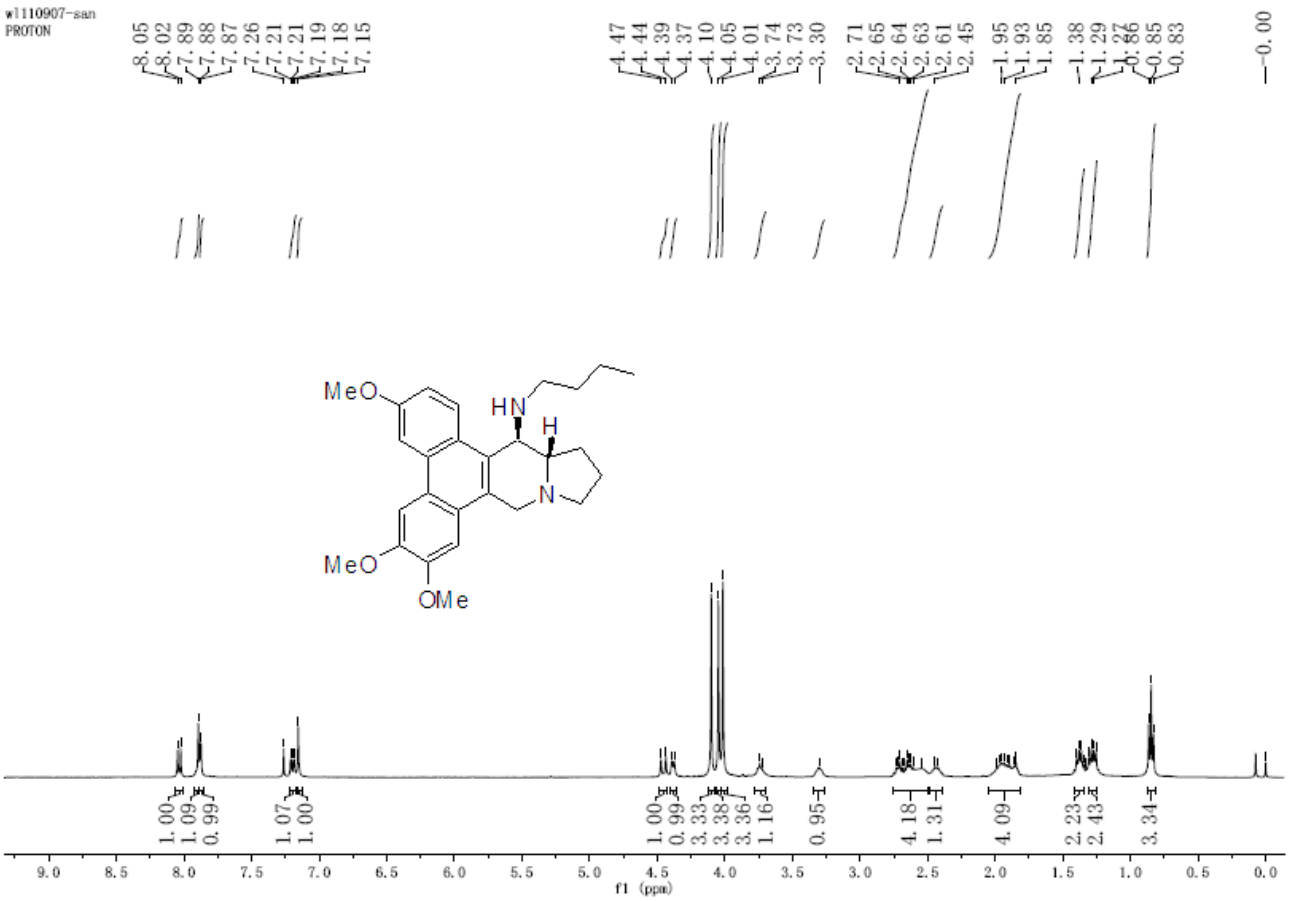
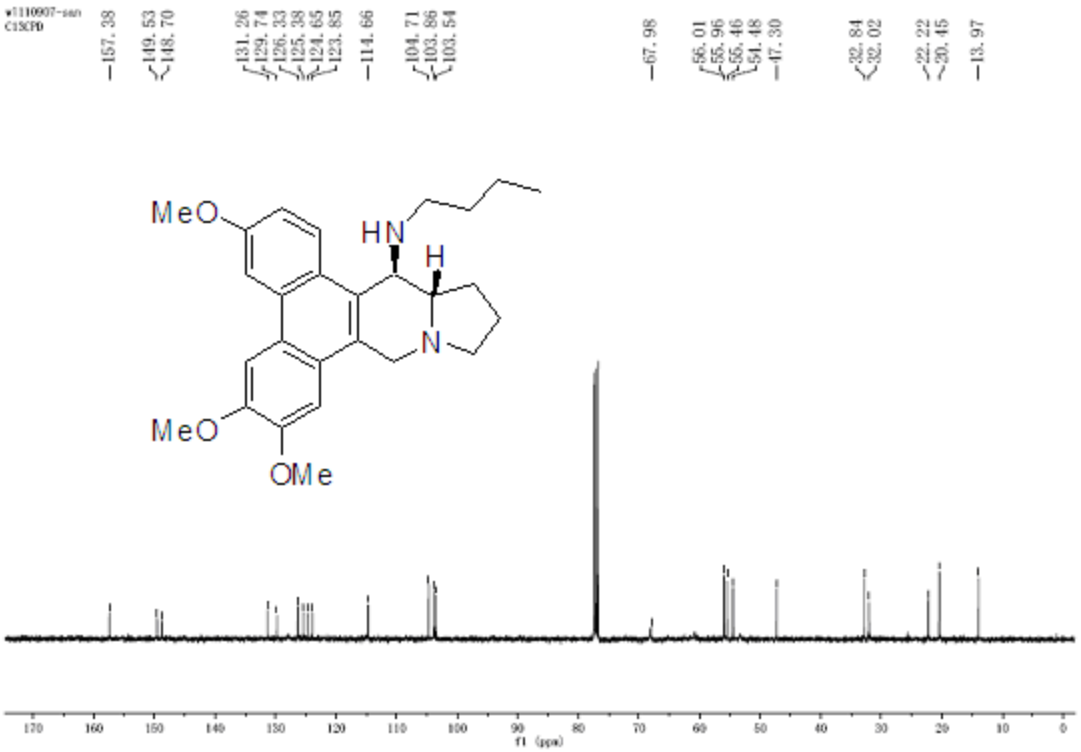
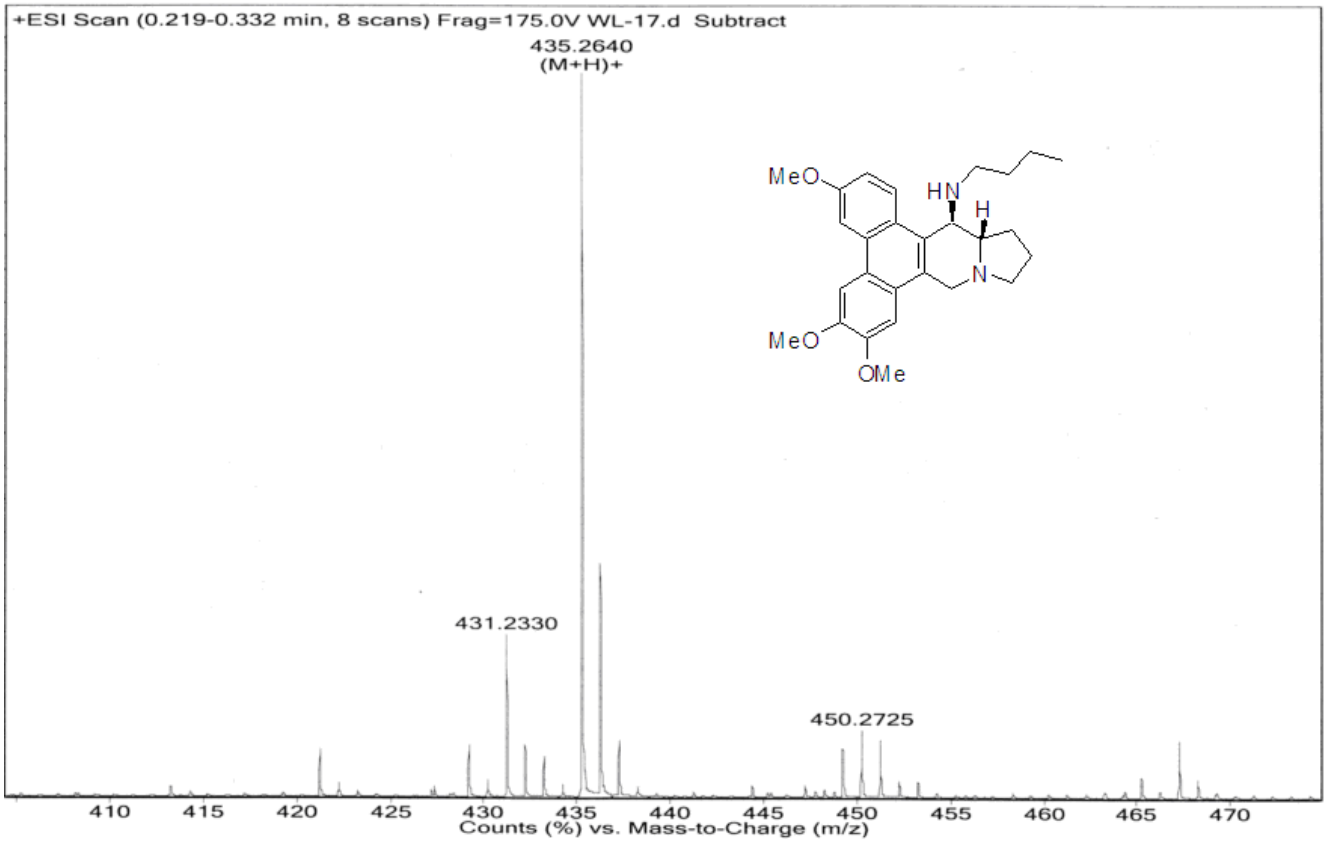
435.2642
(M+H)+
MeO
HN
H
N
MeO
OMe
428 429 430 431 432 433 434 435 436 437 438 439 440 441 442 443 444 445 446 447 448 449 450
Counts (%) vs. Mass-to-Charge (m/z)


w1110907-san
PROTON
8.05 8.02 7.89 7.88 7.87 7.26 7.21 7.21 7.19 7.18 7.15
4.47 4.44 4.39 4.37 4.10 4.05 4.01 3.74 3.73 3.30 2.71 2.65 2.64 2.63 2.61 2.45 1.95 1.93 1.85 1.38 1.29 1.27 0.86 0.85 0.83 0.00
MeO
HN
H
N
MeO
OMe
1.00 1.09 0.99 1.07 1.00 1.00 0.99 3.33 3.38 3.36 1.16 0.95 4.18 1.31 4.09 2.23 2.43 3.34
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


MeO
HN
H
N
MeO
OMe
f1 (ppm)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435.2640
(M+H)+
MeO
HN
H
N
MeO
OMe
431.2330
450.2725
410
415
420
425
430
435
440
445
450
455
460
465
470
Counts (%) vs. Mass-to-Charge (m/z)

Chromatogram

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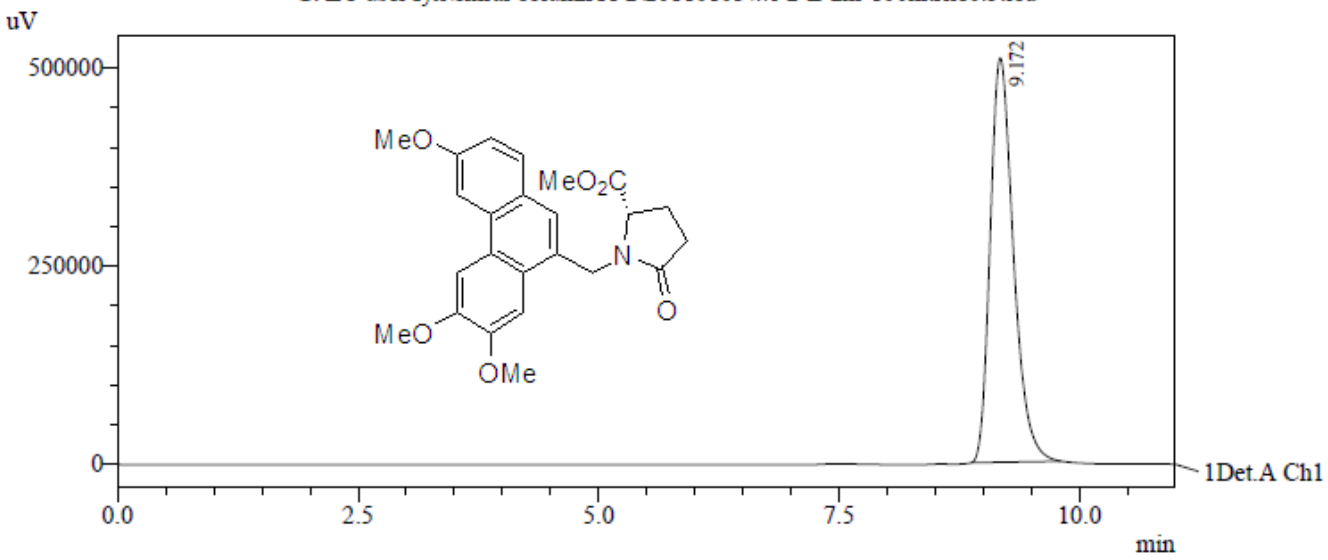


1 Det.A Ch1 / 254nm

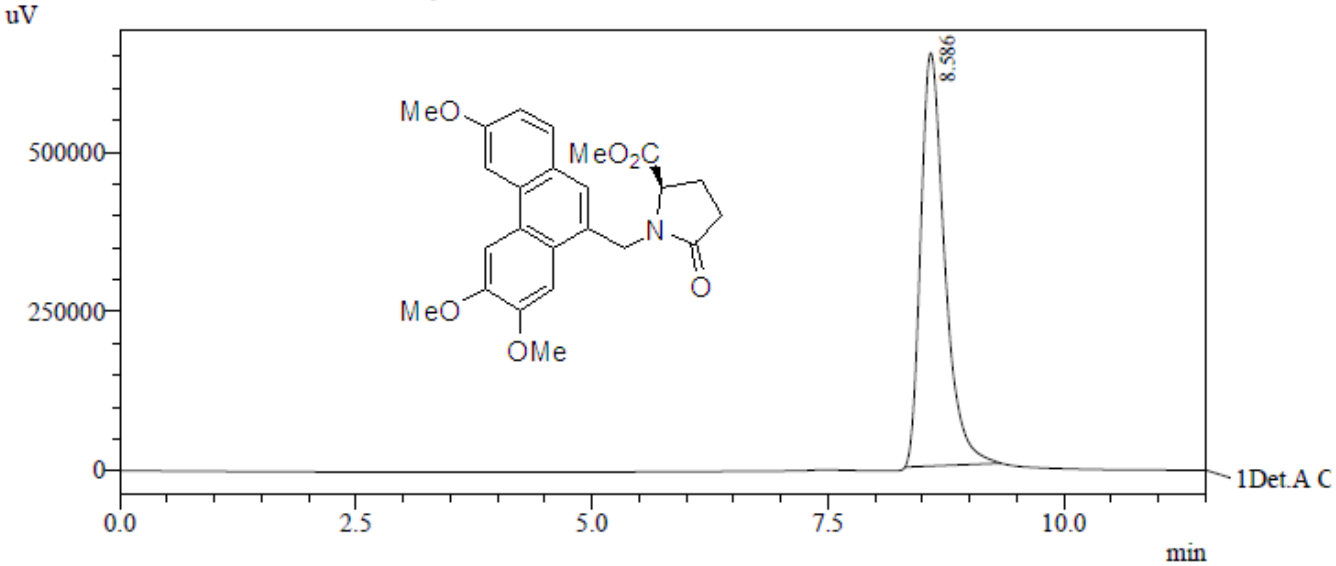
PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.172	8579508	509749	100.000	100.000
Total		8579508	509749	100.000	100.000

Chromatogram

G:\LC user\lyx\chiral column\A-2\20110103\wl-2-D-zhi-100nitrile0.5.lcd

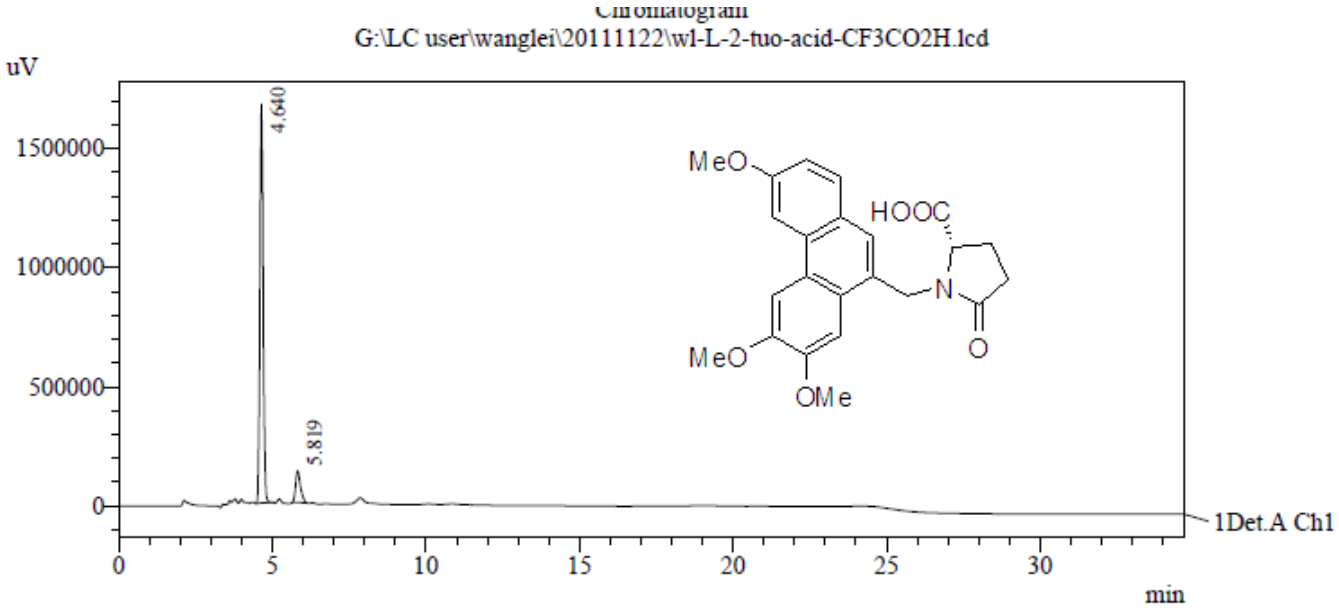


1 Det.A Ch1 / 254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.586	11459813	648475	100.000	100.000
Total		11459813	648475	100.000	100.000

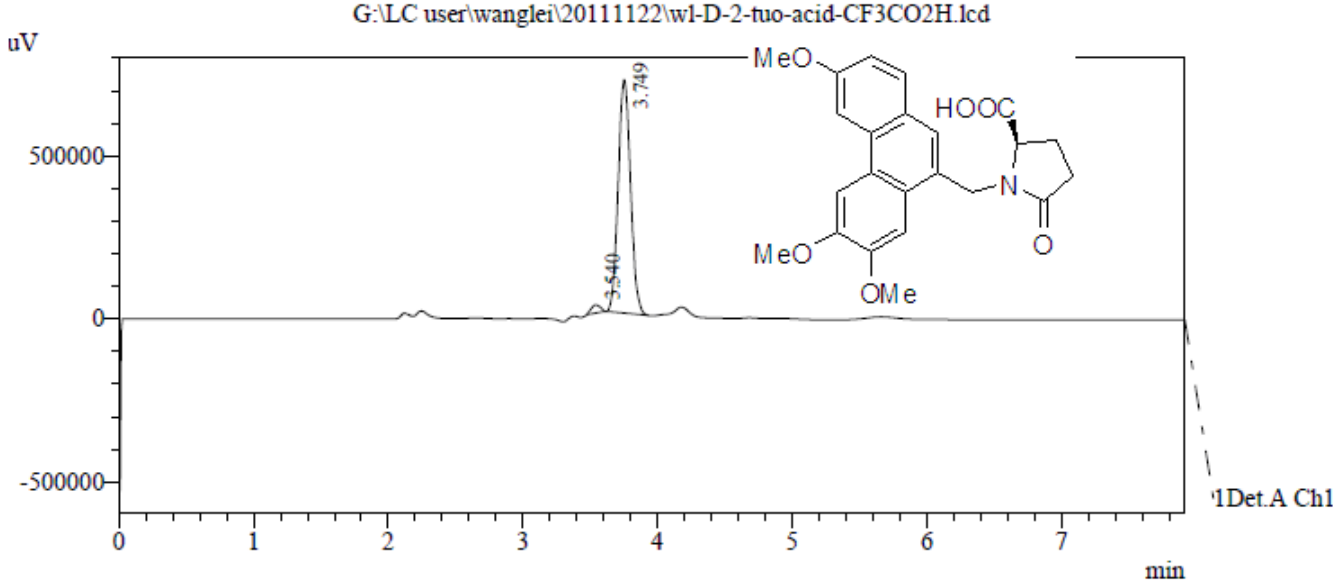


1 Det.A Ch1 / 254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.640	12395895	1674091	89.632	92.638
2	5.819	1433868	133047	10.368	7.362
Total		13829764	1807138	100.000	100.000

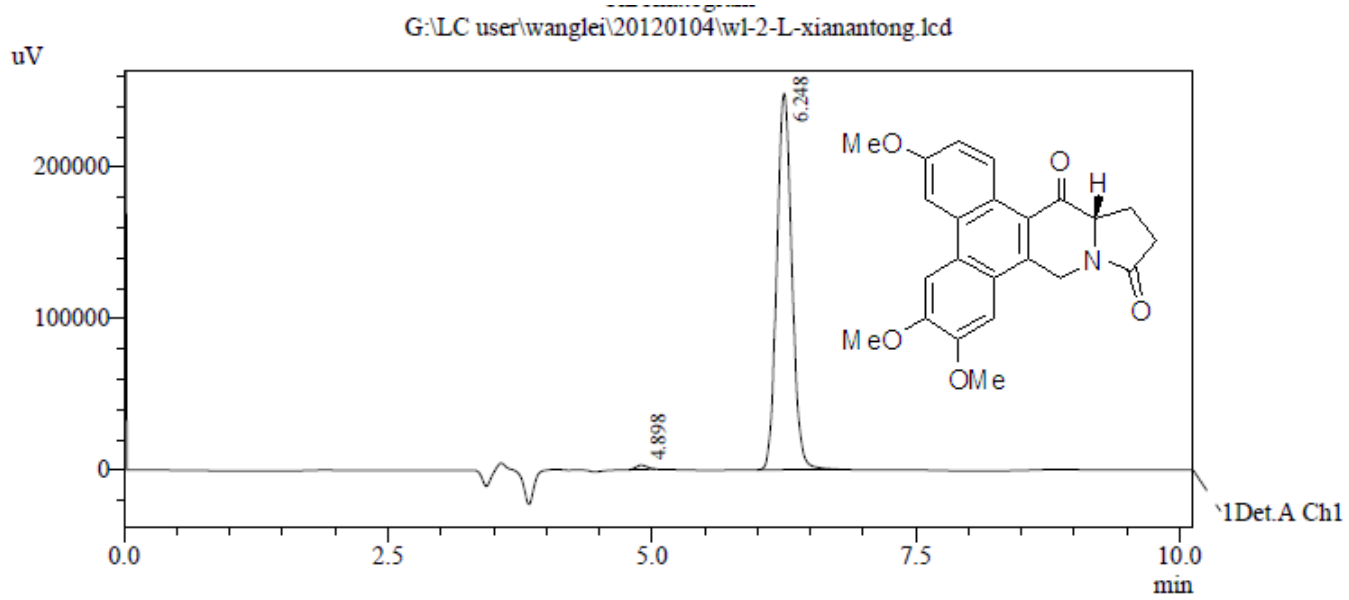


1 Det.A Ch1 / 254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	3.540	118048	24857	2.524	3.353
2	3.749	4559089	716382	97.476	96.647
Total		4677137	741240	100.000	100.000

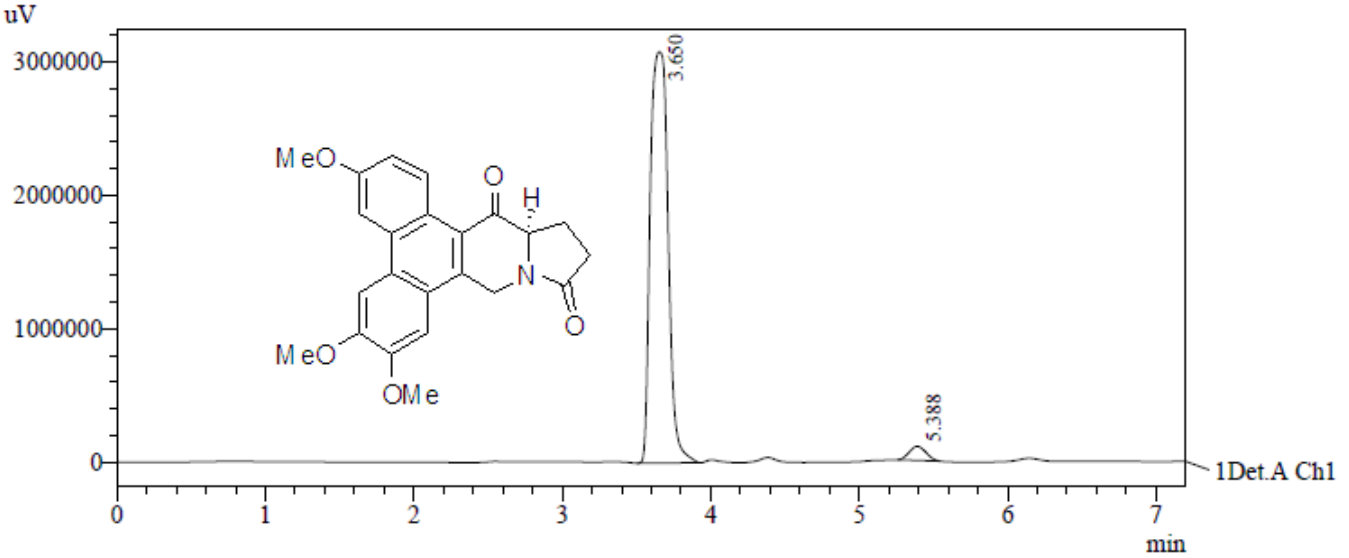


1 Det.A Ch1 / 254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.898	20096	2785	0.808	1.108
2	6.248	2466663	248481	99.192	98.892
Total		2486759	251267	100.000	100.000

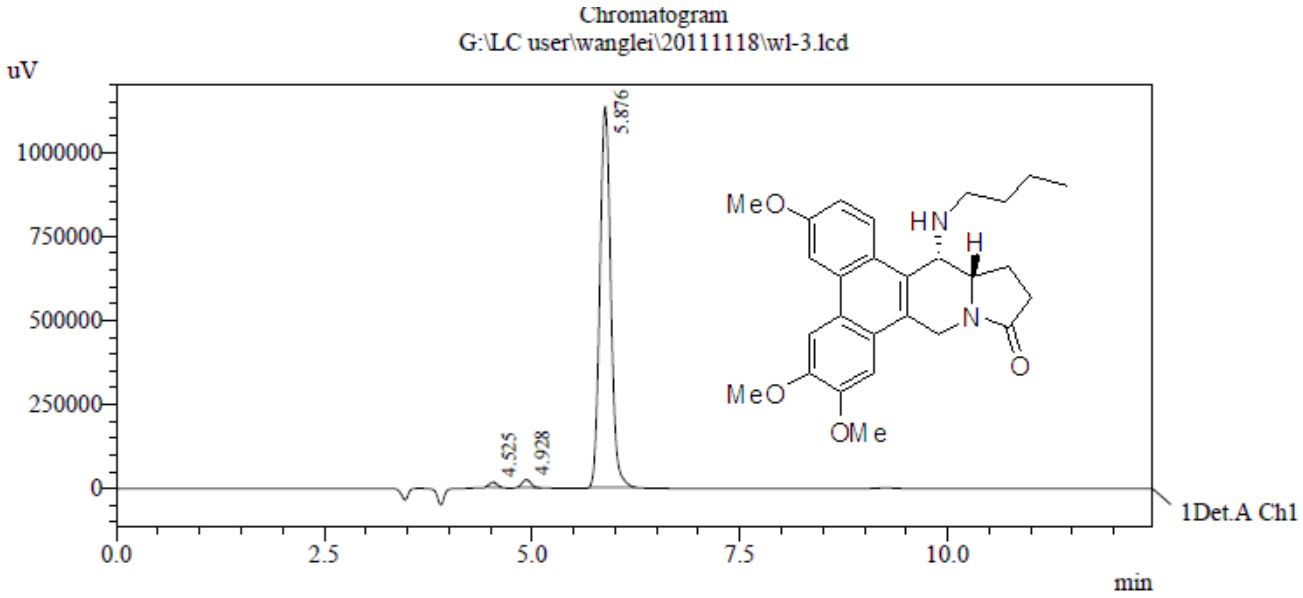


1 Det.A Ch1 / 254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	3.650	25739771	3081900	96.896	96.682
2	5.388	824619	105758	3.104	3.318
Total		26564390	3187658	100.000	100.000

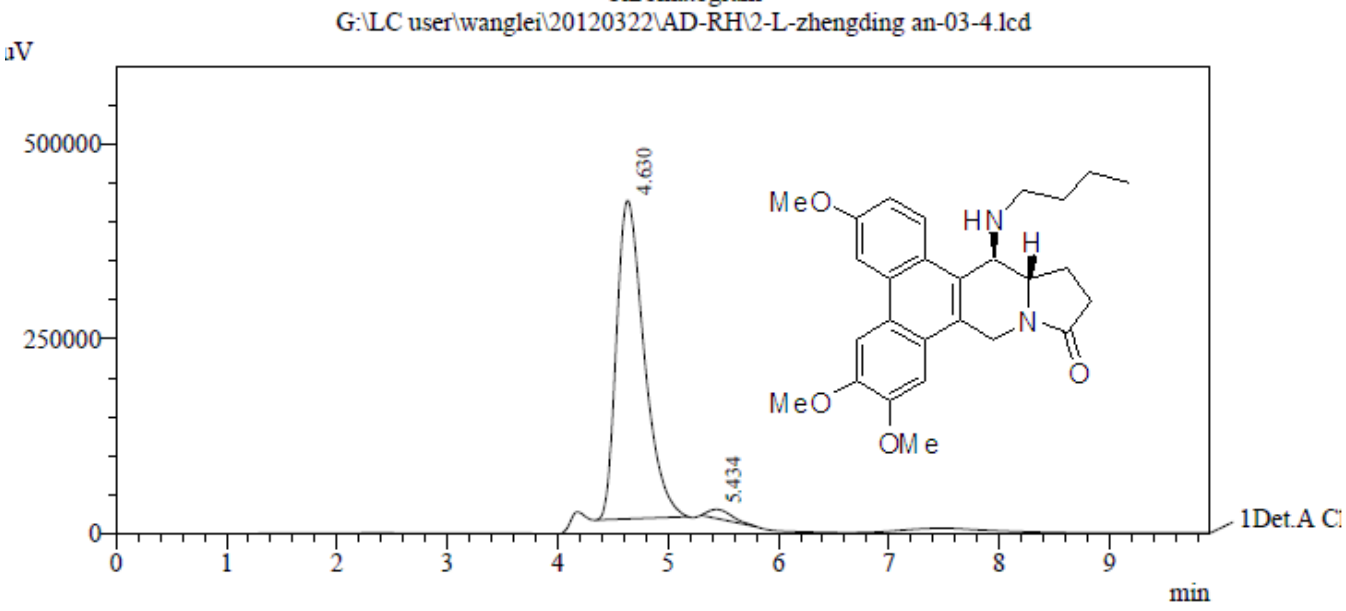


1 Det.A Ch1 / 254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.525	96338	15122	0.908	1.291
2	4.928	161892	23291	1.526	1.989
3	5.876	10350488	1132750	97.566	96.720
Total		10608718	1171164	100.000	100.000

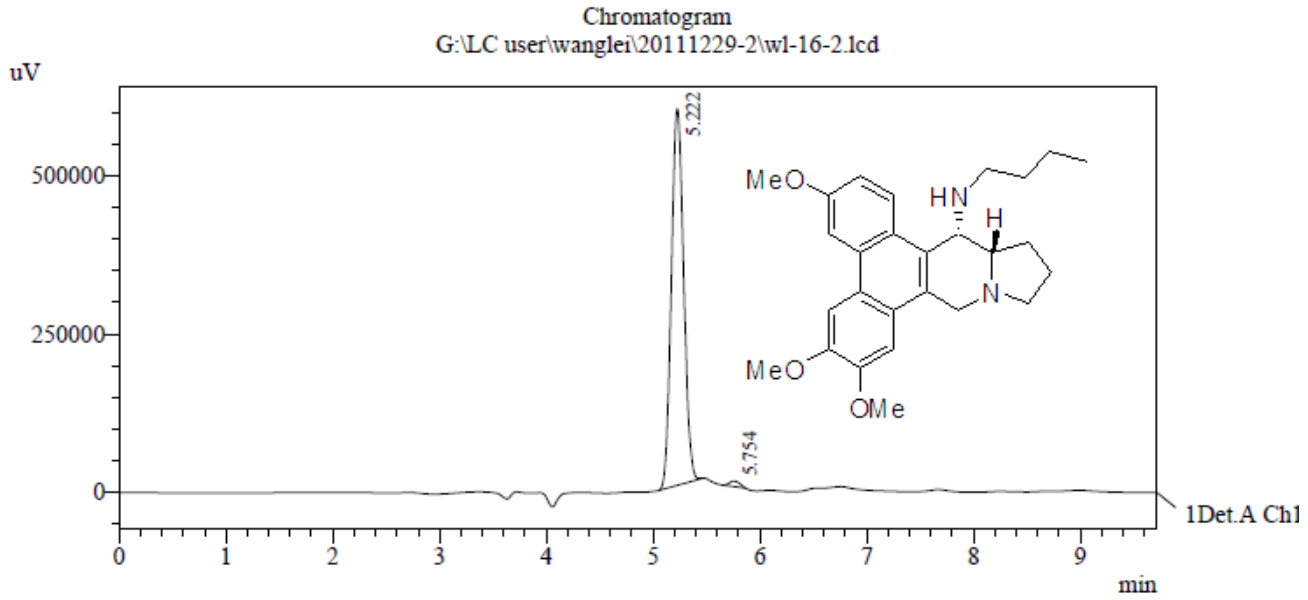


1 Det.A Ch1 / 254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.630	7118848	408689	97.581	97.254
2	5.434	176482	11538	2.419	2.746
Total		7295330	420227	100.000	100.000

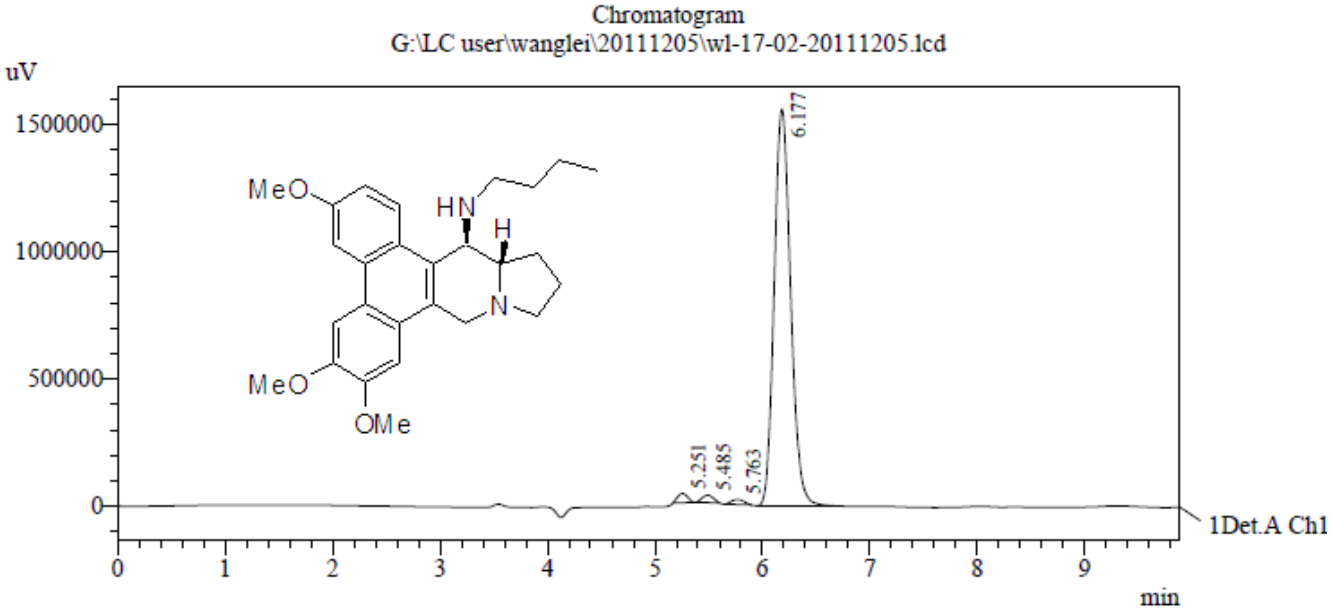


1 Det.A Ch1 / 254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.222	4743384	595180	98.788	98.578
2	5.754	58206	8583	1.212	1.422
Total		4801589	603763	100.000	100.000

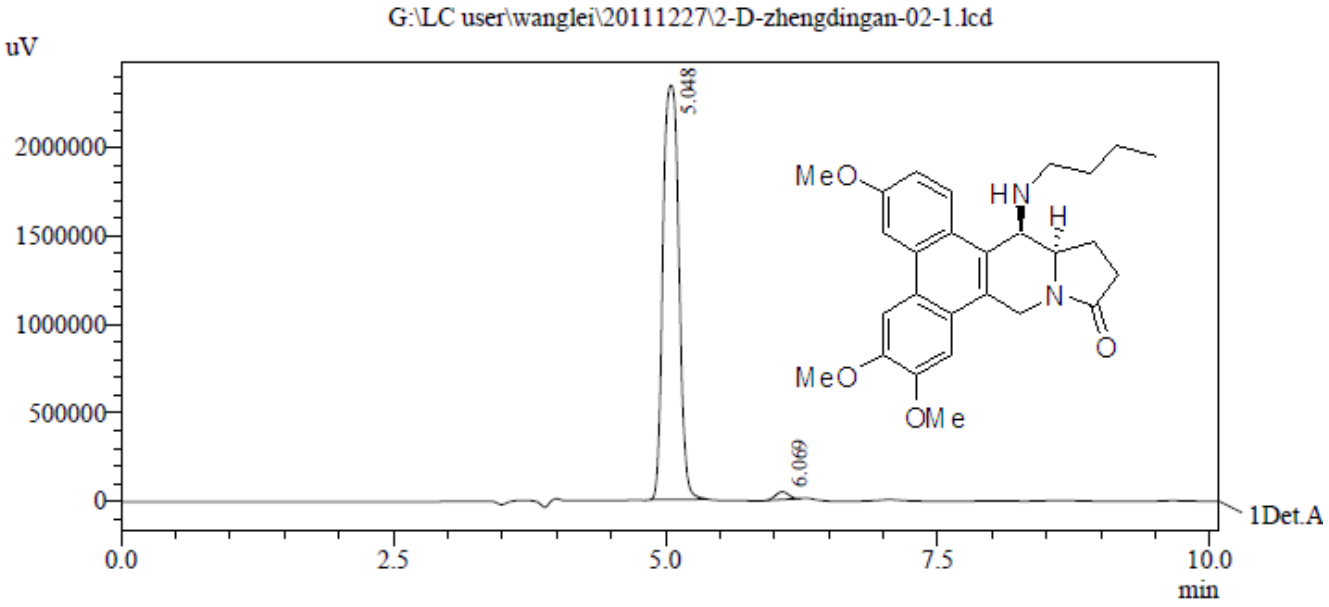


1 Det.A Ch1 / 254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.251	235908	36394	1.370	2.214
2	5.485	208570	28880	1.211	1.757
3	5.763	158923	19621	0.923	1.194
4	6.177	16614380	1558613	96.495	94.835
Total		17217781	1643508	100.000	100.000



1 Det.A Ch1 / 254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.048	23663429	2341534	98.497	98.156
2	6.069	361203	43978	1.503	1.844
Total		24024632	2385511	100.000	100.000

Chromatogram

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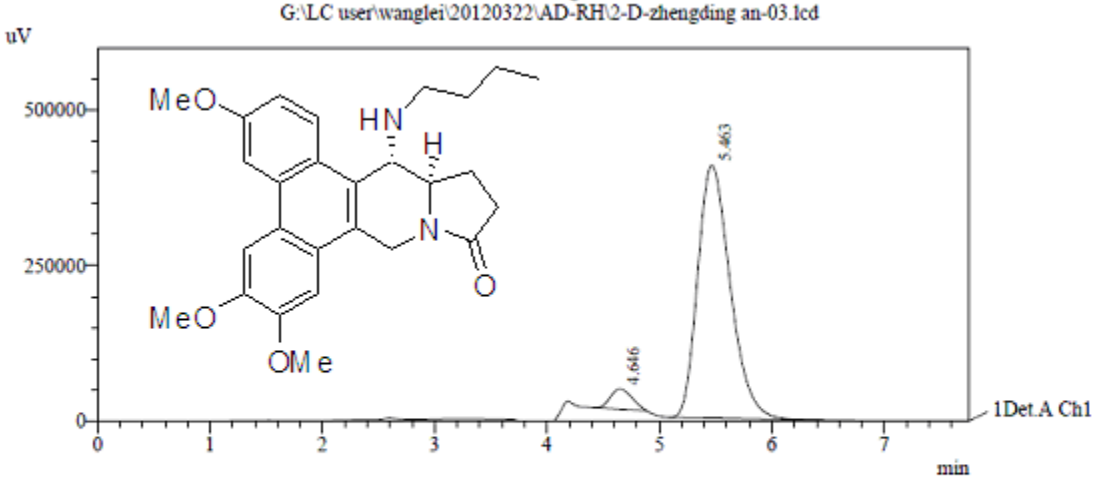

1 Det.A Ch1 / 254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.646	429455	32223	4.987	7.344
2	5.463	8182842	406555	95.013	92.656
Total		8612298	438778	100.000	100.000

Chromatogram

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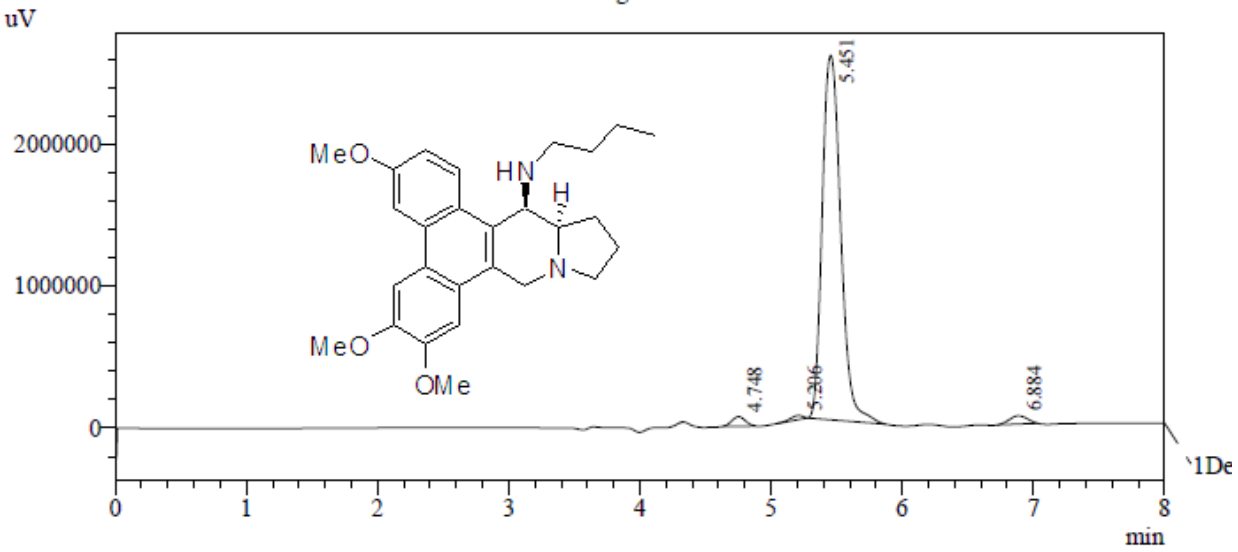


1 Det.A Ch1 / 254nm

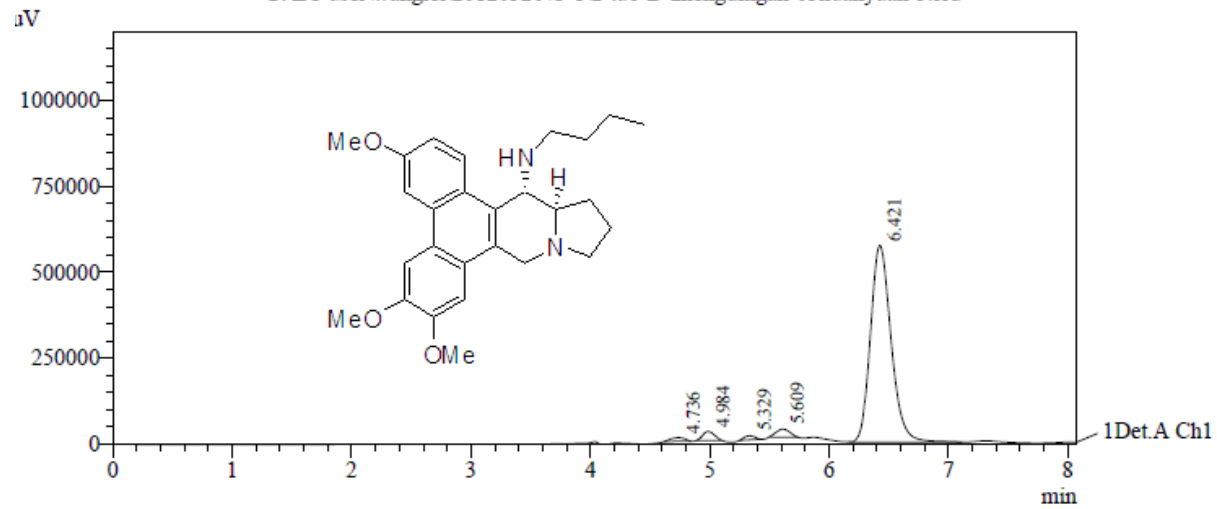
PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.748	477178	67450	1.800	2.474
2	5.206	201930	29495	0.762	1.082
3	5.451	25271083	2571146	95.324	94.304
4	6.884	560577	58367	2.115	2.141
Total		26510768	2726458	100.000	100.000

Chromatogram

G:\LC user\wanglei\20120320\C-1\2-tuo-D-zhengdingan-03huanyuan-3.lcd



1 Det.A Ch1 / 254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.736	91253	10856	1.235	1.685
2	4.984	175094	25945	2.370	4.027
3	5.329	73351	11995	0.993	1.862
4	5.609	188870	23412	2.556	3.634
5	6.421	6859563	572060	92.846	88.792
Total		7388131	644268	100.000	100.000