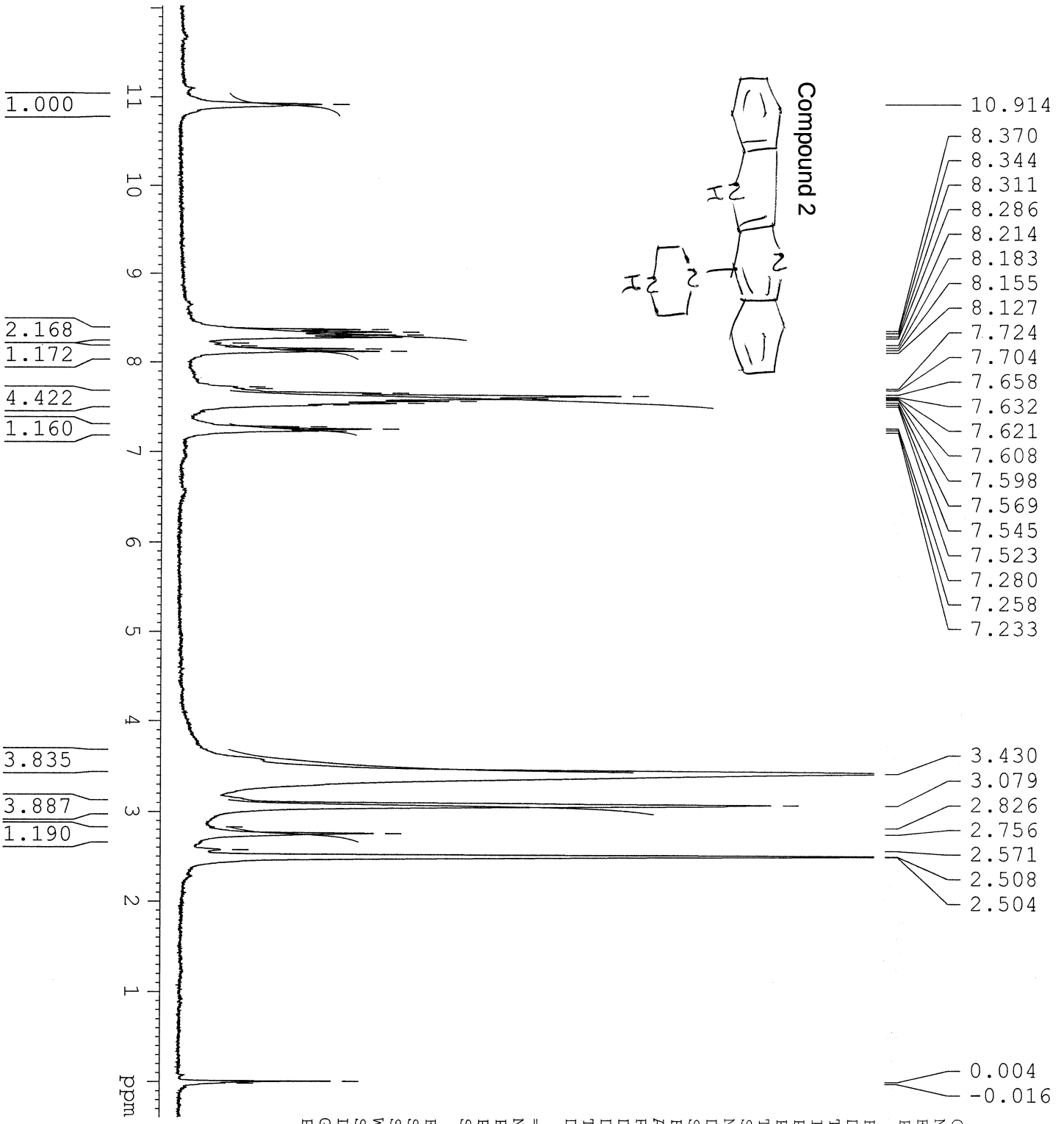
Supporting Information

The anticancer activity and cellular repression of c-MYC by the G-quadruplex-stabilizing 11-piperazinyl quindoline is not dependent on direct targeting of the G-quadruplex in the c-MYC promoter

Peda V. L. Boddupally,[1] Seongmin Hahn,[1] Cristina Beman,[1] Biswanath De,[1] Tracy A. Brooks,[1–3] Vijay Gokhale,[1–3] Laurence H. Hurley[1–3]*

Spectral data ($^{1}H/^{13}C$–NMR, HRMS, and HPLC) for compounds 2–16.


Compound 2
10.914
8.370
8.344
8.311
8.286
8.214
8.183
8.155
8.127
7.724
7.704
7.658
7.632
7.621
7.608
7.598
7.569
7.545
7.523
7.280
7.258
7.233
3.430
3.079
2.826
2.756
2.571
2.508
2.504
0.004
-0.016
1.000
2.168
1.172
4.422
1.160
3.835
3.887
1.190
ppm
Current Data Parameters
NAME VB-GSA-Piperazine
EXPNO 9
PROCNO 3
F2 - Acquisition Parameters
Date_ 20090203
Time_ 11.39
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 574.7
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
========== CHANNEL f1 ==========
NUC1 1H
P1 9.25 usec
PL1 0.00 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
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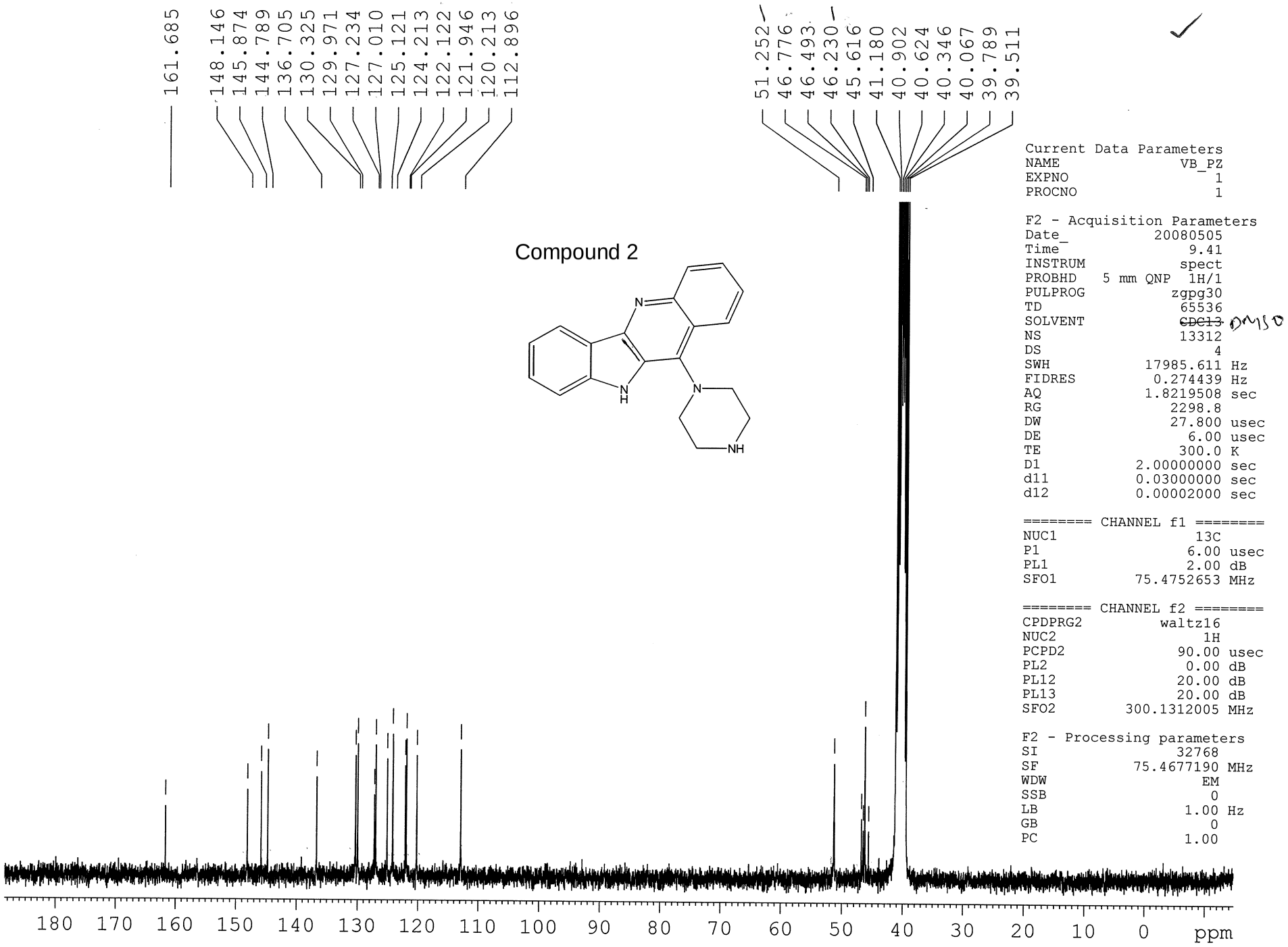
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


161.685
148.146
145.874
144.789
136.705
130.325
129.971
127.234
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125.121
124.213
122.122
121.946
120.213
112.896
51.252
46.776
46.493
46.230
45.616
41.180
40.902
40.624
40.346
40.067
39.789
39.511
Compound 2
N
N
H
N
NH
Current Data Parameters
NAME VB_PZ
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080505
Time 9.41
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PULPROG zgpg30
TD 65536
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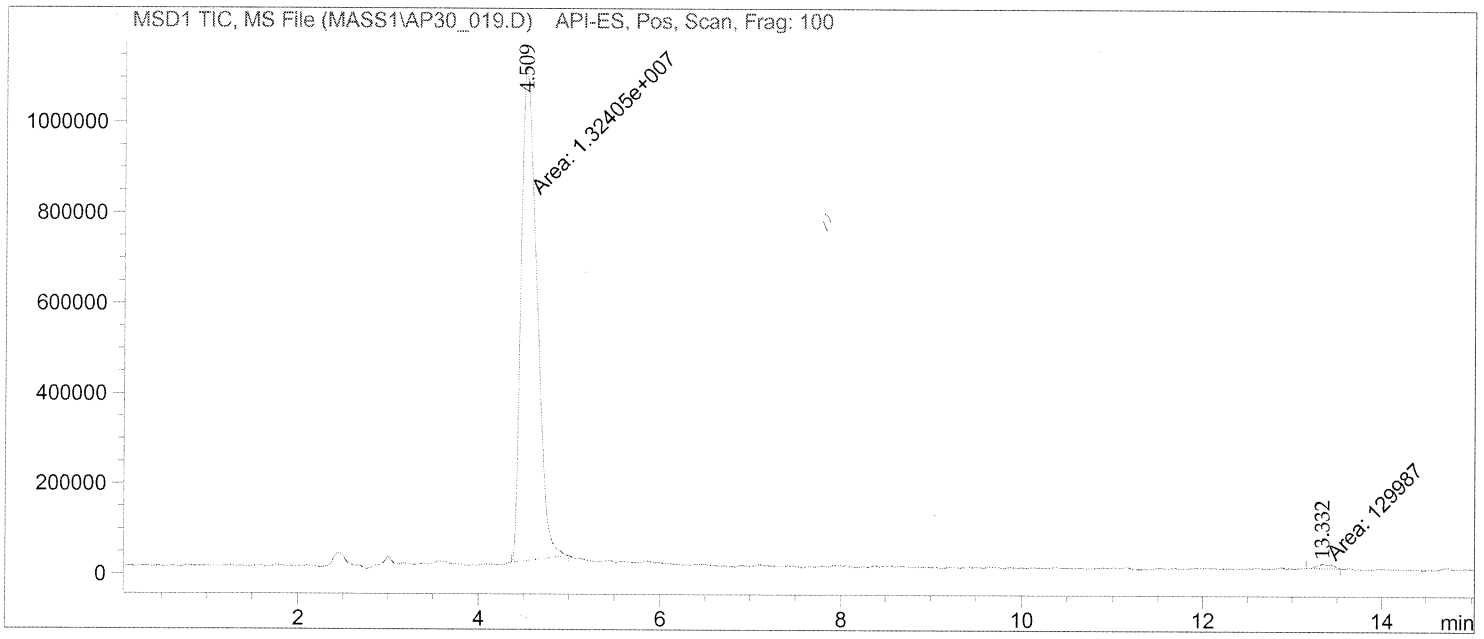
NS 13312
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2298.8
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 2.00 dB
SFO1 75.4752653 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 20.00 dB
PL13 20.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

==========

Injection Date : 4/30/08 7:30:22 PM
Sample Name : VB-pz Vial : 4
Acq. Operator : Karen Inj : 1
Inj Volume : 0.1 µl
Method : D:\HPCHEM\1\METHODS\SCOTT_C.M
Last changed : 4/30/08 7:45:44 PM by Karen
(modified after loading)
Zorbax C18 SB column,3.5u, 4.6 x 150mm, mp=30/70/0175, MeOH:water:formic A; scan 150-500;
flow 0.5mL/min; vcap 2500, frag 100; col temp 40 0.175

==========



==========

Area Percent Report

==========

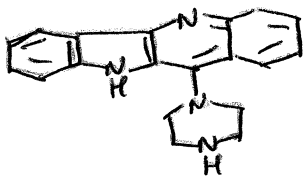
Sorted By : Retention Time
Calib. Data Modified : Tuesday, November 27, 2007 2:17:56 PM
Multiplier : 1.0000
Dilution : 1.0000

Signal 1: MSD1 TIC, MS File

Peak #	RetTime [min]	Sig	Type	Area	Area %	Name
1	4.509	1	MM	1.32405e7	99.0278	?
2	13.332	1	MM	1.29987e5	0.9722	

Totals : 1.33705e7

Compound 2



1 Warnings or Errors :

Warning : Calibration warnings (see calibration table listing)

==========

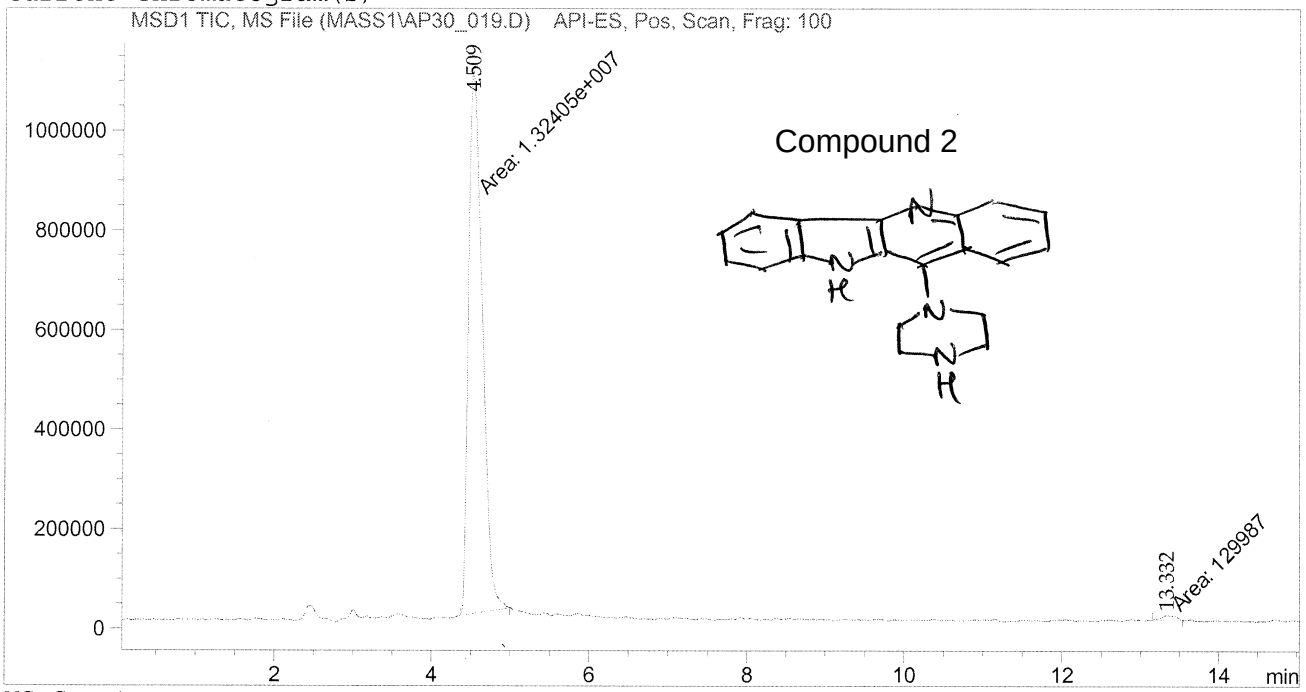
*** End of Report ***

==========

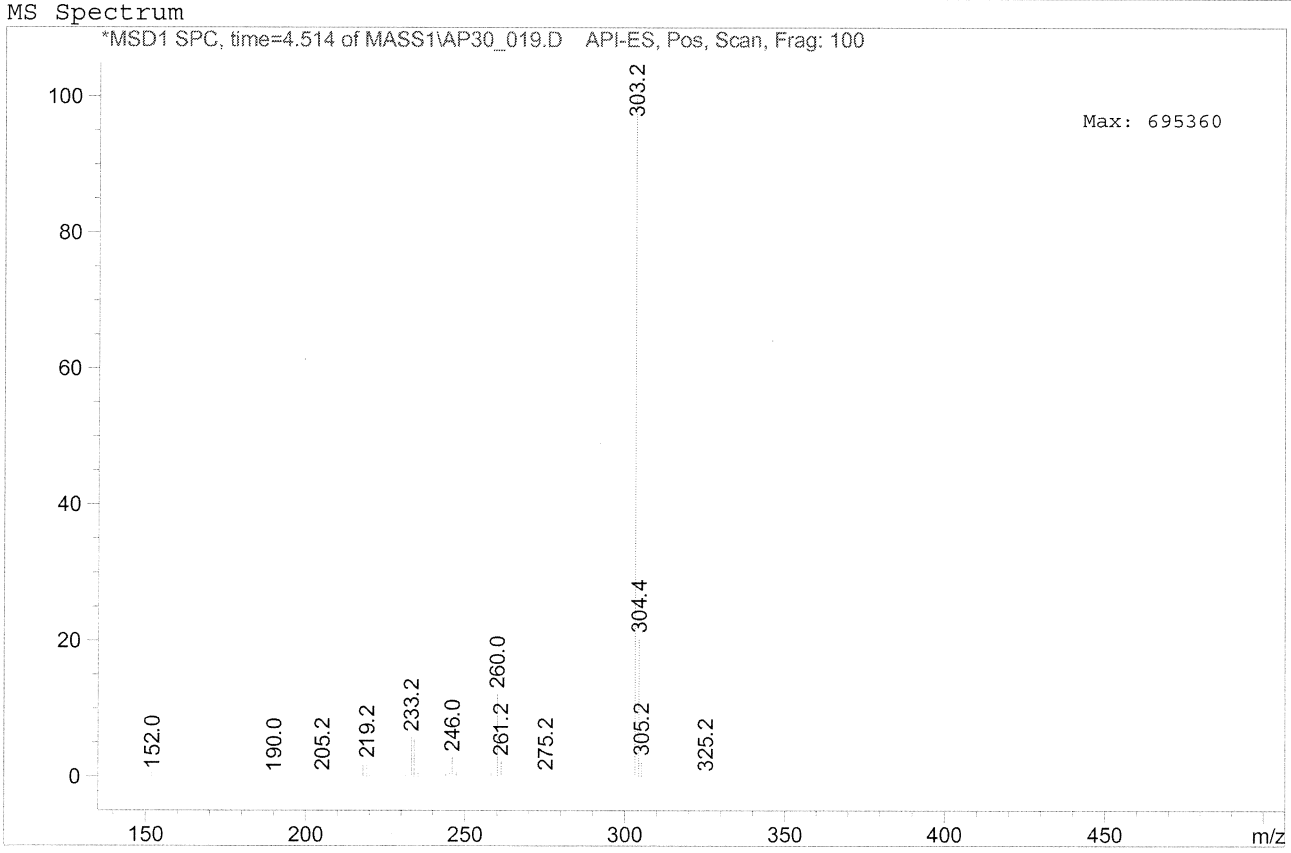
Injection Date : 4/30/08 7:30:22 PM
Sample Name : VB-pz Vial : 4
Acq. Operator : Karen Inj : 1
Inj Volume : 0.1 µl
Method : D:\HPCHEM\1\METHODS\SCOTT_C.M
Last changed : 4/30/08 7:45:44 PM by Karen
(modified after loading)

Zorbax C18 SB column,3.5u, 4.6 x 150mm, mp=30/70/0175, MeOH:water:formic A; scan 150-500; flow 0.5mL/min; vcap 2500, frag 100; col temp 40

Current Chromatogram(s)



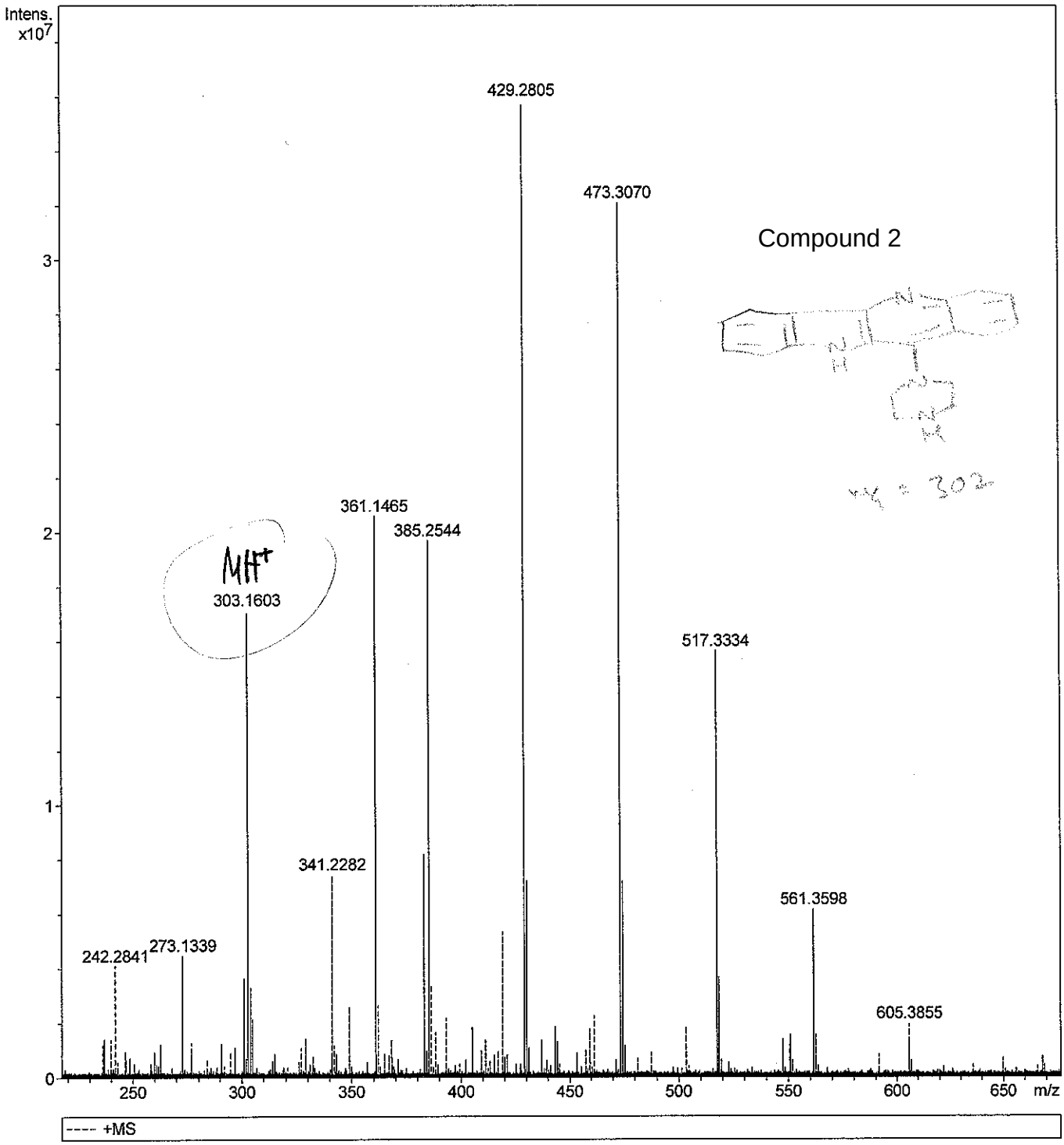
MS Spectrum



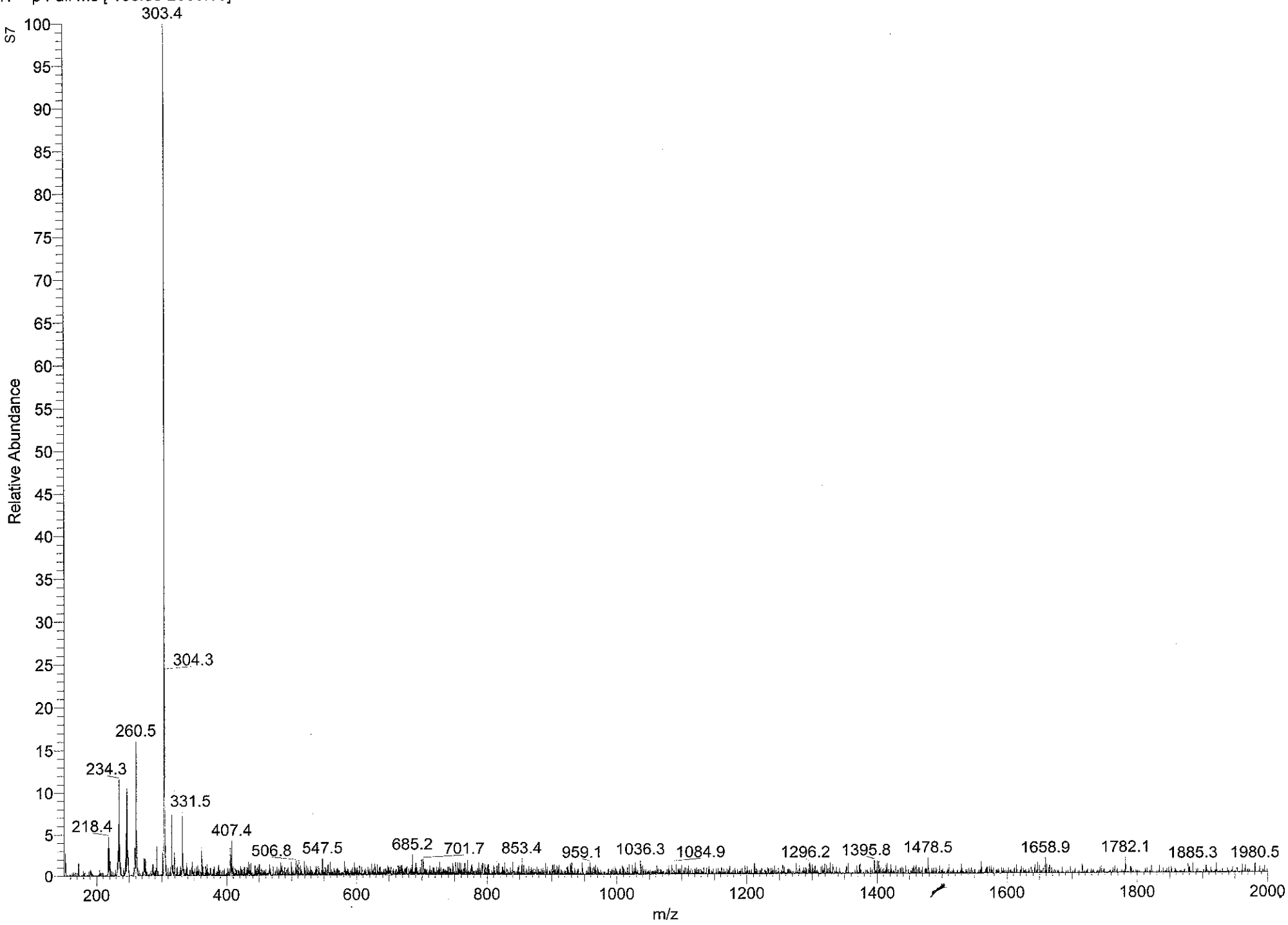
Generic Display Report

Analysis Info

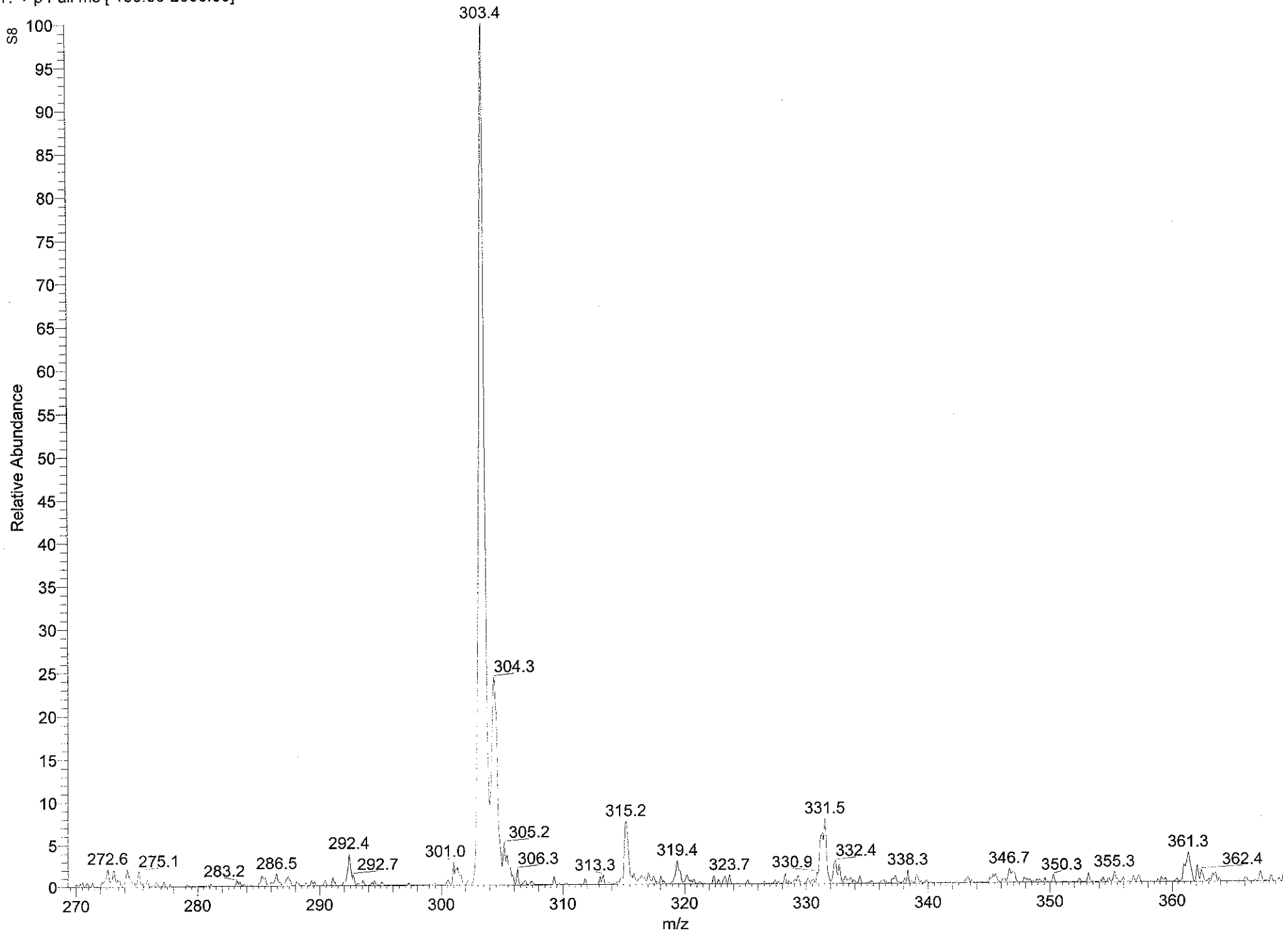
Analysis Name	D:\DATA\Facility_April_08\VB-PZ_000002.d	Acquisition Date	5/2/2008 2:25:45 PM
Method	ESI_101506	Operator	Administrator
Sample Name	VB-PZ	Instrument	apex-Qe
Comment	Venkat Boddupally VB-PZ in MeOH:ACN		



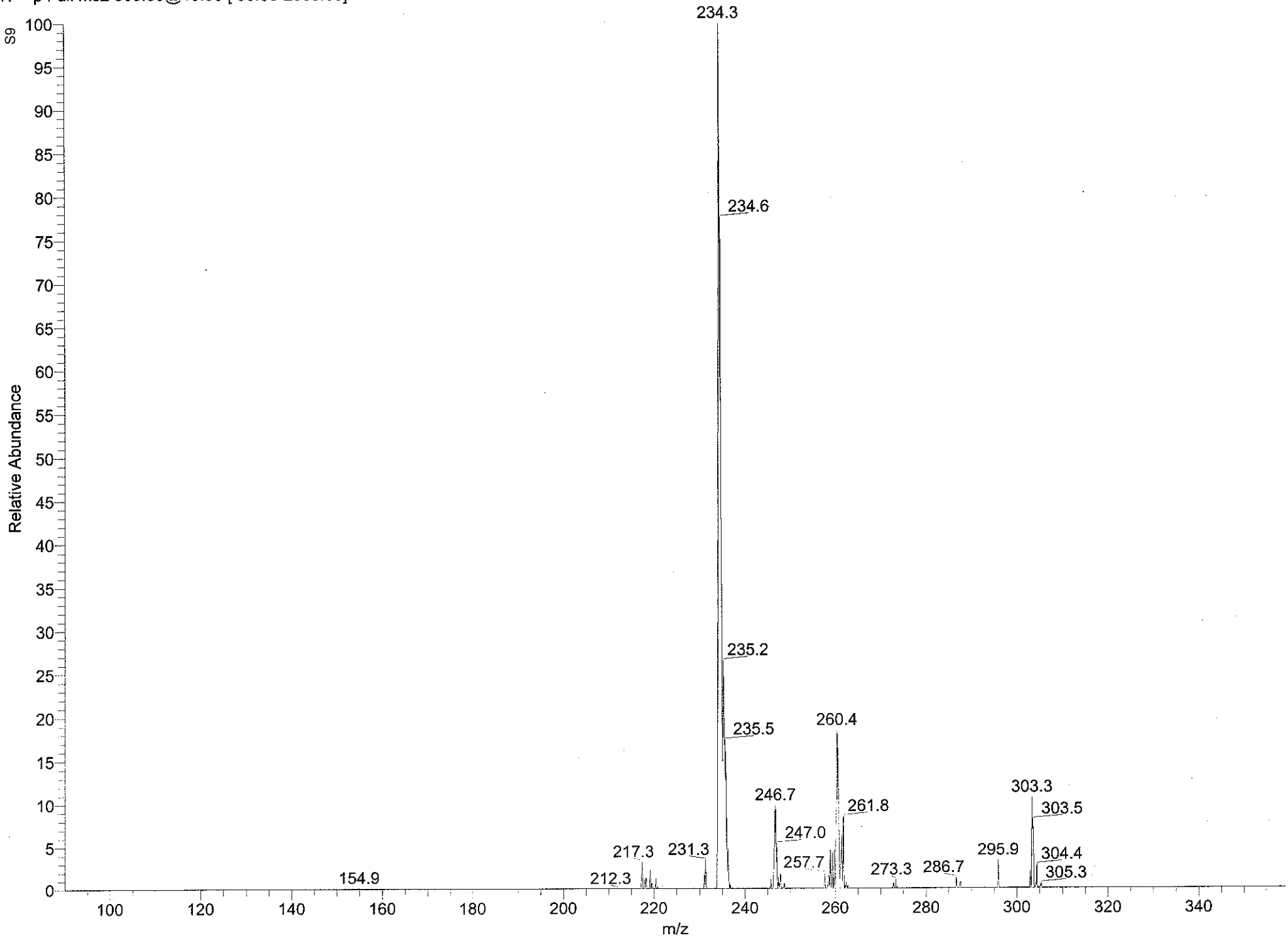
C:\Xcalibur\data\Facility Data\VB-PZ 05/02/2008 09:38:26 AM VB-PZ
Venkat B., MeOH:ACN
VB-PZ #40-43 RT: 1.43-1.53 AV: 4 NL: 1.39E7
T: + p Full ms [150.00-2000.00]



C:\Xcalibur\data\Facility Data\VB-PZ 05/02/2008 09:38:26 AM VB-PZ
Venkat B., MeOH:ACN
VB-PZ #40-43 RT: 1.43-1.53 AV: 4 NL: 1.39E7
T: + p Full ms [150.00-2000.00]



C:\Xcalibur\data\Facility Data\VB-PZ 05/02/2008 09:38:26 AM VB-PZ
Venkat B., MeOH:ACN
VB-PZ #30-32 RT: 1.06-1.15 AV: 3 NL: 5.88E5
T: + p Full ms2 303.30@40.00 [90.00-2000.00]

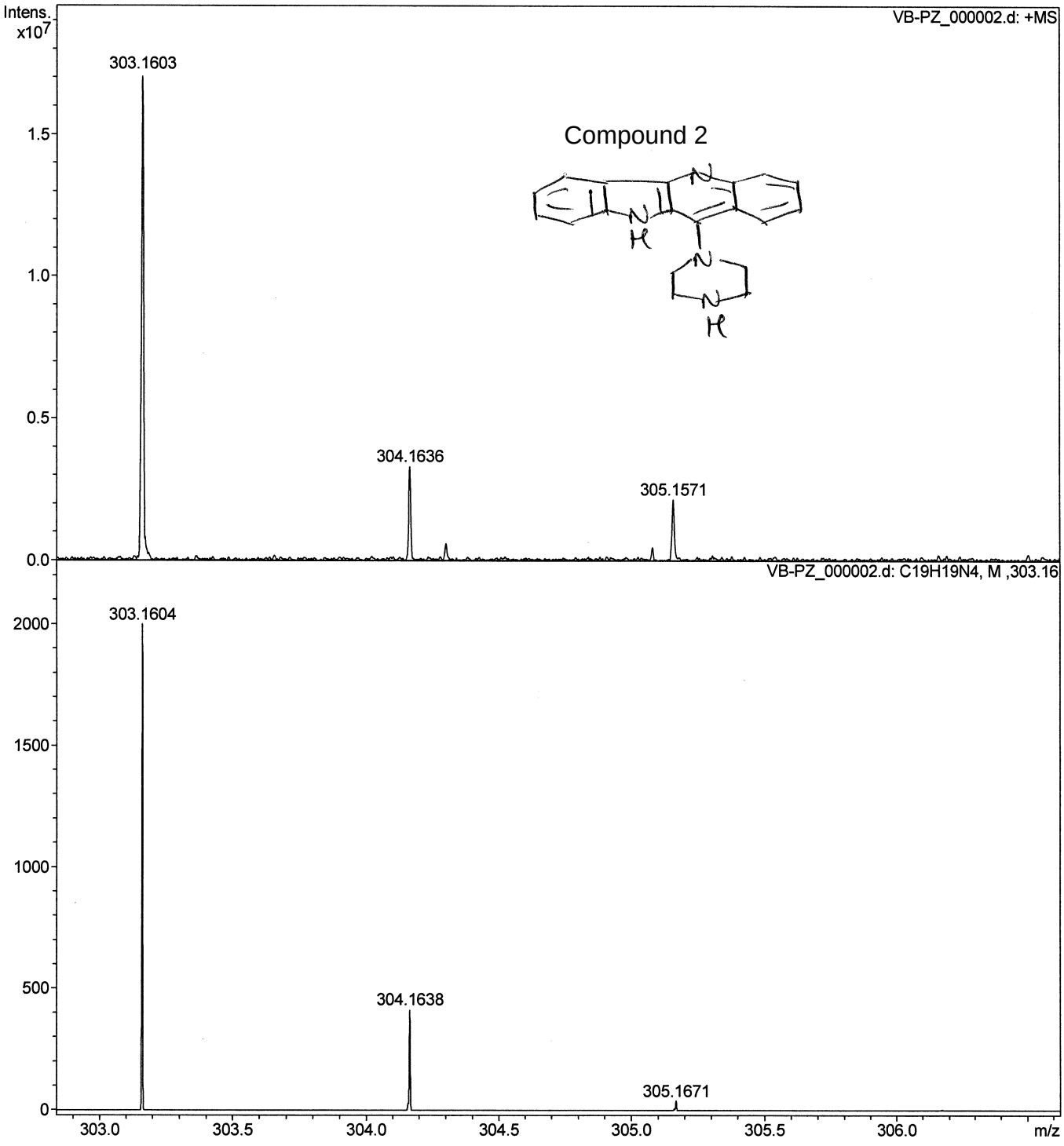


Generic Display Report

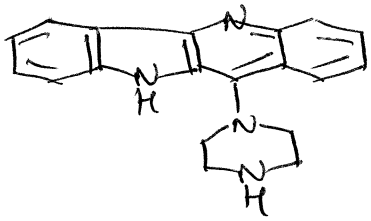
Analysis Info

Analysis Name	D:\DATA\Facility_April_08\VB-PZ_000002.d	Acquisition Date	5/2/2008 2:25:45 PM
Method	ESI_101506	Operator	Administrator
Sample Name	VB-PZ	Instrument	apex-Qe
Comment	Venkat Boddupally VB-PZ in MeOH:ACN		

Compound 2



Compound 2



Generate Molecular Formula

Min C_{12}

Max C_{21}

C 12-21

Generate

Save Results...

Help

Note: for m < 2000 the elements C, H, N, and O are considered implicitly.

Measured m/z 303.1603 Tolerance 2 mDa Charge 1

#	Mol. Formula	m/z	err [mDa]	err [ppm]	err [ppm]	mean err [ppm]	
1	C 18 H 23 O 4	303.1591	-1.24	4.1	-4.1	-2.2	0.
2	C 21 H 21 N 1 O 1	303.1618	1.44	4.7	4.7	7.1	0.
3	C 19 H 19 N 4	303.1604	0.10	0.3	0.3	2.2	0

Automatically locate monoisotopic peak

Maximum number of formulas 200

Check rings plus double bonds

Minimum 0 Maximum 0

Apply nitrogen rule

Electron configuration both

Filter H/C element ratio

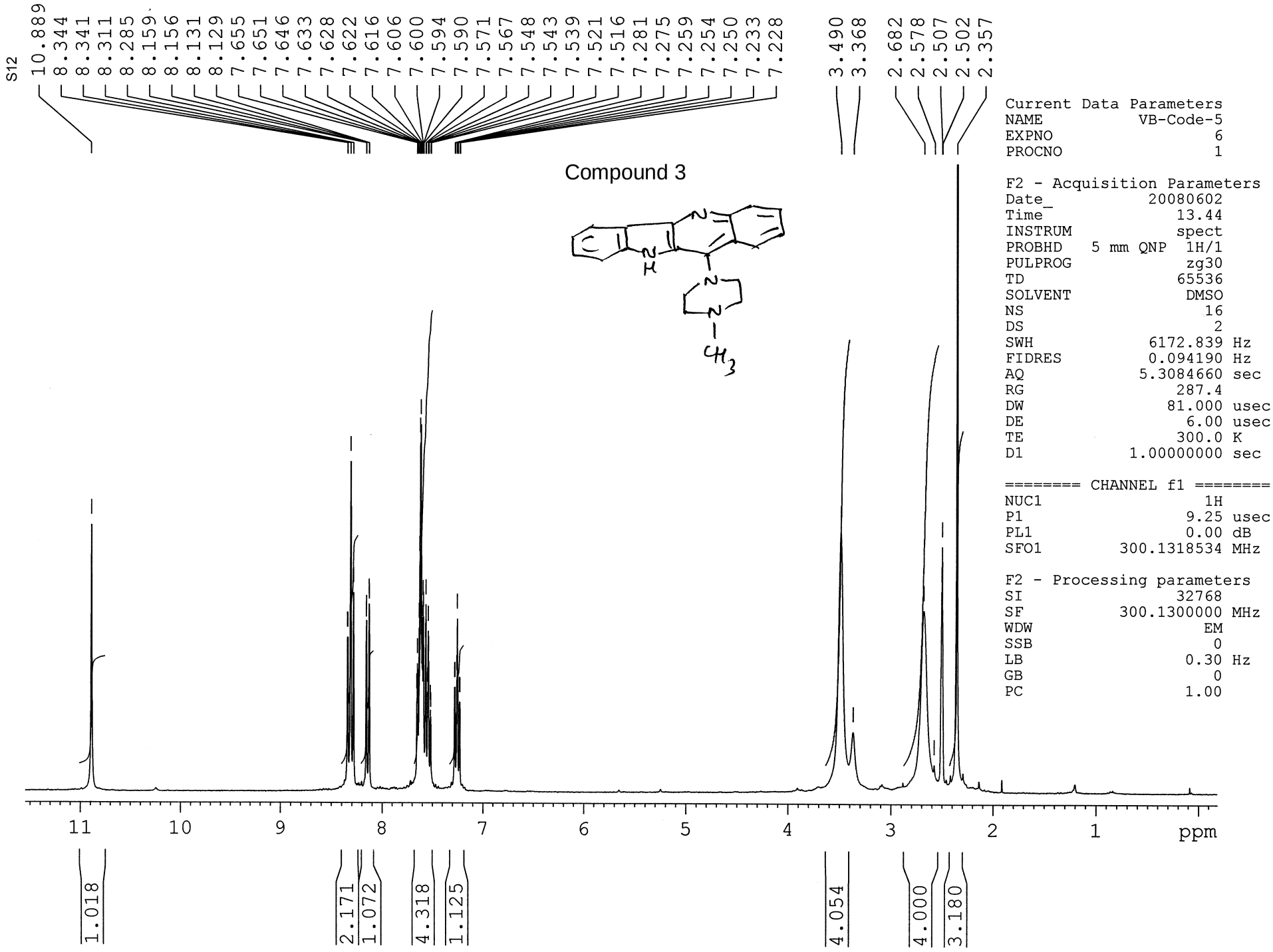
Minimum H/C [illegible] ...mum H/C 3

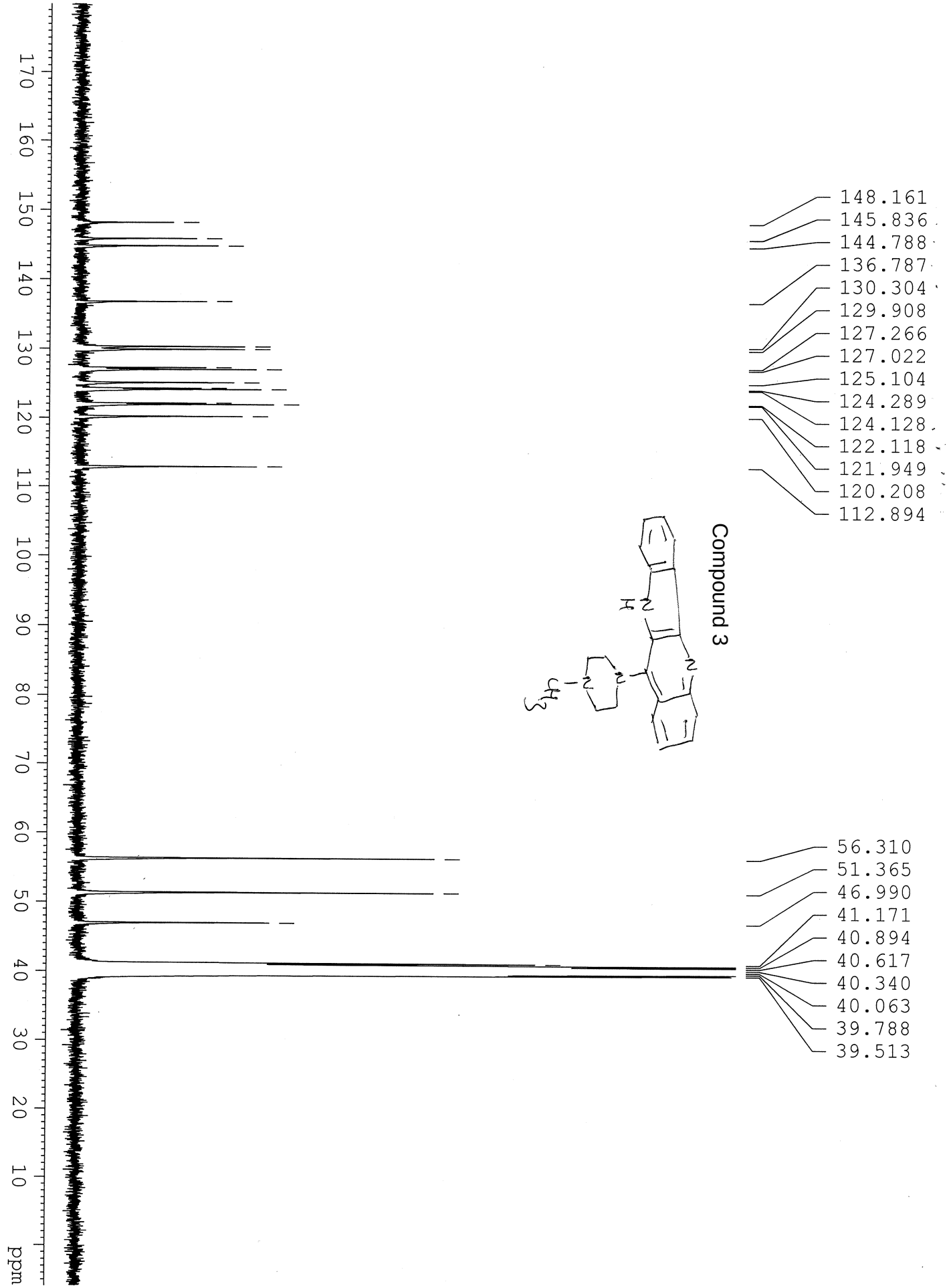
Estimate carbon number

Generate immediately

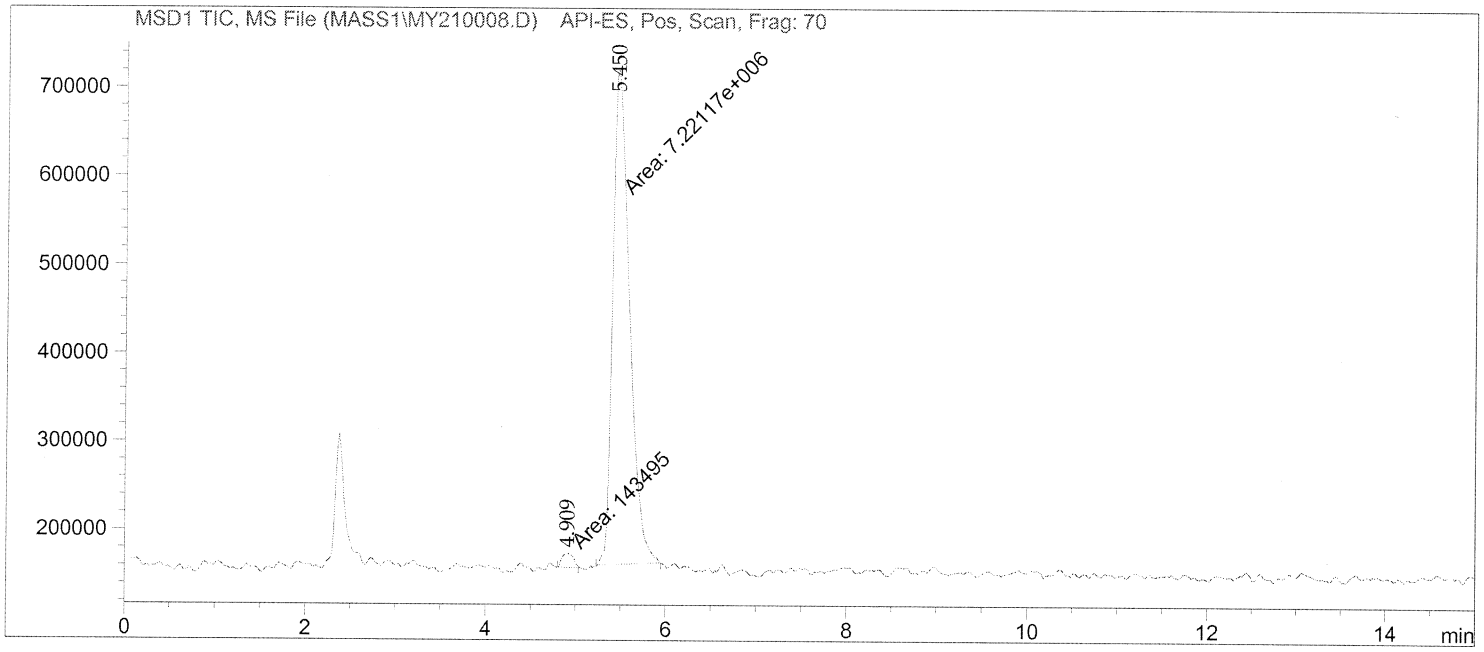
Save for Reporting

Show Pattern


S12
10.889
8.344
8.341
8.311
8.285
8.159
8.156
8.131
8.129
7.655
7.651
7.646
7.633
7.628
7.622
7.616
7.606
7.600
7.594
7.590
7.571
7.567
7.548
7.543
7.539
7.521
7.516
7.281
7.275
7.259
7.254
7.250
7.233
7.228
3.490
3.368
2.682
2.578
2.507
2.502
2.357
Compound 3
Current Data Parameters
NAME VB-Code-5
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080602
Time 13.44
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 287.4
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 9.25 usec
PL1 0.00 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
11
10
9
8
7
6
5
4
3
2
1
ppm
1.018
2.171
1.072
4.318
1.125
4.054
4.000
3.180

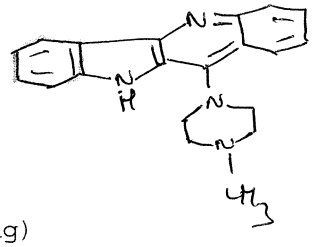

148.161
145.836
144.788
136.787
130.304
129.908
127.266
127.022
125.104
124.289
124.128
122.118
121.949
120.208
112.894
56.310
51.365
46.990
41.171
40.894
40.617
40.340
40.063
39.788
39.513
Compound 3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

```
==========================================================================
Injection Date  : 5/21/08 3:38:02 PM
Sample Name     : VB-N-Me-Pz                              Vial :   4
Acq. Operator   : Karen                                    Inj :   1
                                                  Inj Volume : 0.1 µl
Method          : D:\HPCHEM\1\METHODS\SCOTT_C.M
Last changed    : 5/21/08 3:36:29 PM by Karen
Zorbax C18 SB column,3.5u, 4.6 x 150mm, mp=30/70/0.175, MeOH:water:HAc; scan 150-500; flow
0.5mL/min; vcap 2500, frag 70; col temp 40
==========================================================================
```




```
==========================================================================
                          Area Percent Report
==========================================================================

Sorted By             :      Retention Time
Calib. Data Modified  :      Tuesday, November 27, 2007 2:17:56 PM
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: MSD1 TIC, MS File

Peak RetTime Sig  Type      Area       Area     Name
  #   [min]                            %
----|-------|---|------|----------|--------|--------------------------
   1   4.909  1  MM     1.43495e5    1.9484 ?
   2   5.450  1  MM     7.22117e6   98.0516

Totals :                 7.36467e6

1 Warnings or Errors :

Warning : Calibration warnings (see calibration table listing)

==========================================================================
                          *** End of Report ***
```

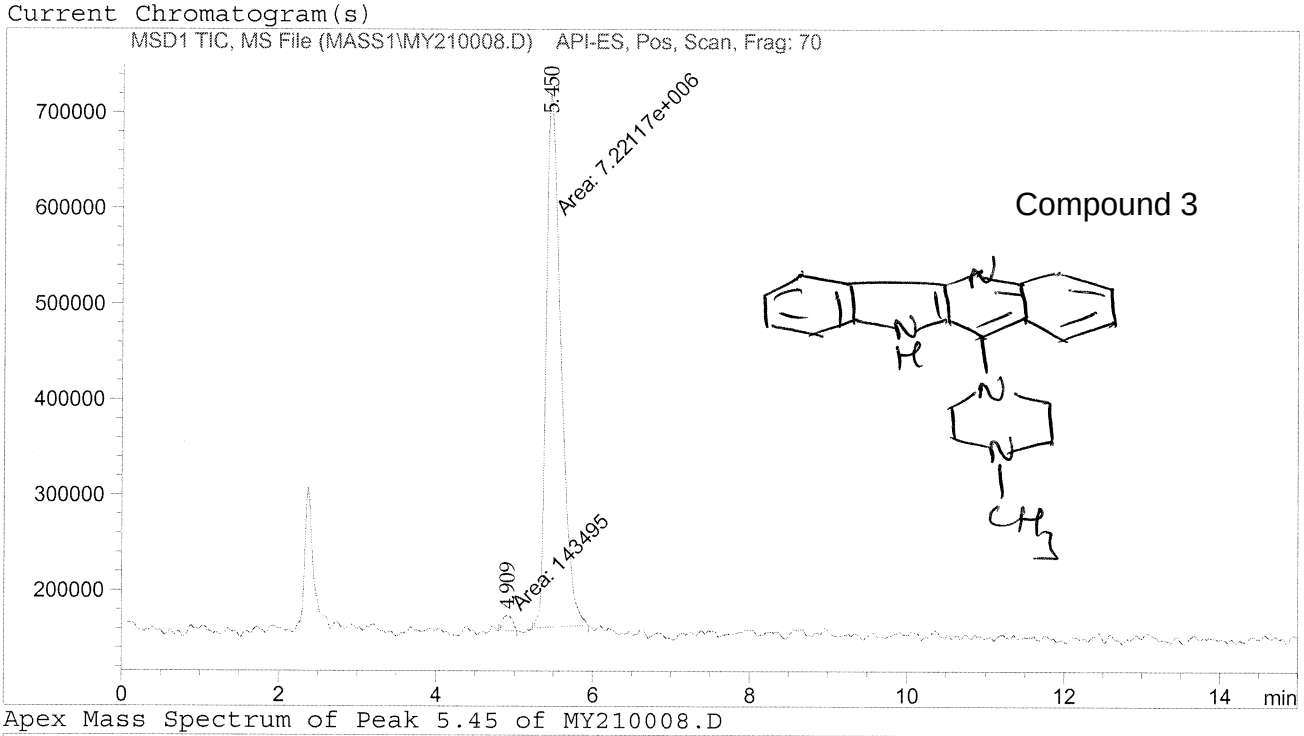
Compound 3



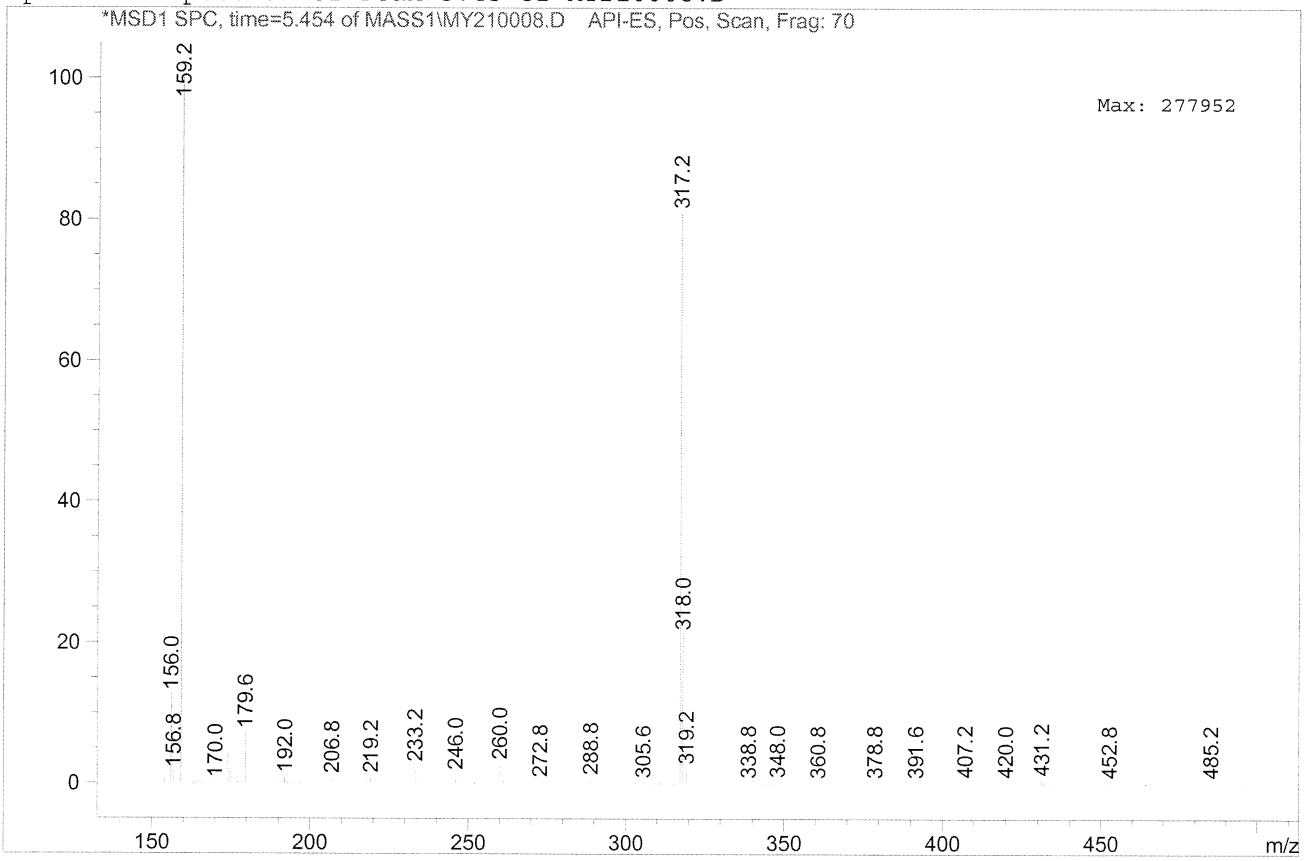
Print of all graphic windows
MeOH

==========
Injection Date : 5/21/08 3:38:02 PM
Sample Name : VB-N-Me-Pz Vial : 4
Acq. Operator : Karen Inj : 1
Inj Volume : 0.1 µl
Method : D:\HPCHEM\1\METHODS\SCOTT_C.M
Last changed : 5/21/08 3:36:29 PM by Karen
Zorbax C18 SB column,3.5u, 4.6 x 150mm, mp=30/70/0.175, MeOH:water:HAc; scan 150-500; flow 0.5mL/min; vcap 2500, frag 70; col temp 40

Current Chromatogram(s)

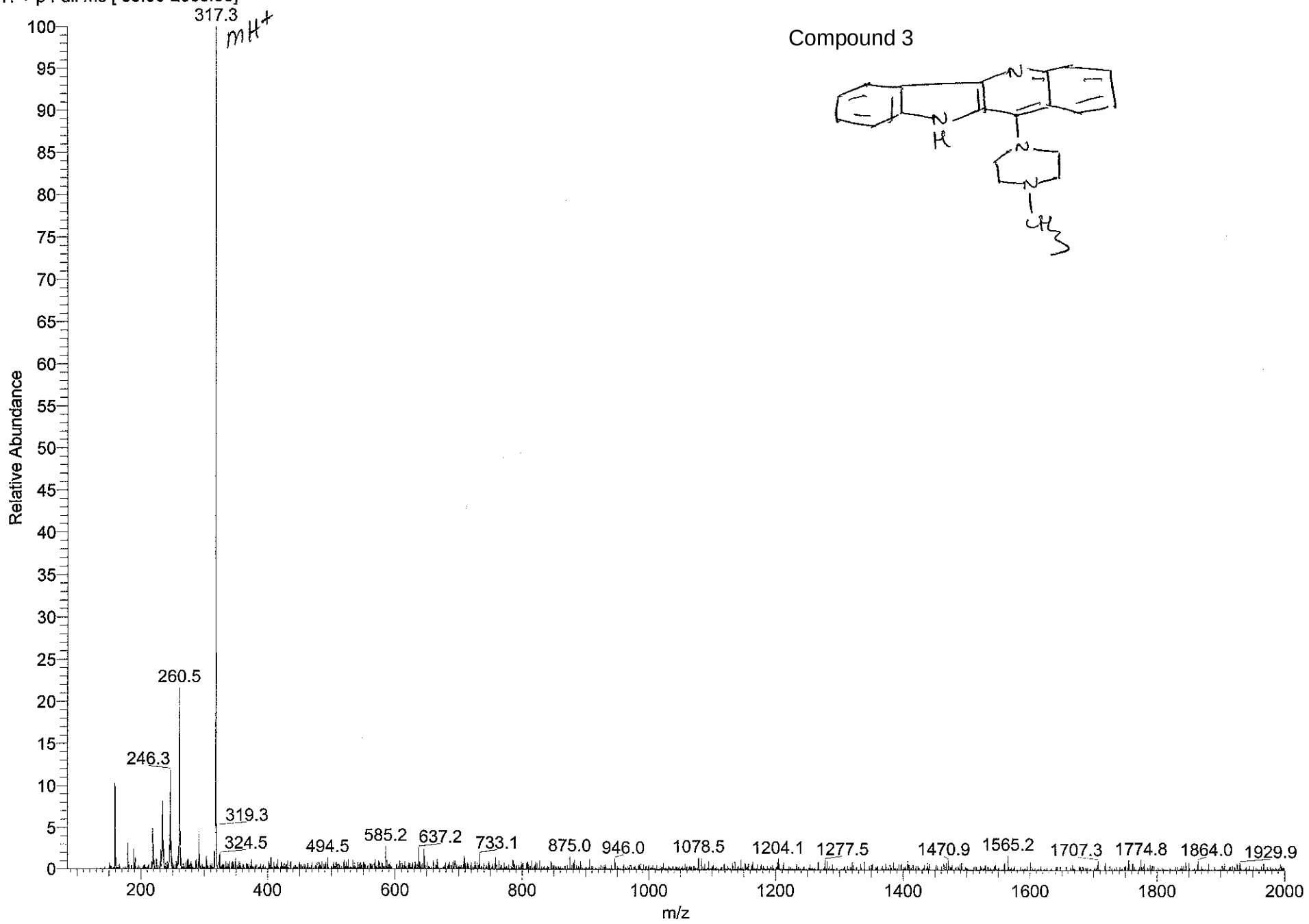


Apex Mass Spectrum of Peak 5.45 of MY210008.D



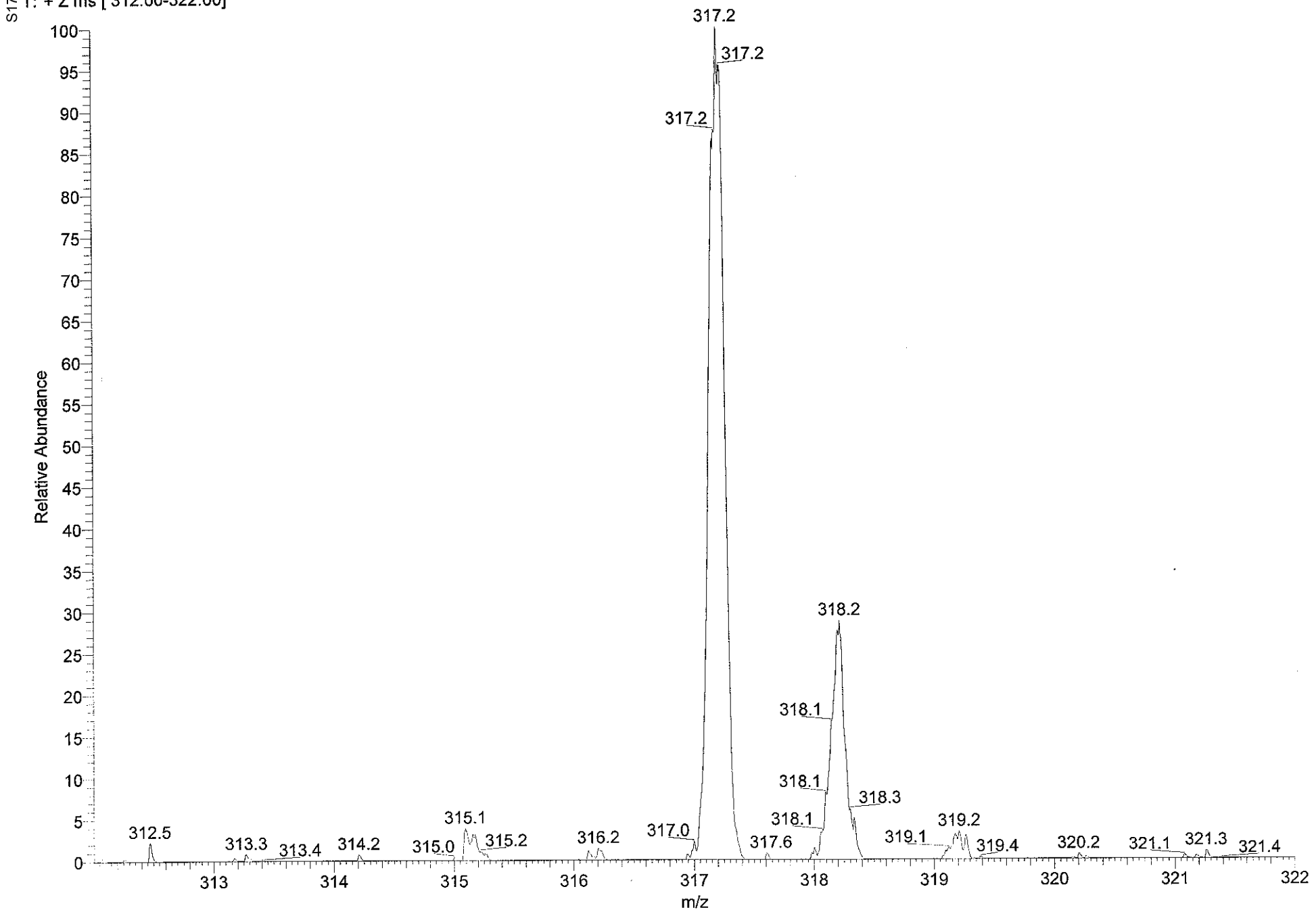
C:\Xcalibur\data\Facility Data\VB_45 05/22/2008 04:29:09 PM VB_45
Venkat Boddupally; MeOH:H2O AcOH
VB_45 #31-34 RT: 0.86-0.95 AV: 4 NL: 7.85E6
T: + p Full ms [85.00-2000.00]

S16

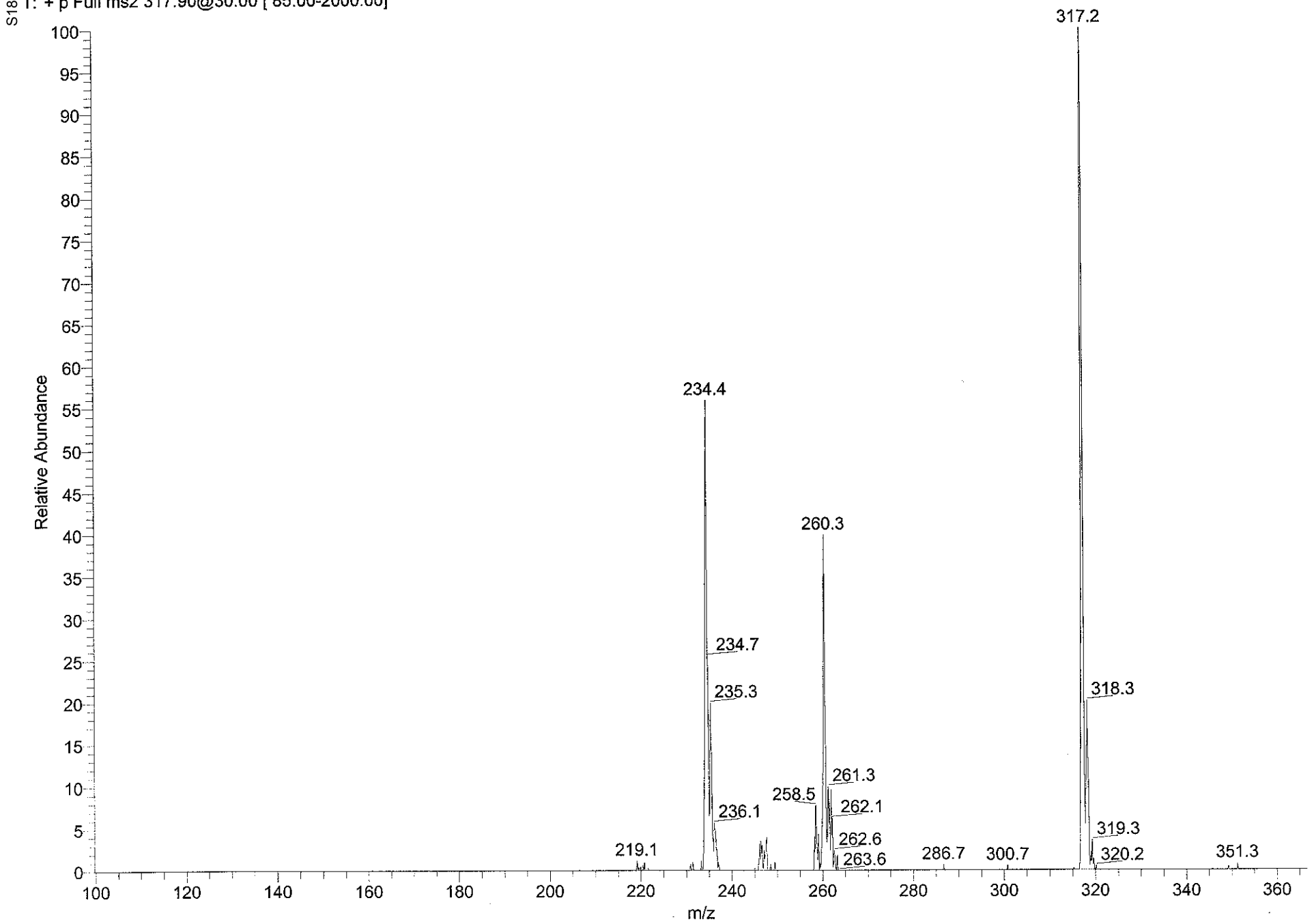


Compound 3

C:\Xcalibur\data\Facility Data\VB_45 05/22/2008 04:29:09 PM VB_45
Venkat Boddupally; MeOH:H2O AcOH
VB_45 #9-16 RT: 0.24-0.36 AV: 8 NL: 2.55E6
T: + Z ms [312.00-322.00]



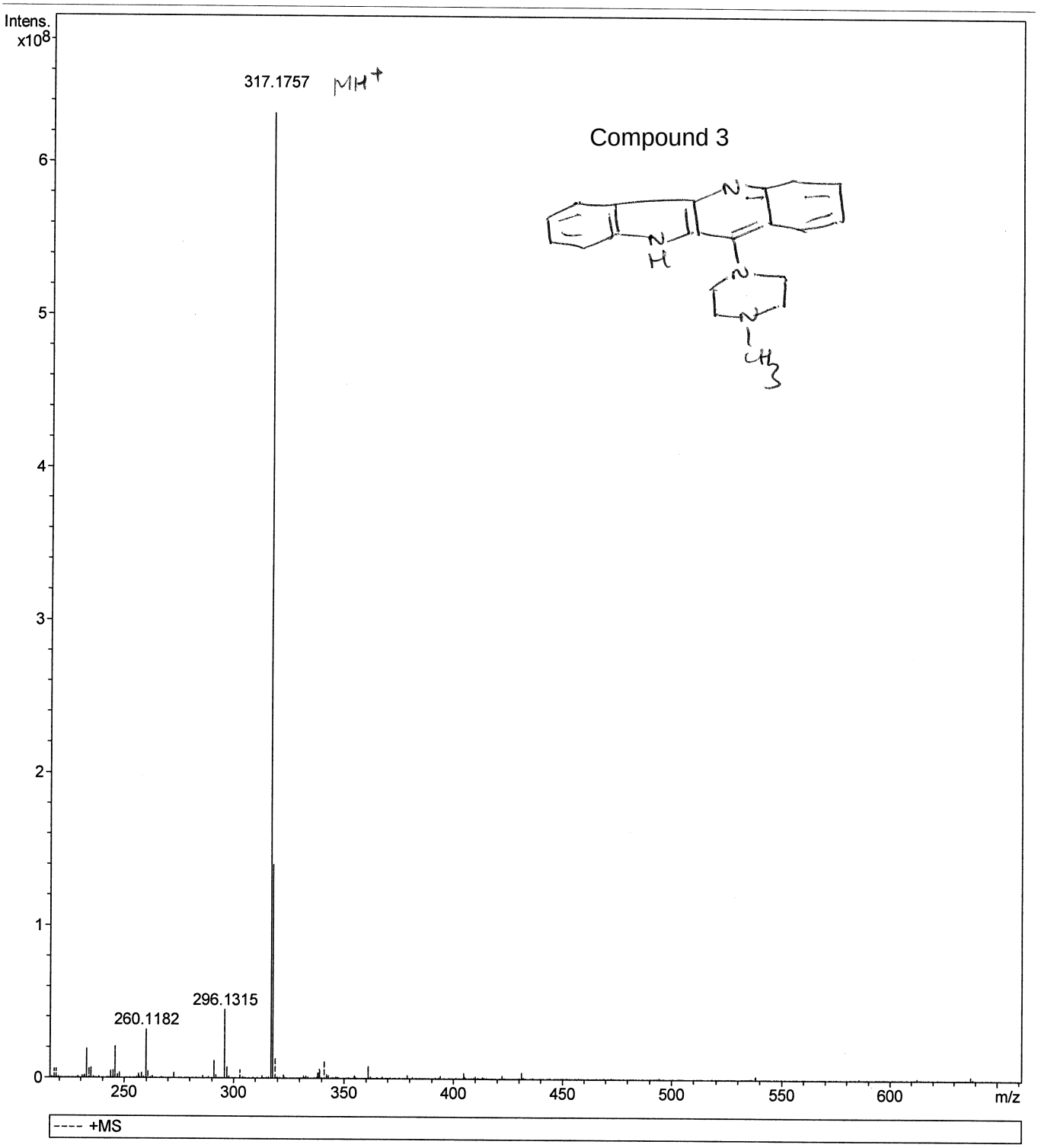
C:\Xcalibur\data\Facility Data\VB_45 05/22/2008 04:29:09 PM VB_45
Venkat Boddupally; MeOH:H2O AcOH
VB_45 #26-29 RT: 0.68-0.79 AV: 4 NL: 4.85E6
T: + p Full ms2 317.90@30.00 [85.00-2000.00]



Generic Display Report

Analysis Info

Analysis Name	D:\DATA\Facility_May_5\VB_45_000001.d	Acquisition Date	5/27/2008 1:04:23 PM
Method	ESI_101506	Operator	Administrator
Sample Name	VB-45	Instrument	apex-Qe
Comment	Venkat B., MeOH:H2O:AcOH		



Generate Molecular Formula

Min C_{14}

Max

C 14-n

Generate

Save Results...

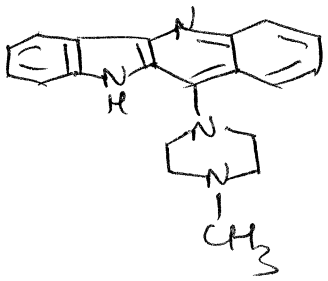
Help

Note: for m < 2000 the elements C, H, N, and O are considered implicitly.

Measured m/z 317.1757 Tolerance 2 mDa Charge 1

#	Mol. Formula	m/z	err [mDa]	|err| [ppm]	err [ppm]	mean err [ppm]	
1	C 19 H 25 O 4	317.1747	-0.95	3.0	-3.0	-3.1	C
2	C 20 H 21 N 4	317.1761	0.35	1.2	1.2	0.9	C
3	C 22 H 23 N 1 O 1	317.1774	1.73	5.5	5.5	5.3	C

Compound 3



Automatically locate monoisotopic peak Maximum number of formulas 200

Check rings plus double bonds Minimum 0 Maximum 0

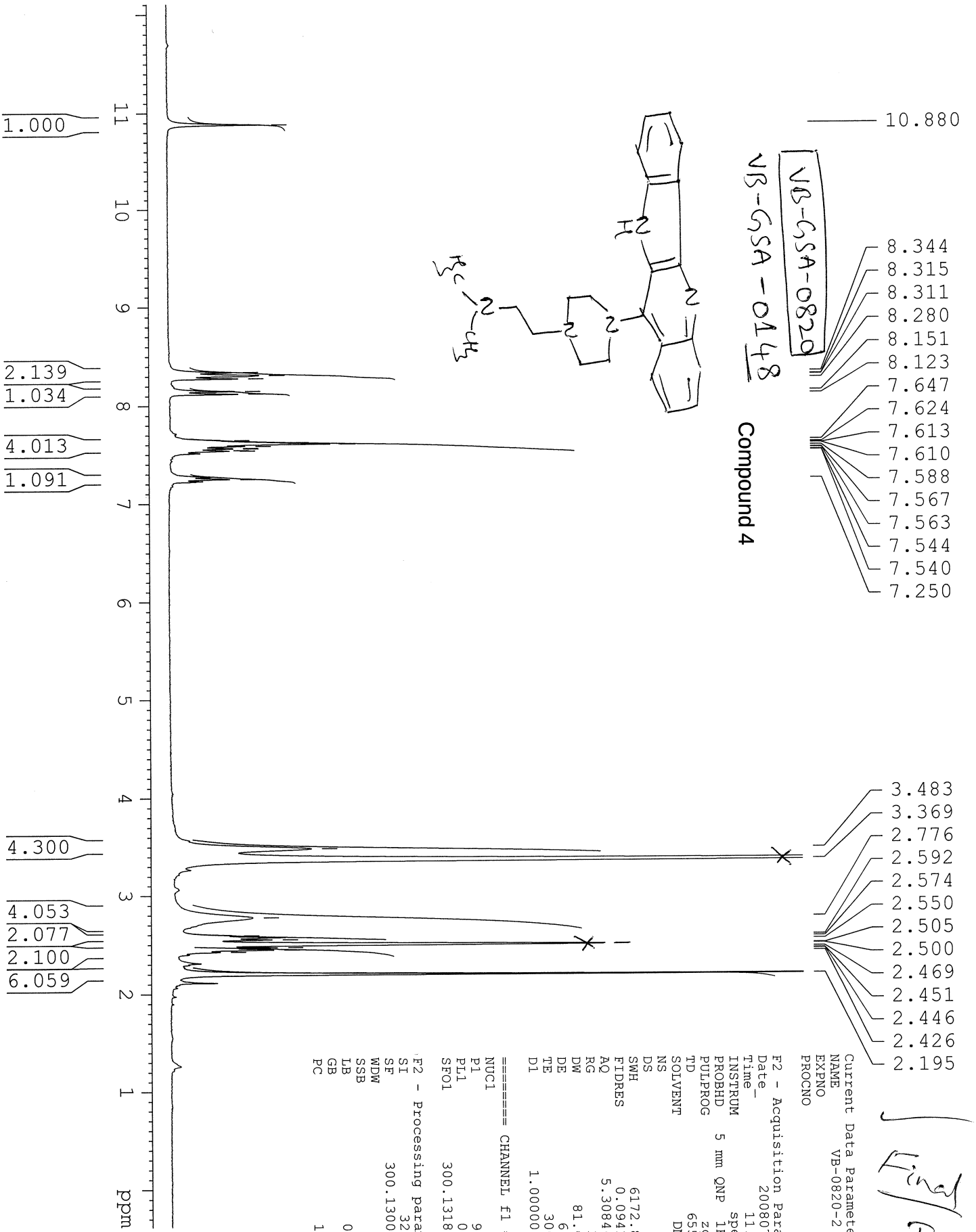
Apply nitrogen rule Electron configuration both

Filter H/C element ratio Minimum H/C 0 Maximum H/C 3

Estimate carbon number Generate immediately

Save for Reporting

Show Pattern


VB-GSA-0820
VB-GSA-0148
Compound 4
10.880
8.344
8.315
8.311
8.280
8.151
8.123
7.647
7.624
7.613
7.610
7.588
7.567
7.563
7.544
7.540
7.250
3.483
3.369
2.776
2.592
2.574
2.550
2.505
2.500
2.469
2.451
2.446
2.426
2.195
1.000
2.139
1.034
4.013
1.091
4.300
4.053
2.077
2.100
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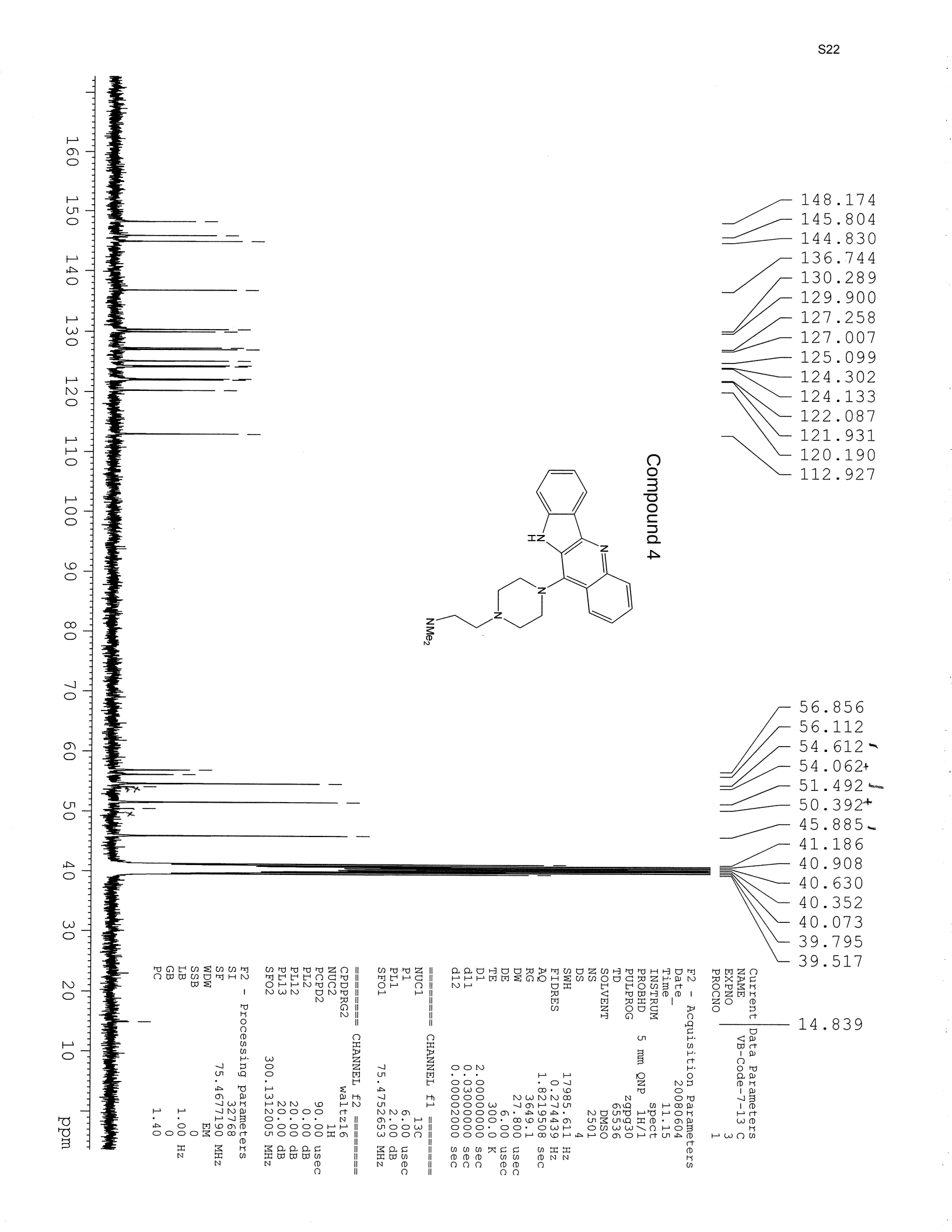
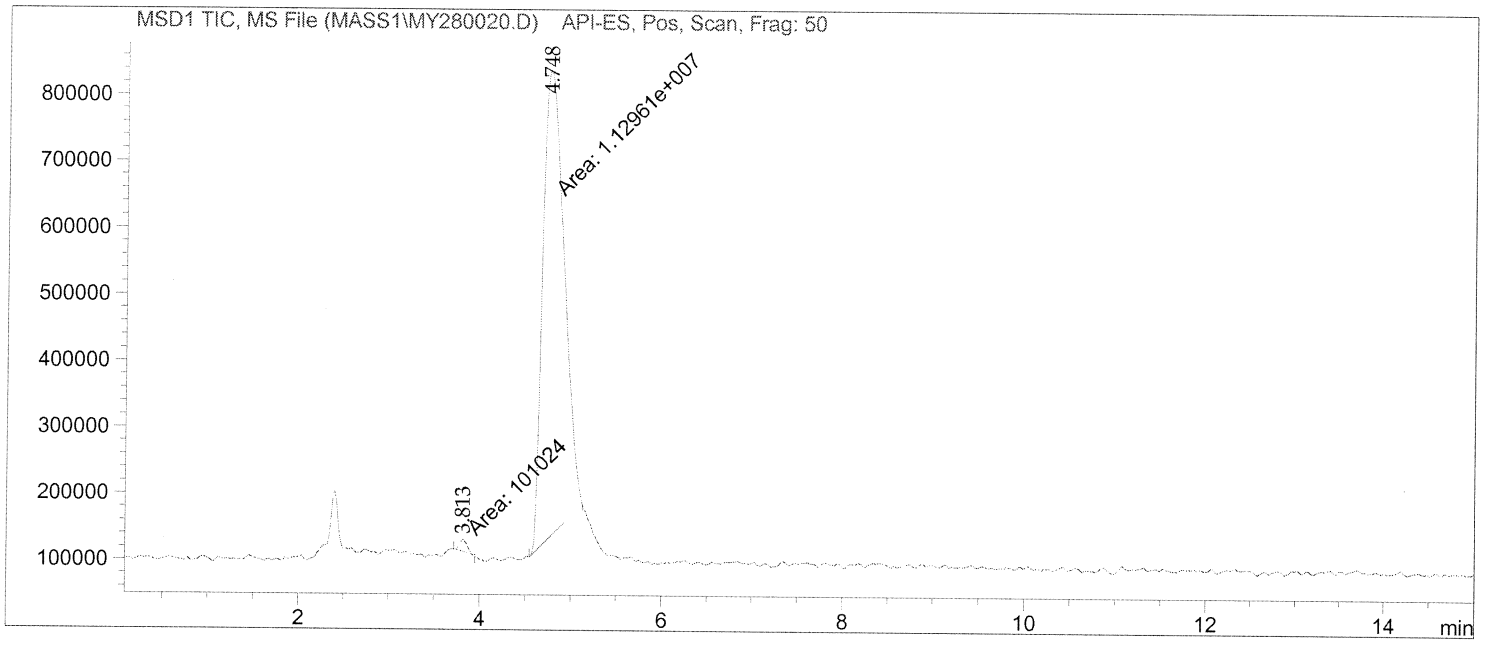
11
10
9
8
7
6
5
4
3
2
1
ppm
Current Data Parameters
NAME VB-0820-2 nd
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080714
Time_ 11.30
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 362
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
========== CHANNEL f1 ==========
NUC1 1H
P1 9.25 usec
PL1 0.00 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

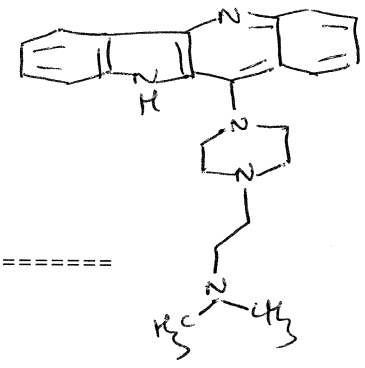

148.174
145.804
144.830
136.744
130.289
129.900
127.258
127.007
125.099
124.302
124.133
122.087
121.931
120.190
112.927
Compound 4
NMe2
56.856
56.112
54.612
54.062
51.492
50.392
45.885
41.186
40.908
40.630
40.352
40.073
39.795
39.517
14.839
Current Data Parameters
NAME VB-Code-7-13 C
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080604
Time_ 11.15
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2501
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 3649.1
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
========== CHANNEL f1 ==========
NUC1 13C
P1 6.00 usec
PL1 2.00 dB
SFO1 75.4752653 MHz
========== CHANNEL f2 ==========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 20.00 dB
PL13 20.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

```
==========================================================================
Injection Date  : 5/28/08 5:04:30 PM
Sample Name     : VB-48-373                              Vial :  13
Acq. Operator   : Karen                                   Inj :   1
                                                  Inj Volume : 0.1 µl
Method          : D:\HPCHEM\1\METHODS\SCOTT_C.M
Last changed    : 5/28/08 5:02:33 PM by Karen
                  (modified after loading)
Zorbax C18 SB column,3.5u, 4.6 x 150mm, mp=40/60/0.150, MeOH:water:HAc; scan 150-500; flow
0.5mL/min; vcap 2500, frag 50; col temp 30
==========================================================================
```




```
==========================================================================
                          Area Percent Report
==========================================================================

Sorted By             :      Retention Time
Calib. Data Modified  :      Tuesday, November 27, 2007 2:17:56 PM
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: MSD1 TIC, MS File

Peak RetTime Sig  Type      Area       Area     Name
  #   [min]                            %
----|-------|---|------|----------|--------|-------------------------
   1   3.813  1   MM     1.01024e5    0.8864 ?
   2   4.748  1   MM     1.12961e7   99.1136

Totals :                  1.13971e7

1 Warnings or Errors :

Warning : Calibration warnings (see calibration table listing)

==========================================================================
                        *** End of Report ***
```

Compound 4



Print of all graphic windows
MeOH

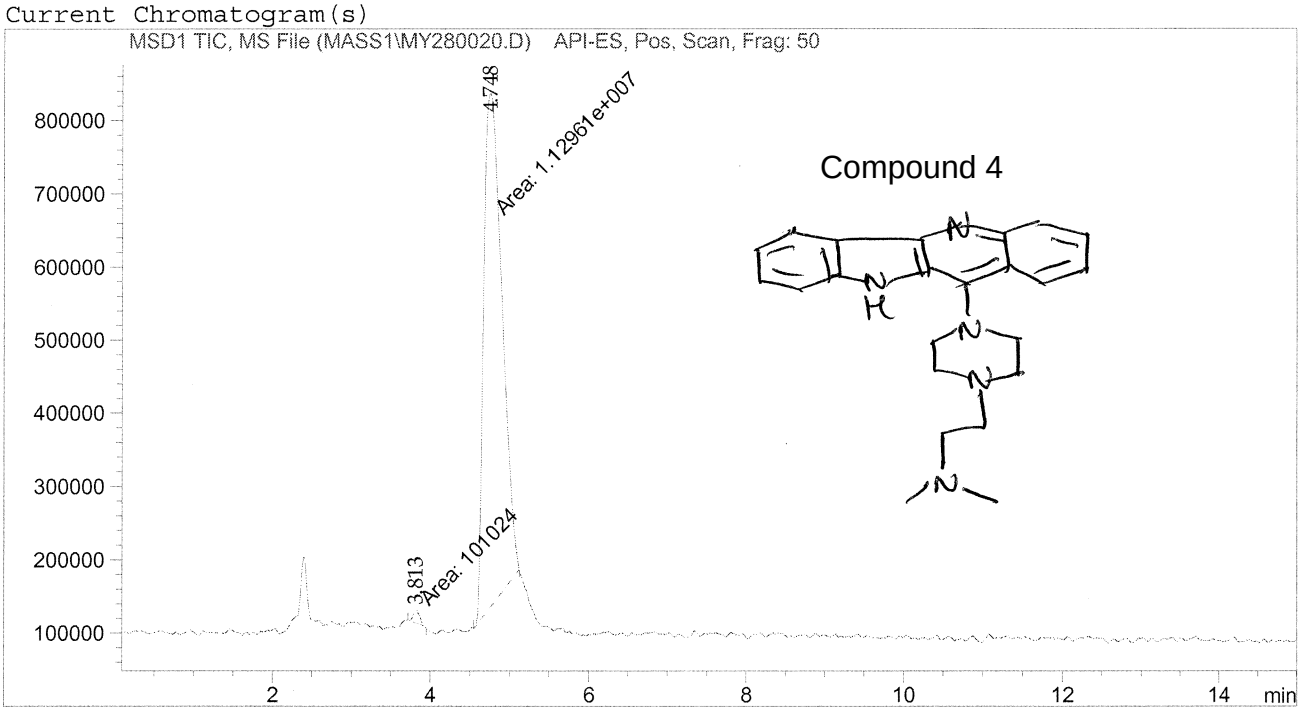
==========

Injection Date : 5/28/08 5:04:30 PM
Sample Name : VB-48-373 Vial : 13
Acq. Operator : Karen Inj : 1
Inj Volume : 0.1 µl

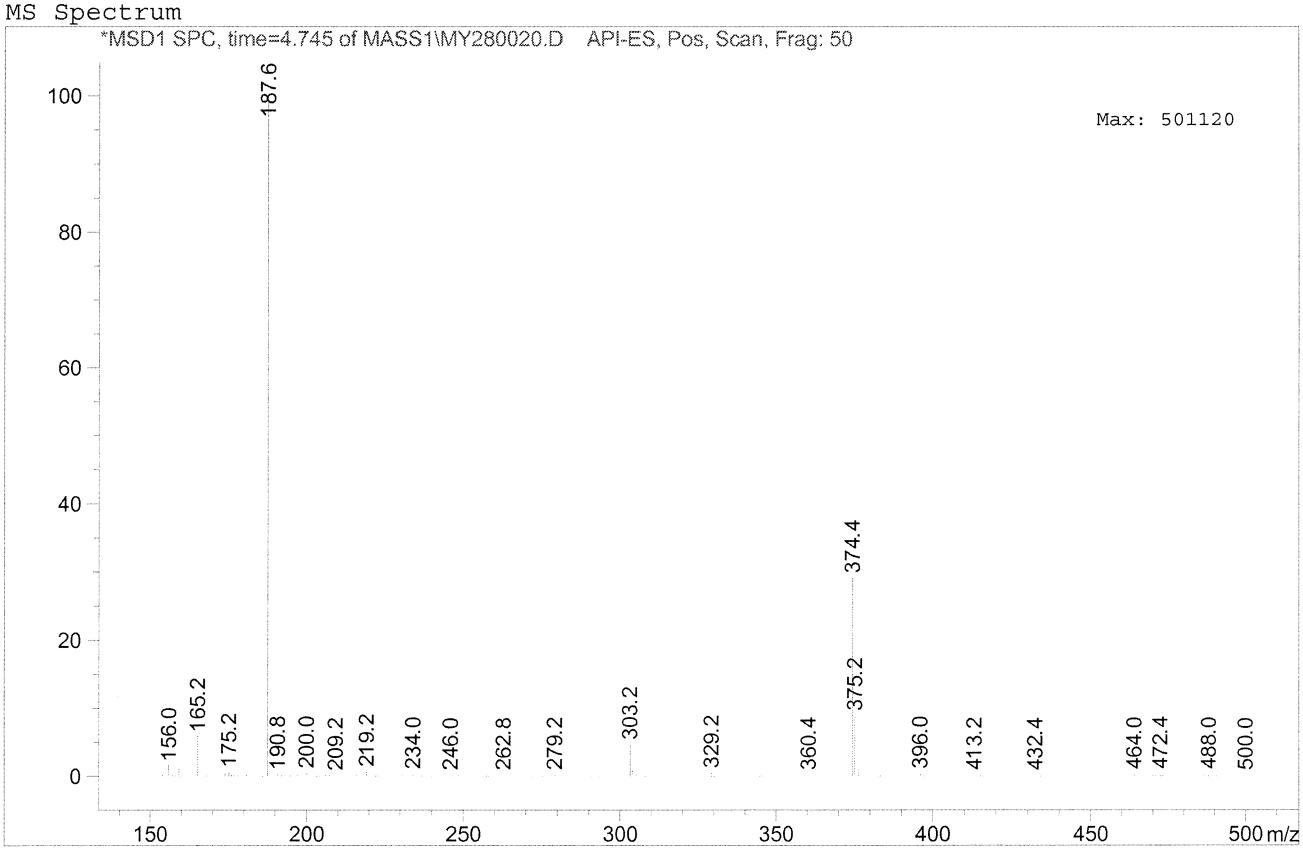
Method : D:\HPCHEM\1\METHODS\SCOTT_C.M
Last changed : 5/28/08 5:02:33 PM by Karen
(modified after loading)

Zorbax C18 SB column,3.5u, 4.6 x 150mm, mp=40/60/0.150, MeOH:water:HAc; scan 150-500; flow 0.5mL/min; vcap 2500, frag 50; col temp 30

Current Chromatogram(s)

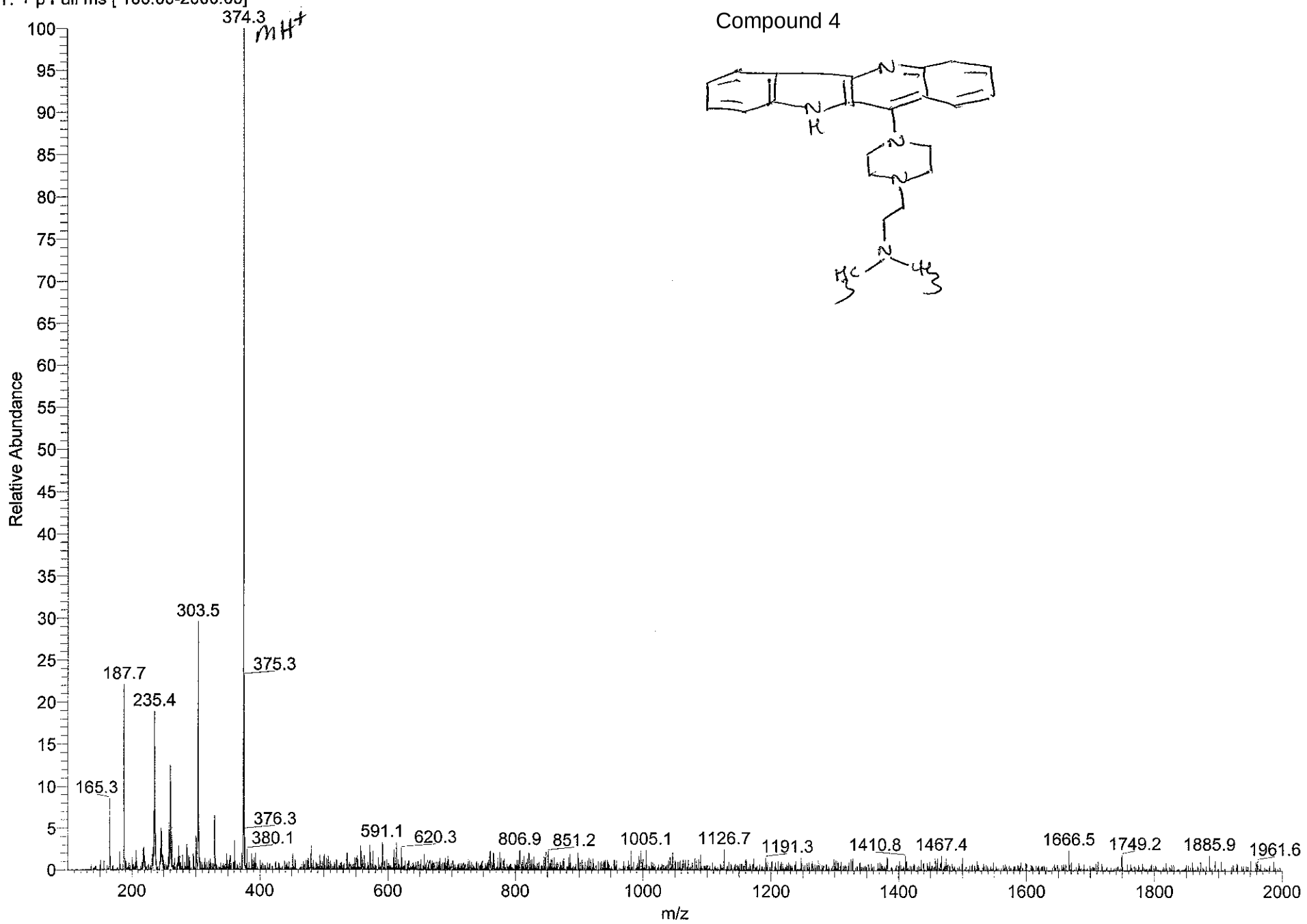


MS Spectrum



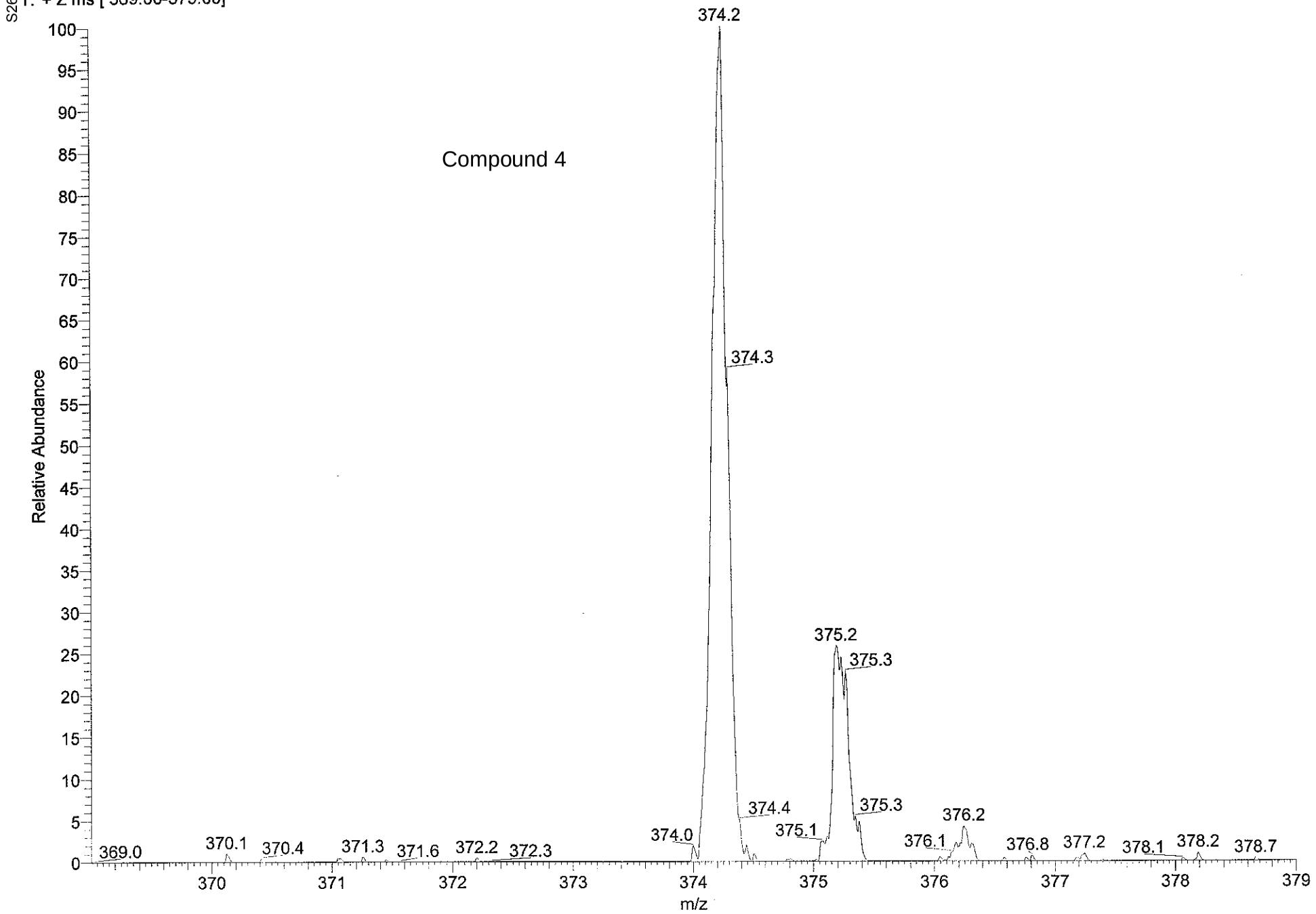
C:\Xcalibur\data\Facility Data\VB_48 05/22/2008 04:40:57 PM VB_48
Venkat Boddupally; MeOH:H2O AcOH
VB_48 #23-27 RT: 0.64-0.77 AV: 5 NL: 8.71E6
T: + p Full ms [100.00-2000.00]

S25



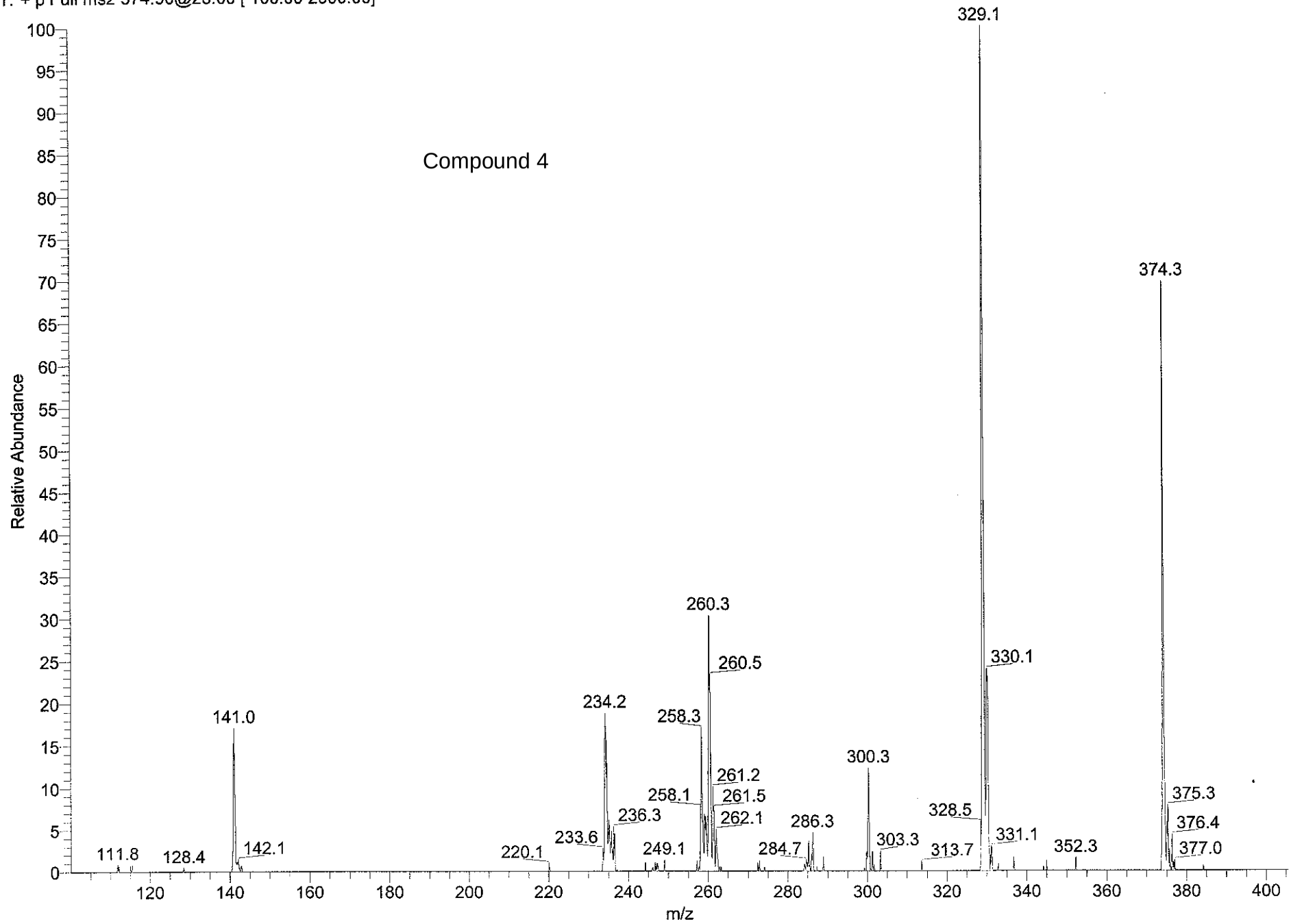
Compound 4

C:\Xcalibur\data\Facility Data\VB_48 05/22/2008 04:40:57 PM VB_48
Venkat Boddupally; MeOH:H2O AcOH
VB_48 #7-13 RT: 0.20-0.30 AV: 7 NL: 3.51E6
T: + Z ms [369.00-379.00]



C:\Xcalibur\data\Facility Data\VB_48 05/22/2008 04:40:57 PM VB_48
Venkat Boddupally; MeOH:H2O AcOH
VB_48 #20-22 RT: 0.53-0.60 AV: 3 NL: 4.85E6
T: + p Full ms2 374.90@28.00 [100.00-2000.00]

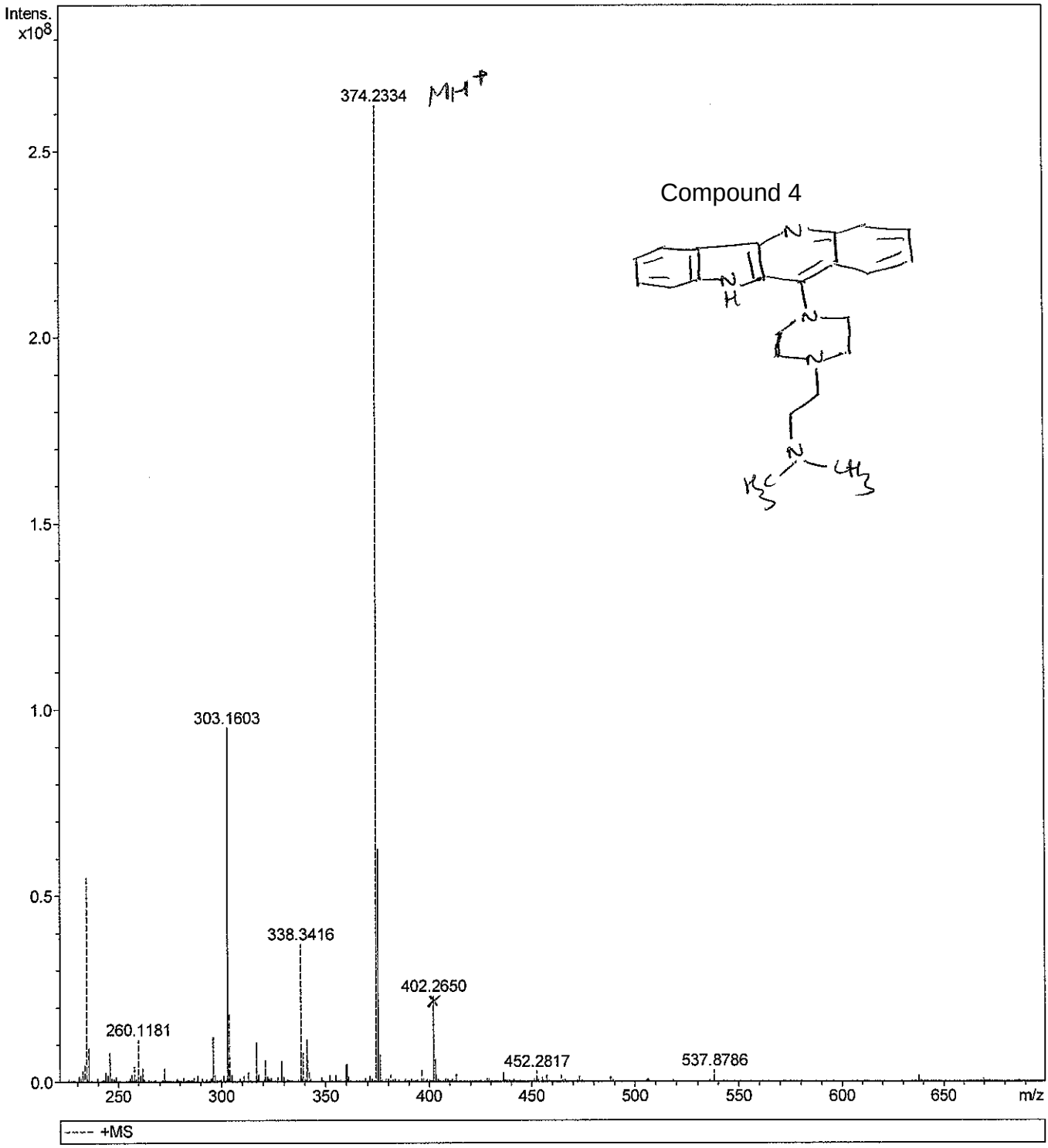
S27



Generic Display Report

Analysis Info

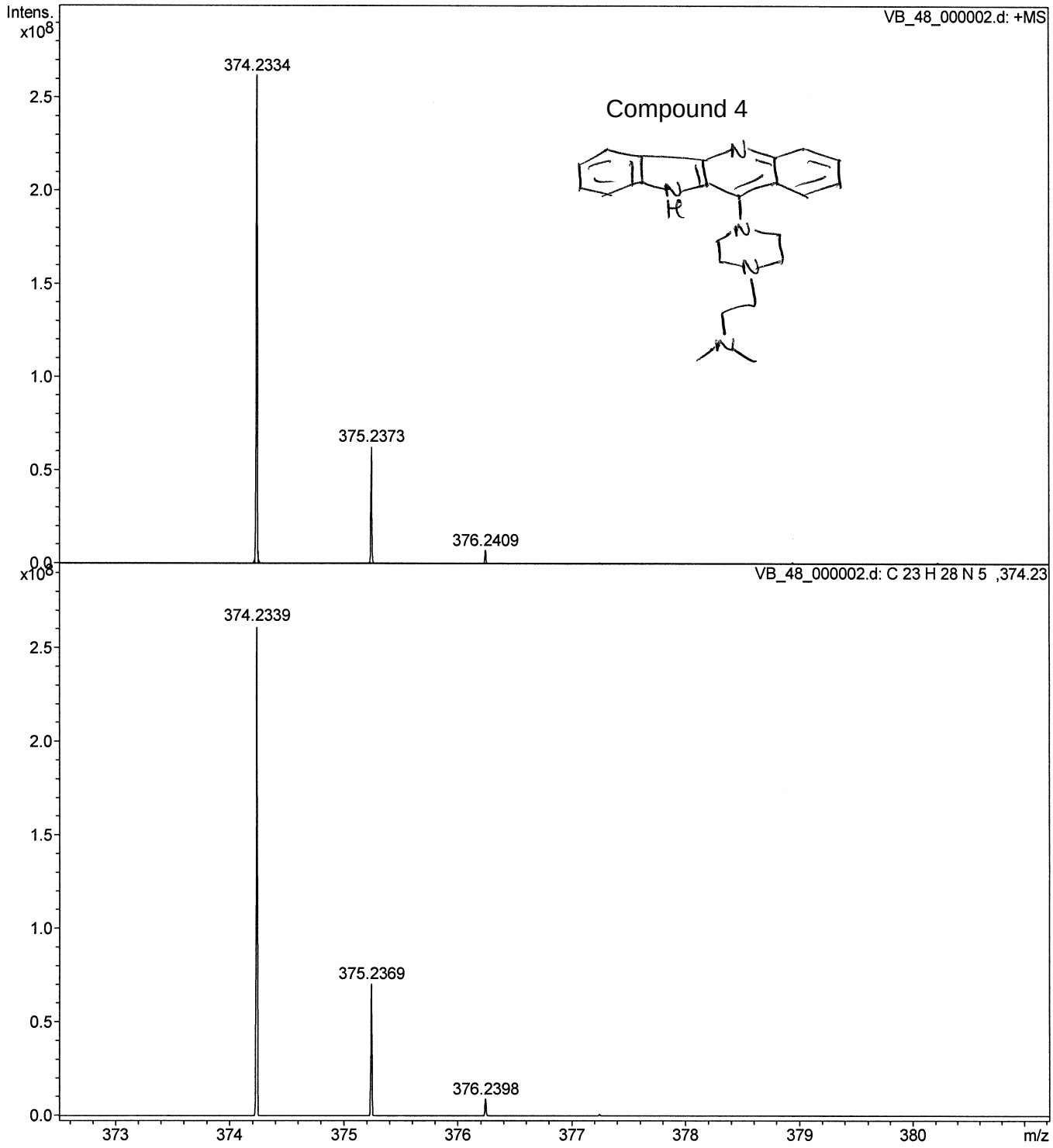
Analysis Name	D:\DATA\Facility_May_5\VB_48_000002.d	Acquisition Date	5/27/2008 1:27:56 PM
Method	ESI_101506	Operator	Administrator
Sample Name	VB-48	Instrument	apex-Qe
Comment	Venkat B., MeOH:H2O:AcOH		



Generic Display Report

Analysis Info

Analysis Name	D:\DATA\Facility_May_5\VB_48_000002.d	Acquisition Date	5/27/2008 1:27:56 PM
Method	ESI_101506	Operator	Administrator
Sample Name	VB-48	Instrument	apex-Qe
Comment	Venkat B., MeOH:H2O:AcOH		



Generate Molecular Formula

Min C_{16}

Max

C 16-n

Generate

Save Results...

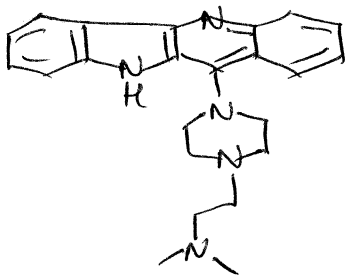
Help

Note: for m < 2000 the elements C, H, N, and O are considered implicitly.

Measured m/z 374.2334 Tolerance 2 mDa Charge 1

#	Mol. Formula	m/z	err [mDa]	lerr[[ppm]	err [ppm]	mean err [ppm]	
1	C 22 H 32 N 1 O 4	374.2326	-0.82	2.2	-2.2	-2.6	C
2	C 23 H 28 N 5	374.2339	0.52	1.4	1.4	0.7	[illegible]
3	C 25 H 30 N 2 O 1	374.2353	1.86	5.0	5.0	4.5	C

Compound 4



Automatically locate monoisotopic peak Maximum number of formulas 200

Check rings plus double bonds Minimum 0 Maximum 0

Apply nitrogen rule Electron configuration both

Filter H/C element ratio Minimum H/C 0 Maximum H/C 3

Estimate carbon number Generate immediately

Save for Reporting

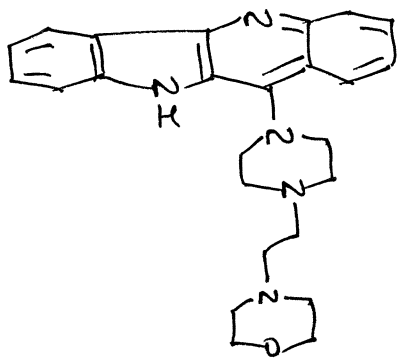
Show Pattern

10.866

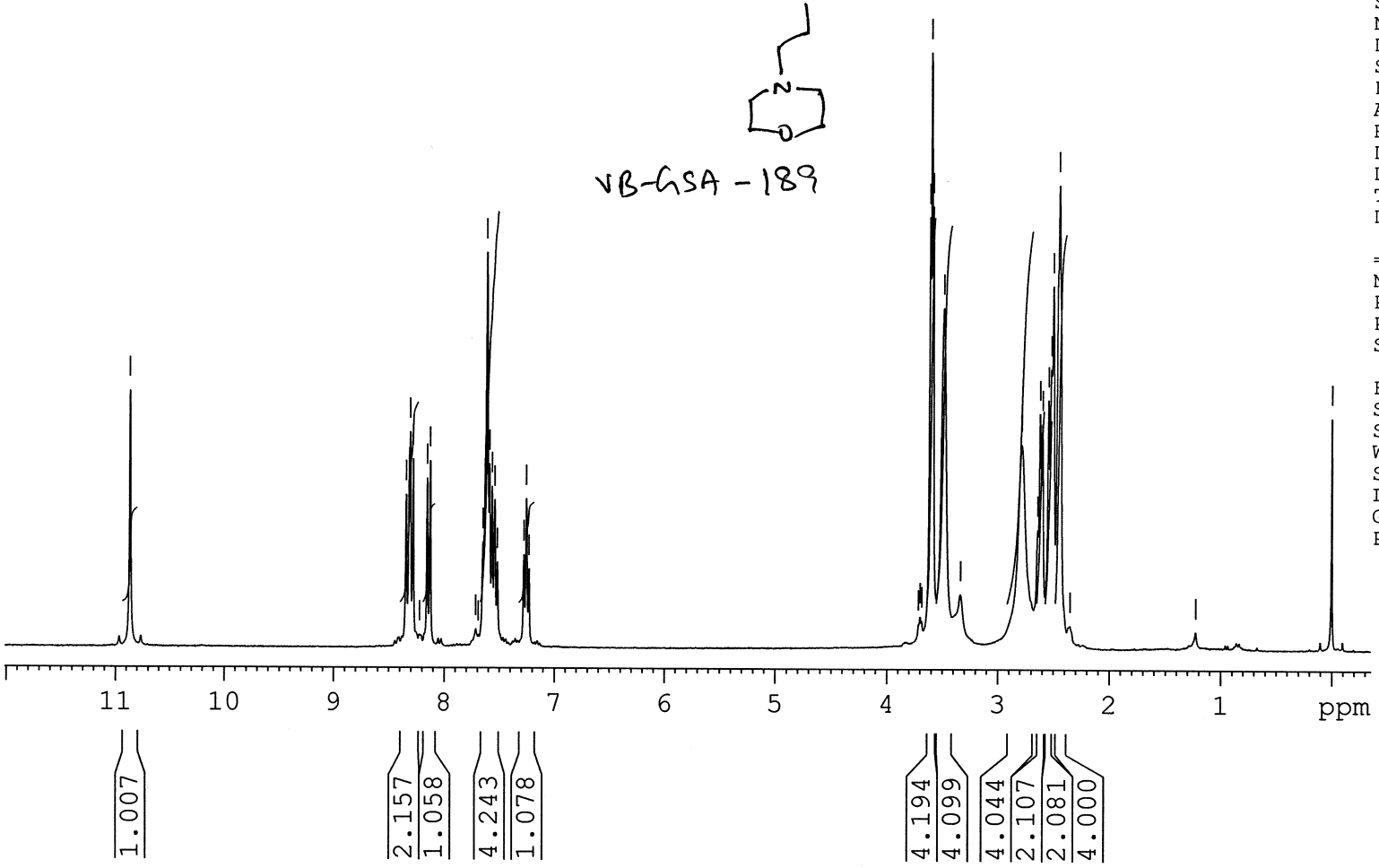
8.345 8.308 8.281 8.221 8.154 8.127 7.715 7.691 7.650 7.615 7.591 7.567 7.543 7.518 7.276 7.255 7.229 3.714 3.700 3.685 3.615 3.600 3.585 3.488 3.334 2.786 2.641 2.622 2.599 2.546 2.523 2.504 2.451 2.352 1.225

0.002

Compound 5



VB-GSA-189



Current Data Parameters

NAME	VB-GSA-189
EXPNO	9
PROCNO	1

F2 - Acquisition Parameters

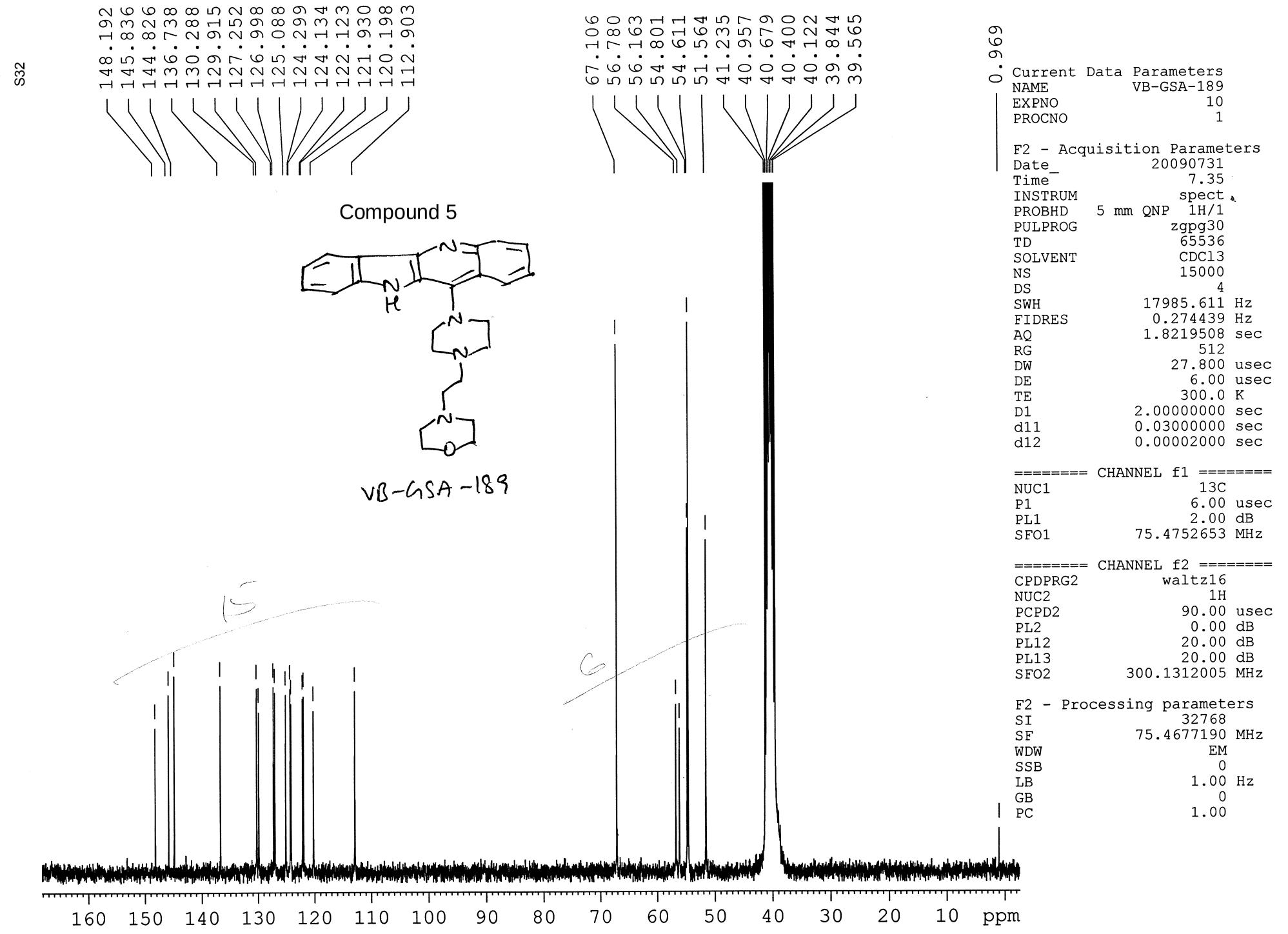
Date_	20090730
Time	15.26
INSTRUM	spect
PROBHD	5 mm QNP 1H/1
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	64
DS	2
SWH	6172.839 Hz
FIDRES	0.094190 Hz
AQ	5.3084660 sec
RG	456.1
DW	81.000 usec
DE	6.00 usec
TE	300.0 K
D1	1.00000000 sec

======== CHANNEL f1 ========

NUC1	1H
P1	9.25 usec
PL1	0.00 dB
SFO1	300.1318534 MHz

F2 - Processing parameters

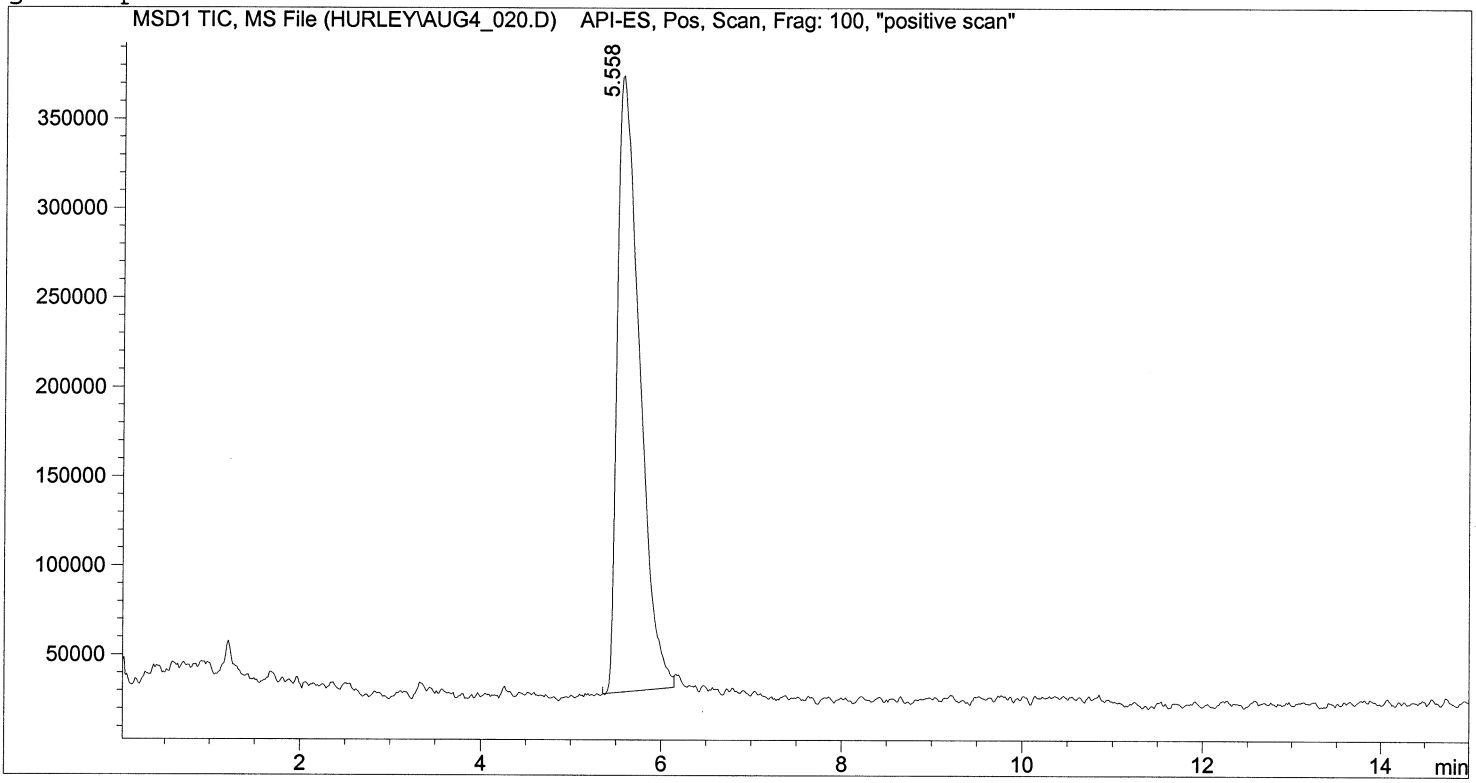
SI	32768
SF	300.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00




```
Current Data Parameters
NAME                  VB-GSA-189
EXPNO                         10
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20090731
Time                        7.35
INSTRUM                    spect
PROBHD    5 mm QNP  1H/1
PULPROG                   zgpg30
TD                         65536
SOLVENT                    CDCl3
NS                         15000
DS                             4
SWH                   17985.611 Hz
FIDRES                 0.274439 Hz
AQ                    1.8219508 sec
RG                           512
DW                        27.800 usec
DE                         6.00 usec
TE                        300.0 K
D1                    2.00000000 sec
d11                   0.03000000 sec
d12                   0.00002000 sec

======== CHANNEL f1 ========
NUC1                         13C
P1                         6.00 usec
PL1                        2.00 dB
SFO1                  75.4752653 MHz

======== CHANNEL f2 ========
CPDPRG2                  waltz16
NUC2                         1H
PCPD2                     90.00 usec
PL2                        0.00 dB
PL12                      20.00 dB
PL13                      20.00 dB
SFO2                 300.1312005 MHz

F2 - Processing parameters
SI                           32768
SF                    75.4677190 MHz
WDW                             EM
SSB                              0
LB                         1.00 Hz
GB                               0
PC                            1.00
```

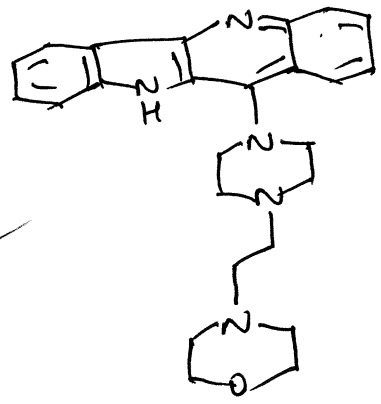
S33

```
==========================================================================
Injection Date  : 8/4/2009 5:51:38 PM
Sample Name     : VB-GSA-189                    Location : Vial 17
Acq. Operator   : Karen                            Inj :   1
Acq. Instrument : Instrument 1                 Inj Volume : 0.1 µl
Method          : C:\HPCHEM\1\METHODS\LC_MS.M
Last changed    : 8/4/2009 5:50:35 PM by Karen
Zorbax SB ODS,20:80:0.25; MeCN/water/formicA, POS, 300-550; frag 100; 30C, cap volt 3000,
gas temp 325
```




```
==========================================================================
                          Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MSD1 TIC, MS File

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]                          %
----|-------|----|-------|----------|----------|--------|
   1   5.558 BB    0.2325 5.91404e6  3.45798e5  100.0000

Totals :                  5.91404e6  3.45798e5

==========================================================================
                          *** End of Report ***
```

Compound 5

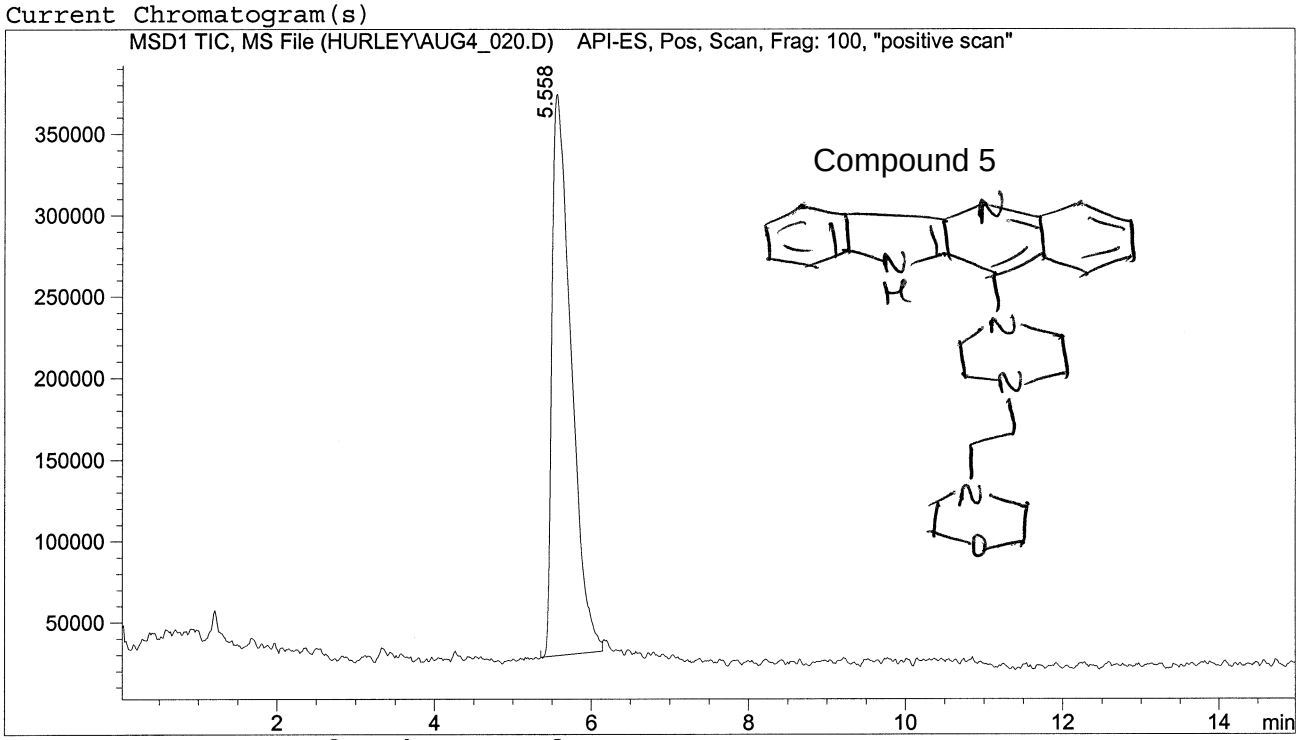


VB-GSA-189
(m/z = 415)

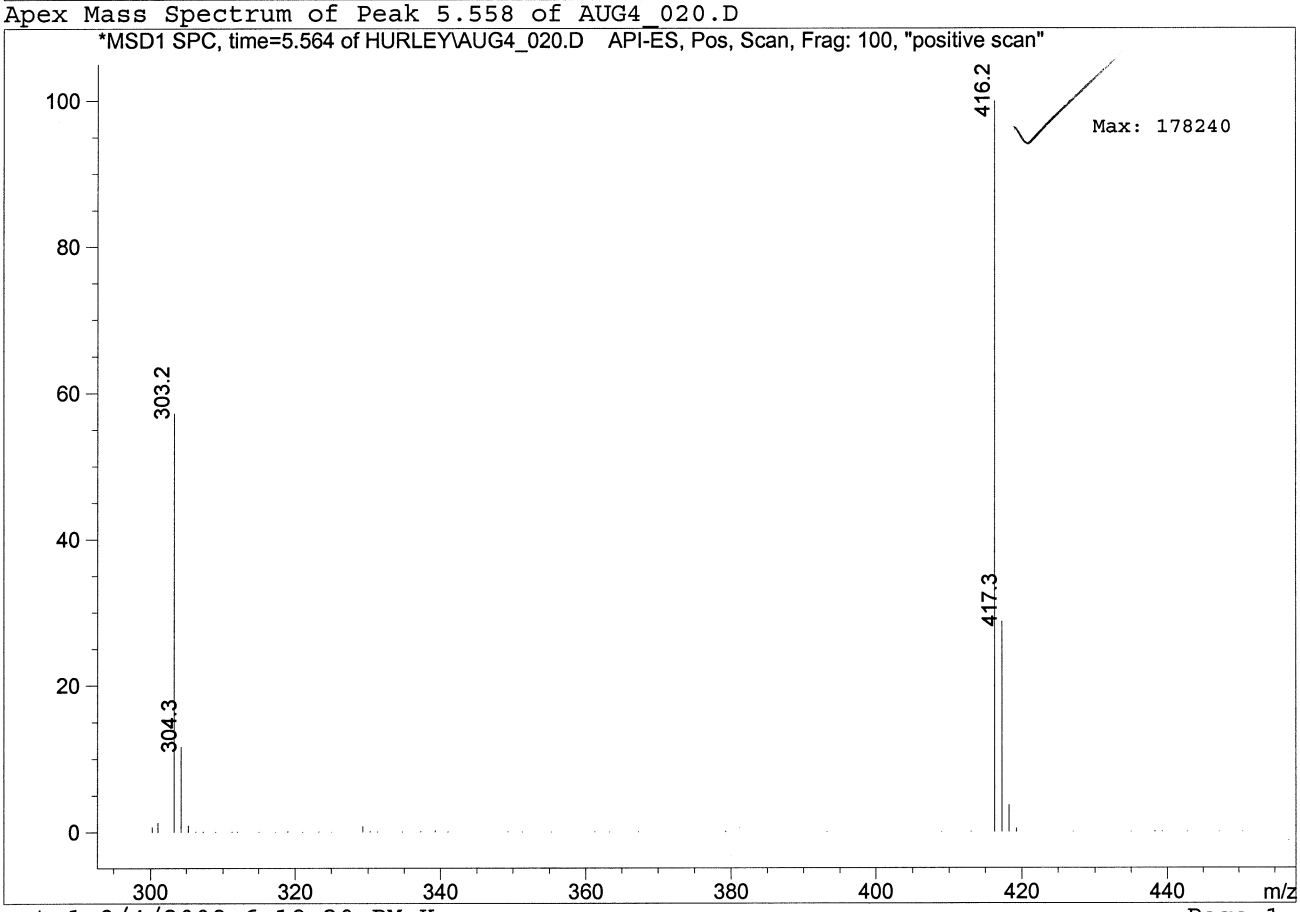
Print of all graphic windows

```
Injection Date  : 8/4/2009 5:51:38 PM
Sample Name     : VB-GSA-189                    Location : Vial 17
Acq. Operator   : Karen                            Inj :   1
Acq. Instrument : Instrument 1                 Inj Volume : 0.1 µl
Method          : C:\HPCHEM\1\METHODS\LC_MS.M
Last changed    : 8/4/2009 5:50:35 PM by Karen
Zorbax SB ODS,20:80:0.25; MeCN/water/formicA, POS, 300-550; frag 100; 30C, cap volt 3000,
gas temp 325
```

Current Chromatogram(s)



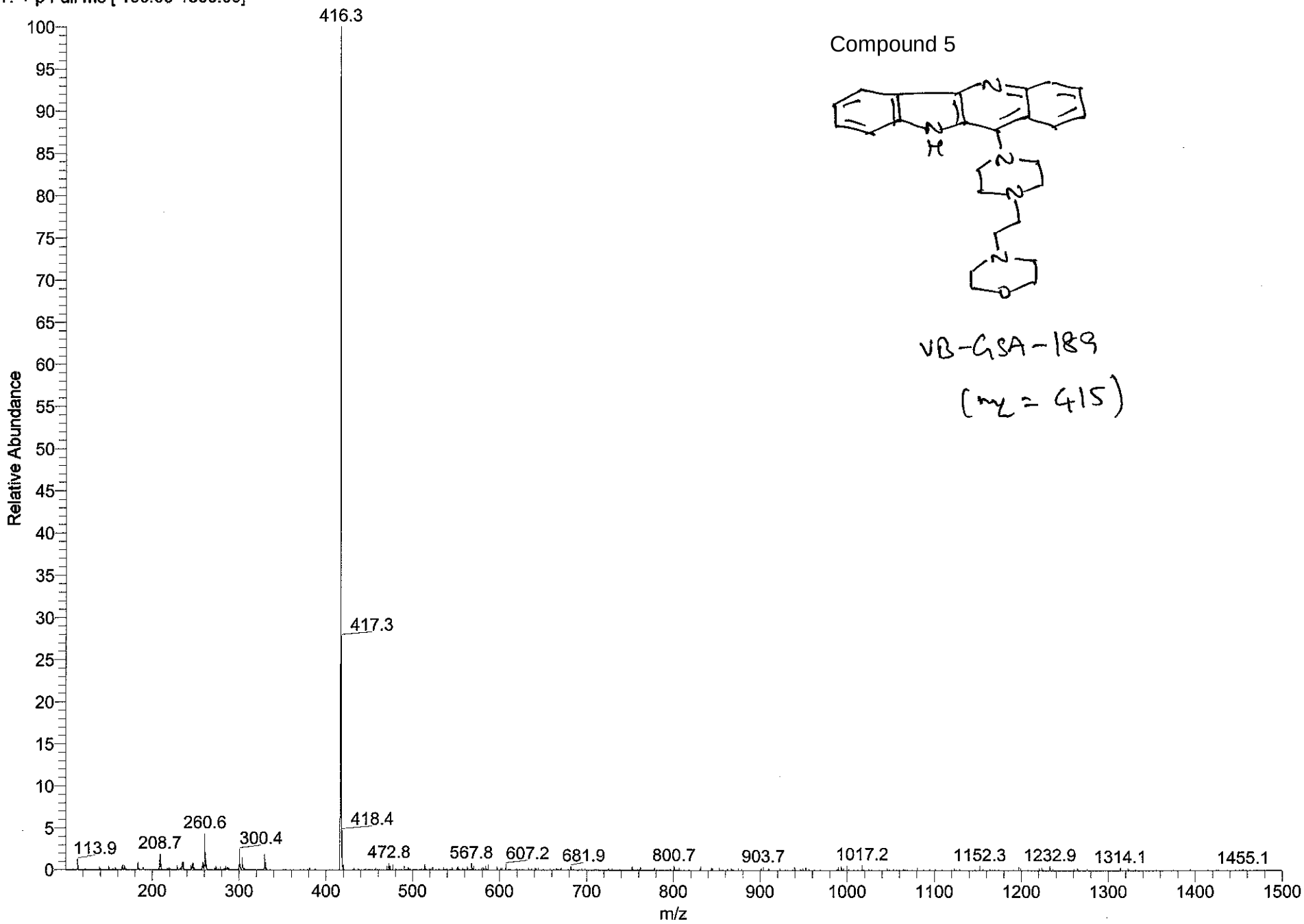
Apex Mass Spectrum of Peak 5.558 of AUG4_020.D



E:\MSLab_LCQ\VB-GSA-189 08/05/2009 04:47:22 PM VB-GSA-189
Venkat B., MeOH:ACN 1:1

VB-GSA-189 #19-21 RT: 0.50-0.55 AV: 3 NL: 8.86E6
T: + p Full ms [100.00-1500.00]

S35



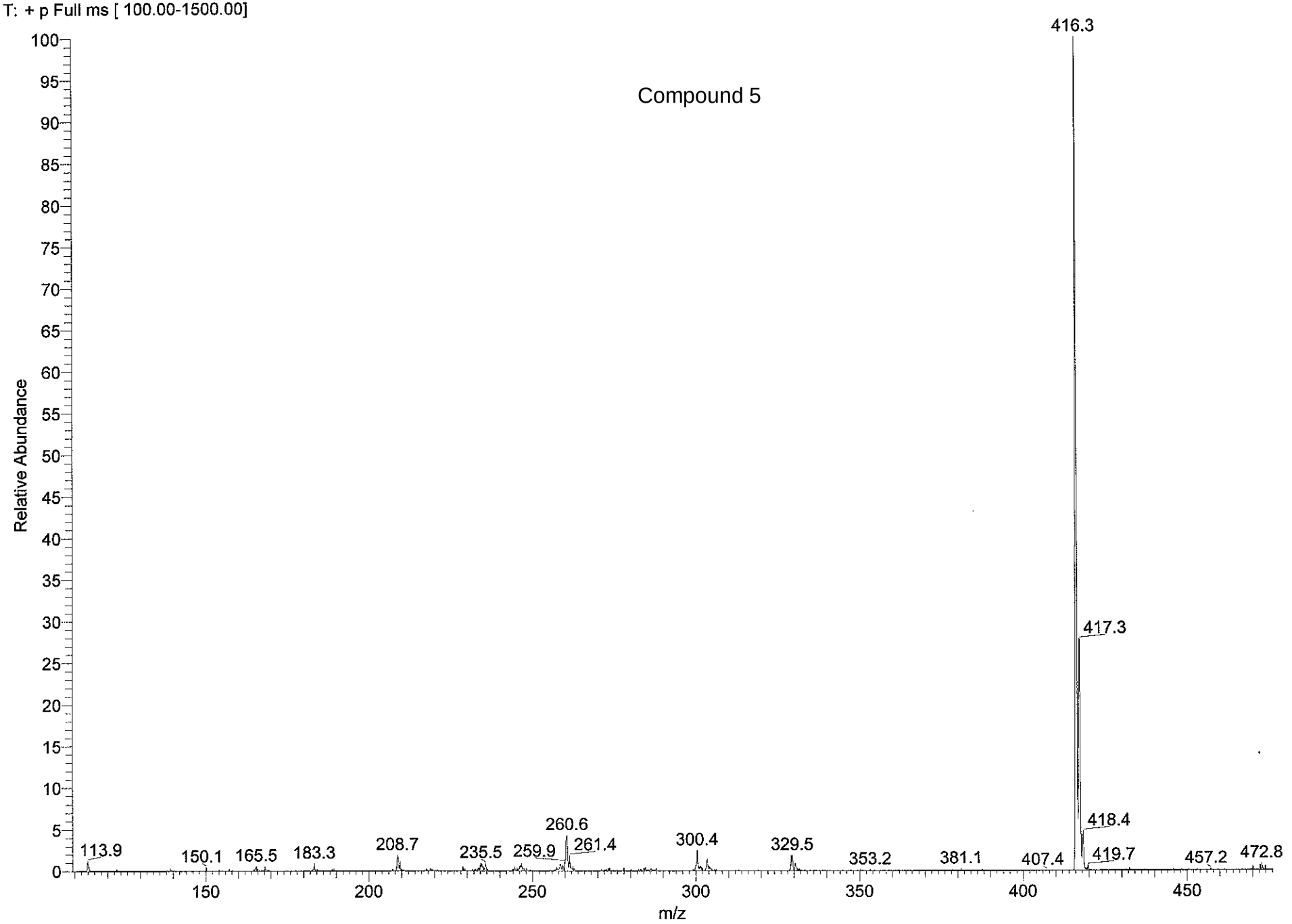
Compound 5

VB-GSA-189

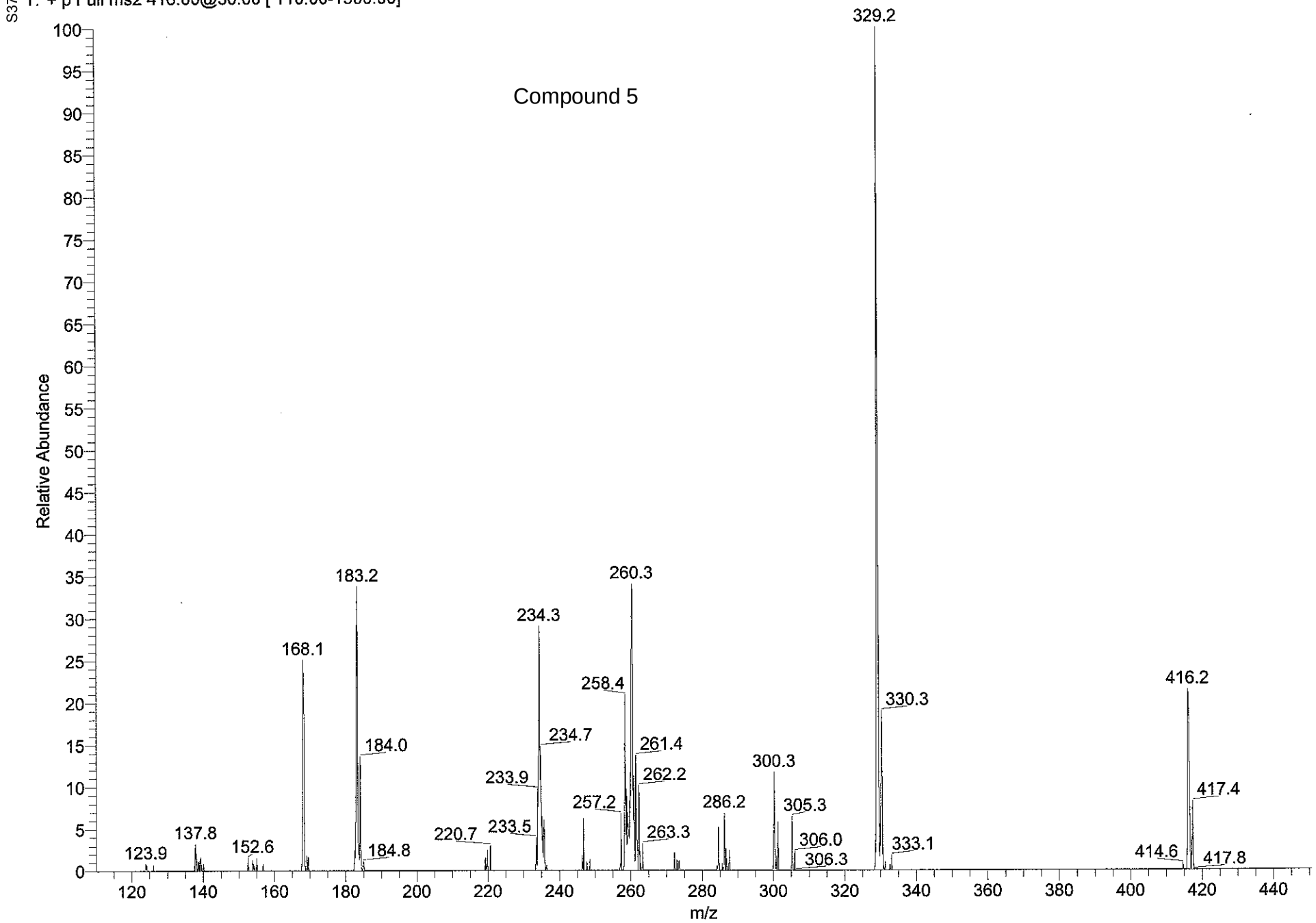
(m/z = 415)

E:\MSLab_LCQ\VB-GSA-189 08/05/2009 04:47:22 PM VB-GSA-189
Venkat B., MeOH:ACN 1:1

VB-GSA-189 #19-21 RT: 0.50-0.55 AV: 3 NL: 8.86E6
T: + p Full ms [100.00-1500.00]

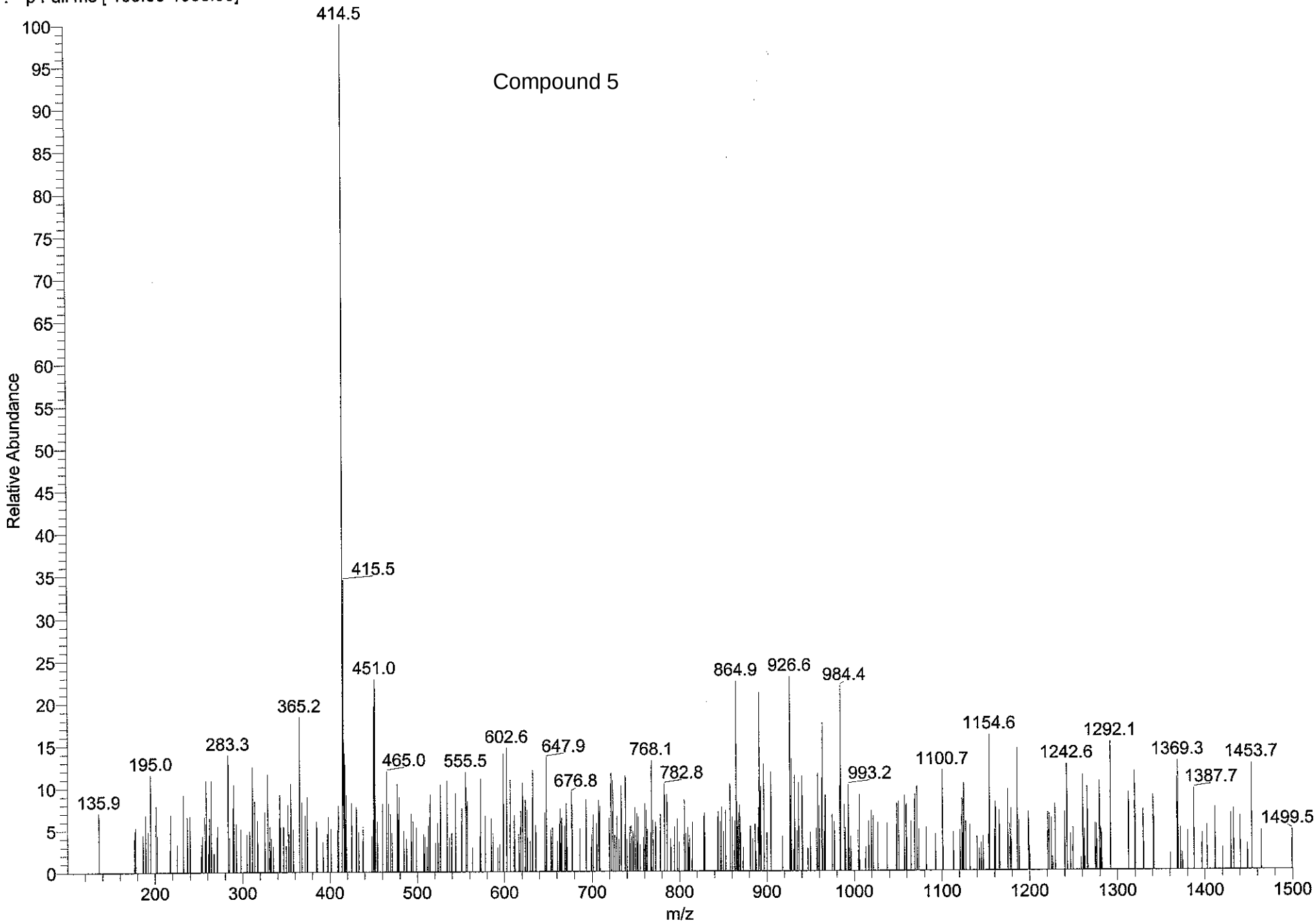


E:\MSLab_LCQ\VB-GSA-189 08/05/2009 04:47:22 PM VB-GSA-189
Venkat B., MeOH:ACN 1:1
VB-GSA-189 #14-15 RT: 0.36-0.39 AV: 2 NL: 2.41E6
T: + p Full ms2 416.00@30.00 [110.00-1500.00]



E:\MSLab_LCQ\VB-GSA-189 08/05/2009 04:47:22 PM VB-GSA-189
Venkat B., MeOH:ACN 1:1
VB-GSA-189 #23-24 RT: 0.63-0.66 AV: 2 NL: 4.32E4
T: - p Full ms [100.00-1500.00]

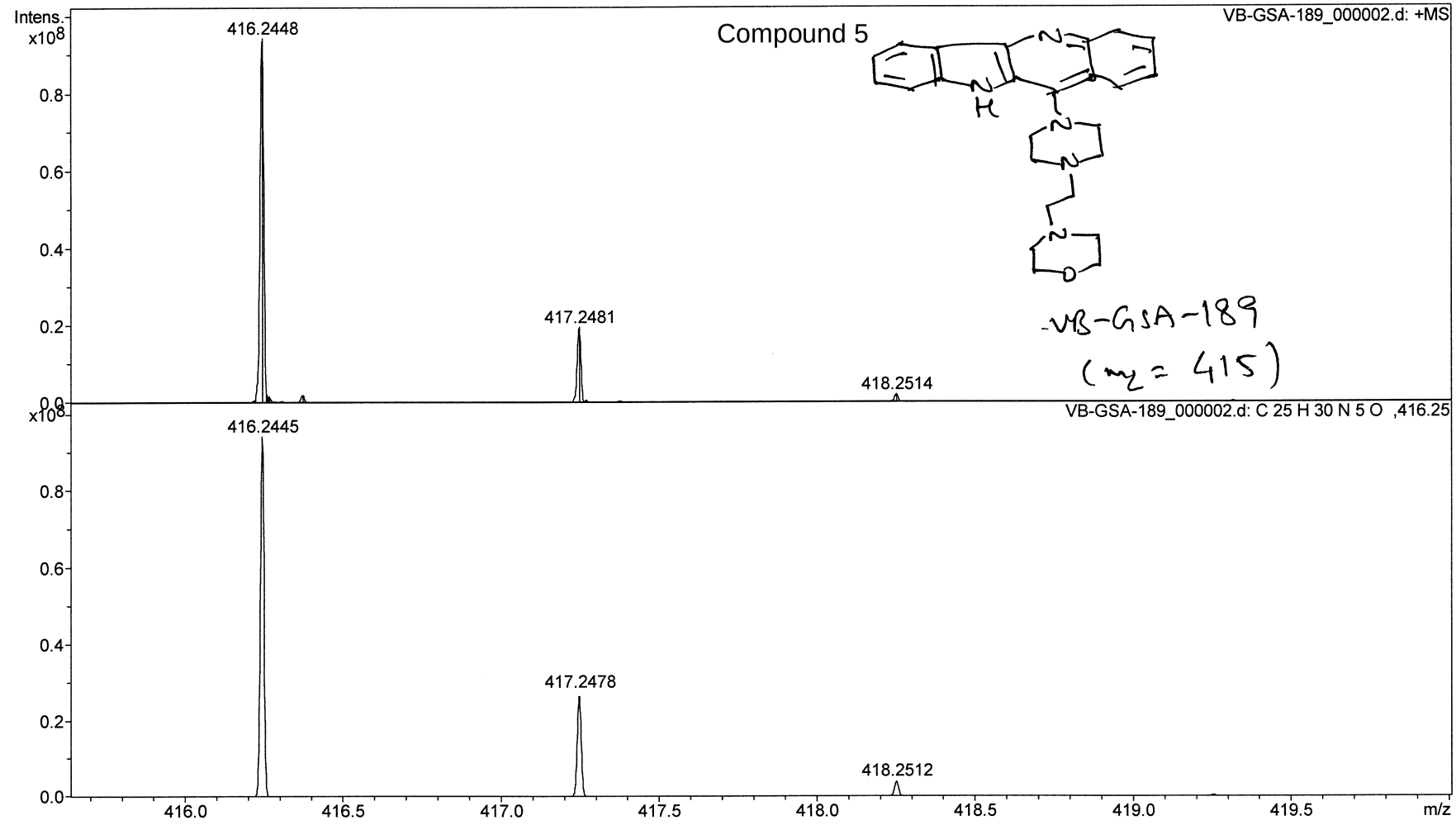
S38



Generic Display Report

Analysis Info

Analysis Name	D:\DATA\Facility_August_09\VB-GSA-189_000002.d	Acquisition Date	8/6/2009 2:44:45 PM
Method	ESI_101506	Operator	
Sample Name	VB-GSA-189	Instrument	apex-Qe
Comment	Venkat B., MeOH:ACN 1:1		



SmartFormula Manually

Min C_{13}

Max

C 13-n

Generate

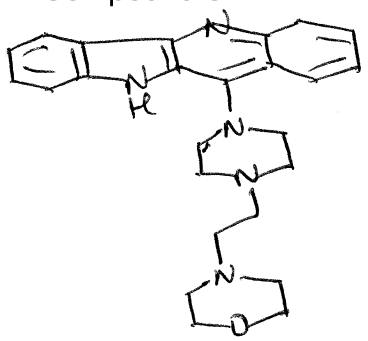
Help

Note: for m < 2000 the elements C, H, N, and O are considered implicitly.

Measured m/z 416.2448 Tolerance 2 mDa Charge 1

#	Mol. Formula	m/z	err [mDa]	|err| [ppm]	err [ppm]	mean err [ppm]	mSigma	Sigma Rank	rdb	N rule	e⁻
1	C 13 H 34 N 7 O 8	416.2463	1.57	3.8	3.8	3.6	21.8	1	0.5	ok	even
2	C 24 H 34 N O 5	416.2431	-1.62	3.9	-3.9	-3.9	36.9	2	8.5	ok	even
3	C 25 H 30 N 5 O	416.2445	-0.28	0.7	-0.7	-0.7	48.2	3	13.5	ok	even

Compound 5



Automatically locate monoisotopic peak Maximum number of formulas 500

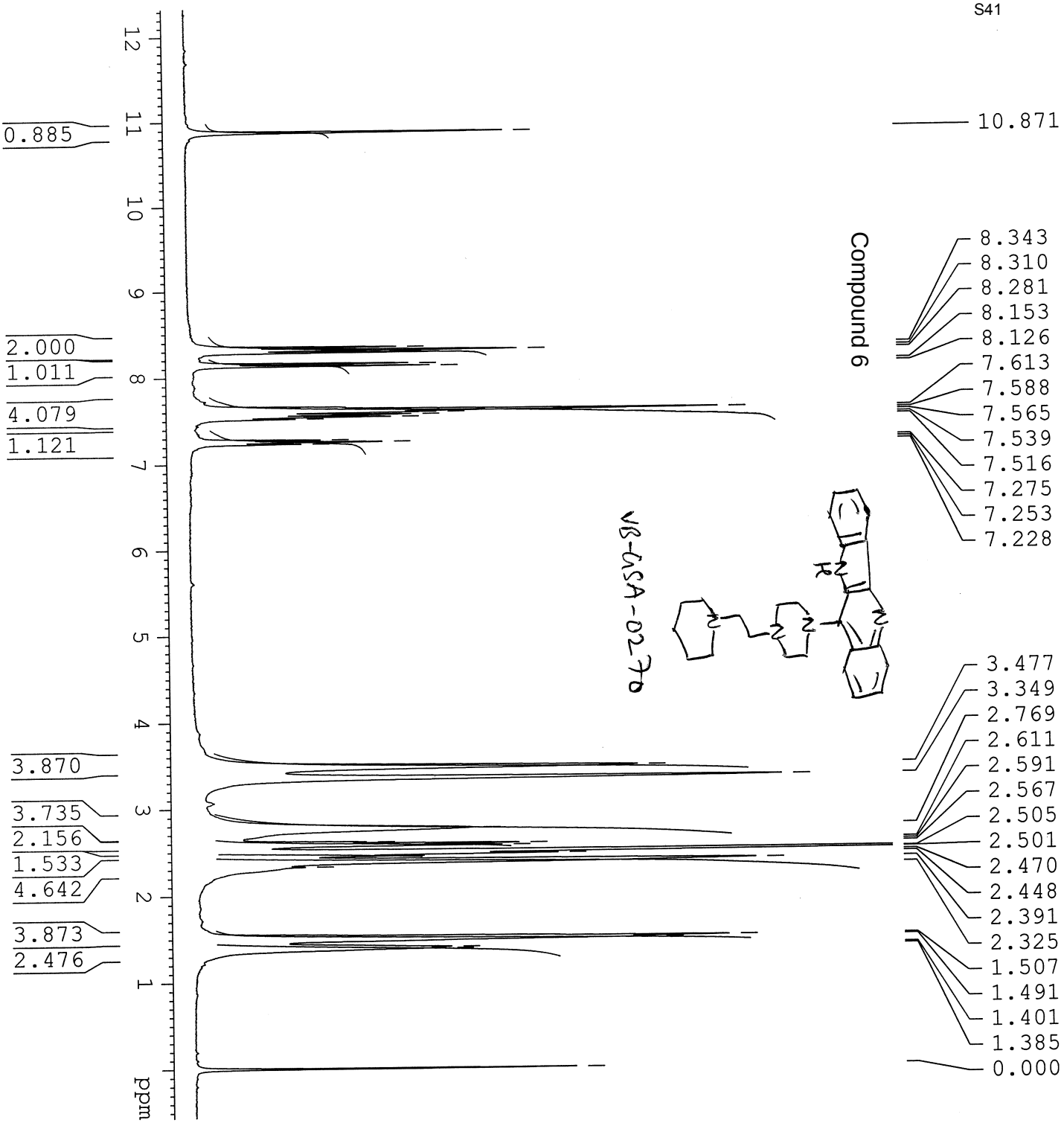
Check rings plus double bonds Minimum -0.5 Maximum 40

Electron configuration even

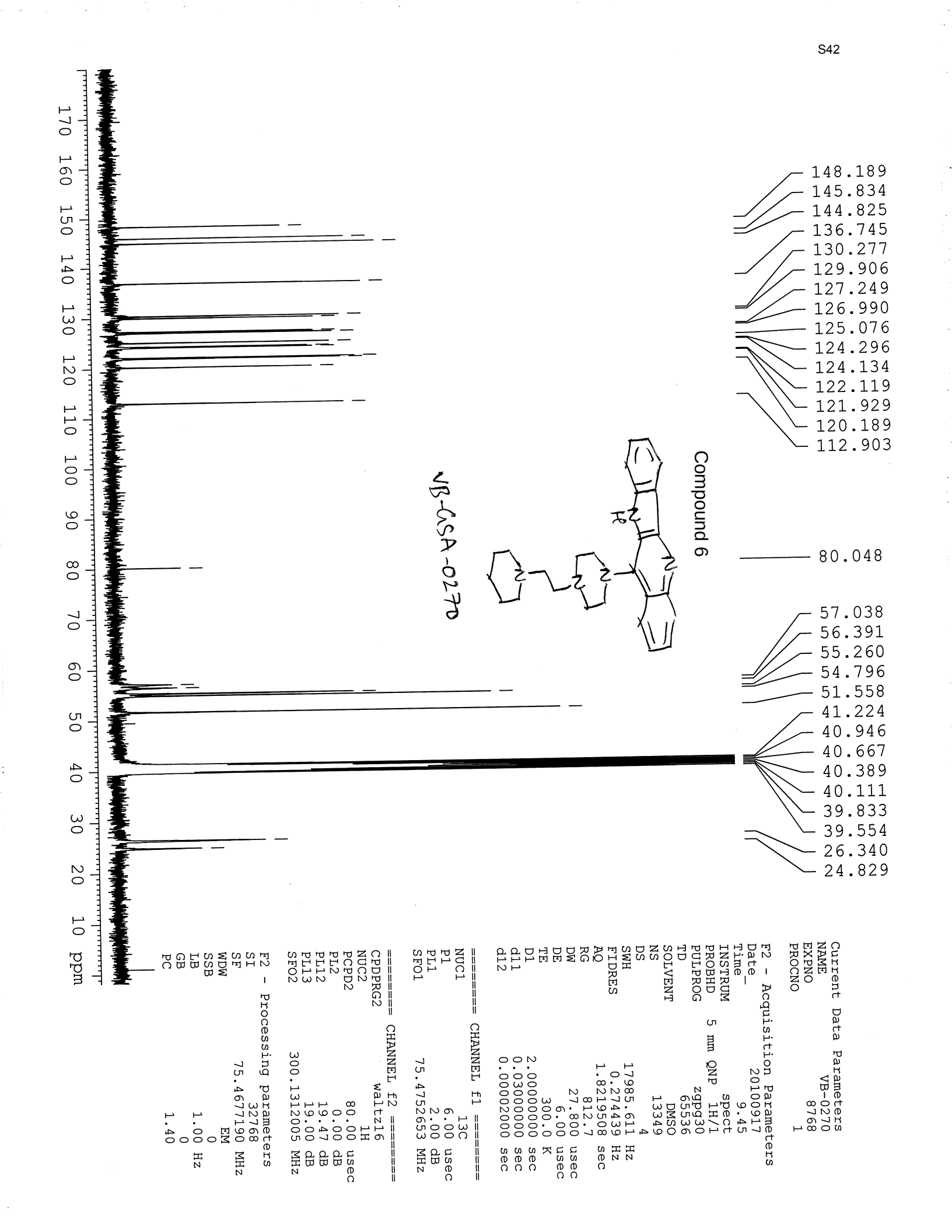
Filter H/C element ratio Minimum H/C 0 Maximum H/C 3

Estimate carbon number Generate immediately

Show Pattern




```
Current Data Parameters
NAME                 VB-CASA-02-70
EXPNO                656565
PROCNO               1

F2 - Acquisition Parameters
Date_                20100827
Time_                14.25
INSTRUM              spect
PROBHD     5 mm QNP  1H/1
PULPROG              zg30
TD                   65536
SOLVENT              DMSO
NS                   64
DS                   2
SWH                  6172.839 Hz
FIDRES               0.094190 Hz
AQ                   5.3084660 sec
RG                   287.4
DW                   81.000 usec
DE                   6.00 usec
TE                   300.0 K
D1                   1.00000000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                   8.50 usec
PL1                  0.00 dB
SFO1                 300.1318534 MHz

F2 - Processing parameters
SI                   32768
SF                   300.1300000 MHz
WDW                  EM
SSB                  0
LB                   0.30 Hz
GB                   0
PC                   1.00
```



Current Data Parameters
NAME VB-0270
EXPNO 8768
PROCNO 1

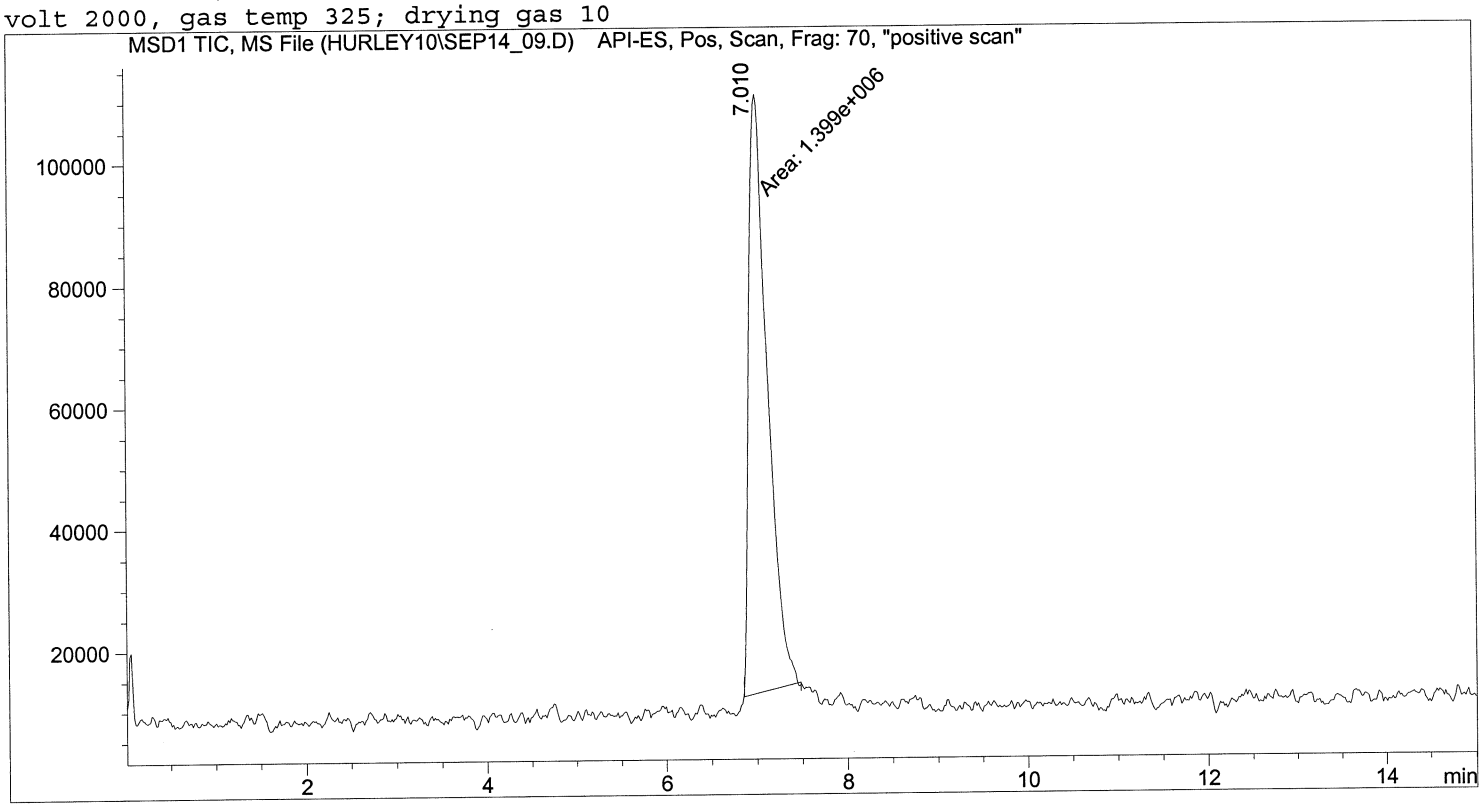
F2 - Acquisition Parameters
Date_ 20100917
Time_ 9.45
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 13349
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 812.7
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 2.00 dB
SFO1 75.4752653 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 19.47 dB
PL13 19.00 dB
SFO2 300.1312005 MHz

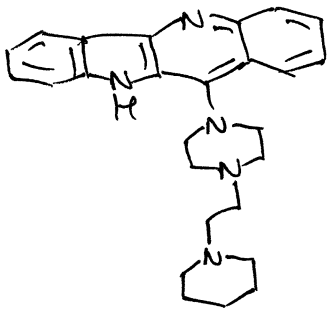
F2 - Processing parameters
SI 32768
SF 75.4677190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Injection Date : 9/14/2010 3:03:03 PM
Sample Name : VB-GSA-0270 Location : Vial 4
Acq. Operator : Karen Inj : 1
Acq. Instrument : Instrument 1 Inj Volume : 0.1 µl
Acq. Method : C:\HPCHEM\1\METHODS\LC_MS.M
Last changed : 9/14/2010 3:01:13 PM by Karen
Analysis Method : C:\HPCHEM\1\METHODS\LC_MS.M
Last changed : 9/16/2010 5:50:56 PM by Karen
Zorbax SB C18, 150 x 4.6, 3.5u,55:45:0.25, MeCN/H2O/formic, POS, 150-400; frag 70; 25C, cap volt 2000, gas temp 325; drying gas 10



Area Percent Report

Compound 6



Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: MSD1 TIC, MS File

Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	7.010	MM	0.2364	1.39900e6	9.86347e4	100.0000
Totals :				1.39900e6	9.86347e4	

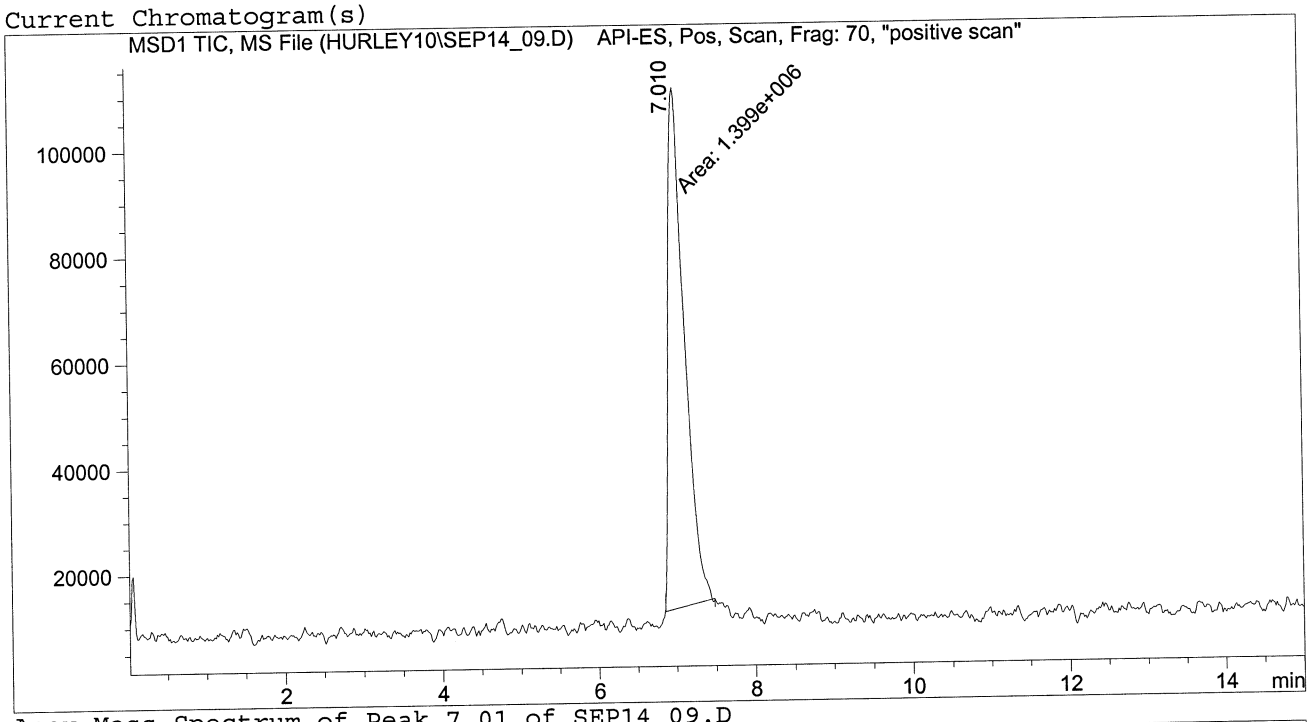
VB-GSA-0270

*** End of Report ***

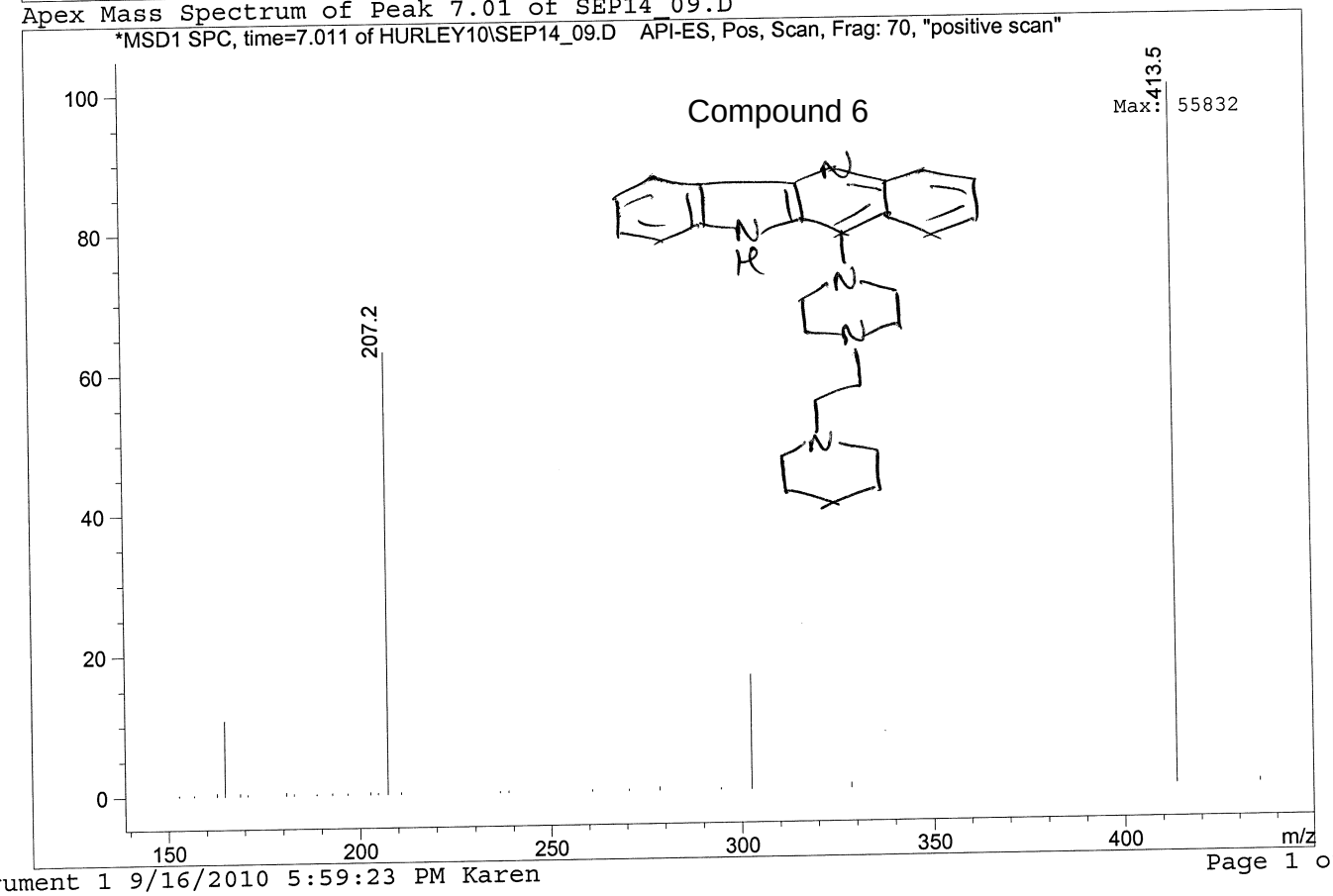
Print of all graphic windows

```
Injection Date  : 9/14/2010 3:03:03 PM
Sample Name     : VB-GSA-0270                    Location : Vial 4
Acq. Operator   : Karen                             Inj :   1
Acq. Instrument : Instrument 1                  Inj Volume : 0.1 µl
Acq. Method     : C:\HPCHEM\1\METHODS\LC_MS.M
Last changed    : 9/14/2010 3:01:13 PM by Karen
Analysis Method : C:\HPCHEM\1\METHODS\LC_MS.M
Last changed    : 9/16/2010 5:50:56 PM by Karen
Zorbax SB C18, 150 x 4.6, 3.5u,55:45:0.25, MeCN/H2O/formic, POS, 150-400; frag 70; 25C,
cap volt 2000, gas temp 325; drying gas 10
```

Current Chromatogram(s)

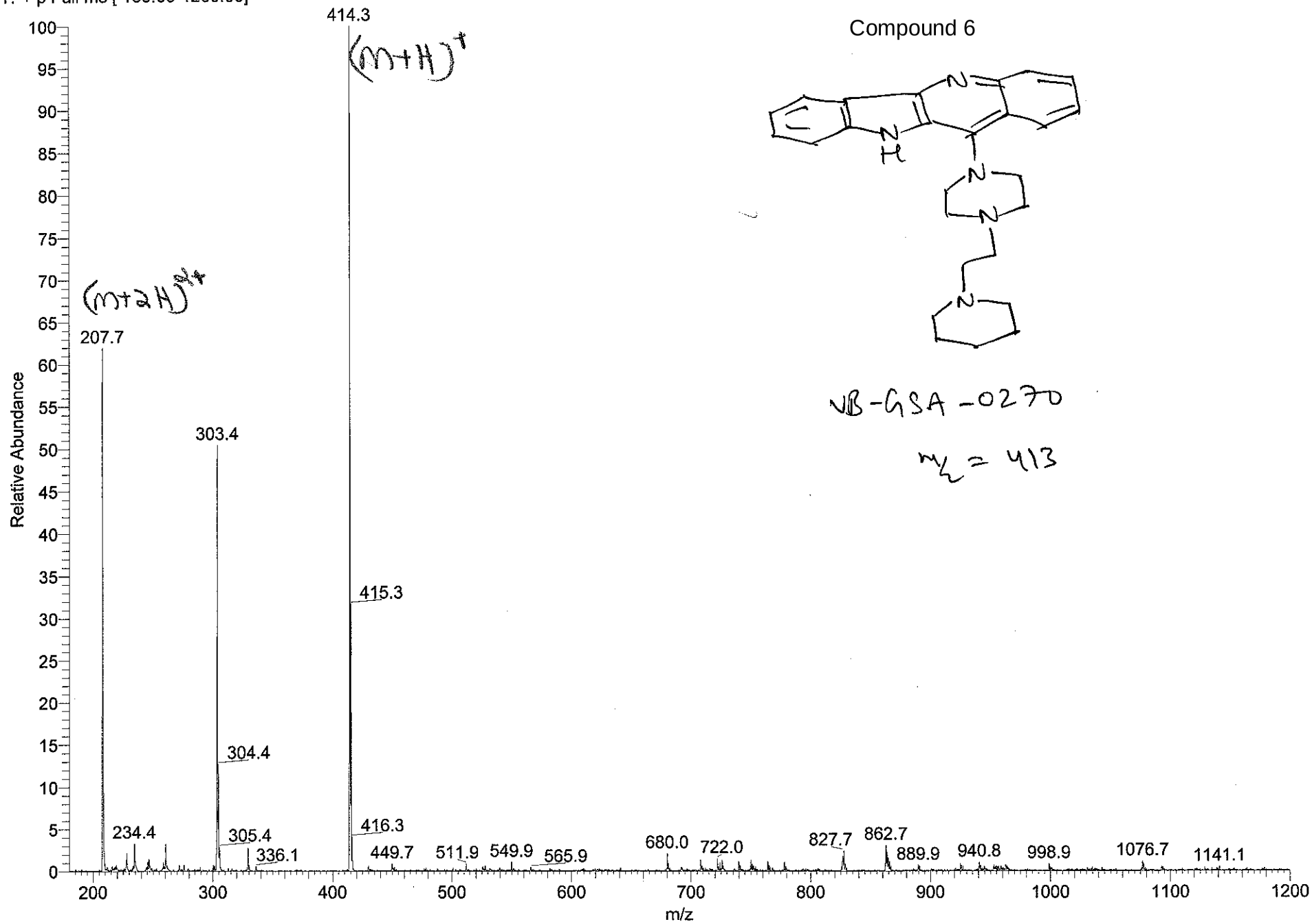


Apex Mass Spectrum of Peak 7.01 of SEP14_09.D



E:\MSLab_LCQ\VB_0270 09/16/2010 11:20:01 AM VB-0270
V. R. C., ACN:H20:FA 1:1:0.1%
VB_0270 #2-12 RT: 0.04-0.24 AV: 11 NL: 6.04E6
T: + p Full ms [180.00-1200.00]

S45



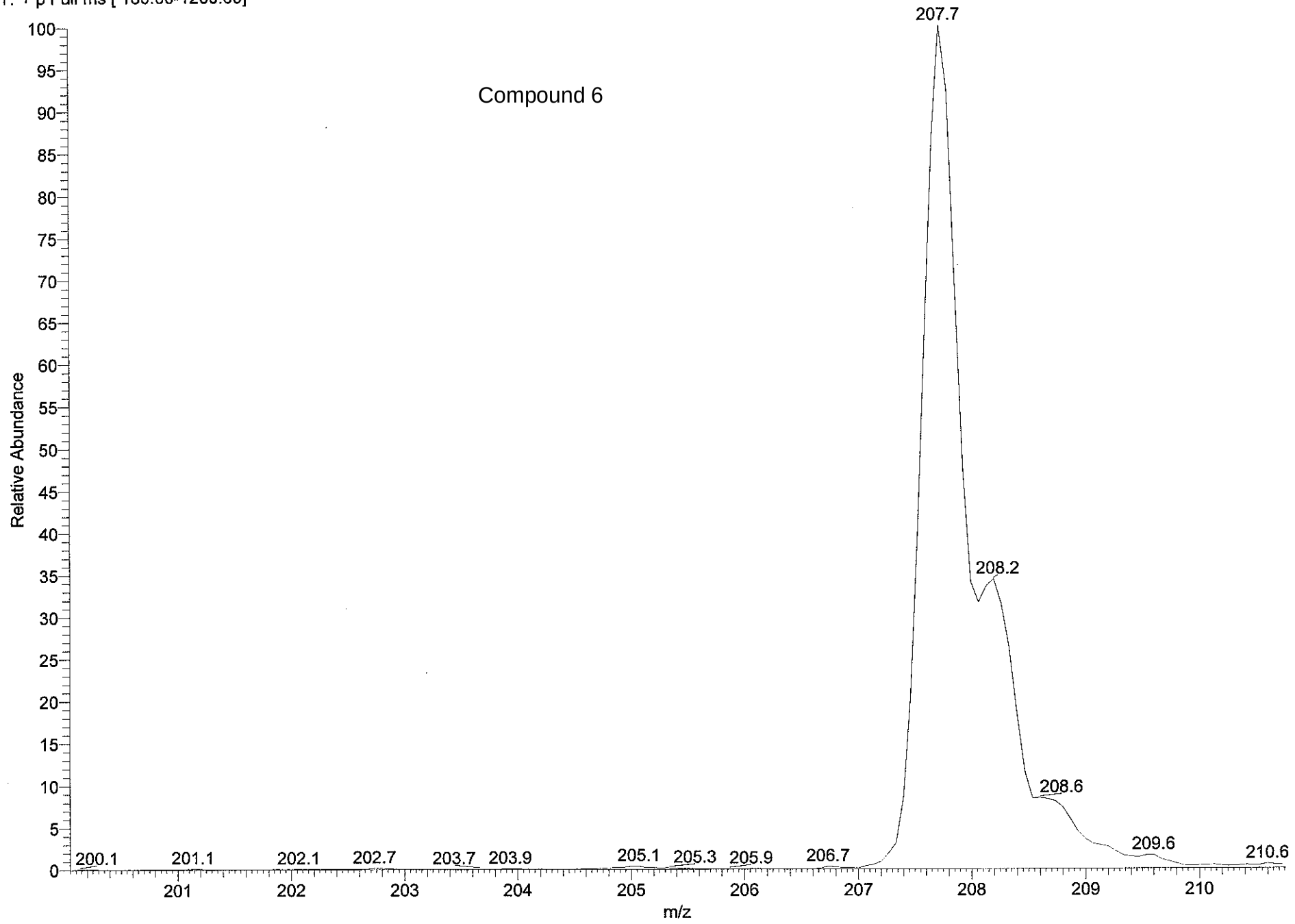
Compound 6

VB-GSA-0270

m/z = 413

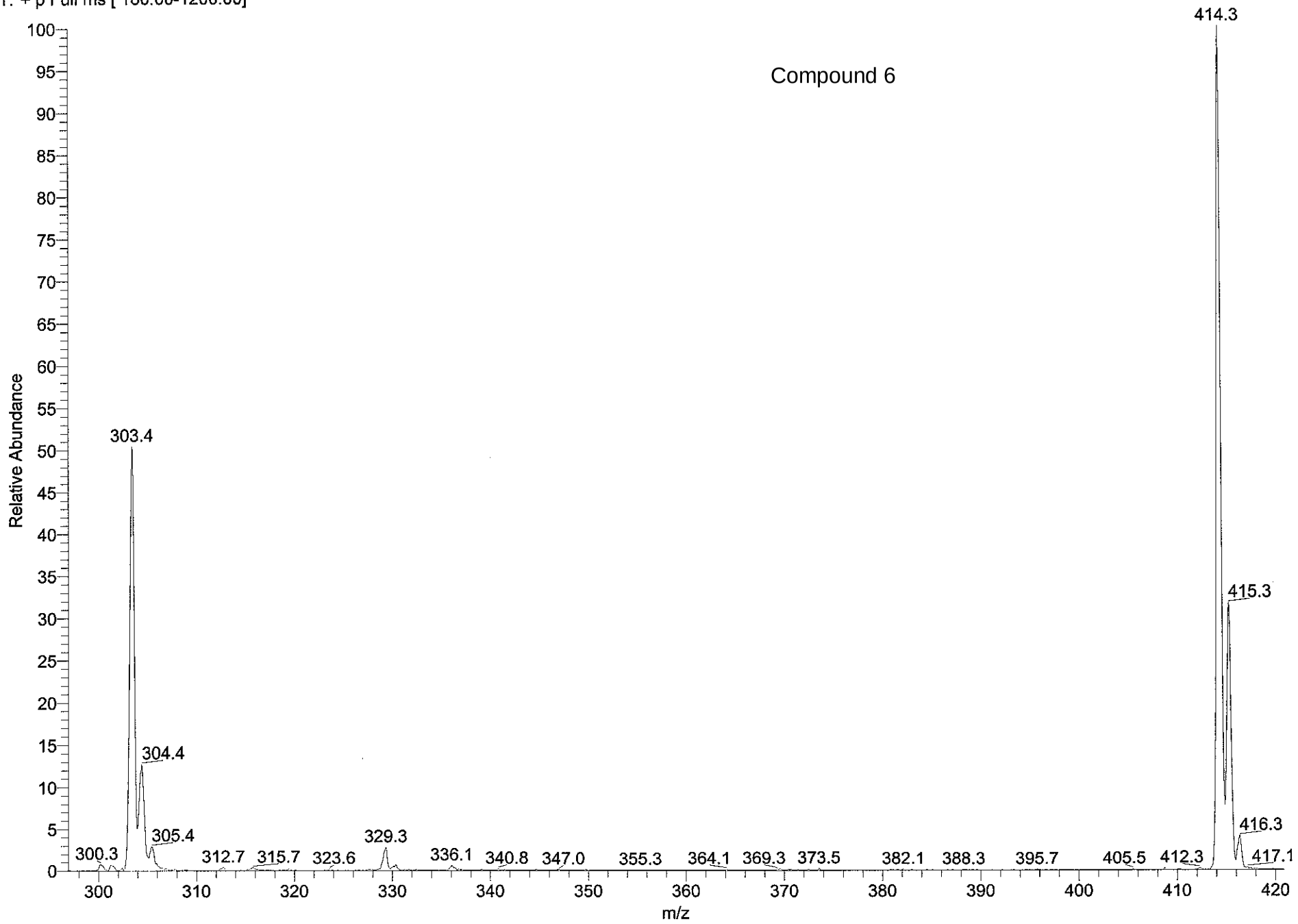
E:\MSLab_LCQ\VB_0270 09/16/2010 11:20:01 AM VB-0270
V. R. C., ACN:H20:FA 1:1:0.1%
VB_0270 #2-12 RT: 0.04-0.24 AV: 11 NL: 3.75E6
T: + p Full ms [180.00-1200.00]

S46



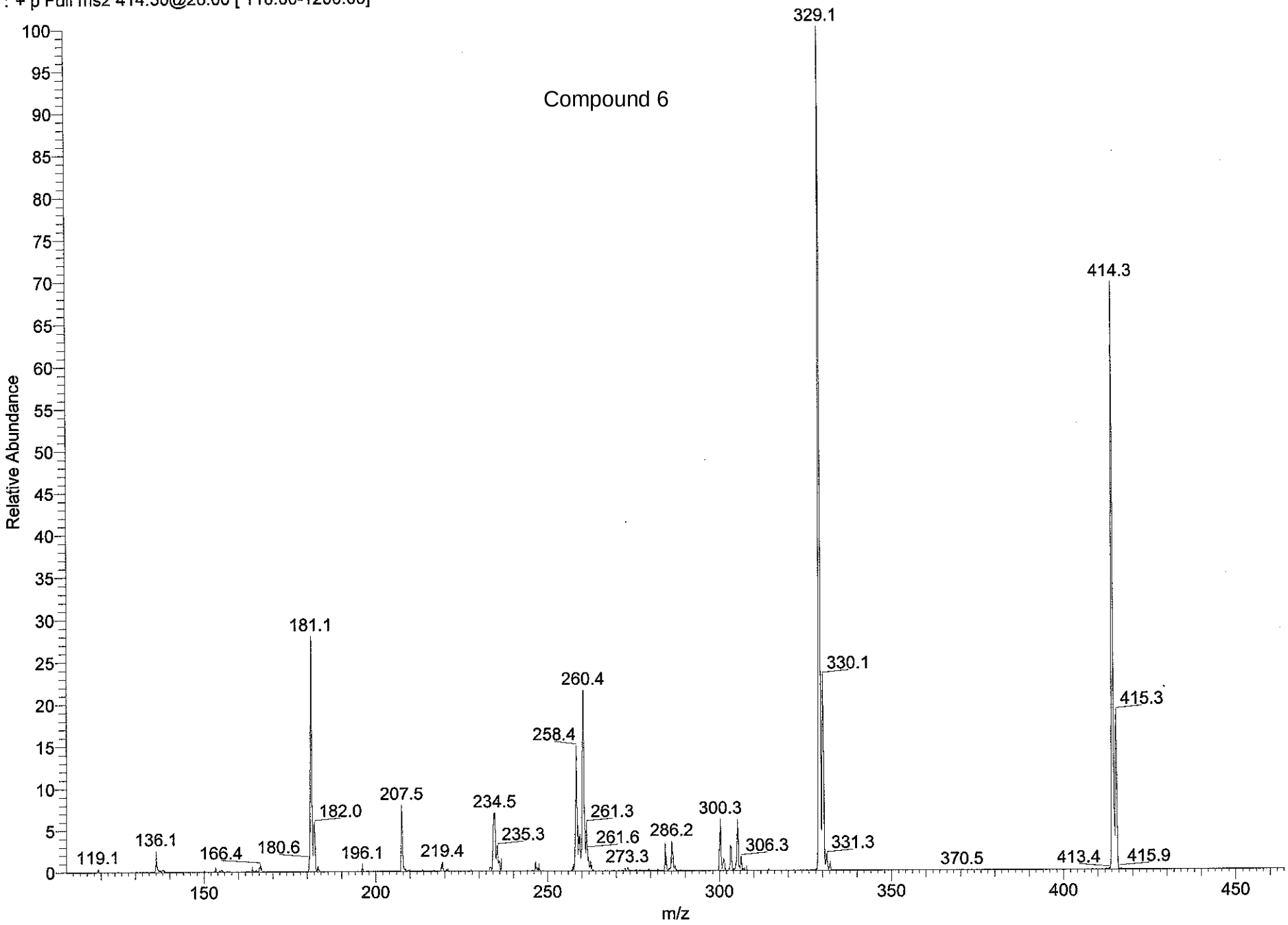
E:\MSLab_LCQ\VB_0270 09/16/2010 11:20:01 AM VB-0270
V. R. C., ACN:H20:FA 1:1:0.1%
VB_0270 #2-12 RT: 0.04-0.24 AV: 11 NL: 6.04E6
T: + p Full ms [180.00-1200.00]

S47

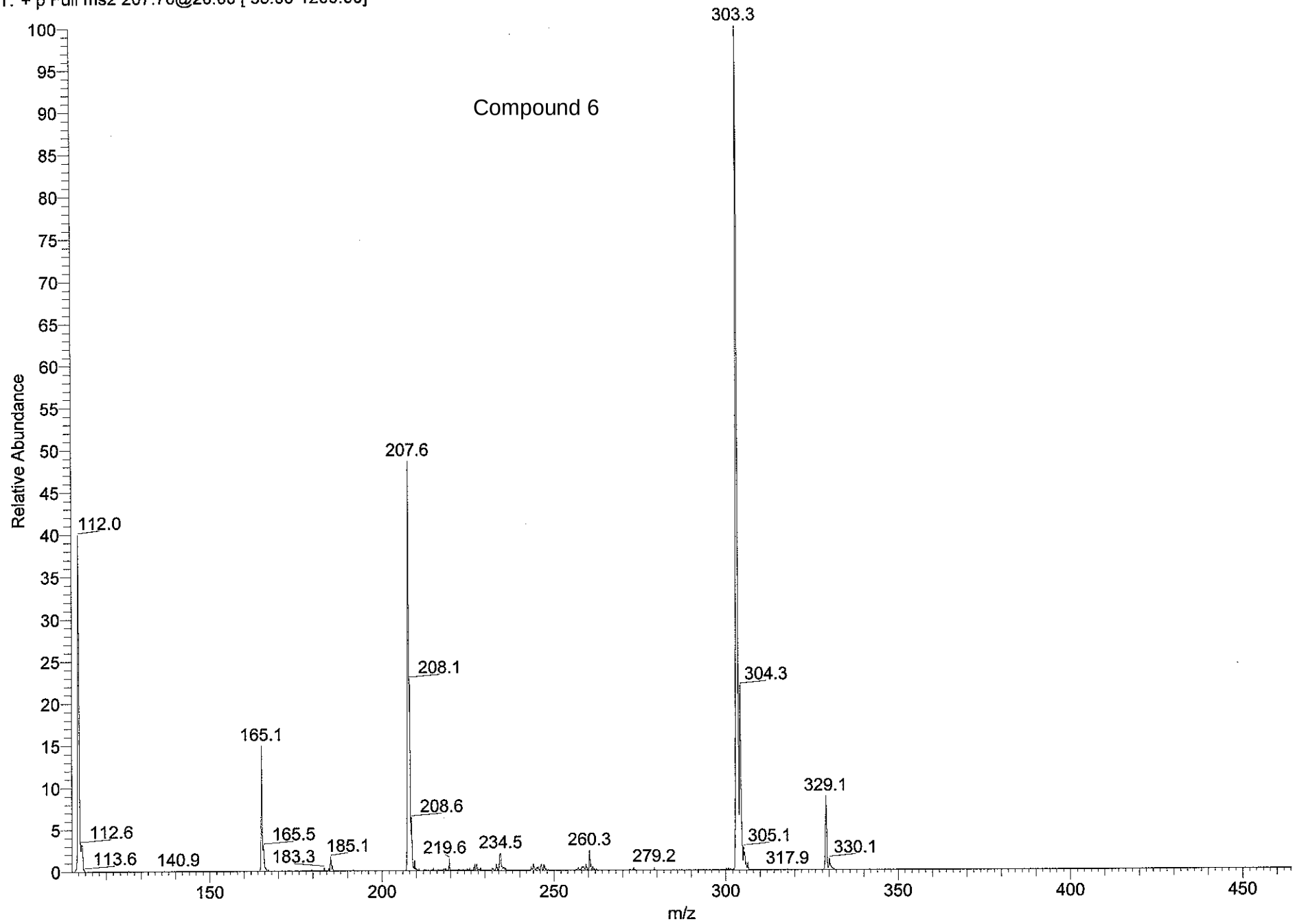


E:\MSLab_LCQ\VB_0270 09/16/2010 11:20:01 AM VB-0270
V. R. C., ACN:H20:FA 1:1:0.1%
VB_0270 #29-49 RT: 0.66-1.16 AV: 21 NL: 1.64E6
T: + p Full ms2 414.30@28.00 [110.00-1200.00]

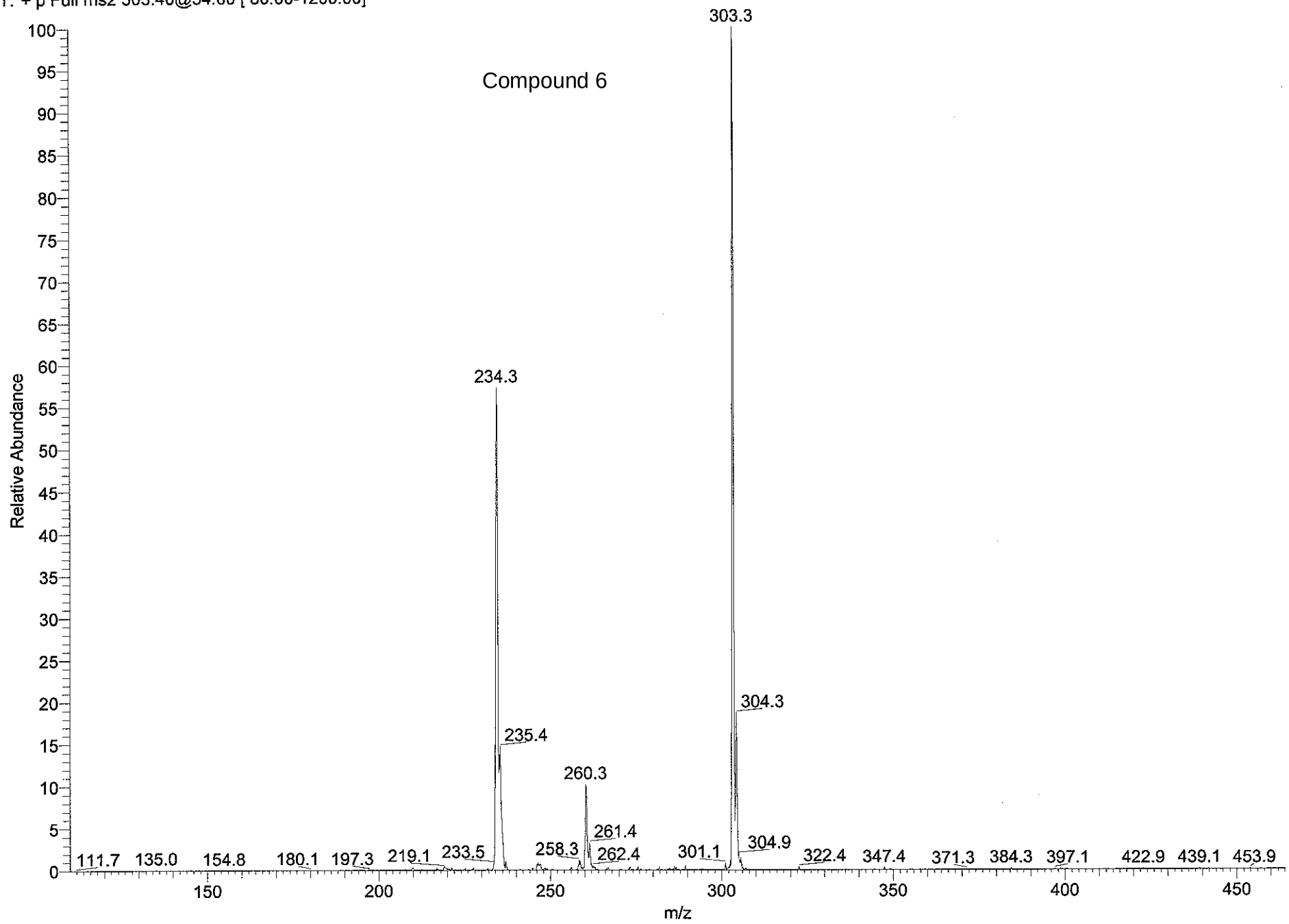
S48



E:\MSLab_LCQ\VB_0270 09/16/2010 11:20:01 AM VB-0270
V. R. C., ACN:H20:FA 1:1:0.1%
VB_0270 #75-89 RT: 1.77-2.12 AV: 15 NL: 5.69E6
T: + p Full ms2 207.70@20.00 [55.00-1200.00]



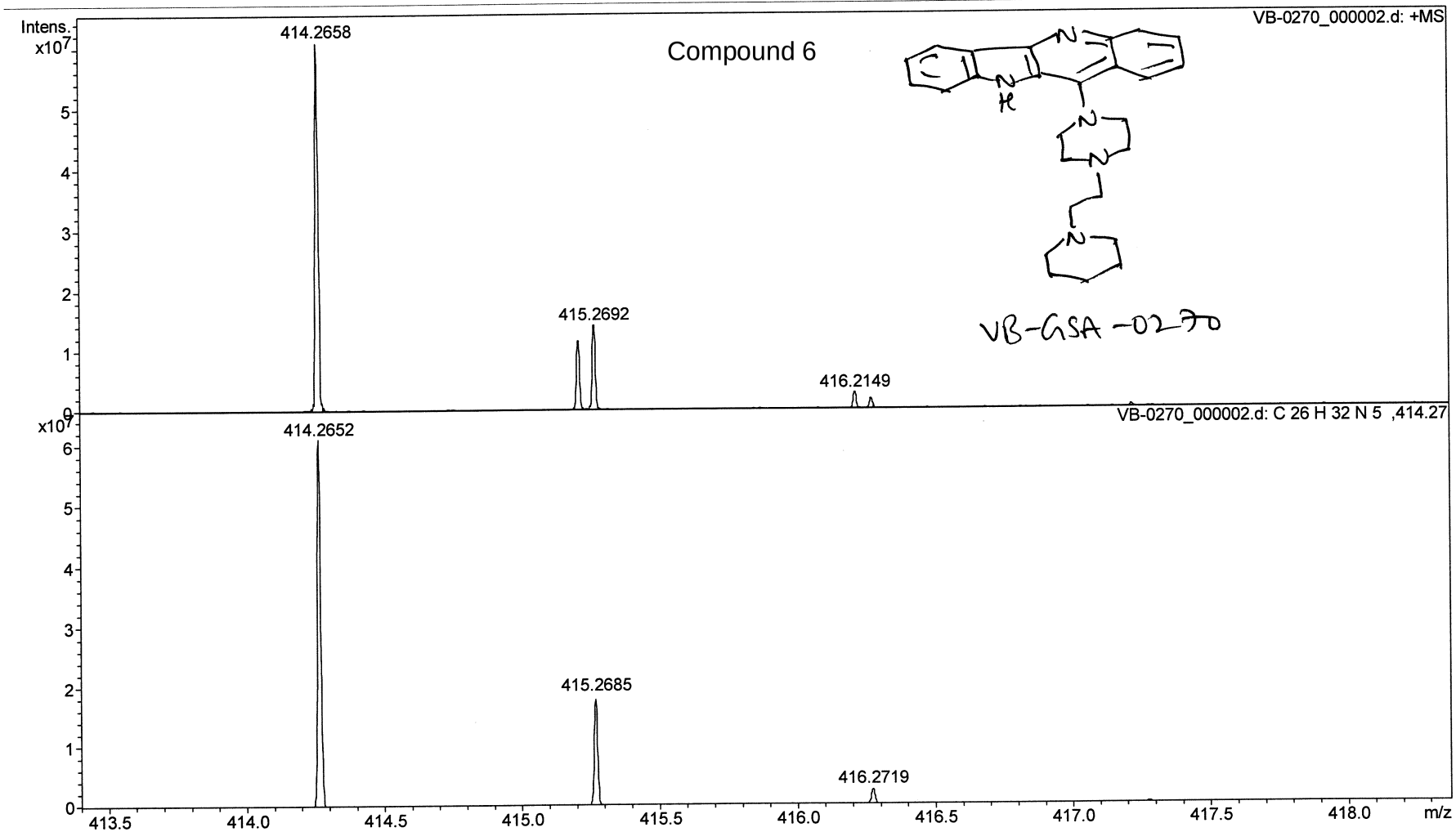
E:\MSLab_LCQ\VB_0270 09/16/2010 11:20:01 AM VB-0270
V. R. C., ACN:H20:FA 1:1:0.1%
VB_0270 #116-131 RT: 2.89-3.37 AV: 16 NL: 1.48E5
T: + p Full ms2 303.40@34.00 [80.00-1200.00]
S50



Generic Display Report

Analysis Info

Analysis Name	D:\DATA\Facility_Sept_10\VB-0270_000002.d	Acquisition Date	9/16/2010 2:04:45 PM
Method	ESI_101506	Operator	
Sample Name	VB-0270	Instrument	apex-Ultra
Comment	V. Chappeta, positive mode, ACN:H2O 1:1:0.1%FA		



SmartFormula Manually

Min C_{15}

Max

C 15-n

Generate

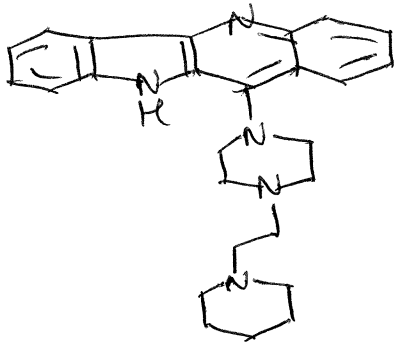
Help

Note: for m < 2000 the elements C, H, N, and O are considered implicitly.

Measured m/z 414.2658 Tolerance 2 mDa Charge 1

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
414.2658	2	C 26 H 32 N 5	100.00	414.2652	-0.6	-1.4	41.5	13.5	even	ok
	1	C 25 H 36 N O 4	62.36	414.2639	-1.9	-4.6	27.7	8.5	even	ok

Compound 6



☐ Automatically locate monoisotopic peak Maximum number of formulas 500

☑ Check rings plus double bonds Minimum -0.5 Maximum 40

Electron configuration even

☑ Filter H/C element ratio Minimum H/C 0 Maximum H/C 3

☑ Estimate carbon number ☑ Generate immediately

Show Pattern

Current Data Parameters
NAME VB-GSA-182
EXPNO 99
PROCNO 1

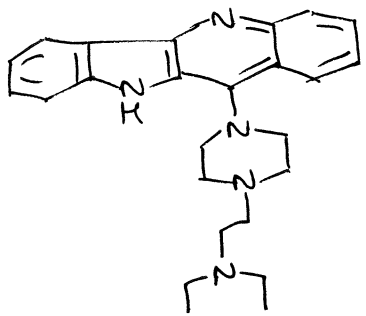
F2 – Acquisition Parameters
Date_ 20091123
Time 15.37
INSTRUM spect
PROBHD 5 mm Dual 13
PULPROG zg30
TD 16384
SOLVENT DMSO
NS 16
DS 2
SWH 6258.772 Hz
FIDRES 0.382005 Hz
AQ 1.3089329 sec
RG 181
DW 79.888 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec

========== CHANNEL f1 ==========
NUC1 1H
P1 13.40 usec
PL1 0.00 dB
SFO1 499.4828750 MHz

F2 – Processing parameters
SI 32768
SF 499.4800000 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00

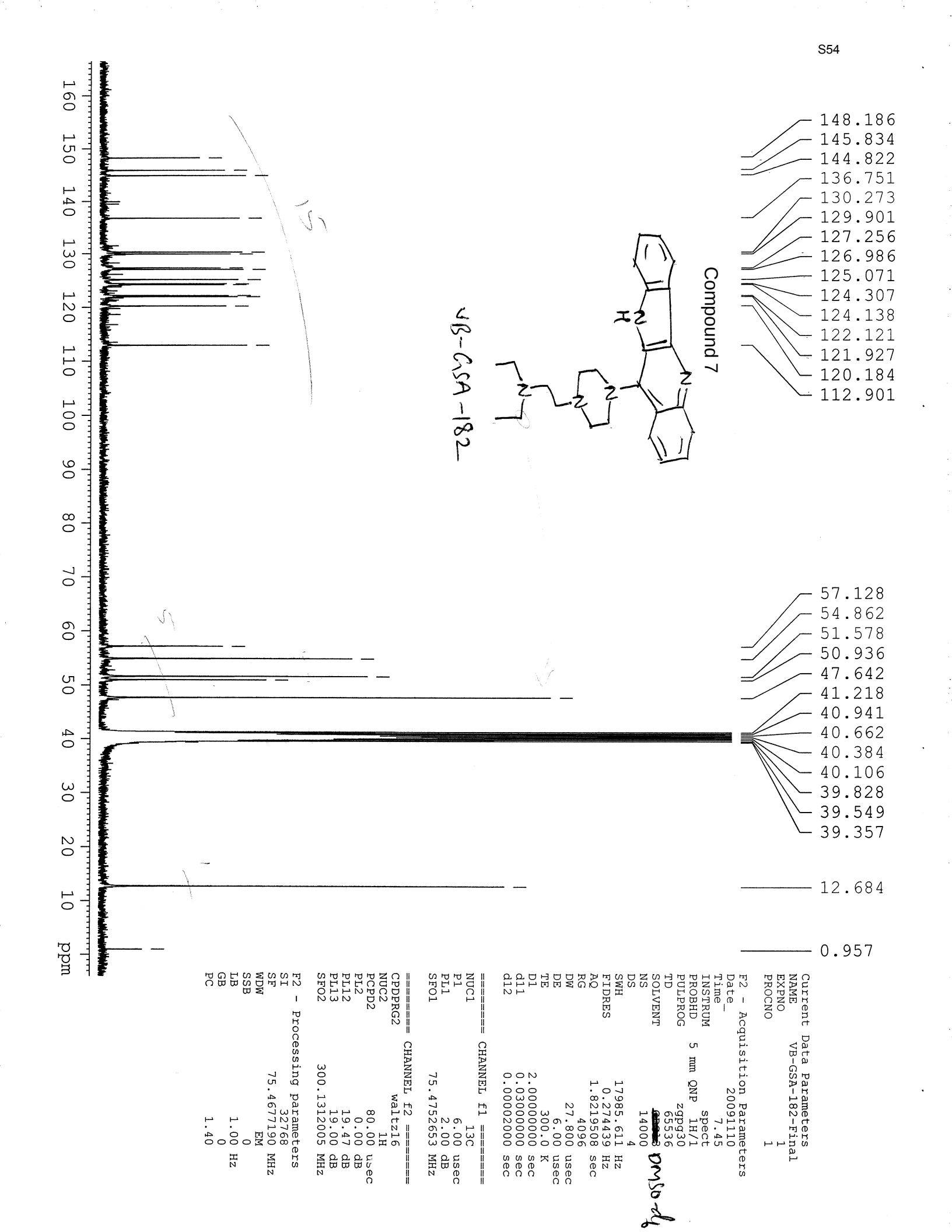
DRX-500

Compound 7



VB-GSA-182

(DMSO-d_6 ; 500 MHz)


148.186
145.834
144.822
136.751
130.273
129.901
127.256
126.986
125.071
124.307
124.138
122.121
121.927
120.184
112.901
Compound 7
VB-GSA-182
57.128
54.862
51.578
50.936
47.642
41.218
40.941
40.662
40.384
40.106
39.828
39.549
39.357
12.684
0.957
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
Current Data Parameters
NAME VB-GSA-182-Final
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20091110
Time_ 7.45
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT DMSO-d6
NS 14000
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 4096
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
========== CHANNEL f1 ==========
NUC1 13C
P1 6.00 usec
PL1 2.00 dB
SFO1 75.4752653 MHz
========== CHANNEL f2 ==========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 19.47 dB
PL13 19.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

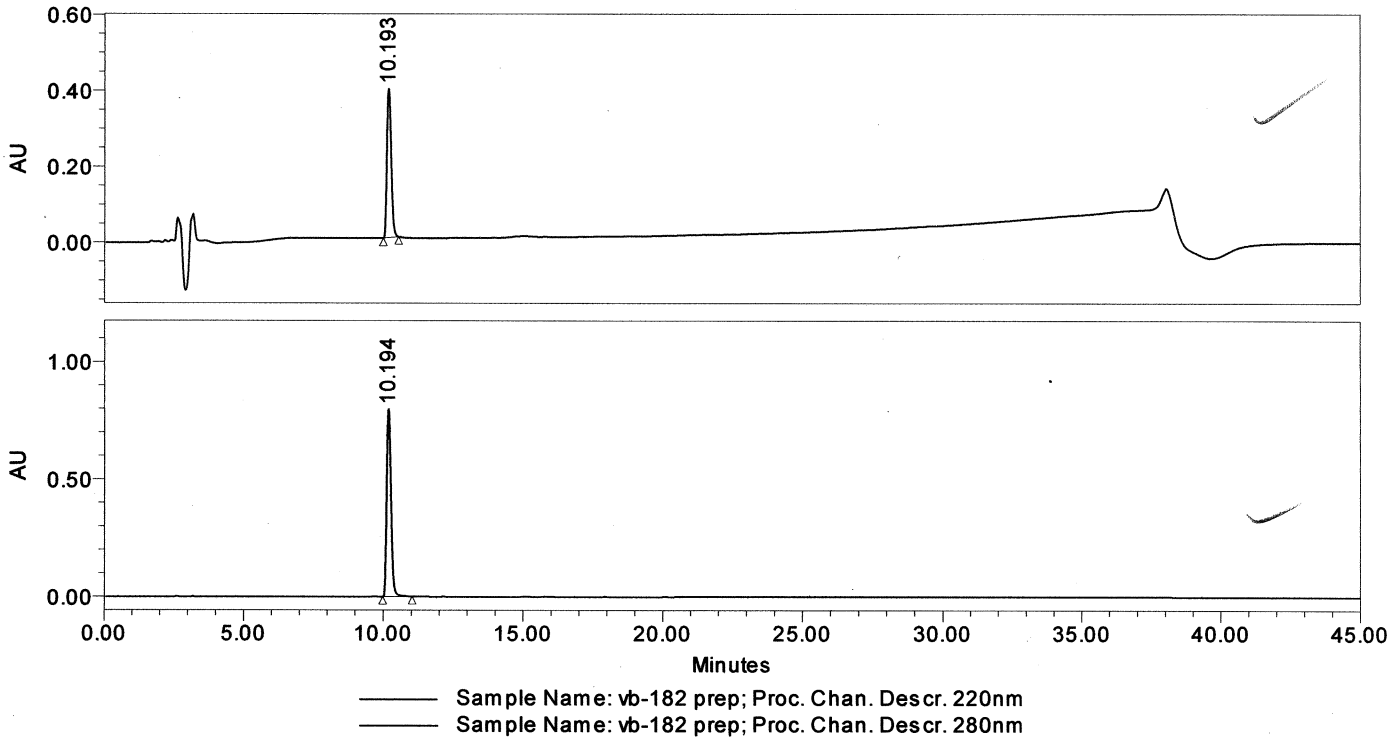
Empower software

Dual Channel Summary

Reported by User: Jatinder J. (Jatinder) Project Name: BIO5_HPLC1

SAMPLE INFORMATION

Sample Name:	vb-182 prep	Acquired By:	Jatinder
Sample Type:	Unknown	Date Acquired:	9/29/2009 11:57:13 AM
Vial:	58	Acq. Method Set:	10_90B_in
Injection #:	1	Date Processed:	9/29/2009 1:28:21 PM, 9/29/2009
Injection Volume:	10.00 ul	Processing Method	Peptide_general
Run Time:	45.0 Minutes	Channel Name:	2487Channel 1, 2487Channel 2
Sample Set Name	Prime_Run	Proc. Chnl. Descr.:	220nm, 280nm



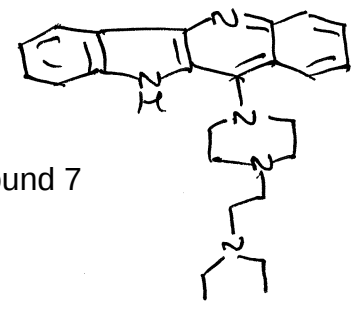
Channel 220 nm
Channel: 2487Channel 1

	RT	Area (µV*sec)	% Area	Channel
1	10.193	4.29e+006	100.00	2487Channel 1

Channel 280 nm
Channel: 2487Channel 2

	RT	Area (µV*sec)	% Area	Channel
1	10.194	8.95e+006	100.00	2487Channel 2

NOTES:



Compound 7

VB-GSA-182

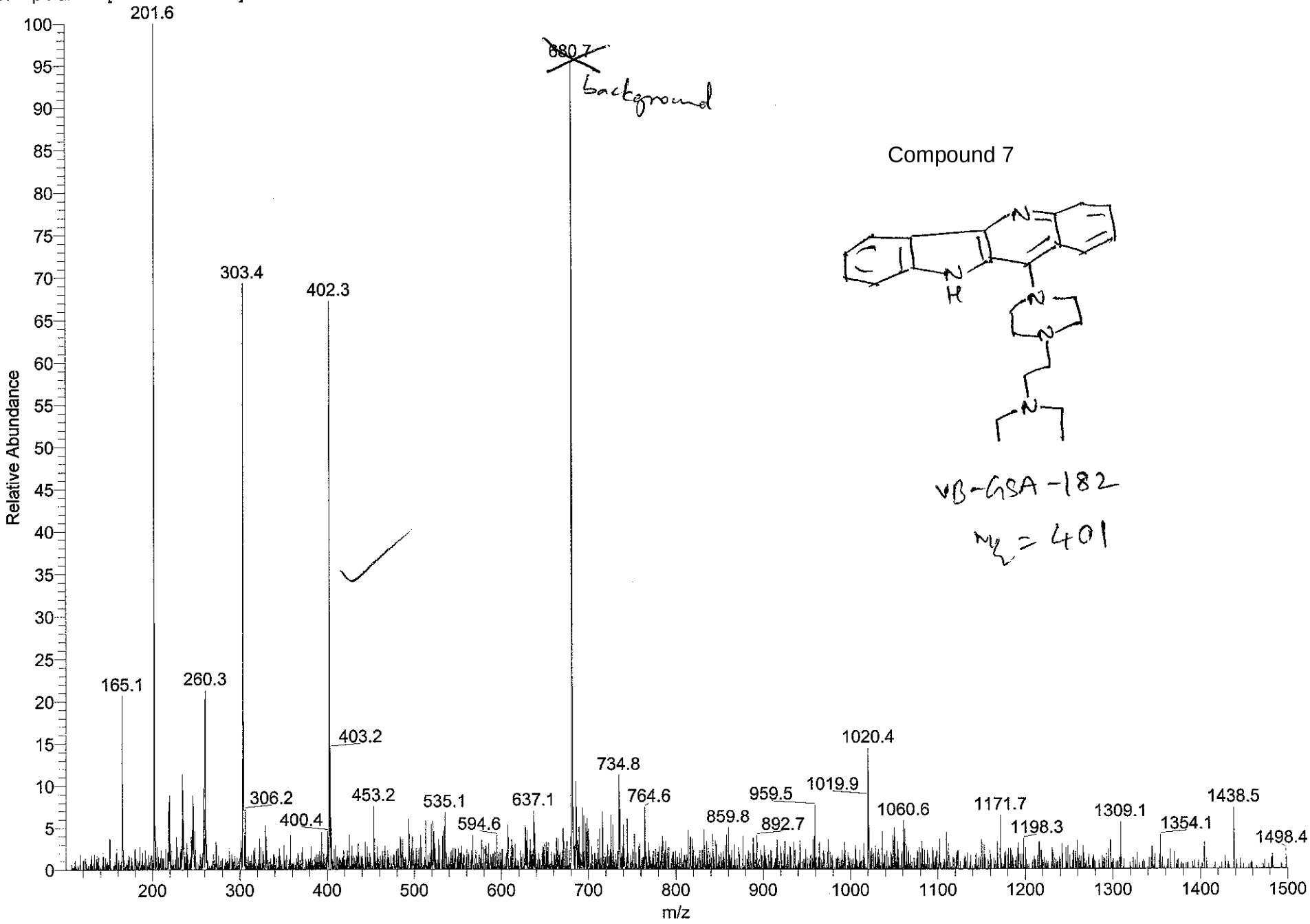
E:\MSLab_LCQ\VB-182
Venkat Boddupally, MeOH:H2O 1:1

11/12/2009 04:02:57 PM

VB-182

VB-182 #29-30 RT: 0.89-0.92 AV: 2 NL: 2.61E5
T: + p Full ms [100.00-1500.00]

S56

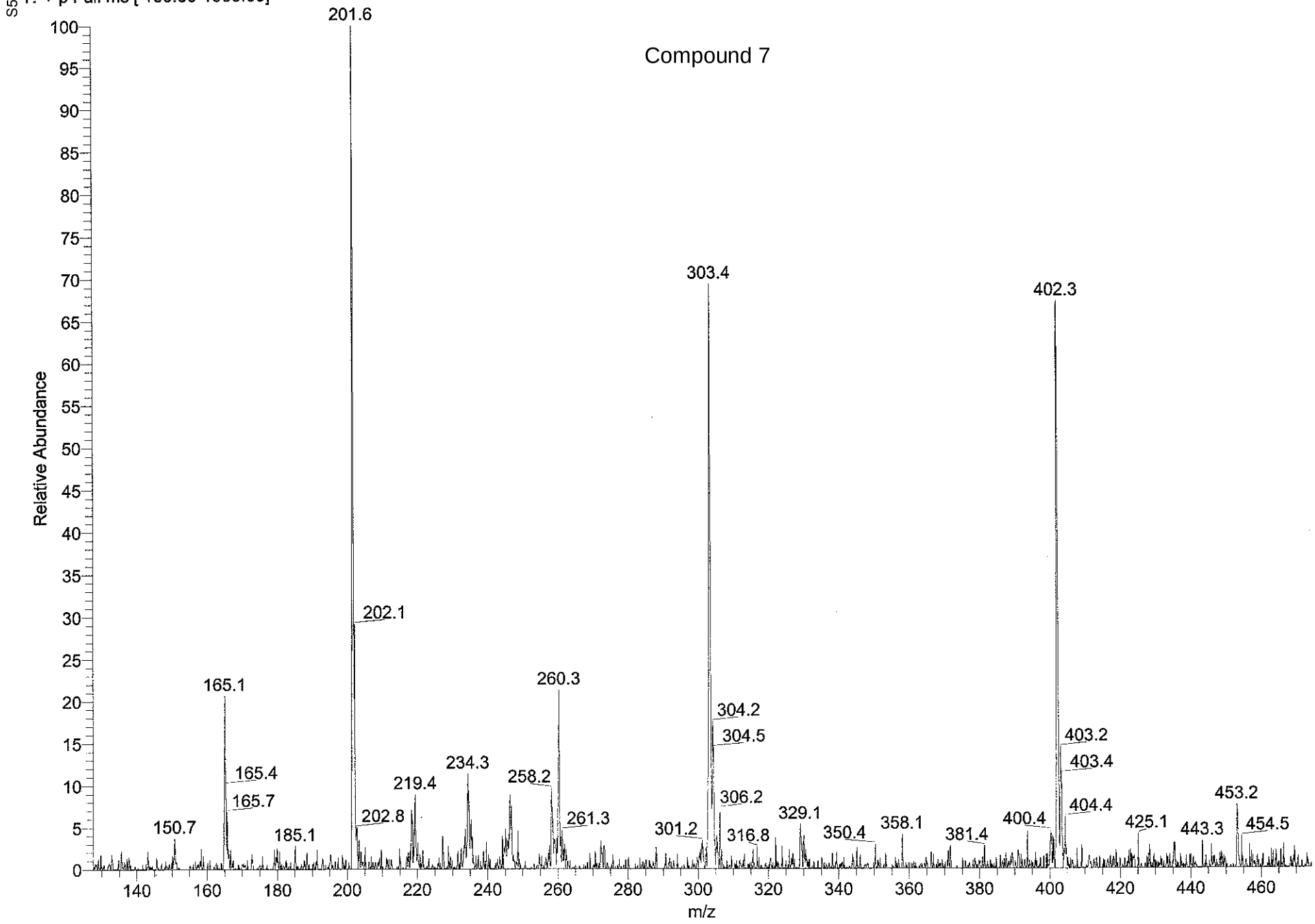


Compound 7

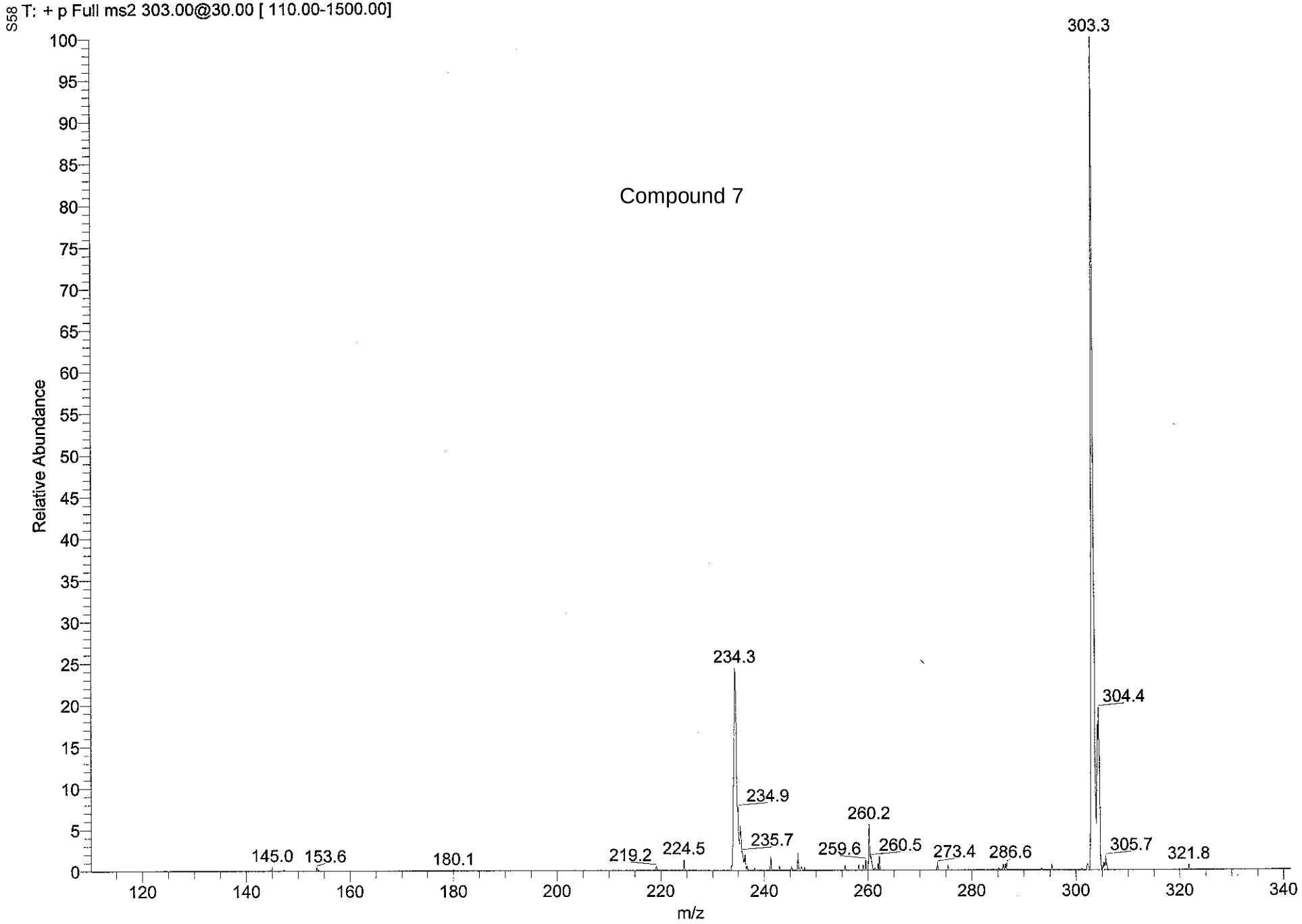
VB-GSA-182

MW = 401

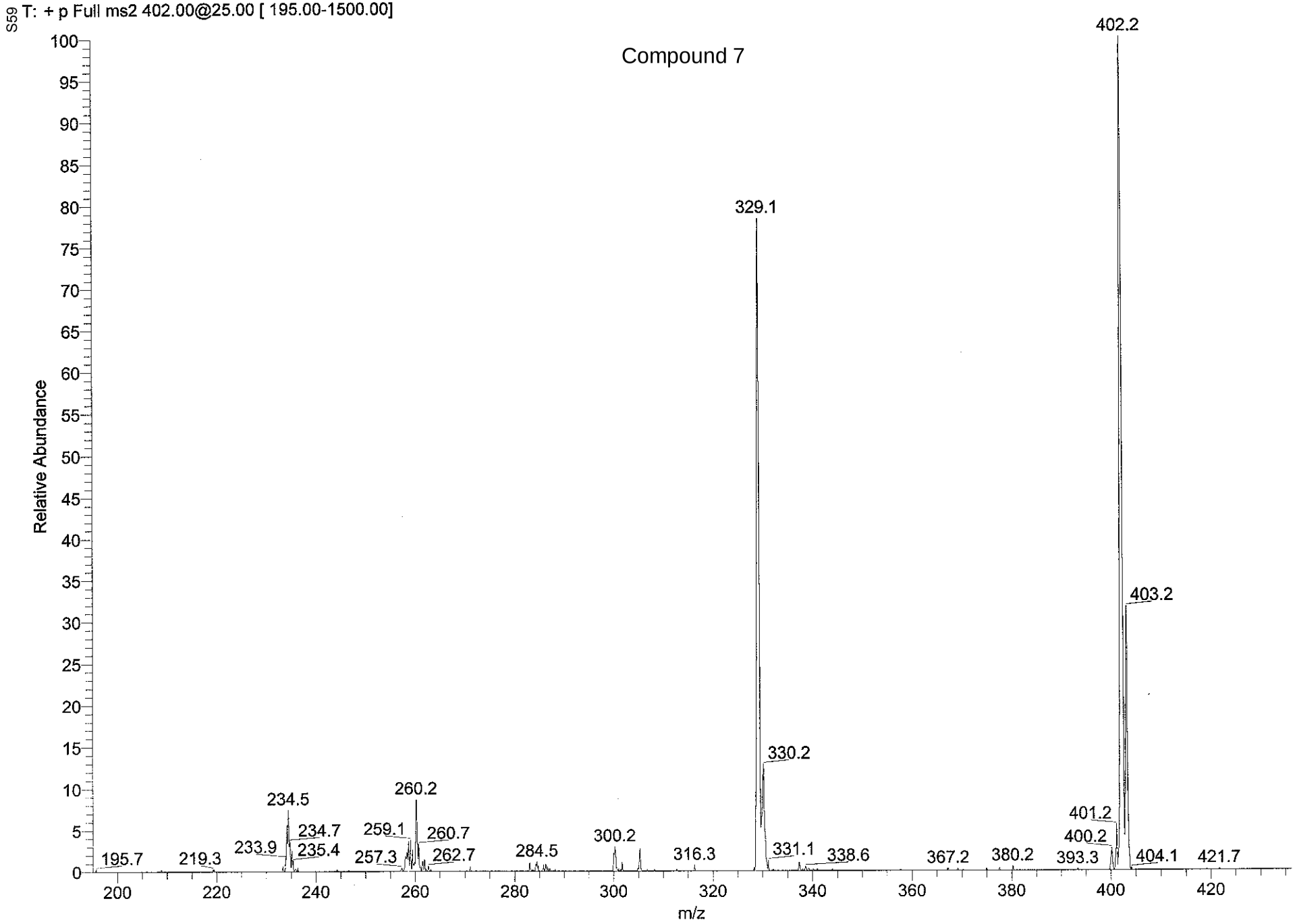
E:\MSLab_LCQ\VB-182 11/12/2009 04:02:57 PM VB-182
Venkat Boddupally, MeOH:H2O 1:1
VB-182 #29-30 RT: 0.89-0.92 AV: 2 NL: 2.61E5
T: + p Full ms [100.00-1500.00]



E:\MSLab_LCQ\VB-182 11/12/2009 04:02:57 PM VB-182
Venkat Boddupally, MeOH:H2O 1:1
VB-182 #24-25 RT: 0.73-0.77 AV: 2 NL: 8.29E4
T: + p Full ms2 303.00@30.00 [110.00-1500.00]



E:\MSLab_LCQ\VB-182 11/12/2009 04:02:57 PM VB-182
Venkat Boddupally, MeOH:H2O 1:1
VB-182 #9-10 RT: 0.26-0.29 AV: 2 NL: 1.09E5
T: + p Full ms2 402.00@25.00 [195.00-1500.00]

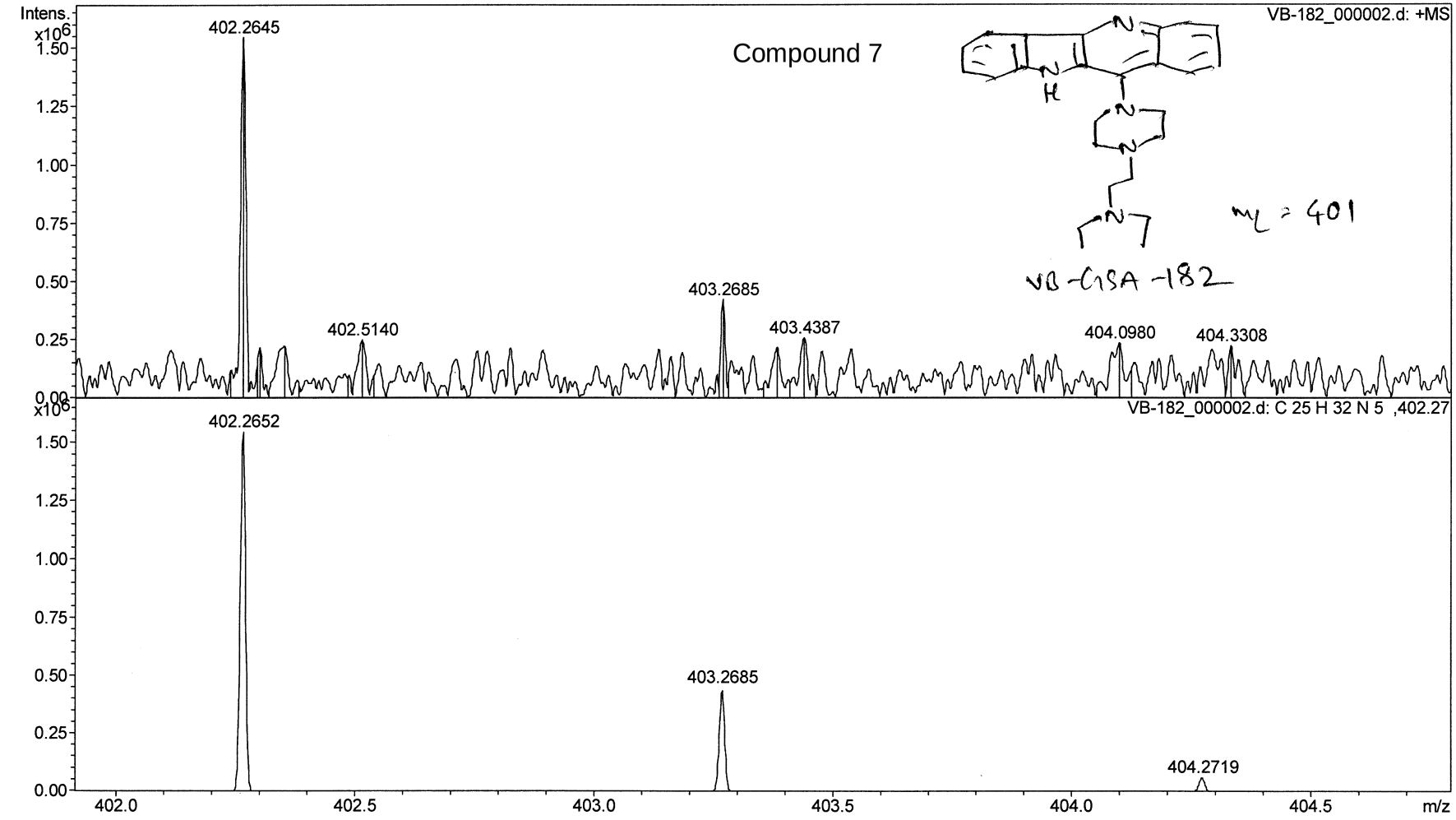


S60

Generic Display Report

Analysis Info

Analysis Name	D:\DATA\Facility_Nov_09\VB-182_000002.d	Acquisition Date	11/13/2009 10:17:15 AM
Method	ESI_101506	Operator	
Sample Name	VB-182	Instrument	apex-Qe
Comment	Venkat B., ACN:H2O 1:1:0.1%FA		



SmartFormula Manually

Min C_{18}

Max

C 18-n

Generate

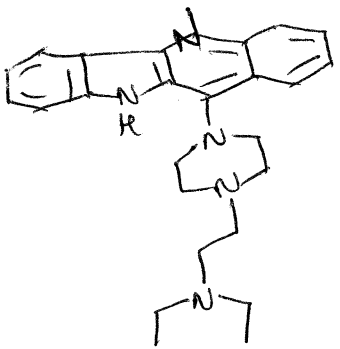
Help

Note: for m < 2000 the elements C, H, N, and O are considered implicitly.

Measured m/z 402.2645 Tolerance 2 mDa Charge 1

#	Mol. Formula	m/z	err [mDa]	|err| [ppm]	err [ppm]	mean err [ppm]	mSigma	Sigma Rank	rdb	N rule	e⁻
1	C 24 H 36 N O 4	402.2639	-0.60	1.5	-1.5	-1.9	24.9	1	7.5	ok	even
2	C 25 H 32 N 5	402.2652	0.73	1.8	1.8	1.4	26.0	2	12.5	ok	even

Compound 7



☐ Automatically locate monoisotopic peak Maximum number of formulas 500

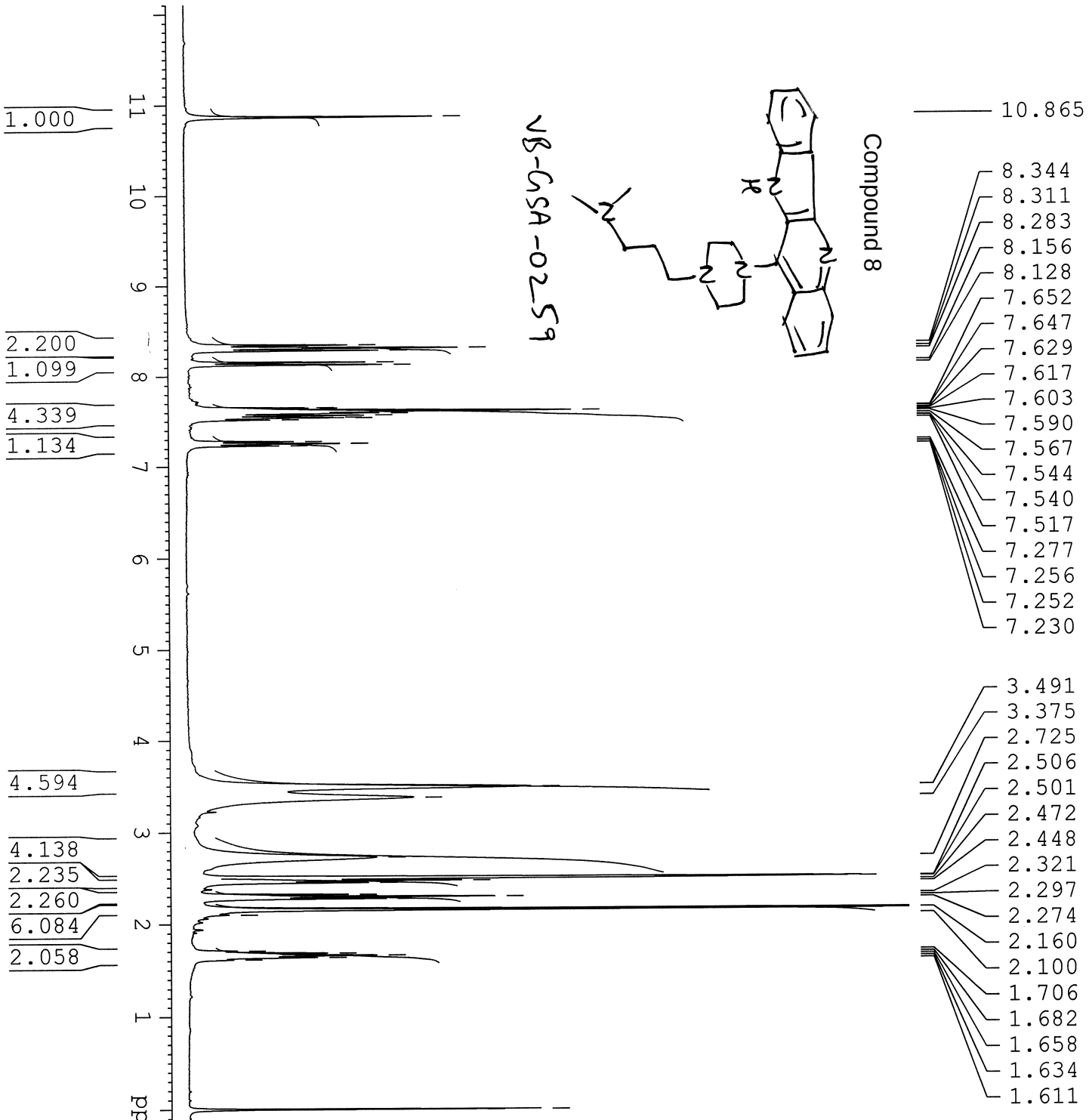
☑ Check rings plus double bonds Minimum -0.5 Maximum 40

Electron configuration even

☑ Filter H/C element ratio Minimum H/C 0 Maximum H/C 3

☑ Estimate carbon number ☑ Generate immediately

Show Pattern

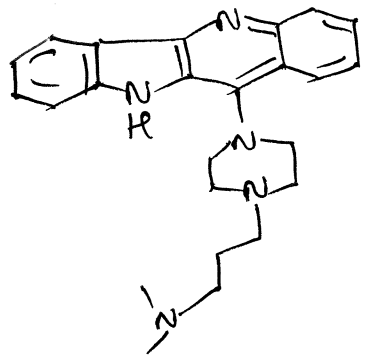

Compound 8
VB-GSA-0259
10.865
8.344
8.311
8.283
8.156
8.128
7.652
7.647
7.629
7.617
7.603
7.590
7.567
7.544
7.540
7.517
7.277
7.256
7.252
7.230
3.491
3.375
2.725
2.506
2.501
2.472
2.448
2.321
2.297
2.274
2.160
2.100
1.706
1.682
1.658
1.634
1.611
1.000
2.200
1.099
4.339
1.134
4.594
4.138
2.235
2.260
6.084
2.058
ppm
Current Data Parameters
NAME VB-GSA-0259
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100802
Time_ 10.26
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 362
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 8.50 usec
PL1 0.00 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

```
Current Data Parameters
NAME         VB-GSA-0259
EXPNO               1019
PROCNO                 1

F2 - Acquisition Parameters
Date_           20100810
Time               10.03
INSTRUM             spect
PROBHD   5 mm QNP  1H/1
PULPROG           zgpg30
TD                 65536
SOLVENT             DMSO
NS                 16000
DS                     4
SWH           17985.611 Hz
FIDRES         0.274439 Hz
AQ             1.8219508 sec
RG                  1024
DW                27.800 usec
DE                 6.00 usec
TE                300.0 K
D1            2.00000000 sec
d11           0.03000000 sec
d12           0.00002000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                 6.00 usec
PL1                2.00 dB
SFO1          75.4752653 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             80.00 usec
PL2                0.00 dB
PL12              19.47 dB
PL13              19.00 dB
SFO2         300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF            75.4677190 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

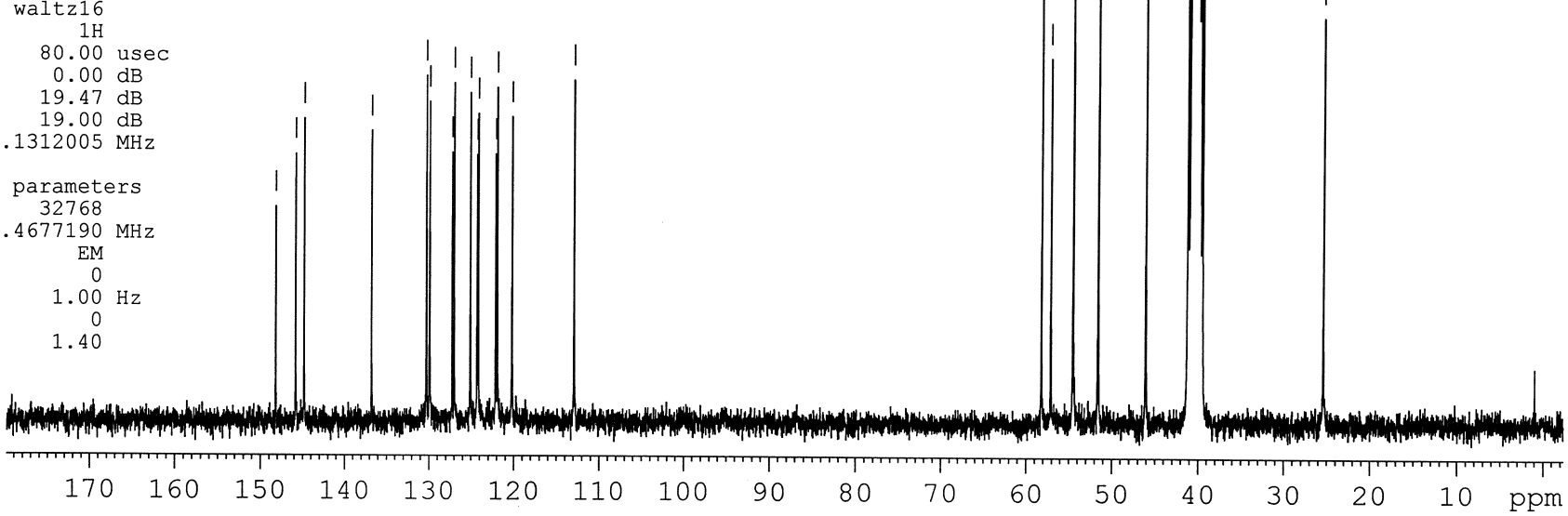
148.183 145.829 144.822 136.768 130.285 129.900 127.241 127.000 125.083 124.292 124.140 122.112 121.931 120.193 112.903

58.209 57.118 54.515 51.595 46.095 41.214 40.935 40.657 40.379 40.102 39.824 39.545 25.410

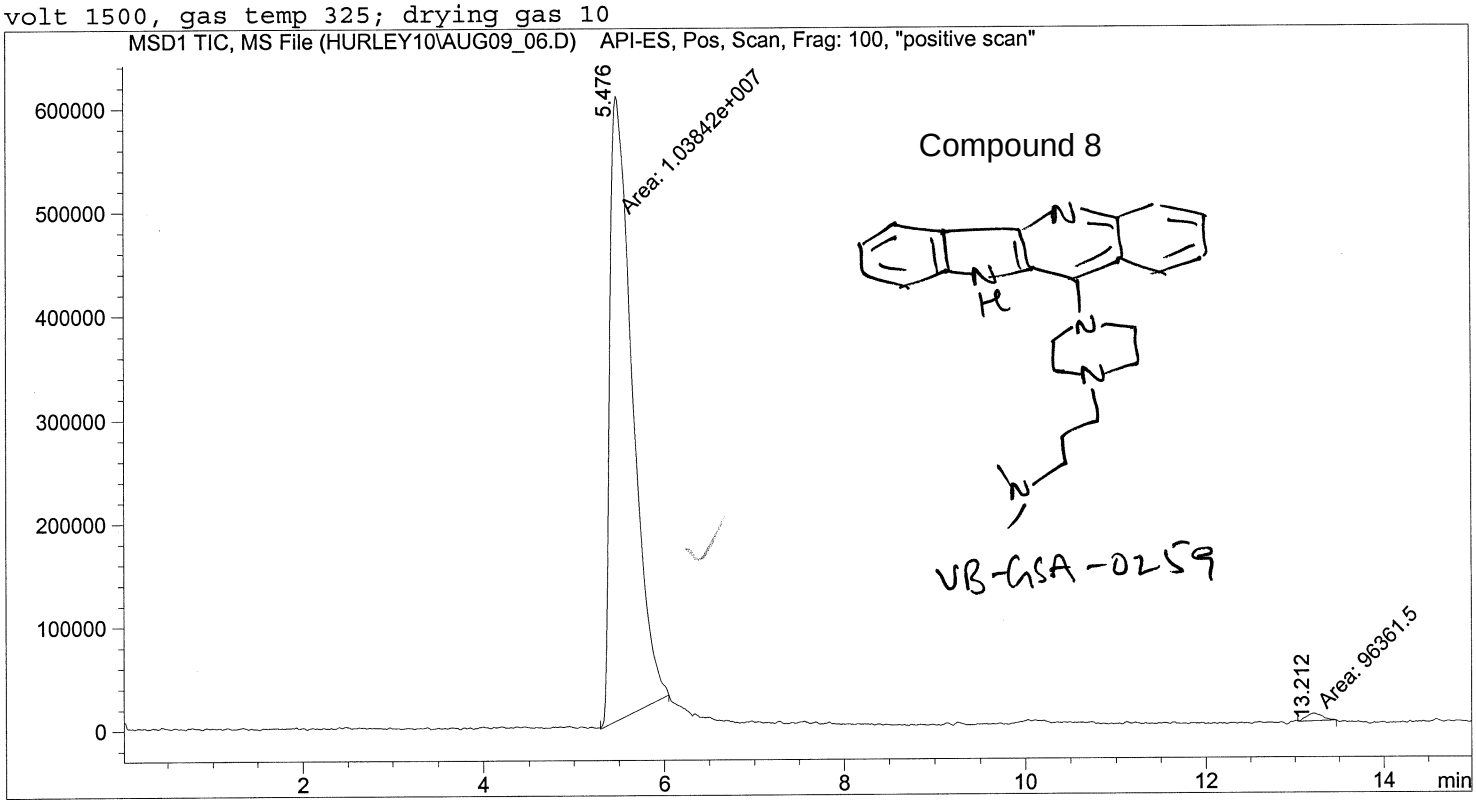
Compound 8



VB-GSA-0259



```
==========================================================================
Injection Date  : 8/9/2010 1:40:08 PM
Sample Name     : VB-GSA-0259                    Location : Vial 1
Acq. Operator   : Karen                             Inj :   1
Acq. Instrument : Instrument 1                  Inj Volume : 0.1 µl
Method          : C:\HPCHEM\1\METHODS\LC_MS.M
Last changed    : 8/9/2010 1:39:00 PM by Karen
Zorbax SB C18, 150 x 4.6, 3.5u,25:75:0.25, MeOH/H2O/formic, POS, 150-500; frag 100; 25C, cap
volt 1500, gas temp 325; drying gas 10
```

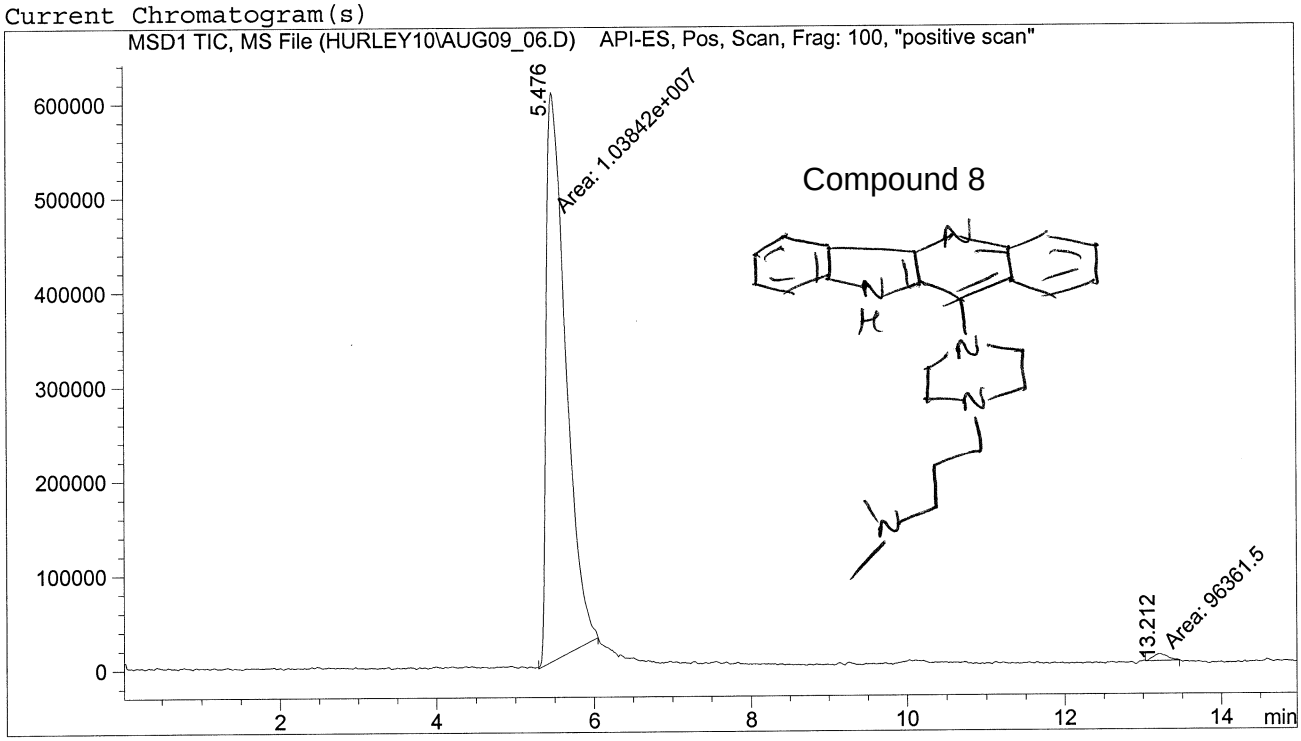



```
==========================================================================
                          Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MSD1 TIC, MS File

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]                          %
----|-------|----|-------|----------|----------|--------|
   1   5.476 MM    0.2862 1.03842e7  6.04644e5   99.0806
   2  13.212 MM    0.2124 9.63615e4  7560.06982   0.9194

Totals :                  1.04806e7  6.12204e5

==========================================================================
                          *** End of Report ***
```

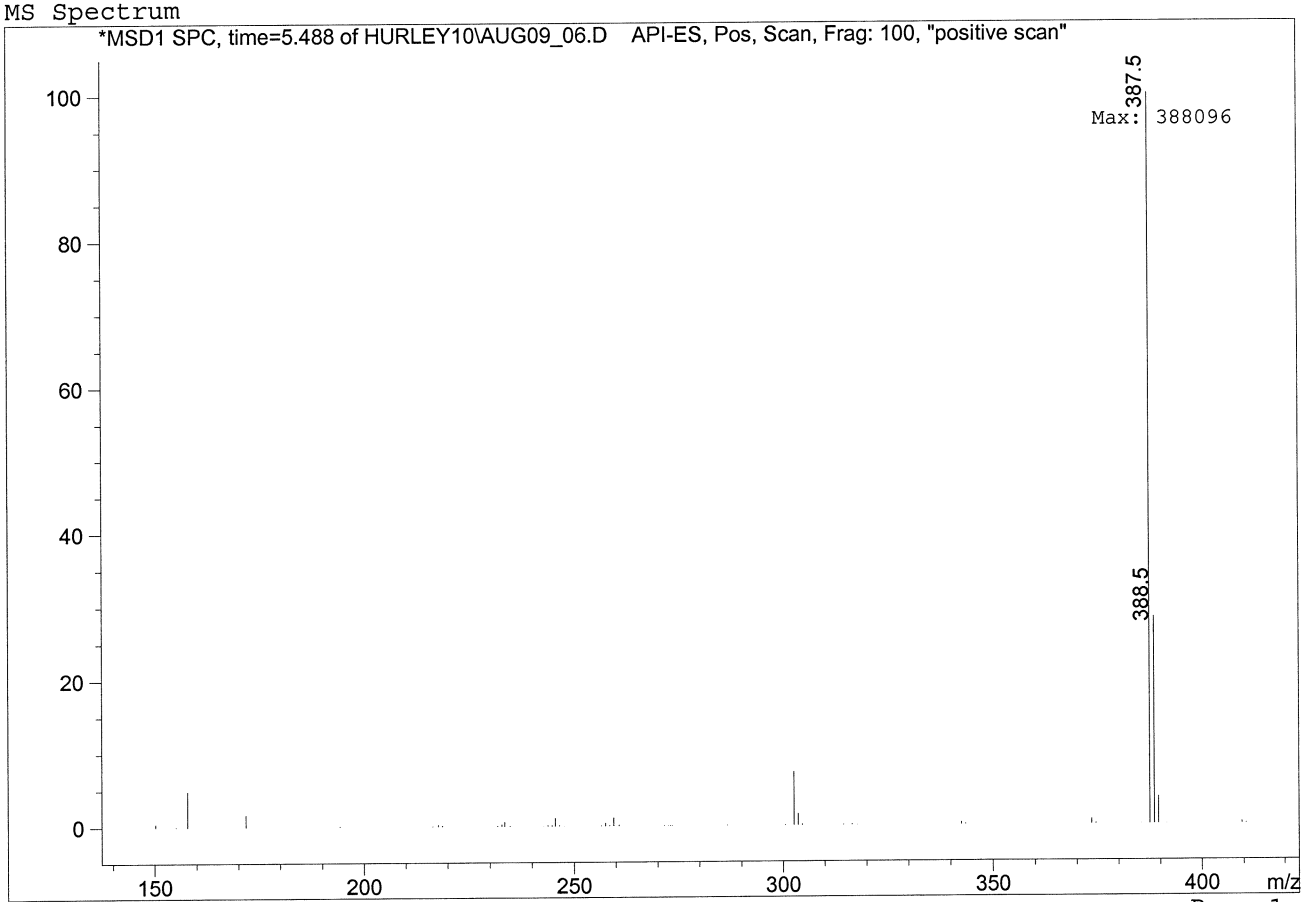
Print of all graphic windows

Injection Date : 8/9/2010 1:40:08 PM
Sample Name : VB-GSA-0259 Location : Vial 1
Acq. Operator : Karen Inj : 1
Acq. Instrument : Instrument 1 Inj Volume : 0.1 µl
Method : C:\HPCHEM\1\METHODS\LC_MS.M
Last changed : 8/9/2010 1:39:00 PM by Karen
Zorbax SB C18, 150 x 4.6, 3.5u,25:75:0.25, MeOH/H2O/formic, POS, 150-500; frag 100; 25C, cap volt 1500, gas temp 325; drying gas 10

Current Chromatogram(s)

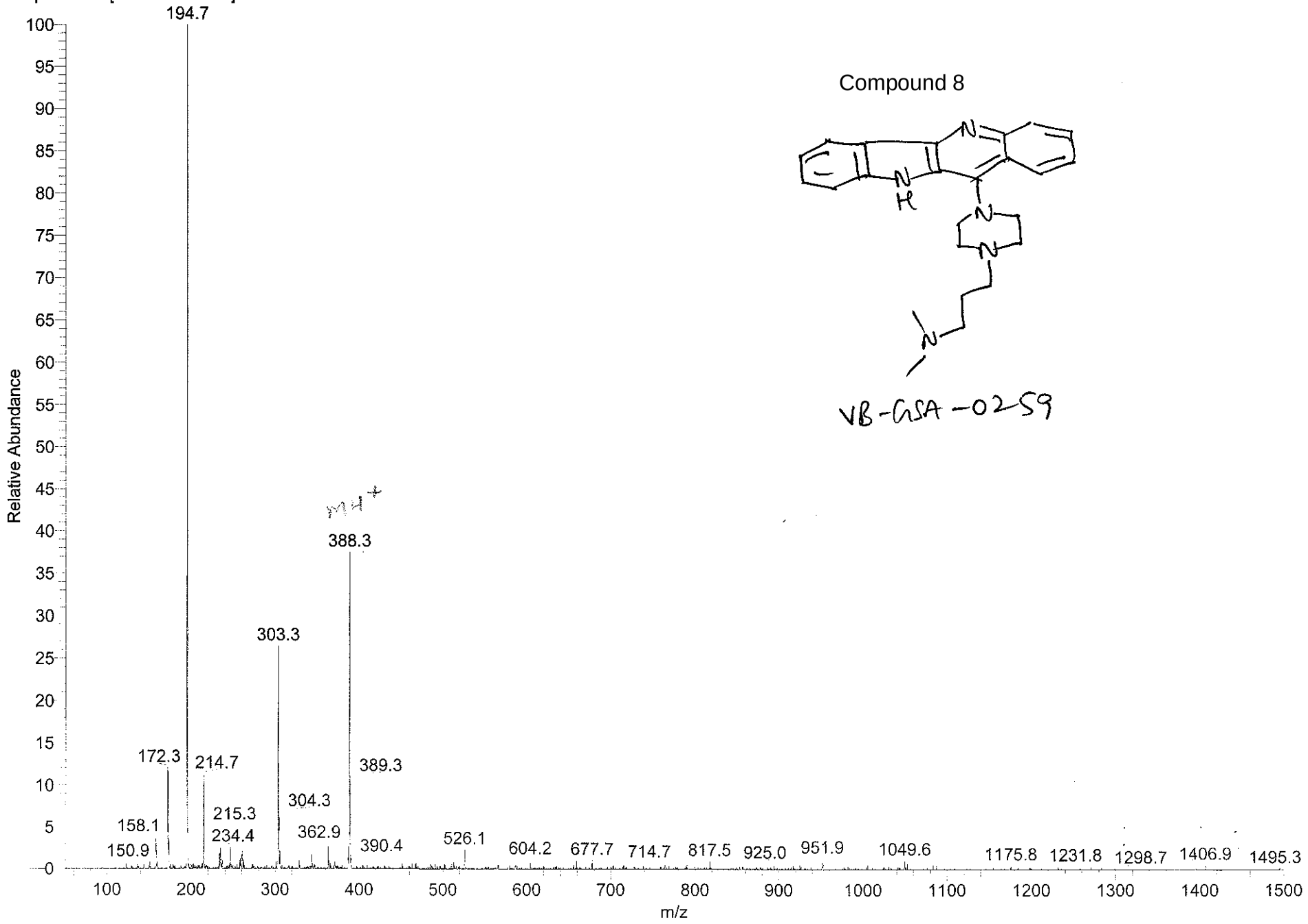


MS Spectrum



E:\MSLab_LCQ\VB-0259 08/11/2010 09:44:40 AM VB-0259
Venkat B., ACN:MeOH 1:1
VB-0259 #39-41 RT: 1.19-1.25 AV: 3 NL: 4.56E6
T: + p Full ms [50.00-1500.00]

S66

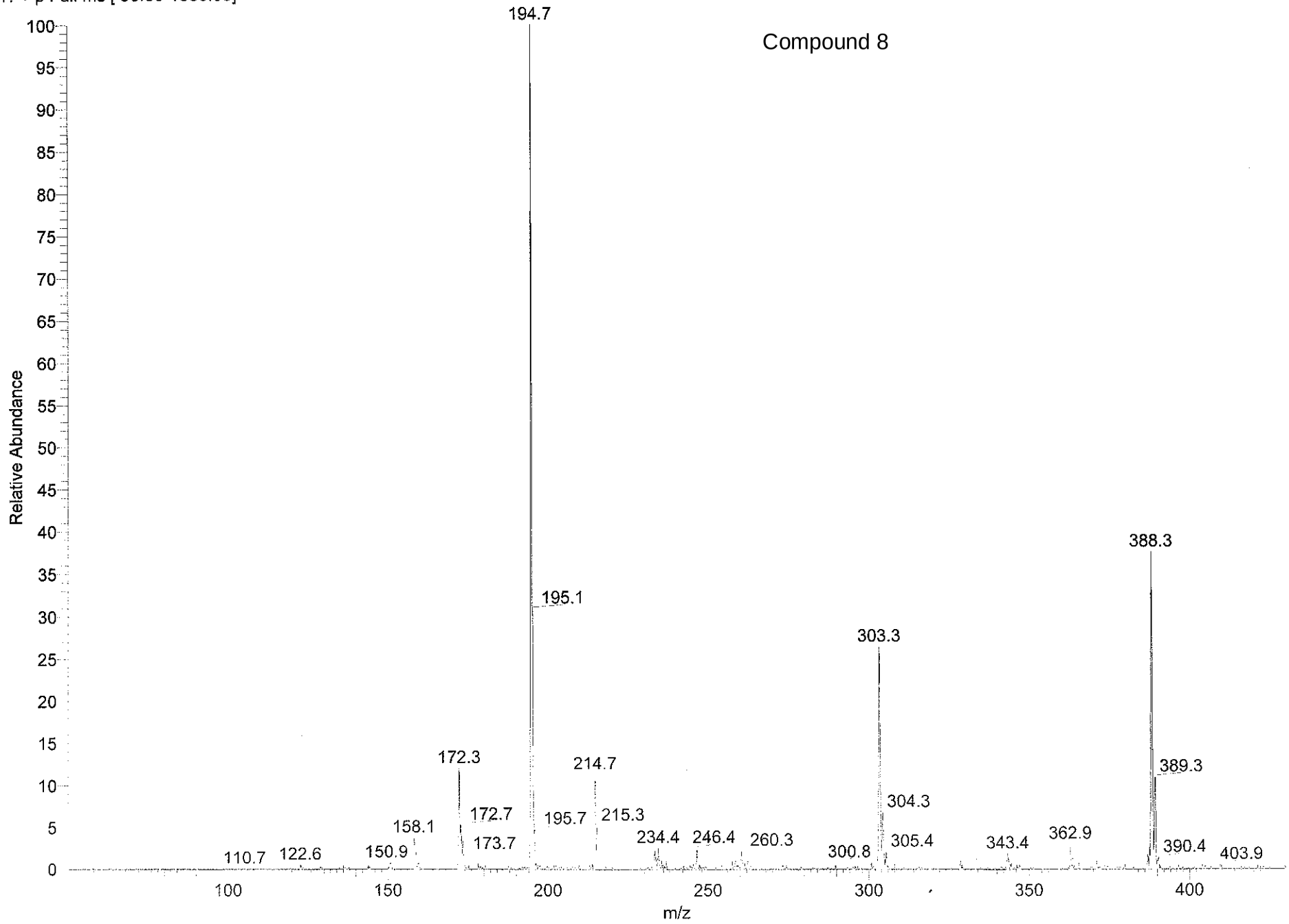


Compound 8

VB-CSA-0259

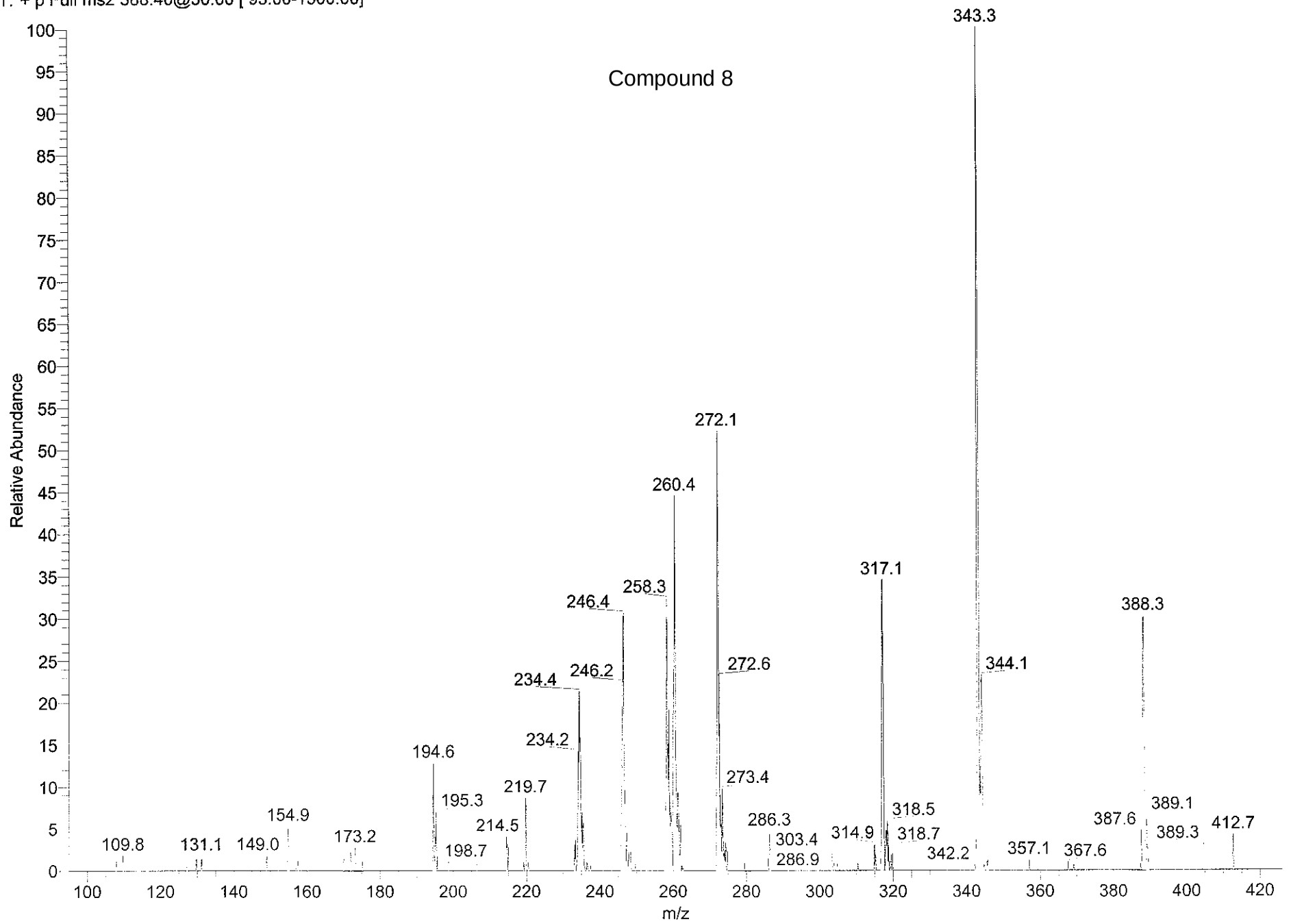
E:\MSLab_LCQ\VB-0259 08/11/2010 09:44:40 AM VB-0259
Venkat B., ACN:MeOH 1:1
VB-0259 #39-41 RT: 1.19-1.25 AV: 3 NL: 4.56E6
T: + p Full ms [50.00-1500.00]

S67



E:\MSLab_LCQ\VB-0259
Venkat B., ACN:MeOH 1:1
VB-0259 #8-9 RT: 0.24-0.27 AV: 2 NL: 6.21E4
T: + p Full ms2 388.40@30.00 [95.00-1500.00]

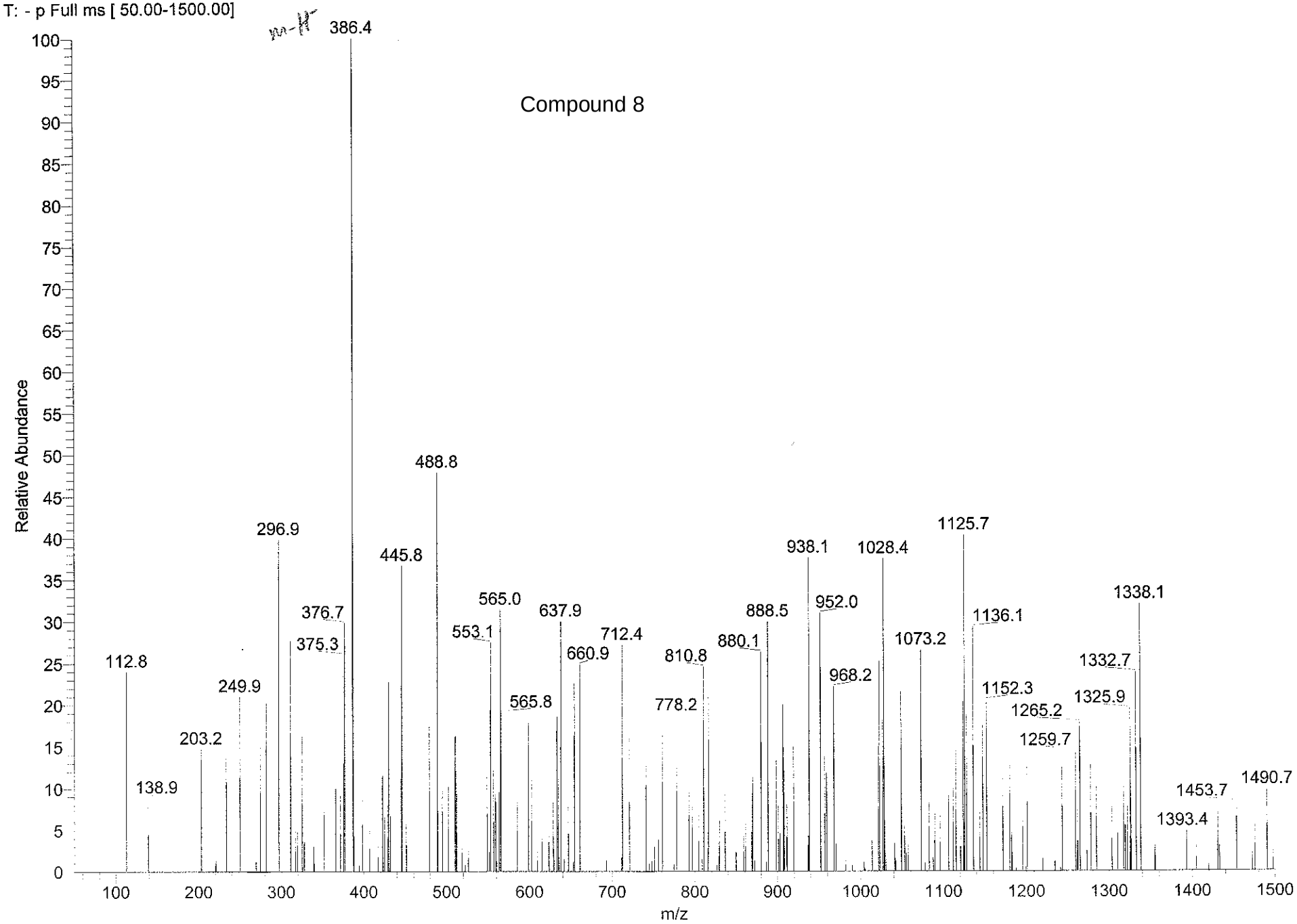
08/11/2010 09:44:40 AM VB-0259



E:\MSLab_LCQ\VB-0259
Venkat B., ACN:MeOH 1:1
VB-0259 #28-33 RT: 0.85-1.00 AV: 6 NL: 4.91E3
T: - p Full ms [50.00-1500.00]

08/11/2010 09:44:40 AM VB-0259

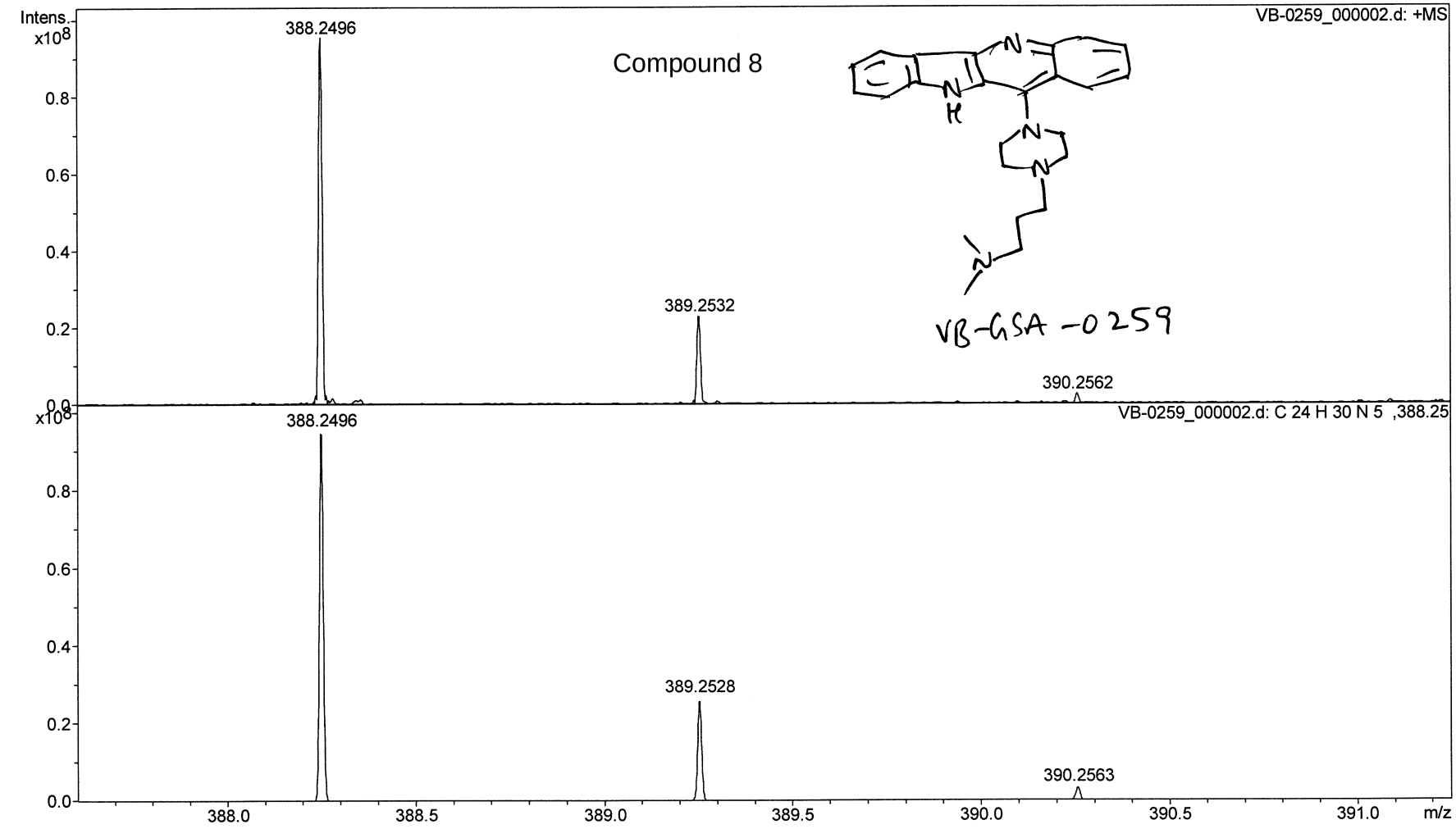
S69



Generic Display Report

Analysis Info

Analysis Name	D:\DATA\Facility_Aug_10\VB-0259_000002.d	Acquisition Date	8/11/2010 11:07:25 AM
Method	ESI_101506	Operator	
Sample Name	VB-0259	Instrument	apex-Ultra
Comment	Venkat B., positive mode, ACN:H2O 1:1:0.1%FA		



SmartFormula Manually

Min C_{16}

Max

C 16-n

Generate

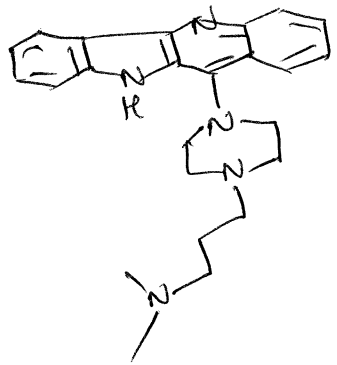
Help

Note: for m < 2000 the elements C, H, N, and O are considered implicitly.

Measured m/z 388.2496 Tolerance 2 mDa Charge 1

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
388.2496	2	C 24 H 30 N 5	100.00	388.2496	-0.0	-0.1	22.1	12.5	even	ok
	1	C 23 H 34 N O 4	62.33	388.2482	-1.4	-3.6	11.2	7.5	even	ok

Compound 8



☐ Automatically locate monoisotopic peak Maximum number of formulas 500

☑ Check rings plus double bonds Minimum -0.5 Maximum 40

Electron configuration even

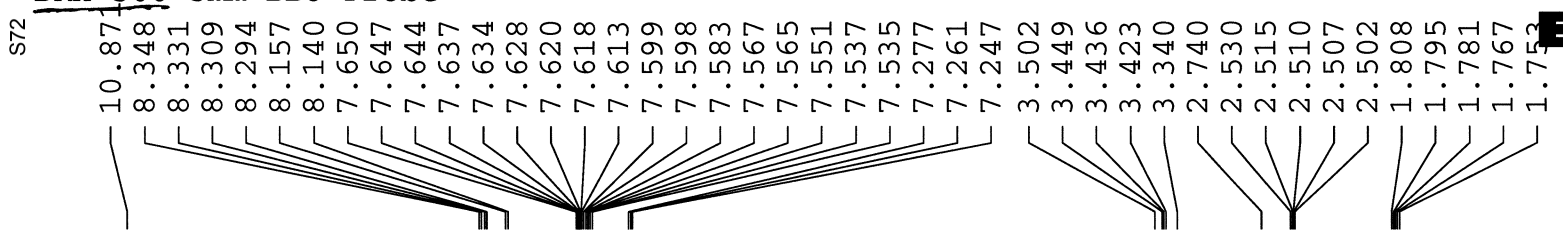
☑ Filter H/C element ratio Minimum H/C 0 Maximum H/C 3

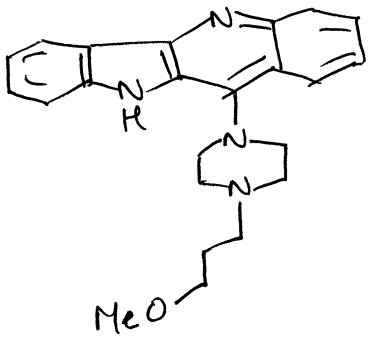
☑ Estimate carbon number ☑ Generate immediately

Show Pattern

DRX-500

Standard 1D 1H Spectrum
DRX-500 5mm BBO Probe





Compound 9

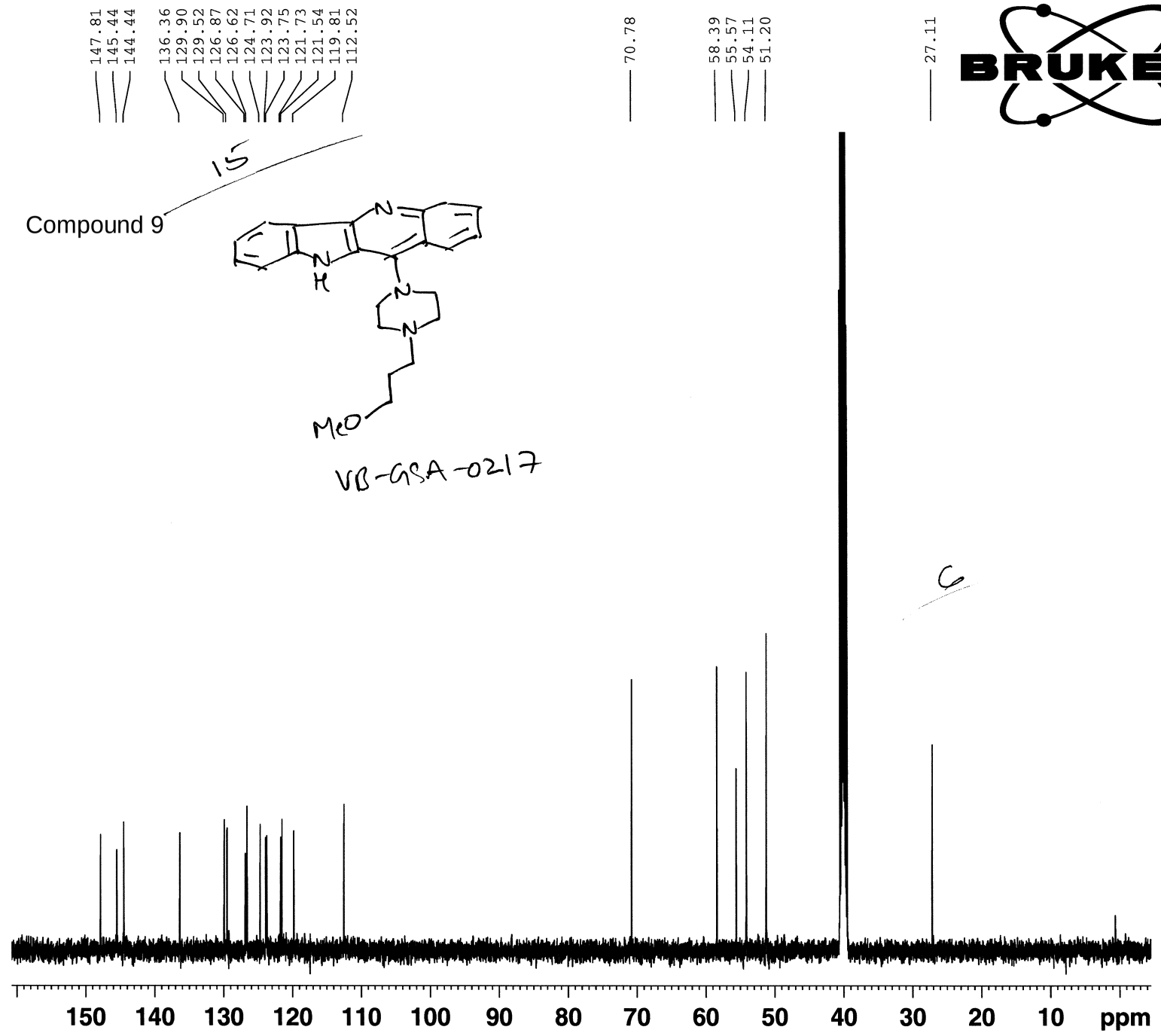
VB-GSA-0217

Current Data Parameters
NAME VB-GSA-0217
EXPNO 100
PROCNO 1

F2 - Acquisition Paramete
Date_ 20091223
Time 11.45
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 16
DS 4
SWH 6250.000 H
FIDRES 0.190735 H
AQ 2.6215701 s
RG 203.2
DW 80.000 u
DE 6.00 u
TE 298.0 K
D1 0.00000000 s
TD0 1

======== CHANNEL f1 =====
NUC1 1H
P1 12.50 u
PL1 -2.00 d
SFO1 499.4829469 M

F2 - Processing parameter
SI 32768
SF 499.4800000 M
WDW EM
SSB 0
LB 0.20 H
GB 0
PC 1.00



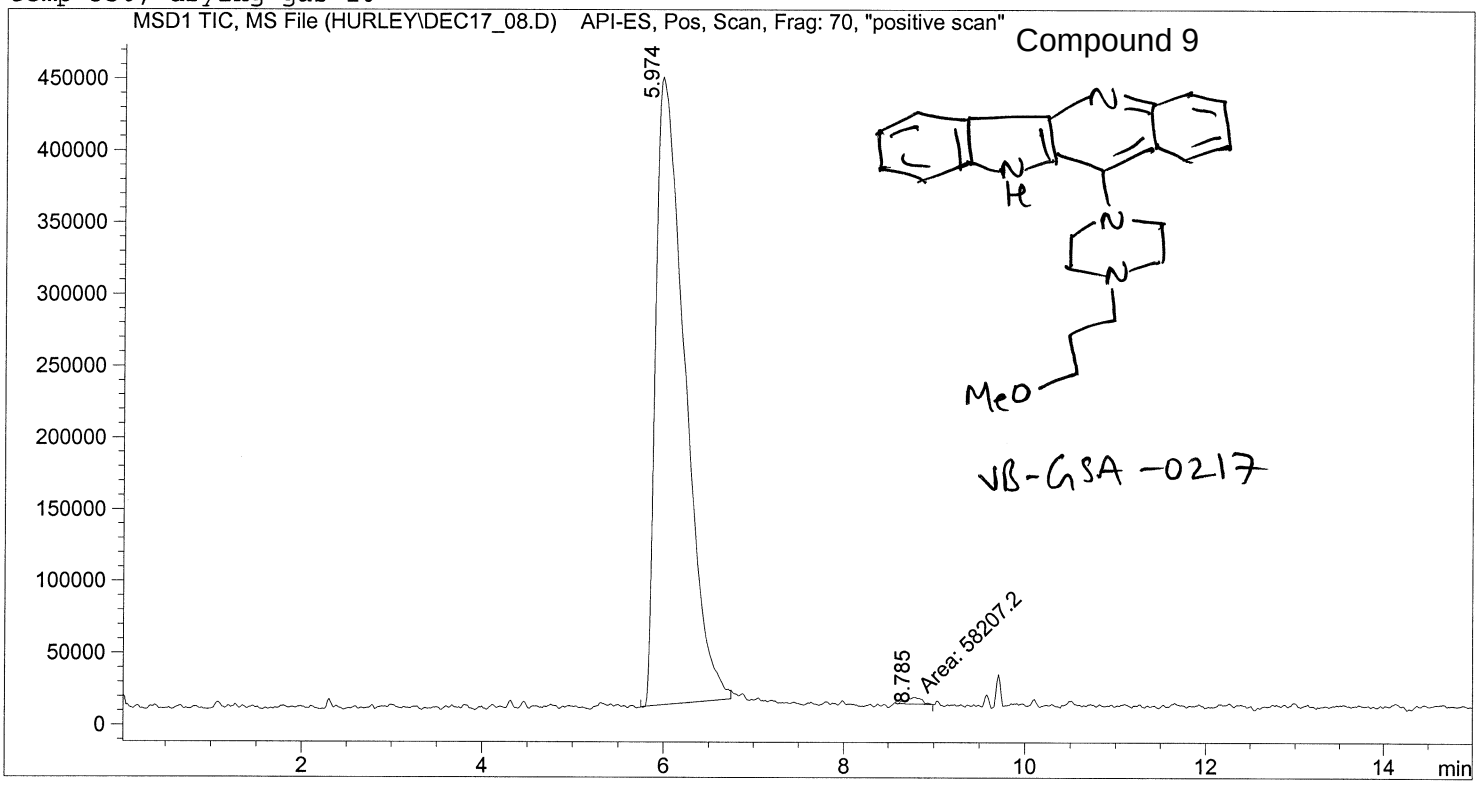
DRX-500

BRUKER

```
Current Data Parameters
NAME          VB-GSA-0217
EXPNO                 101
PROCNO                  1

F2 - Acquisition Parameter
Date_            20091223
Time                14.16
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG           zgpg30
TD                 65536
SOLVENT             DMSO
NS                  1520
DS                     4
SWH           30030.029 Hz
FIDRES         0.458222 Hz
AQ             1.0912410 se
RG                2896.3
DW                16.650 us
DE                 6.00 us
TE                298.3 K
D1             0.69999999 se
d11            0.03000000 se
DELTA          0.59999996 se
TD0                    1

======== CHANNEL f1 ======
NUC1                  13C
P1                 5.00 us
PL1                0.00 dB
SFO1         125.6069050 MH

======== CHANNEL f2 ======
CPDPRG2          waltz16
NUC2                  1H
PCPD2             80.00 us
PL2               -2.00 dB
PL12              18.00 dB
PL13              18.00 dB
SFO2         499.4819980 MH

F2 - Processing parameters
SI                 32768
SF           125.5943460 MH
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                  1.40
```

run w/acid S74

```
==========================================================================
Injection Date  : 12/17/2009 3:37:55 PM
Sample Name     : VB-GSA-0217                    Location : Vial 2
Acq. Operator   : Karen                             Inj :   1
Acq. Instrument : Instrument 1                  Inj Volume : 0.1 µl
Method          : C:\HPCHEM\1\METHODS\LC_MS.M
Last changed    : 12/17/2009 3:36:54 PM by Karen
Zorbax SB ODS,35:65:0.25; MeOH/water/formicA, POS, 300-500; frag 70; 25C, cap volt 2500, gas
temp 350; drying gas 10
```

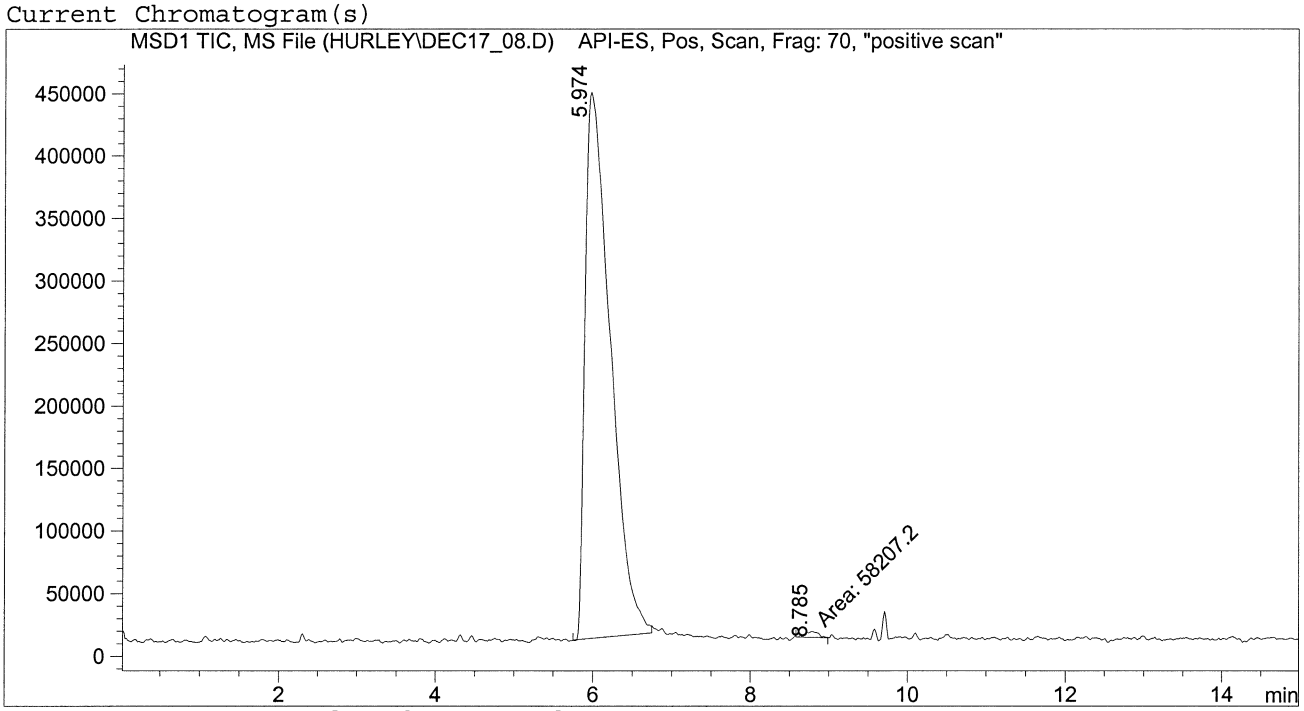



```
==========================================================================
                          Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MSD1 TIC, MS File

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]                          %
----|-------|----|-------|----------|----------|--------|
   1   5.974 PB    0.3145 9.65067e6  4.37089e5   99.4005
   2   8.785 MM    0.2062 5.82072e4  4705.27588   0.5995

Totals :                  9.70888e6  4.41795e5

==========================================================================
                          *** End of Report ***
```

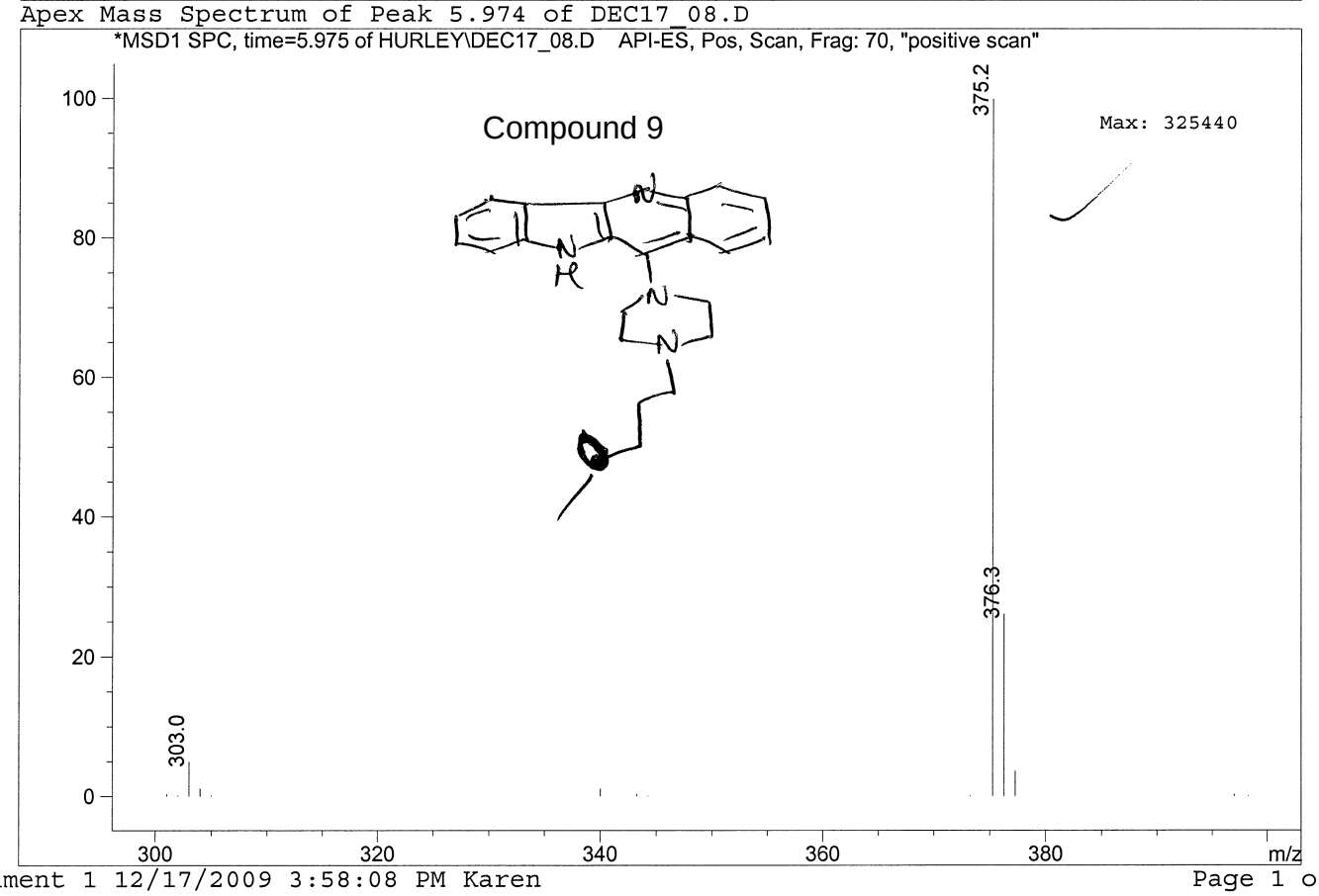
Print of all graphic windows
run w/acid


```
==========================================================================
Injection Date  : 12/17/2009 3:37:55 PM
Sample Name     : VB-GSA-0217                        Location : Vial 2
Acq. Operator   : Karen                                 Inj :   1
Acq. Instrument : Instrument 1                   Inj Volume : 0.1 µl
Method          : C:\HPCHEM\1\METHODS\LC_MS.M
Last changed    : 12/17/2009 3:36:54 PM by Karen
Zorbax SB ODS,35:65:0.25; MeOH/water/formicA, POS, 300-500; frag 70; 25C, cap volt 2500, gas
temp 350; drying gas 10
```

Current Chromatogram(s)



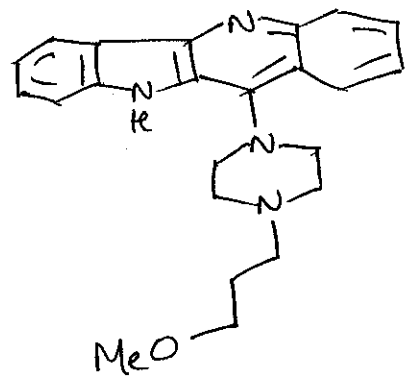
Apex Mass Spectrum of Peak 5.974 of DEC17_08.D



E:\MSLab_LCQ\VB-GSA-0217 12/21/2009 04:38:55 PM VB-GSA-0217
Venkat B., ACN:H2O 1:1:0.1%FA
VB-GSA-0217 #60-63 RT: 1.60-1.68 AV: 4 NL: 7.24E6
T: + p Full ms [100.00-1500.00]

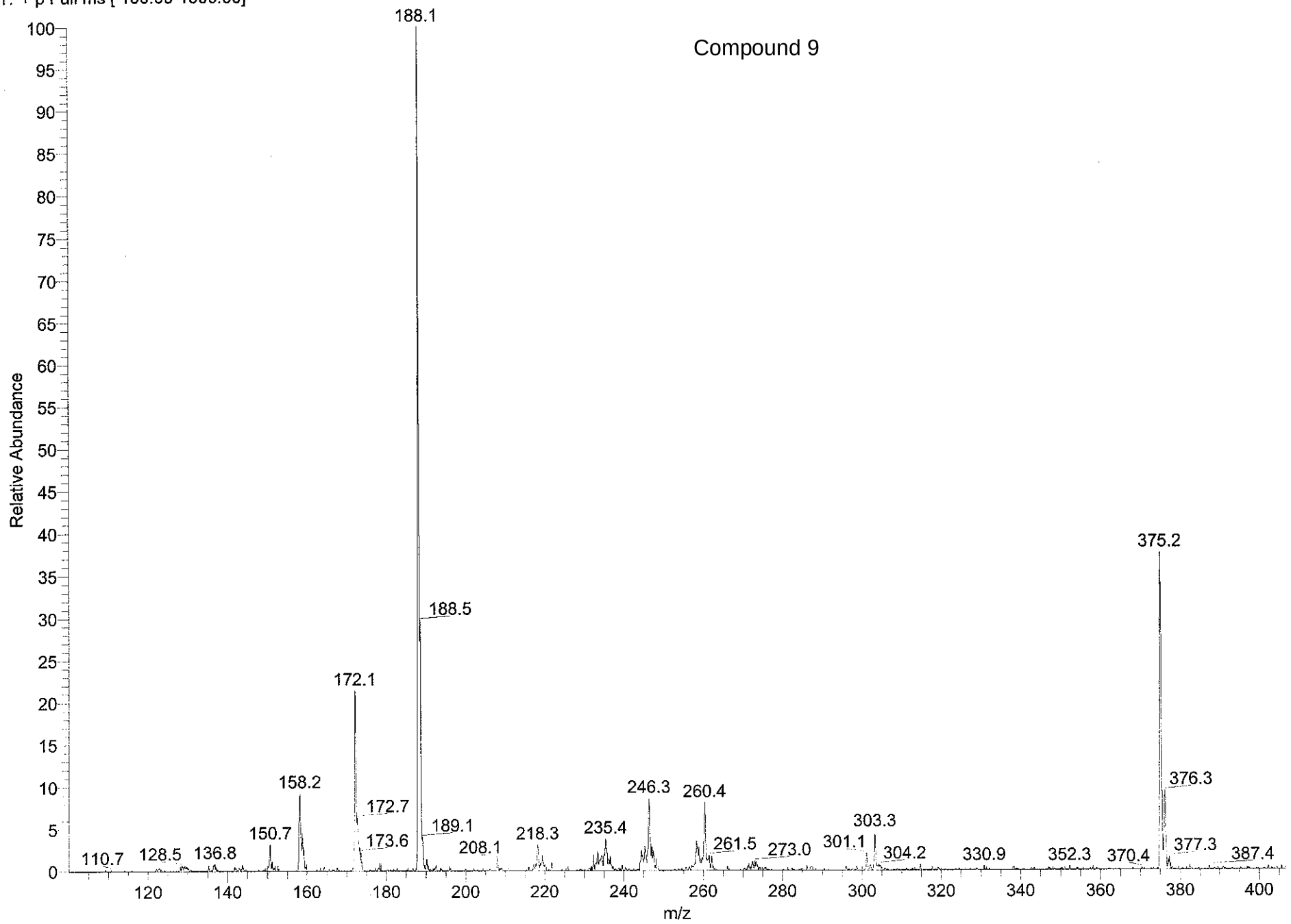
S76

Compound 9

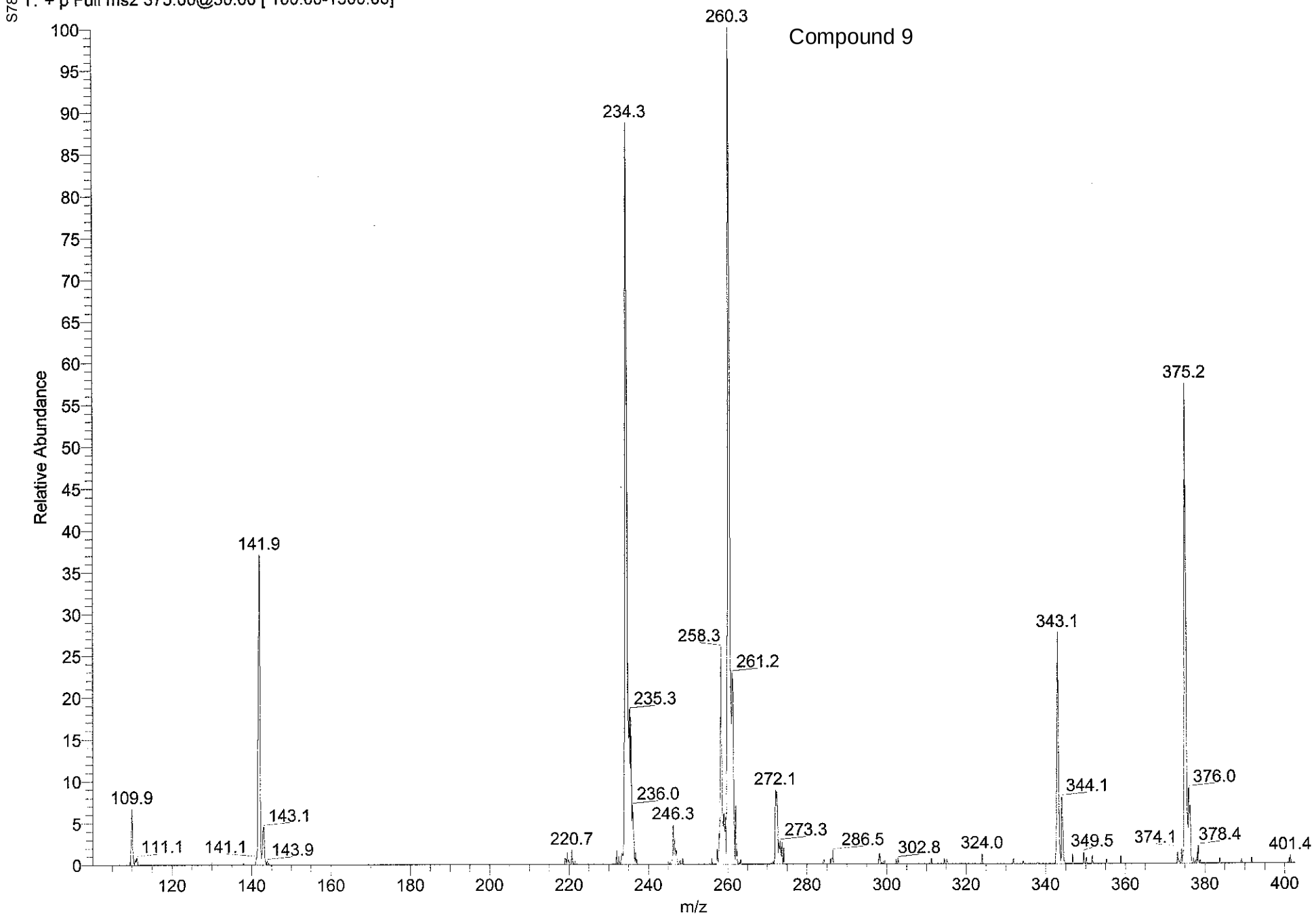


VB-GSA-0217

E:\MSLab_LCQ\VB-GSA-0217 12/21/2009 04:38:55 PM VB-GSA-0217
Venkat B., ACN:H2O 1:1:0.1%FA
VB-GSA-0217 #60-63 RT: 1.60-1.68 AV: 4 NL: 7.24E6
T: + p Full ms [100.00-1500.00]



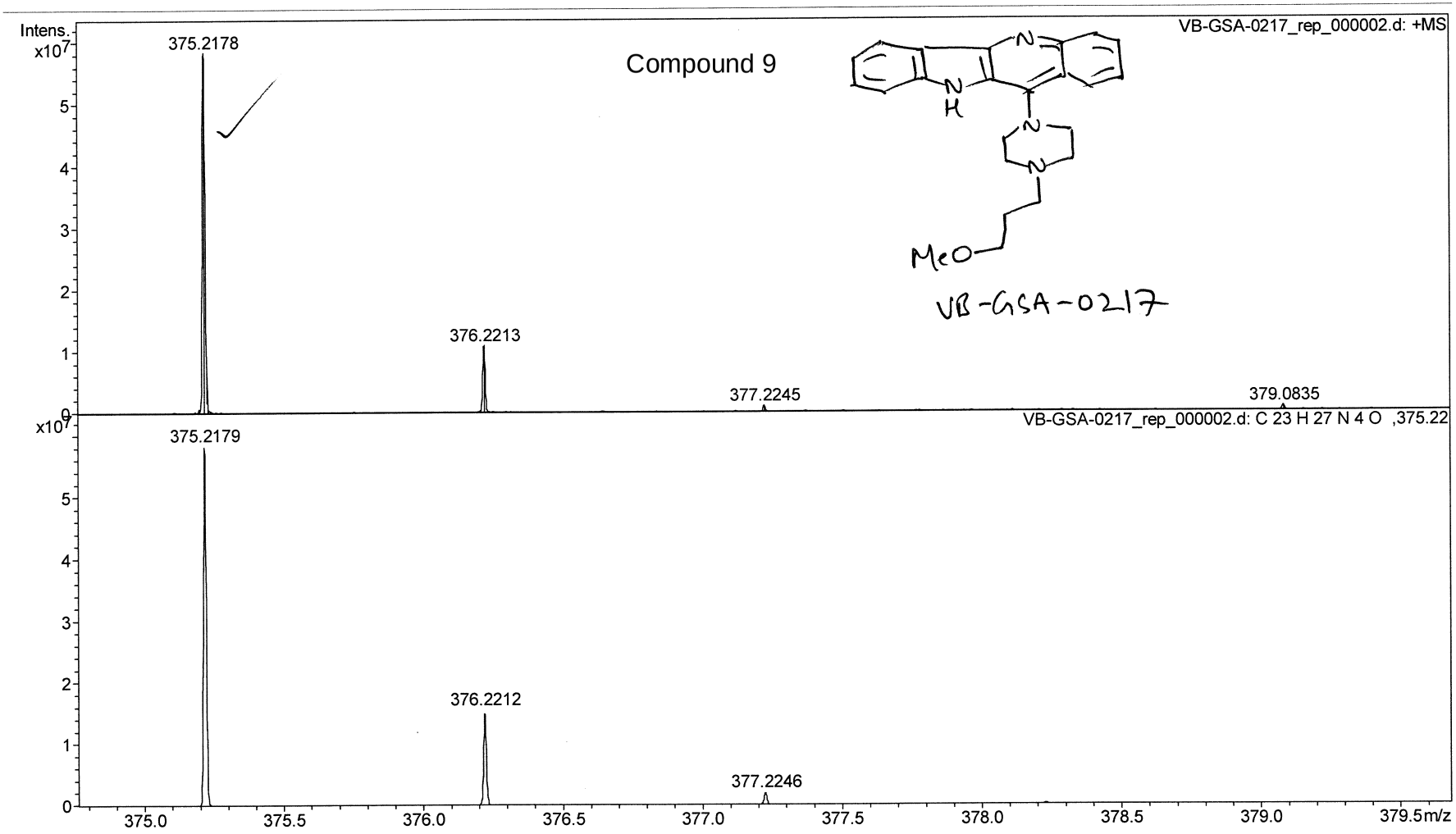
E:\MSLab_LCQ\VB-GSA-0217 12/21/2009 04:38:55 PM VB-GSA-0217
Venkat B., ACN:H2O 1:1:0.1%FA
VB-GSA-0217 #10-12 RT: 0.27-0.33 AV: 3 NL: 5.30E5
T: + p Full ms2 375.00@30.00 [100.00-1500.00]



Generic Display Report

Analysis Info

Analysis Name	D:\DATA\Facility_Dec_09\VB-GSA-0217_rep_000002.d	Acquisition Date	12/22/2009 10:29:39 AM
Method	ESI_101506	Operator	
Sample Name	VB-GSA-0217	Instrument	apex-Qe
Comment	Venkat B., ACN:H2O 1:1:0.1%FA		



SmartFormula Manually

Min C_{11}

Max

C 11-n

Generate

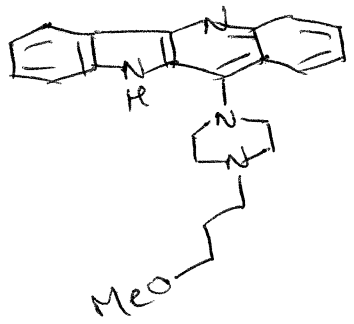
Help

Note: for m < 2000 the elements C, H, N, and O are considered implicitly.

Measured m/z 375.2178 Tolerance 2 mDa Charge 1

#	Mol. Formula	m/z	err [mDa]	|err| [ppm]	err [ppm]	mean err [ppm]	mSigma	Sigma Rank	rdb	N rule	e⁻
1	C 22 H 31 O 5	375.2166	-1.22	3.3	-3.3	-3.3	32.6	1	7.5	ok	even
2	C 23 H 27 N 4 O	375.2179	0.12	0.3	0.3	0.2	44.2	2	12.5	ok	even

Compound 9



☐ Automatically locate monoisotopic peak Maximum number of formulas 500

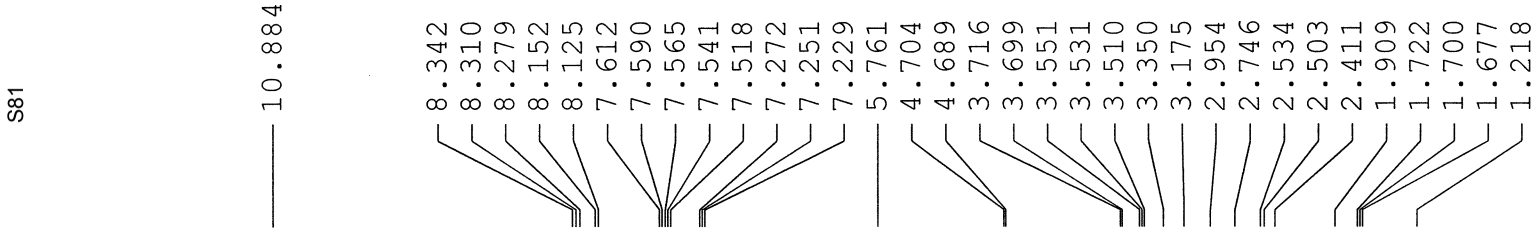
☑ Check rings plus double bonds Minimum -0.5 Maximum 40

Electron configuration even

☑ Filter H/C element ratio Minimum H/C 0 Maximum H/C 3

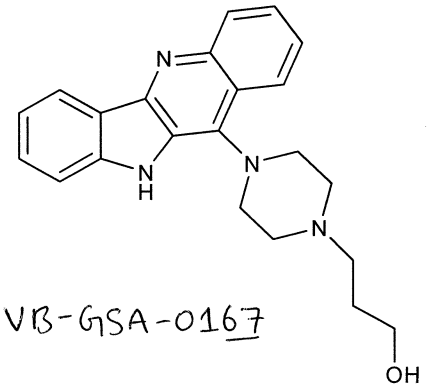
☑ Estimate carbon number ☑ Generate immediately

Show Pattern



Final

Compound 10



VB-GSA-0167

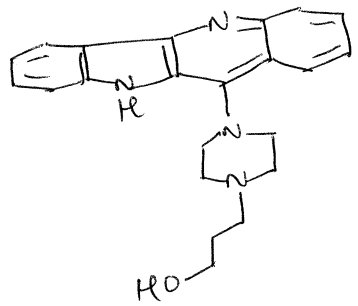
```
Current Data Parameters
NAME         VB-GSA-0167
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20080722
Time               11.46
INSTRUM            spect
PROBHD   5 mm QNP  1H/1
PULPROG            zg30
TD                65536
SOLVENT            DMSO
NS                   16
DS                    2
SWH            6172.839 Hz
FIDRES         0.094190 Hz
AQ             5.3084660 sec
RG                  512
DW                81.000 usec
DE                 6.00 usec
TE                300.0 K
D1             1.00000000 sec

======== CHANNEL f1 ========
NUC1                1H
P1                9.25 usec
PL1               0.00 dB
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF          300.1300000 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```

148.173
145.807
144.812
136.736
130.306
129.896
127.233
127.020
125.108
124.277
124.142
122.091
121.945
120.204
112.898

60.295
56.255
55.787
54.538
51.556
41.183
40.905
40.627
40.349
40.071
39.792
39.514
30.541

VB-GSA-0167

Compound 10



Current Data Parameters
NAME VB-GSA-0167-13C-Final
EXPNO 2
PROCNO 1

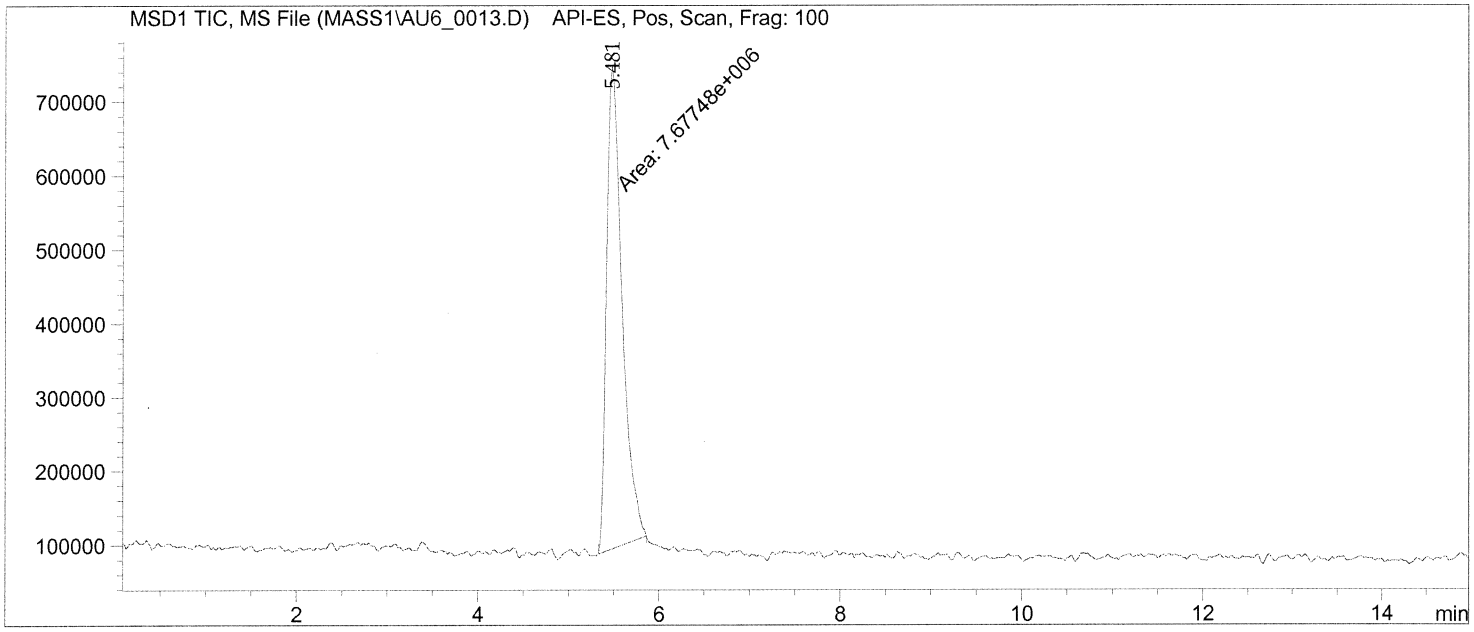
F2 - Acquisition Parameters
Date_ 20080728
Time 8.04
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 16000
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 724.1
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 2.00 dB
SFO1 75.4752653 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 20.00 dB
PL13 20.00 dB
SFO2 300.1312005 MHz

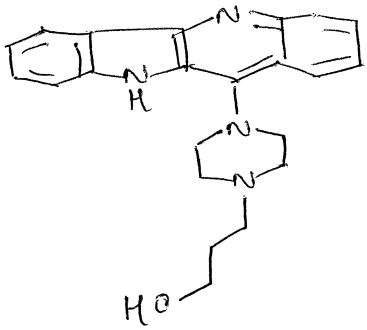
F2 - Processing parameters
SI 32768
SF 75.4677190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

```
==========================================================================
Injection Date   : 8/6/08 4:43:49 PM
Sample Name      : VB-GSA-0167                          Vial :  11
Acq. Operator    : Karen                                 Inj :   1
                                                  Inj Volume : 0.1 µl
Method           : D:\HPCHEM\1\METHODS\SCOTT_C.M
Last changed     : 8/6/08 4:25:49 PM by Karen
                   (modified after loading)
Zorbax C18 SB column,3.5u, 4.6 x 150mm, mp=30/70/0.25, MeOH:HOH:HAc; scan 100-500; flow 0.
5mL/min; vcap 2500, frag 100; col temp 45
==========================================================================
```




```
==========================================================================
                          Area Percent Report
==========================================================================

Sorted By             :      Retention Time
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: MSD1 TIC, MS File

Peak RetTime Sig Type    Area       Height      Area
  #   [min]                                      %
----|-------|---|----|----------|----------|--------|
   1   5.481  1  MM   7.67748e6  6.57356e5  100.0000

Totals :              7.67748e6  6.57356e5

==========================================================================
                          *** End of Report ***
```

Compound 10



Print of all graphic windows
in MeCN/MeOH

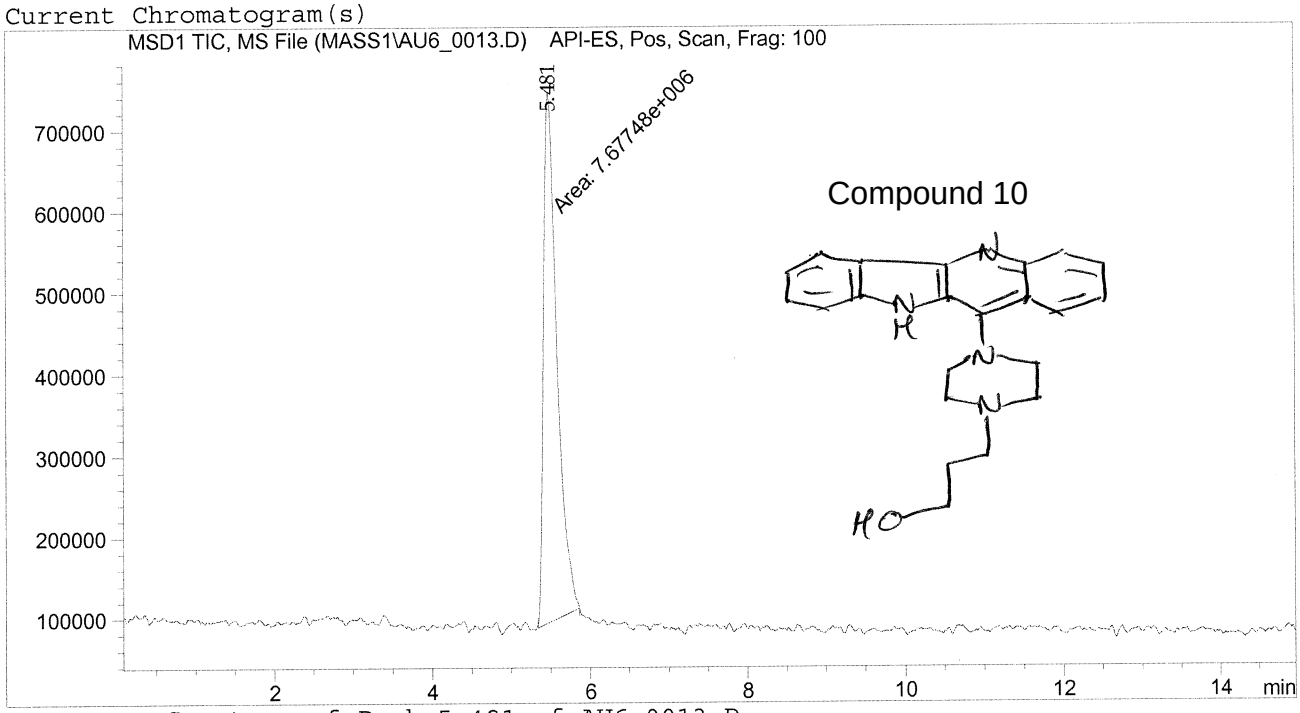
==========

Injection Date : 8/6/08 4:43:49 PM
Sample Name : VB-GSA-0167 Vial : 11
Acq. Operator : Karen Inj : 1
Inj Volume : 0.1 µl

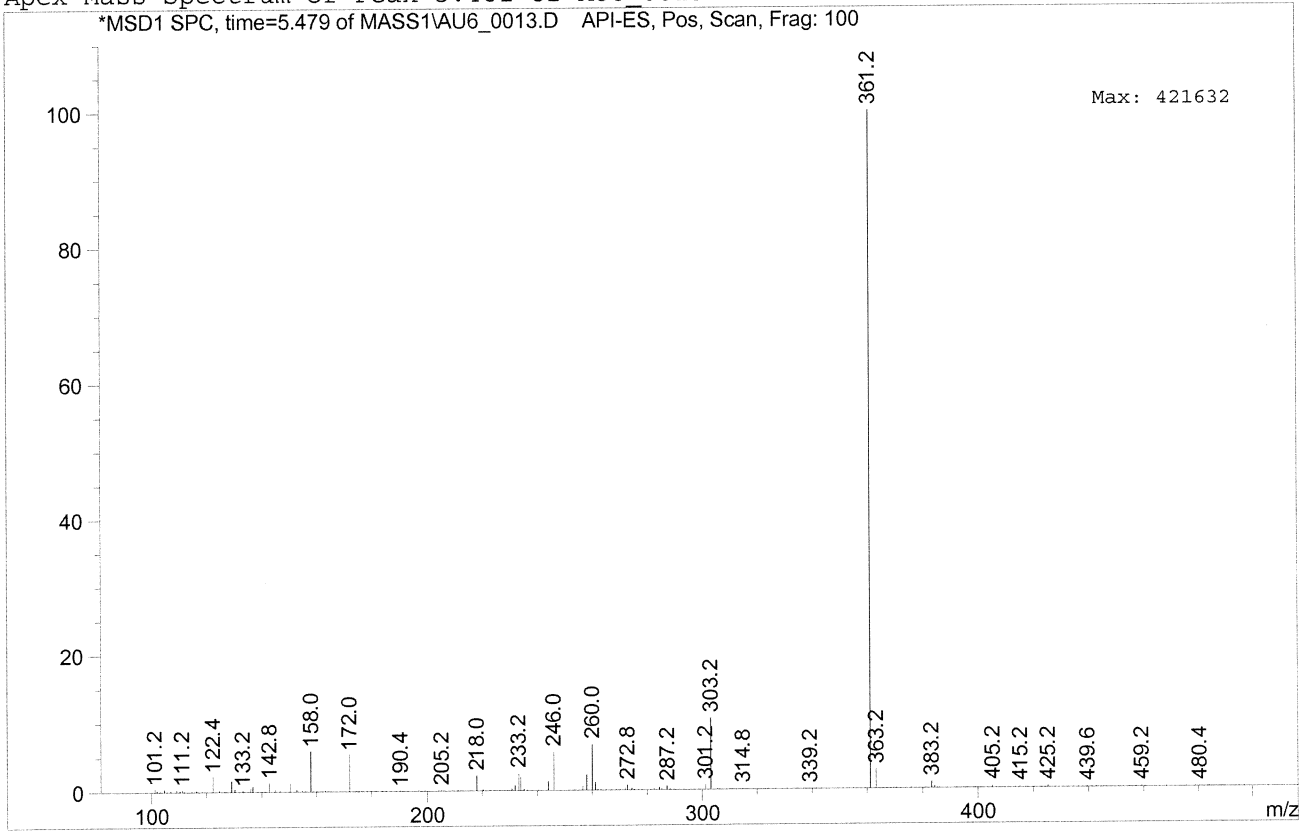
Method : D:\HPCHEM\1\METHODS\SCOTT_C.M
Last changed : 8/6/08 4:25:49 PM by Karen
(modified after loading)

Zorbax C18 SB column,3.5u, 4.6 x 150mm, mp=30/70/0.25, MeOH:HOH:HAc; scan 100-500; flow 0.5mL/min; vcap 2500, frag 100; col temp 45

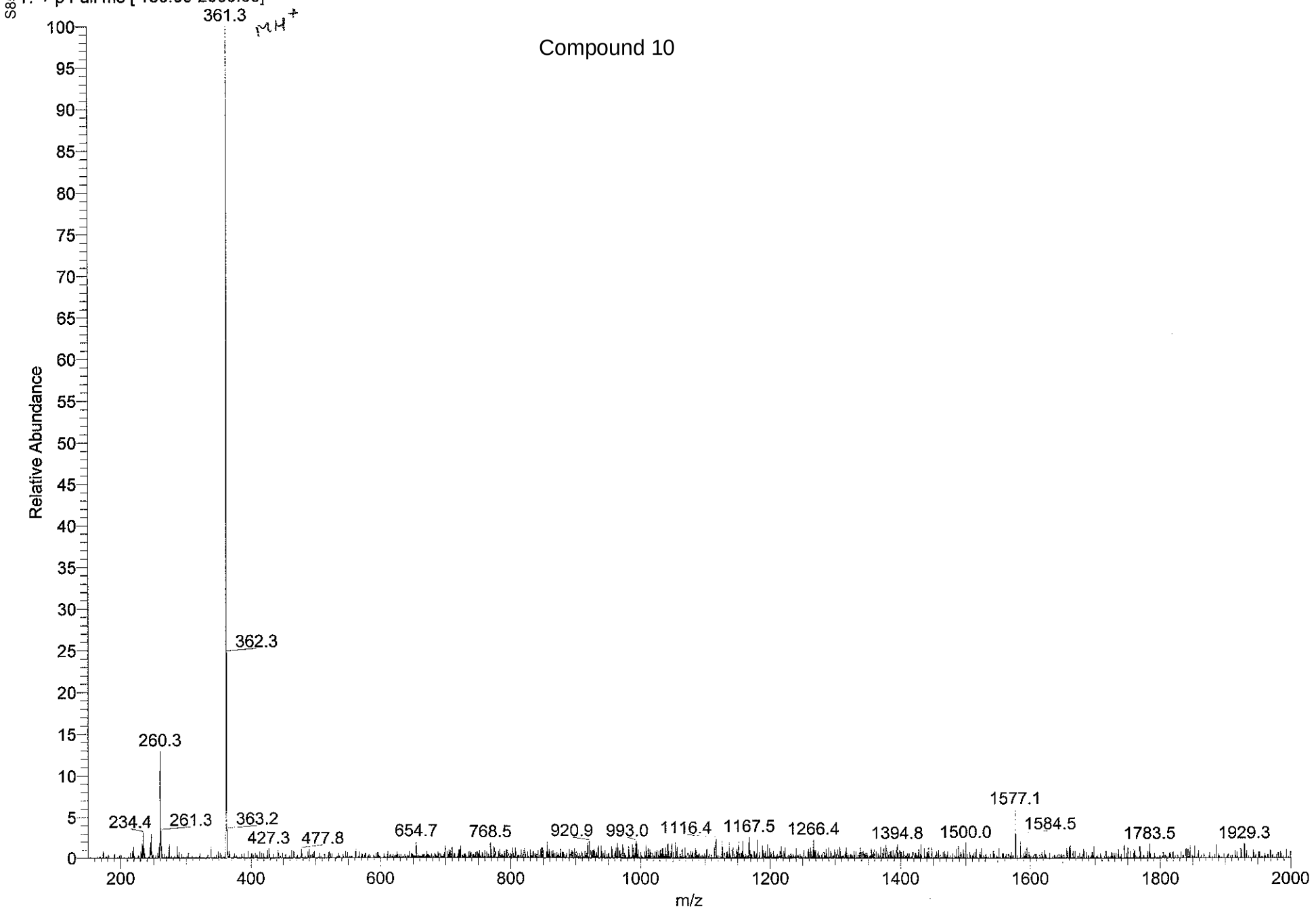
Current Chromatogram(s)



Apex Mass Spectrum of Peak 5.481 of AU6_0013.D



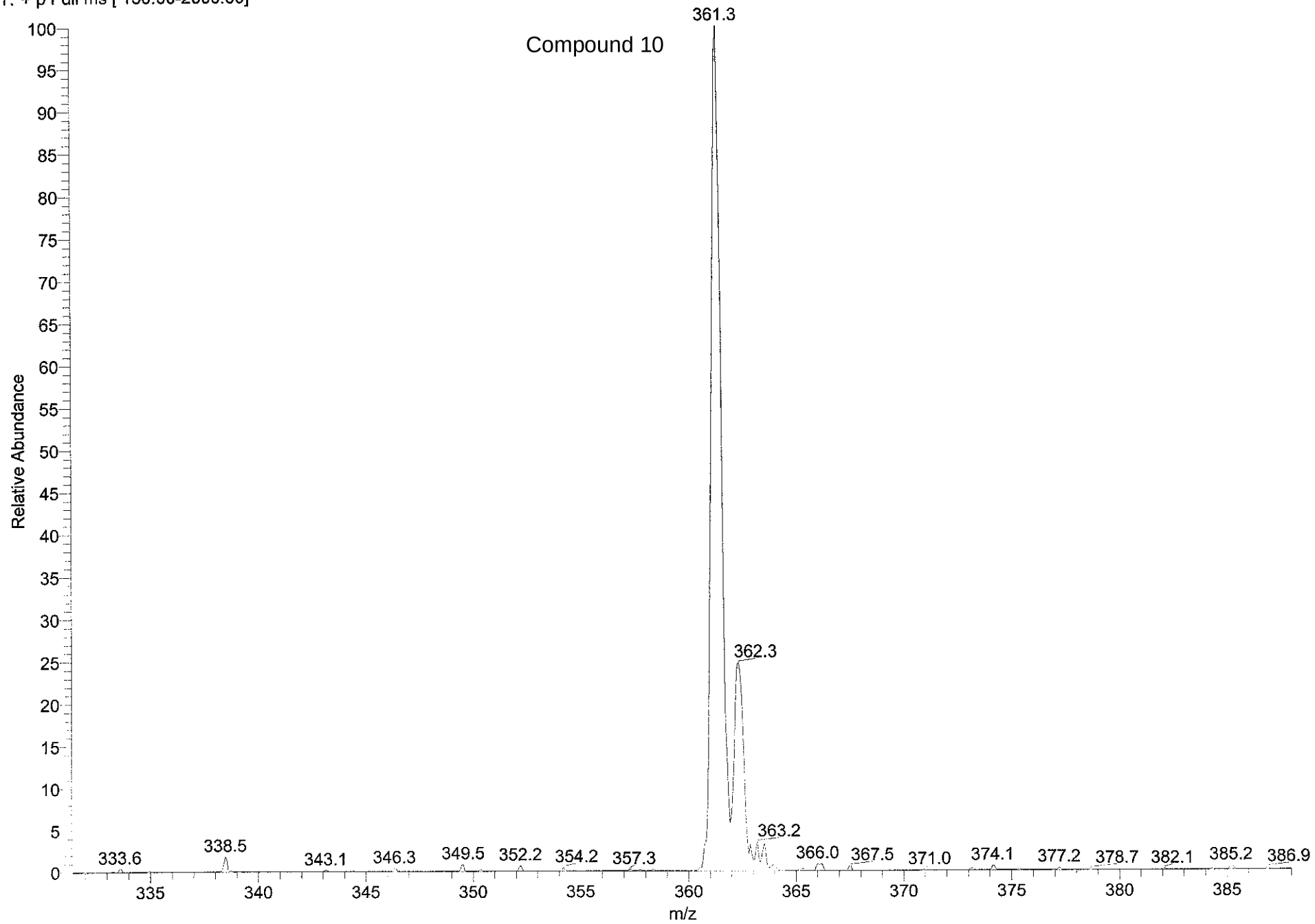
C:\Xcalibur\data\Facility Data\VB-0167 07/24/2008 04:13:01 PM VB-0167
Venkat B., MeOH:ACN
VB-0167 #28-32 RT: 0.94-1.08 AV: 5 NL: 5.66E5
T: + p Full ms [150.00-2000.00]



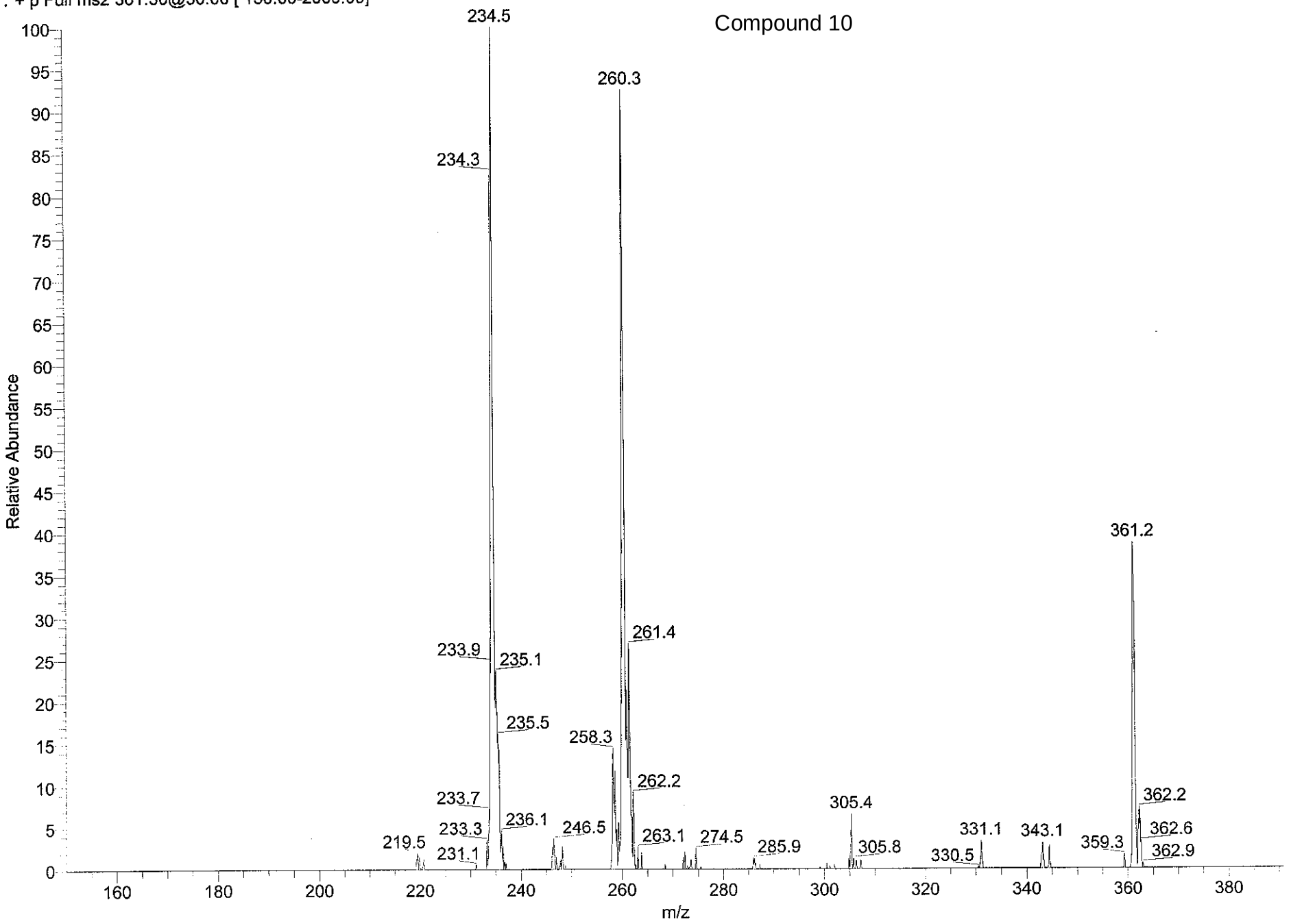
C:\Xcalibur\data\Facility Data\VB-0167 07/24/2008 04:13:01 PM VB-0167
Venkat B., MeOH:ACN

VB-0167 #28-32 RT: 0.94-1.08 AV: 5 NL: 5.66E5
T: + p Full ms [150.00-2000.00]

S86



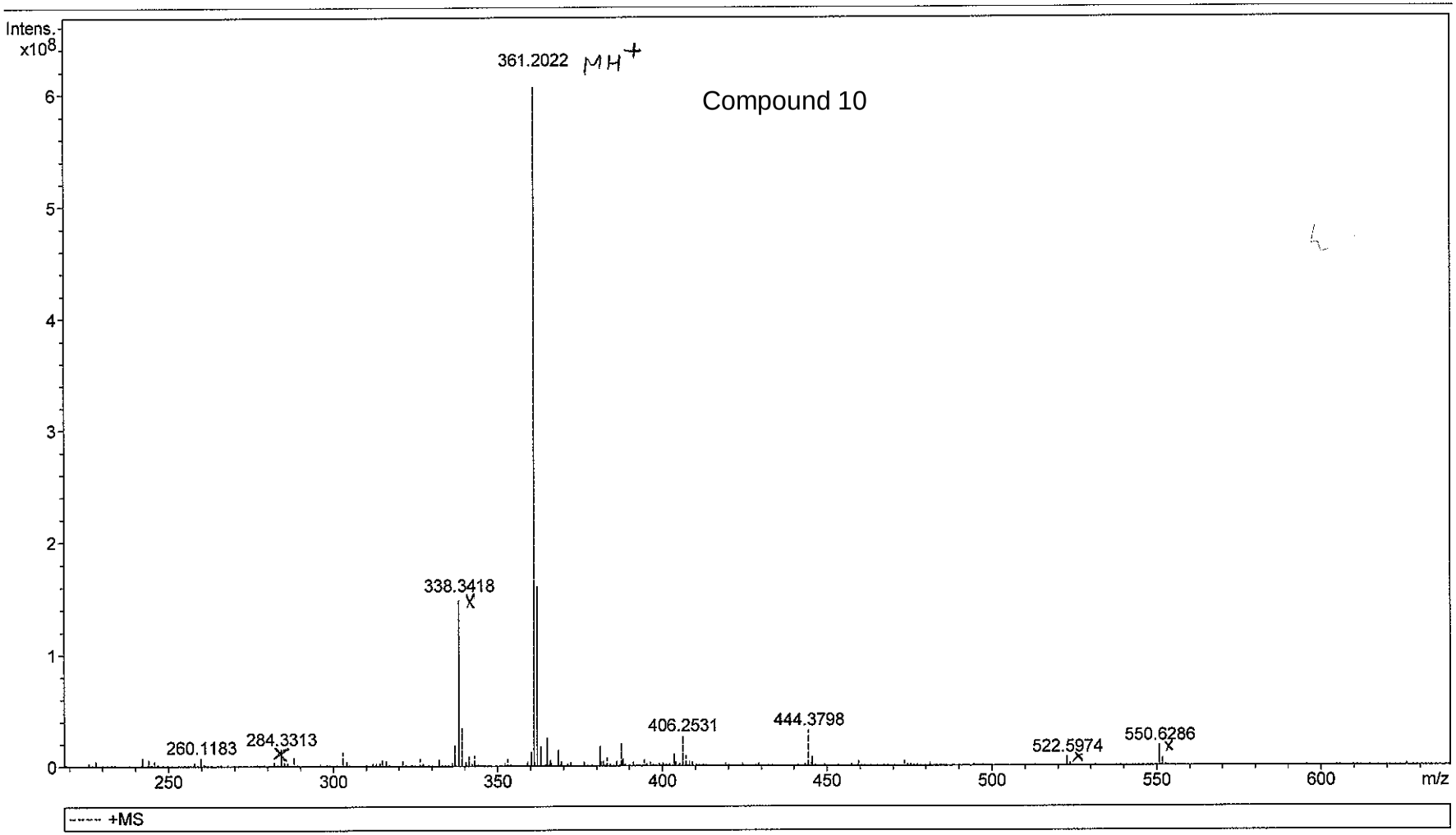
C:\Xcalibur\data\Facility Data\VB-0167 07/24/2008 04:13:01 PM VB-0167
Venkat B., MeOH:ACN
VB-0167 #17-18 RT: 0.56-0.60 AV: 2 NL: 8.97E5
T: + p Full ms2 361.30@30.00 [150.00-2000.00]
S87



Generic Display Report

Analysis Info

Analysis Name	D:\DATA\Facility_July_08\VB-0167_000002.d	Acquisition Date	7/28/2008 10:56:53 AM
Method	ESI_101506	Operator	Administrator
Sample Name	VB-0167	Instrument	apex-Qe
Comment	Venkat B., MeOH:ACN		

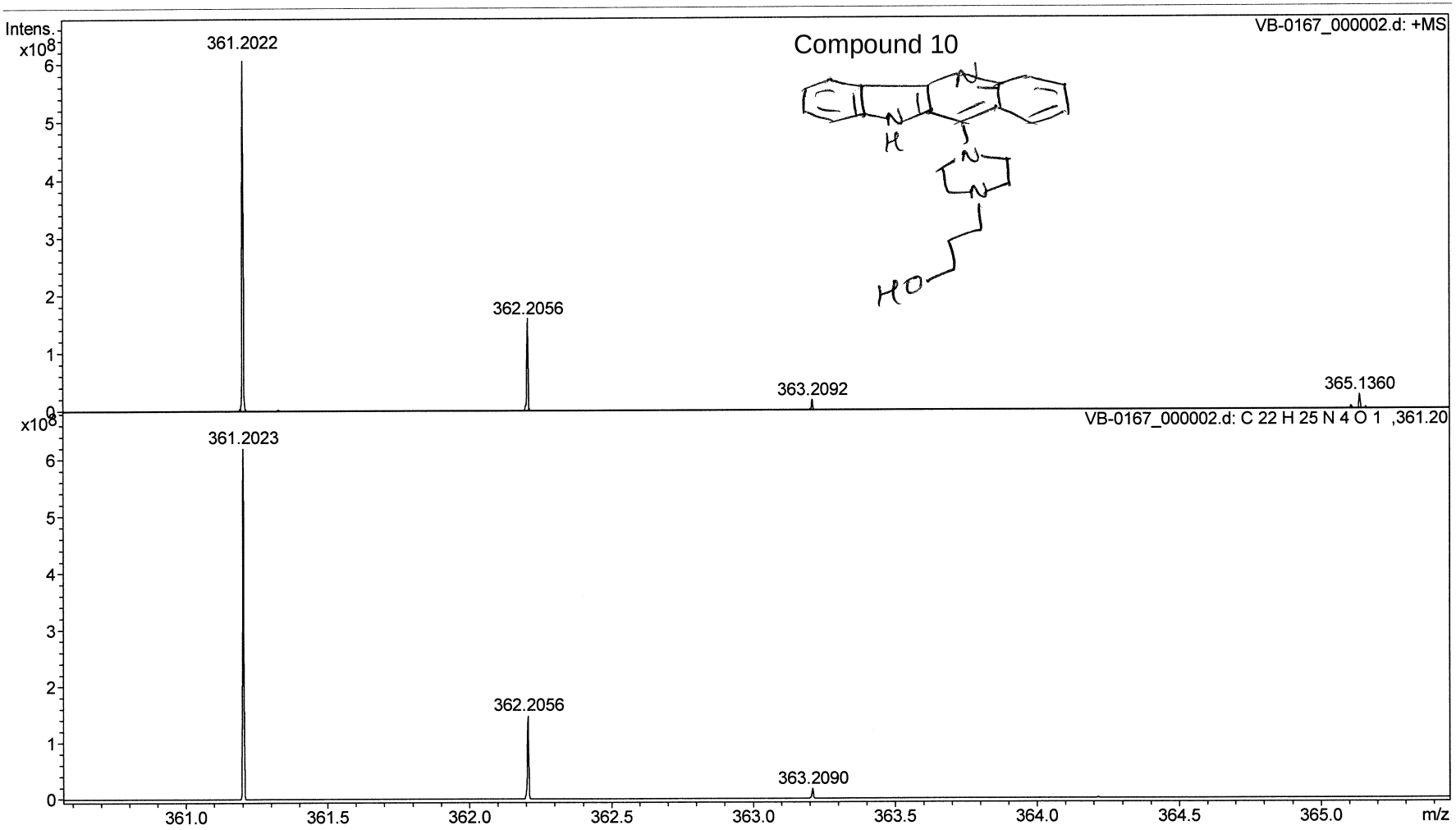


x in background

Generic Display Report

Analysis Info

Analysis Name	D:\DATA\Facility_July_08\VB-0167_000002.d	Acquisition Date	7/28/2008 10:56:53 AM
Method	ESI_101506	Operator	Administrator
Sample Name	VB-0167	Instrument	apex-Qe
Comment	Venkat B., MeOH:ACN		



Generate Molecular Formula

Min C_{17}

Max

C 17-n

Generate | Save Results... | Help

Note: for m < 2000 the elements C, H, N, and O are considered implicitly.

Measured m/z 361.2022 Tolerance 2 mDa Charge 1

#	Mol. Formula	m/z	err [mDa]	|err| [ppm]	err [ppm]	mean err [ppm]	Sigma
1	C 22 H 25 N 4 O 1	361.2023	0.08	0.2	0.2	-0.1	0.0030
2	C 21 H 29 O 5	361.2010	-1.25	3.5	-3.5	-3.5	0.0158

☐ Automatically locate monoisotopic peak Maximum number of formulas 200

☐ Check rings plus double bonds Minimum 0 Maximum 0

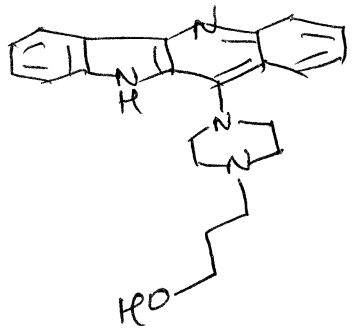
☑ Apply nitrogen rule Electron configuration even

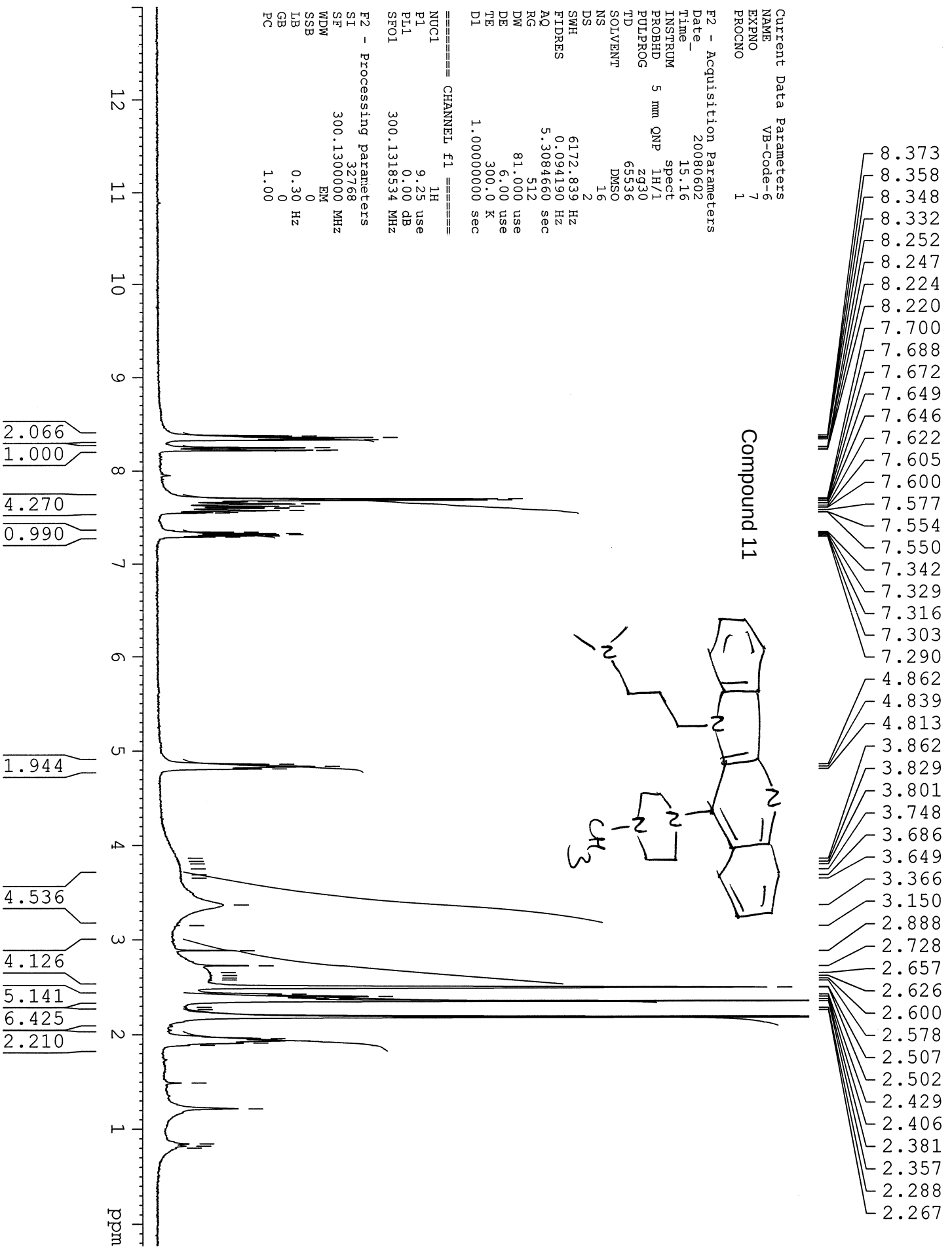
☐ Filter H/C element ratio Minimum H/C 0 Maximum H/C 3

☑ Estimate carbon number ☐ Generate immediately

Save for Reporting | Show Pattern

Compound 10




Compound 11
Current Data Parameters
NAME VB-Code-6
EXPNO 7
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080602
Time_ 15.16
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 512
DW 81.000 use
DE 6.00 use
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 9.25 use
PL1 0.00 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.373
8.358
8.348
8.332
8.252
8.247
8.224
8.220
7.700
7.688
7.672
7.649
7.646
7.622
7.605
7.600
7.577
7.554
7.550
7.342
7.329
7.316
7.303
7.290
4.862
4.839
4.813
3.862
3.829
3.801
3.748
3.686
3.649
3.366
3.150
2.888
2.728
2.657
2.626
2.600
2.578
2.507
2.502
2.429
2.406
2.381
2.357
2.288
2.267
2.066
1.000
4.270
0.990
1.944
4.536
4.126
5.141
6.425
2.210
12
11
10
9
8
7
6
5
4
3
2
1
ppm

Current Data Parameters
NAME VB-Code-6
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080529
Time 10.15
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 14000
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2048
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 2.00 dB
SFO1 75.4752653 MHz

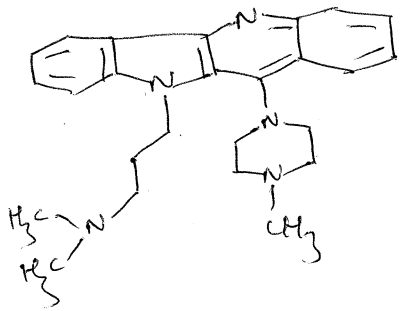
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 20.00 dB
PL13 20.00 dB
SFO2 300.1312005 MHz

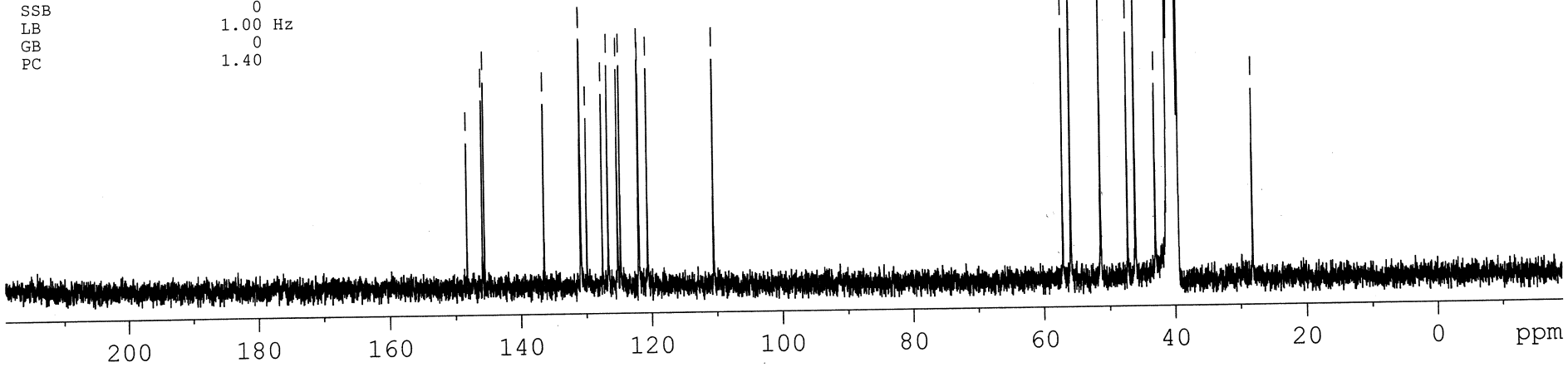
F2 - Processing parameters
SI 32768
SF 75.4677190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

148.270
145.924
145.593
136.493
130.909
130.831
129.940
127.563
126.648
125.224
124.790
122.004
121.916
120.610
110.515

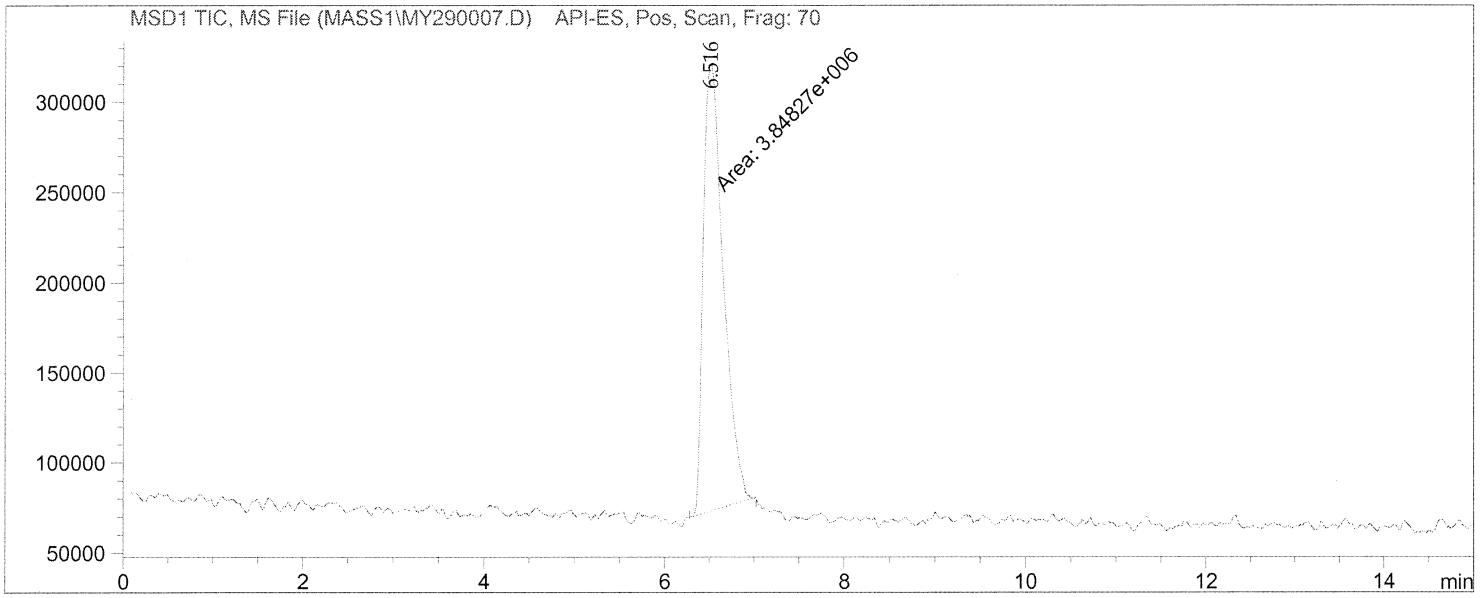
57.111
55.906
51.369
47.221
46.030
42.959
41.180
40.902
40.624
40.346
40.068
39.790
39.512
28.166

Compound 11



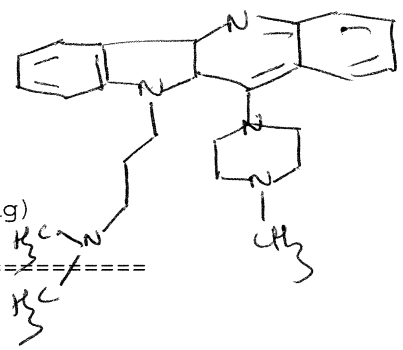


```
==========================================================================
Injection Date  : 5/29/08 3:32:48 PM
Sample Name     : VB-2-arms                              Vial :  13
Acq. Operator   : Karen                                   Inj :   1
                                                  Inj Volume : 0.1 µl
Acq. Method     : D:\HPCHEM\1\METHODS\SCOTT_C.M
Last changed    : 5/29/08 3:12:04 PM by Karen
                  (modified after loading)
Analysis Method : D:\HPCHEM\1\METHODS\SCOTT_C.M
Last changed    : 5/29/08 3:49:22 PM by Karen
                  (modified after loading)
Zorbax C18 SB column,3.5u, 4.6 x 150mm, mp=30/70/0.175, MeOH:water:HAc; scan 150-500; flow
0.5mL/min; vcap 2500, frag 70; col temp 35
==========================================================================
```



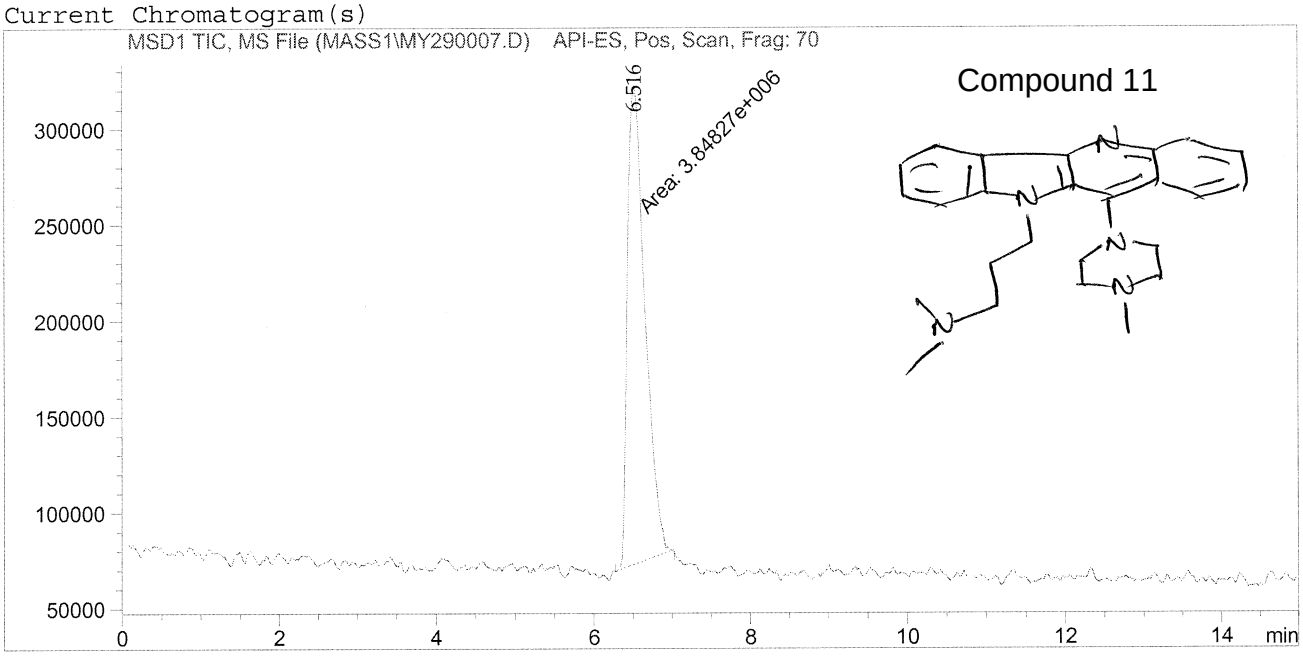

```
==========================================================================
                          Area Percent Report
==========================================================================

Sorted By             :      Retention Time
Calib. Data Modified  :      Tuesday, November 27, 2007 2:17:56 PM
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: MSD1 TIC, MS File

Peak RetTime Sig  Type      Area       Area     Name
  #   [min]                            %
----|-------|---|------|-----------|--------|--------------------------
   1   6.516  1  MM     3.84827e6  100.0000

Totals :                 3.84827e6


1 Warnings or Errors :

Warning : Calibration warnings (see calibration table listing)

==========================================================================
                          *** End of Report ***
```

Compound 11

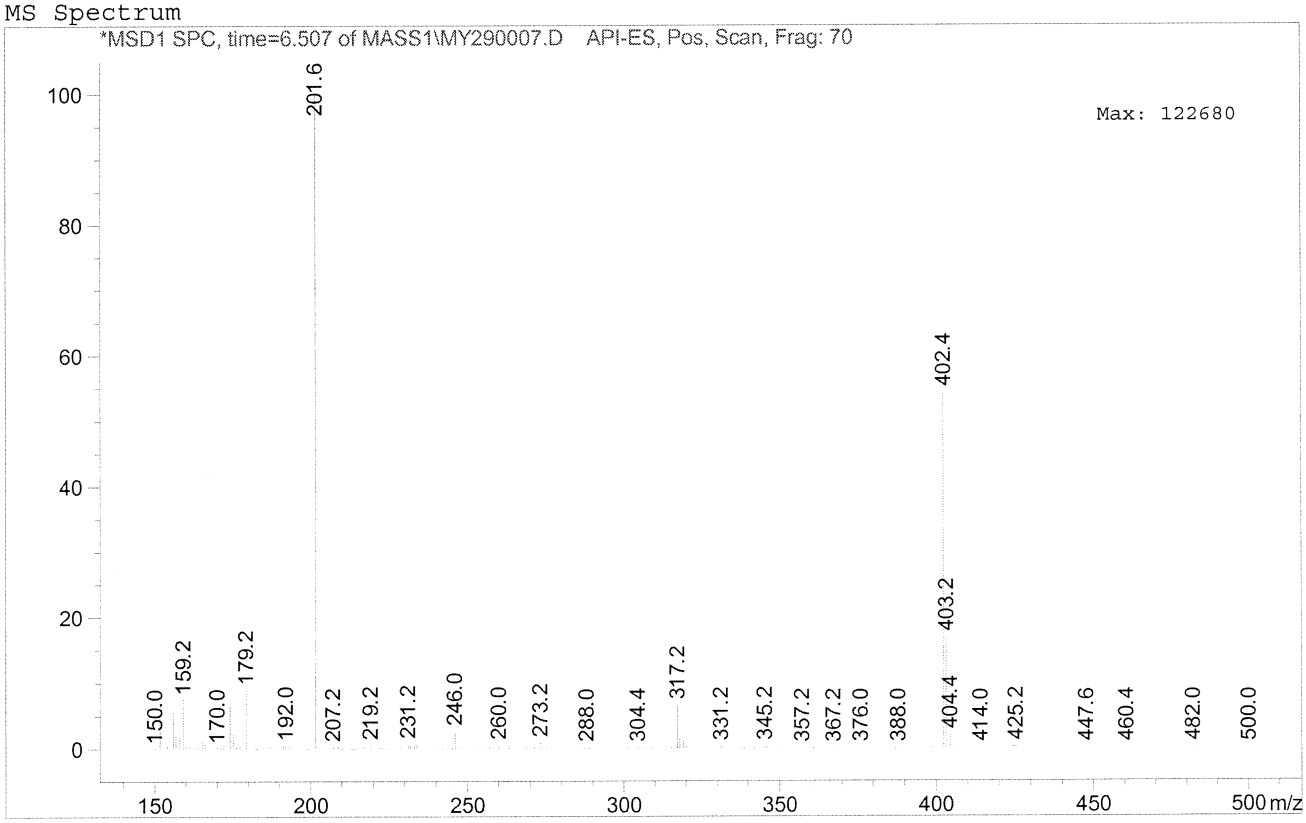


```
==========================================================================
Injection Date  : 5/29/08 3:32:48 PM
Sample Name     : VB-2-arms                                  Vial :  13
Acq. Operator   : Karen                                       Inj :   1
                                                      Inj Volume : 0.1 µl
Acq. Method     : D:\HPCHEM\1\METHODS\SCOTT_C.M
Last changed    : 5/29/08 3:12:04 PM by Karen
                  (modified after loading)
Analysis Method : D:\HPCHEM\1\METHODS\SCOTT_C.M
Last changed    : 5/29/08 3:49:22 PM by Karen
                  (modified after loading)
Zorbax C18 SB column,3.5u, 4.6 x 150mm, mp=30/70/0.175, MeOH:water:HAc; scan 150-500; flow 0.
5mL/min; vcap 2500, frag 70; col temp 35
```

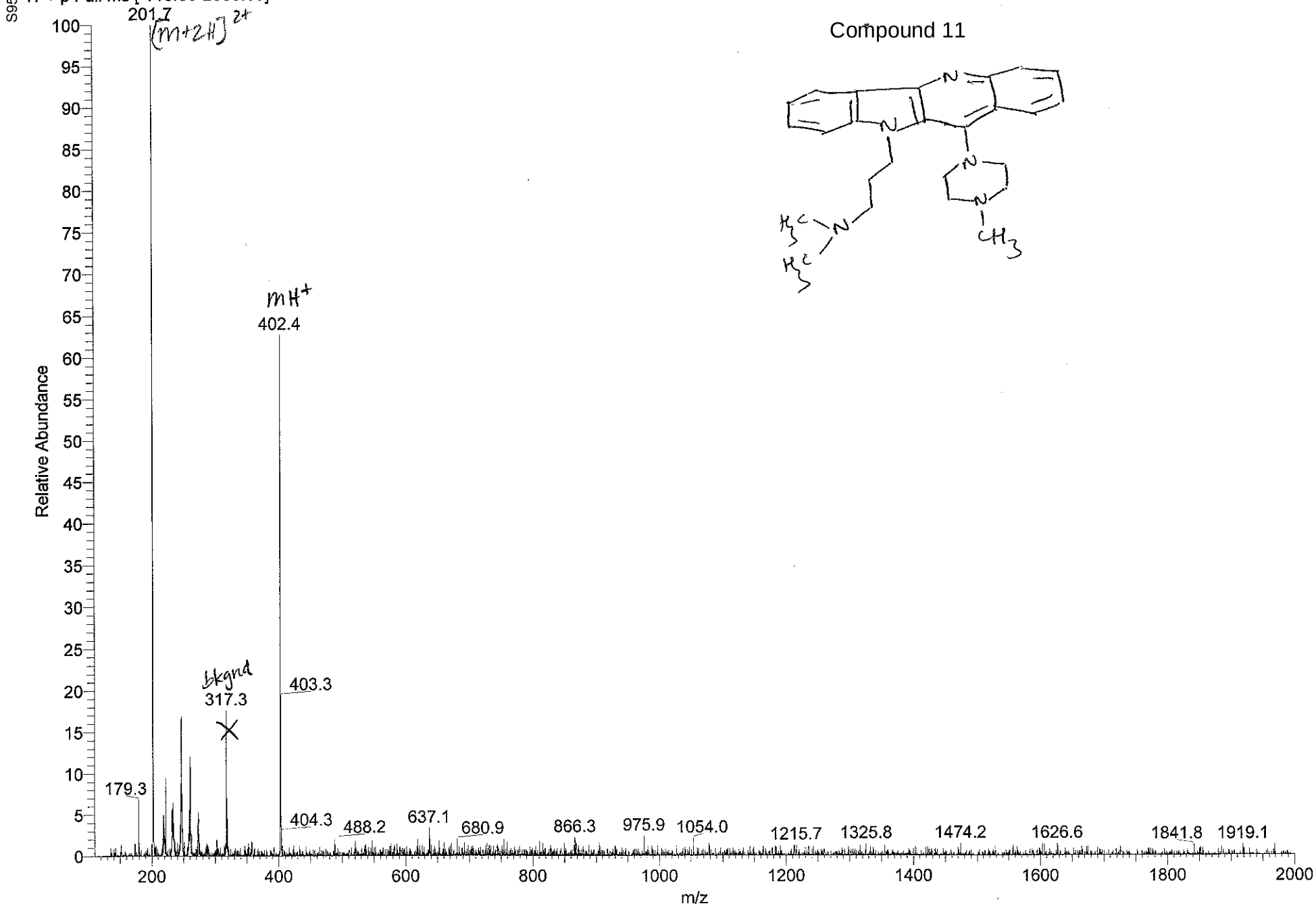
Current Chromatogram(s)



MS Spectrum



C:\Xcalibur\data\Facility Data\VB_46 05/22/2008 04:34:34 PM VB_46
Venkat Boddupally; MeOH:H2O AcOH
VB_46 #44-49 RT: 1.22-1.38 AV: 6 NL: 3.48E6
T: + p Full ms [110.00-2000.00]

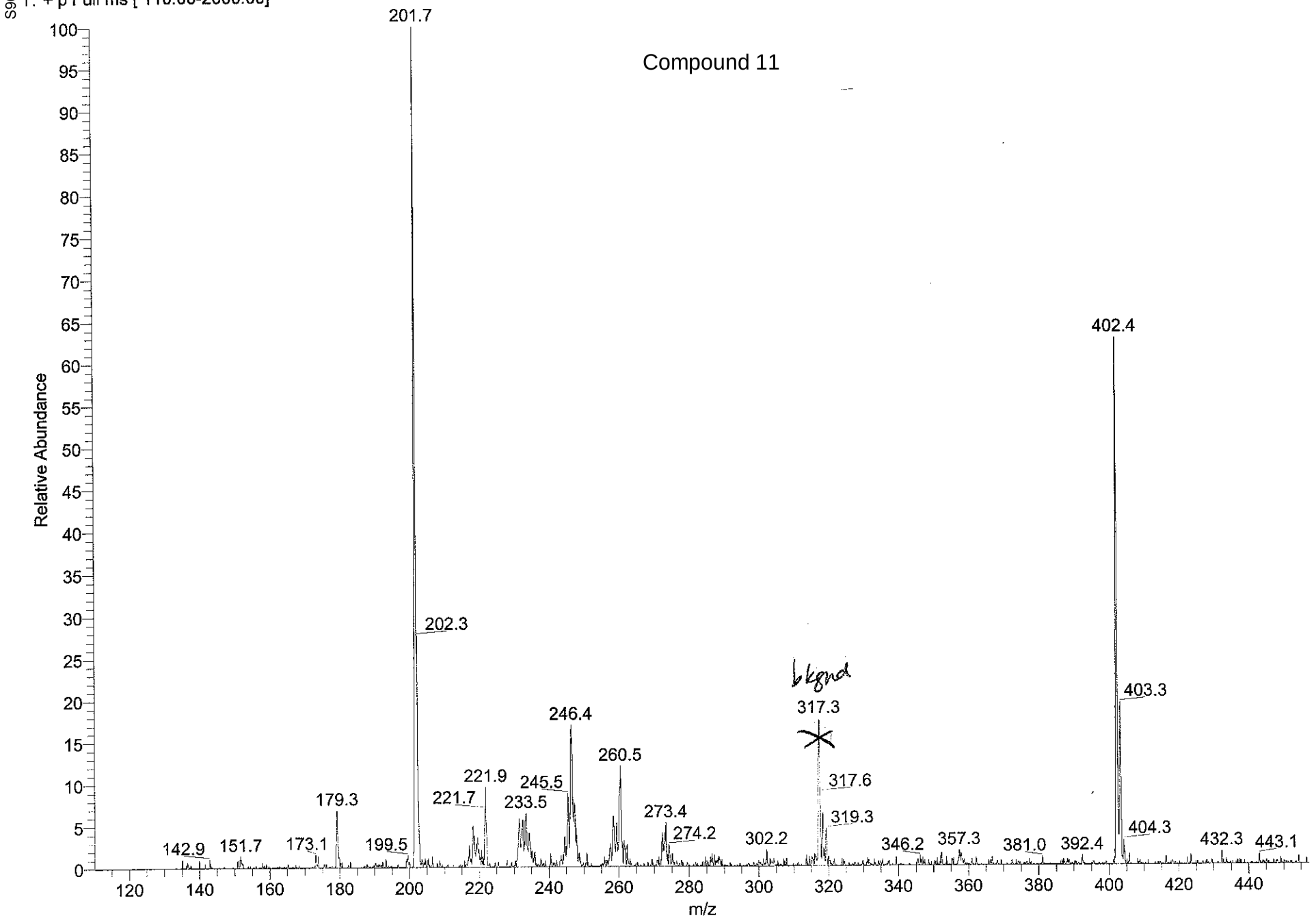


Compound 11

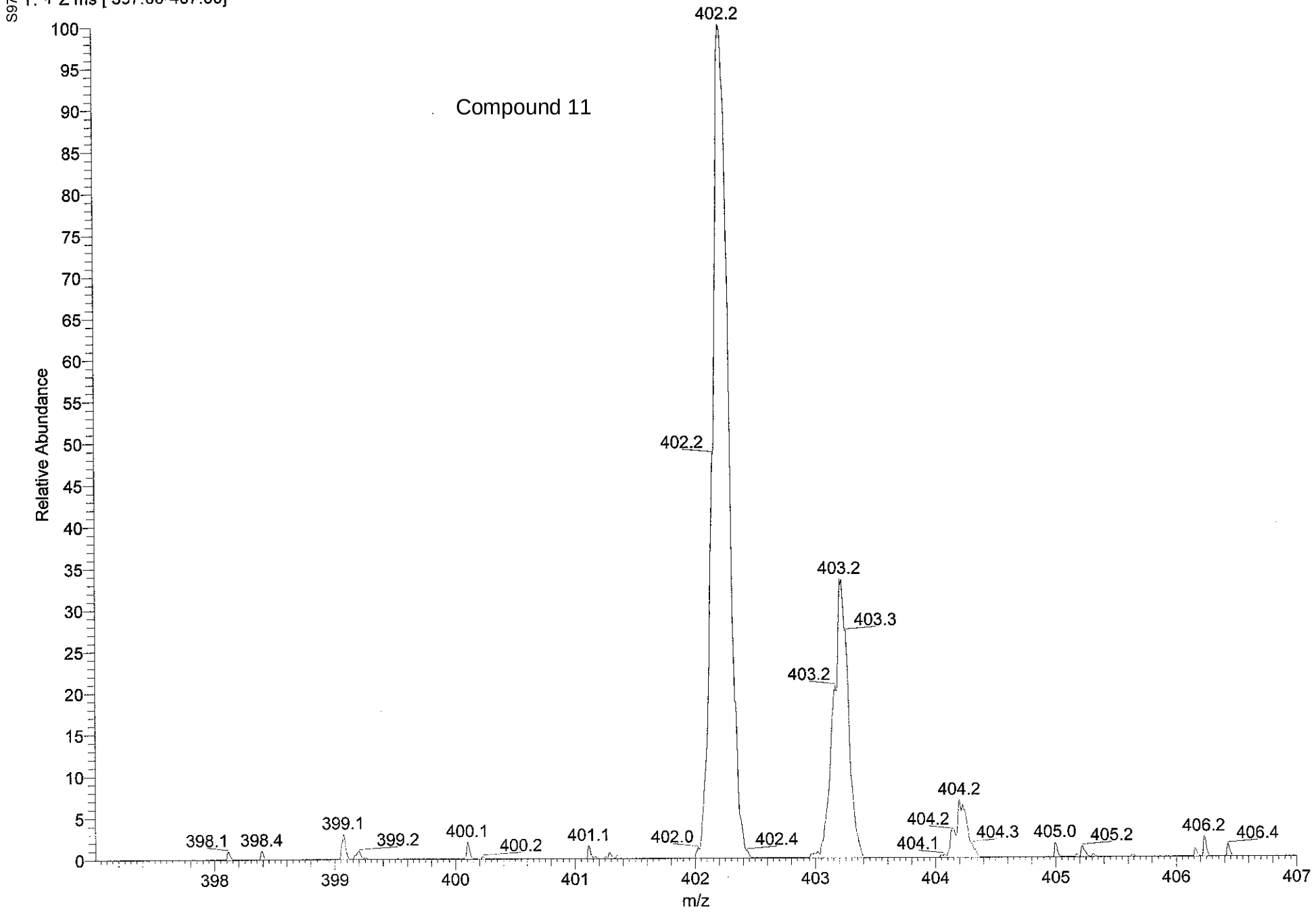
C:\Xcalibur\data\Facility Data\VB_46
Venkat Boddupally; MeOH:H2O AcOH

05/22/2008 04:34:34 PM VB_46

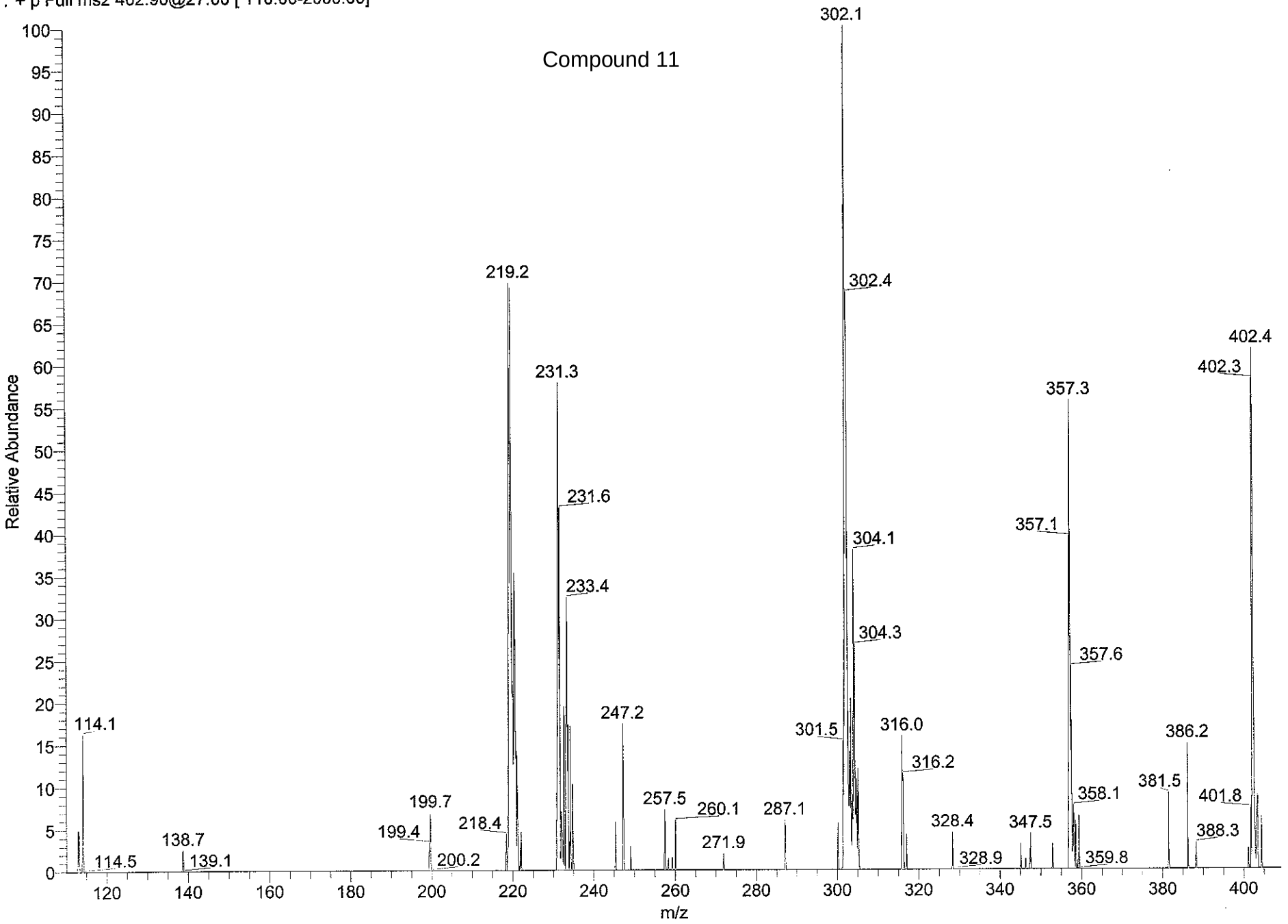
VB_46 #44-49 RT: 1.22-1.38 AV: 6 NL: 3.48E6
T: + p Full ms [110.00-2000.00]



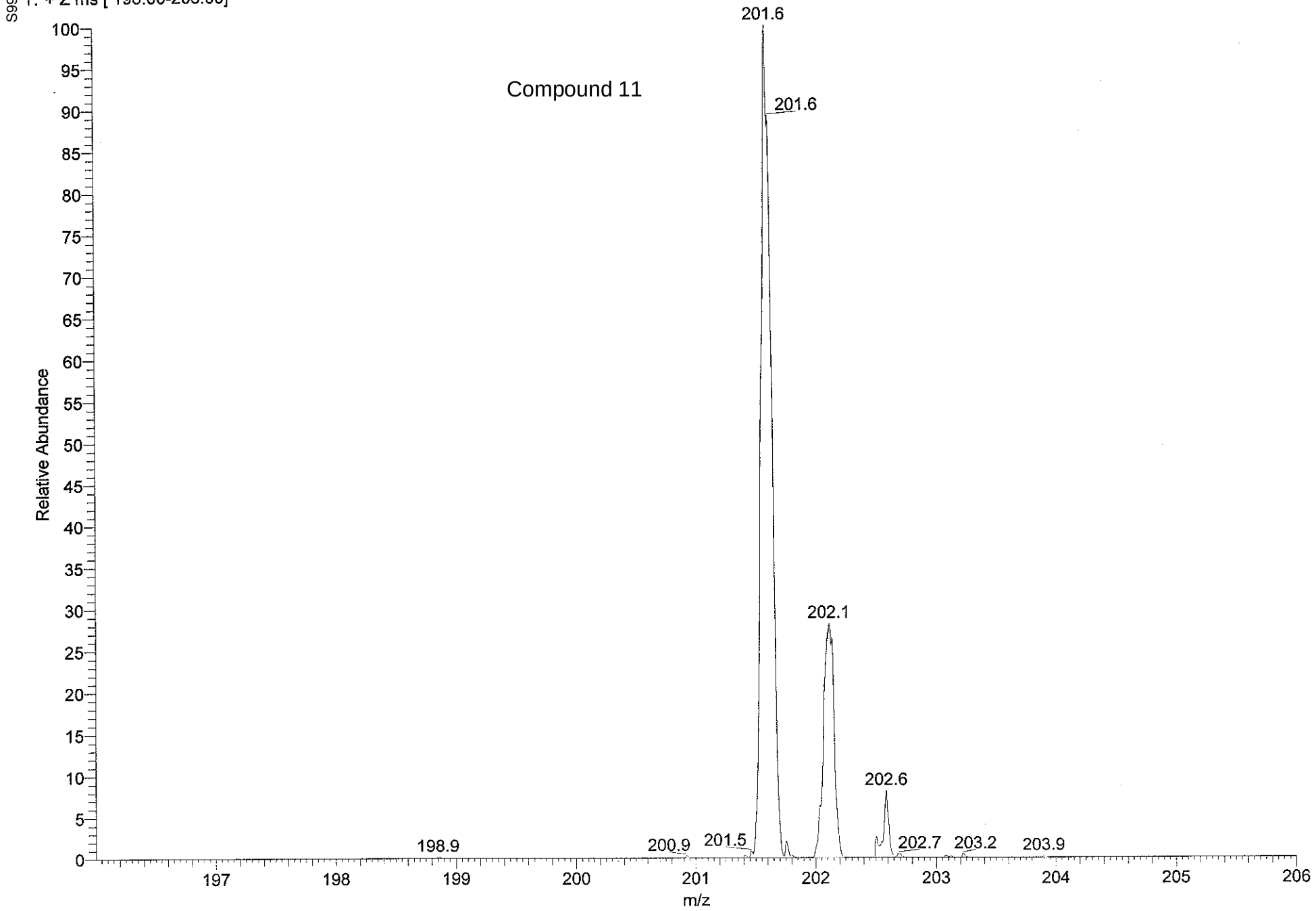
C:\Xcalibur\data\Facility Data\VB_46 05/22/2008 04:34:34 PM VB_46
Venkat Boddupally; MeOH:H2O AcOH
VB_46 #8-14 RT: 0.21-0.31 AV: 7 NL: 1.13E6
T: + Z ms [397.00-407.00]



C:\Xcalibur\data\Facility Data\VB_46 05/22/2008 04:34:34 PM VB_46
Venkat Boddupally; MeOH:H2O AcOH
VB_46 #30-33 RT: 0.86-0.97 AV: 4 NL: 3.56E5
T: + p Full ms2 402.90@27.00 [110.00-2000.00]



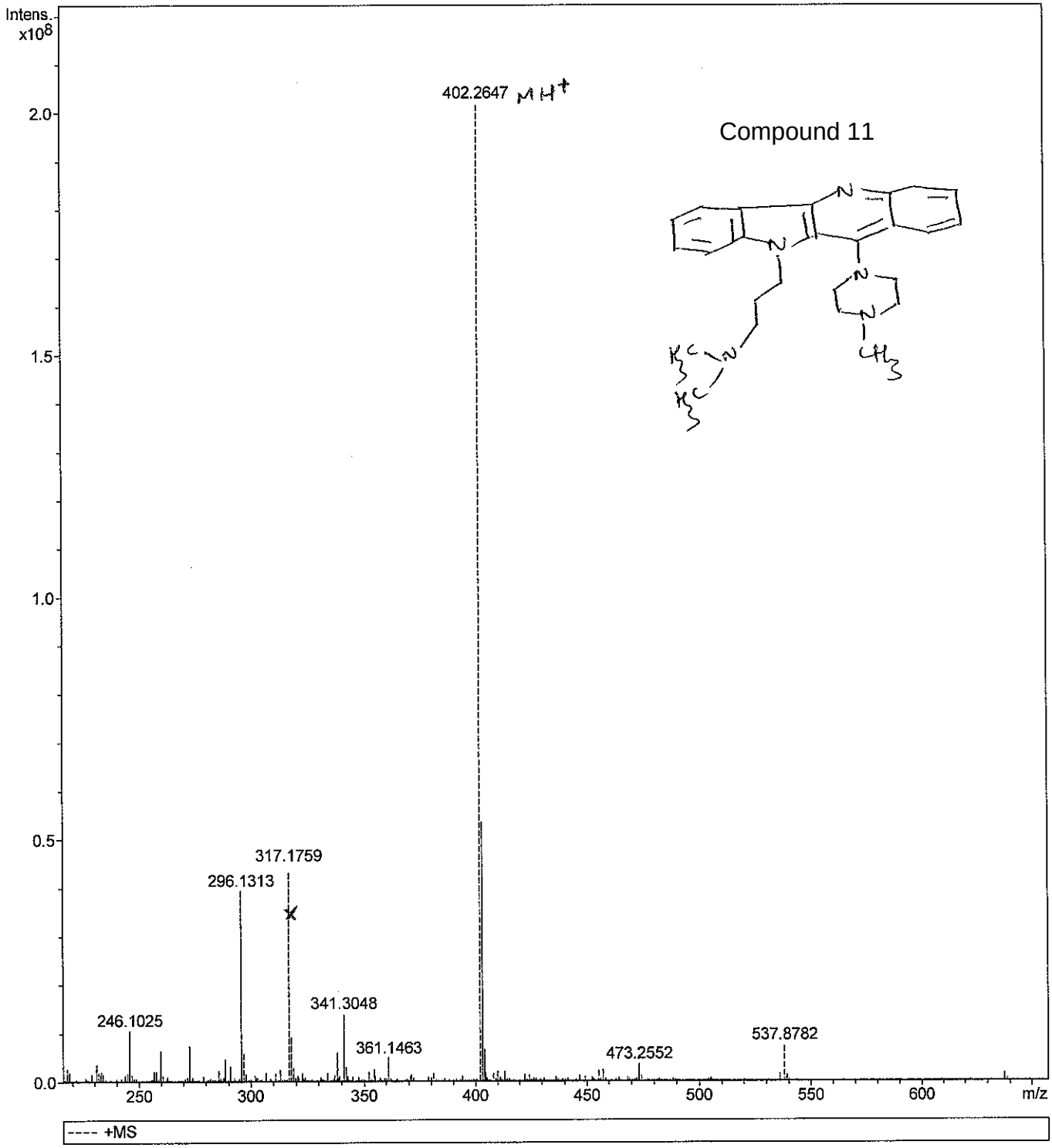
C:\Xcalibur\data\Facility Data\VB_46 05/22/2008 04:34:34 PM VB_46
Venkat Boddupally; MeOH:H2O AcOH
VB_46 #38-42 RT: 1.12-1.19 AV: 5 NL: 2.24E6
T: + Z ms [196.00-206.00]



Generic Display Report

Analysis Info

Analysis Name	D:\DATA\Facility_May_5\VB_46_000001.d	Acquisition Date	5/27/2008 1:14:23 PM
Method	ESI_101506	Operator	Administrator
Sample Name	VB-46	Instrument	apex-Qe
Comment	Venkat B., MeOH:H2O:AcOH		

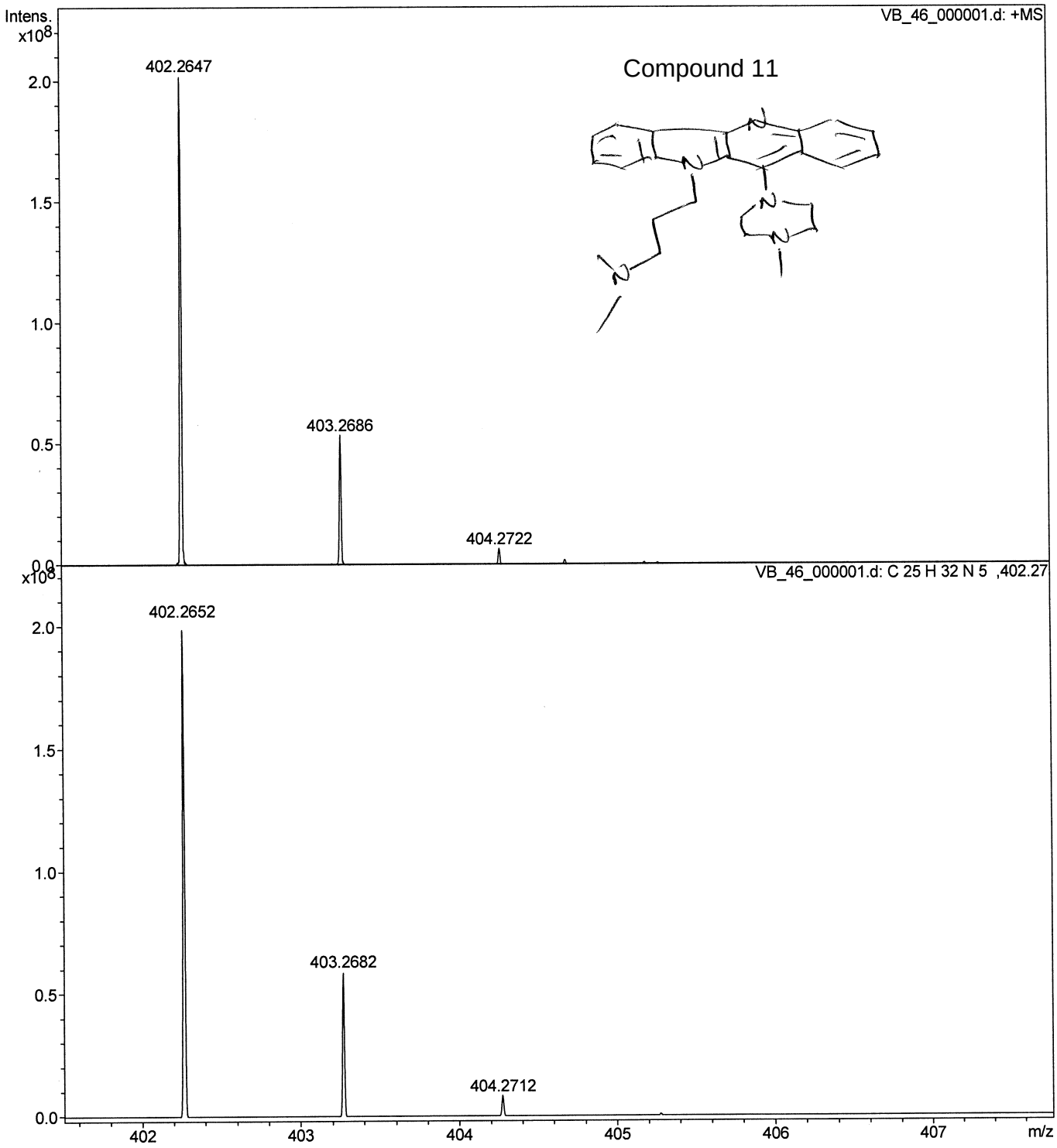


x Carryover

Generic Display Report

Analysis Info

Analysis Name	D:\DATA\Facility_May_5\VB_46_000001.d	Acquisition Date	5/27/2008 1:14:23 PM
Method	ESI_101506	Operator	Administrator
Sample Name	VB-46	Instrument	apex-Qe
Comment	Venkat B., MeOH:H2O:AcOH		



Generate Molecular Formula

Min C_{18}

Max

C 18-n

Generate

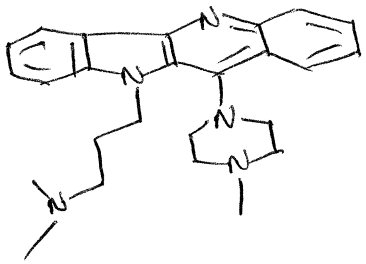
Save Results...

Help

Note: for m < 2000 the elements C, H, N, and O are considered implicitly.

Measured m/z 402.2647 Tolerance 2 mDa Charge 1

#	Mol. Formula	m/z	err [mDa]	|err| [ppm]	err [ppm]	mean err [ppm]	
1	C 24 H 36 N 1 O 4	402.2639	-0.83	2.1	-2.1	-2.5	C
2	C 25 H 32 N 5	402.2652	0.51	1.3	1.3	0.6	C
3	C 27 H 34 N 2 O 1	402.2666	1.85	4.6	4.6	4.1	C



Automatically locate monoisotopic peak Maximum number of formulas 200

Check rings plus double bonds Minimum 0 Maximum 0

Apply nitrogen rule Electron configuration both

Filter H/C element ratio Minimum H/C 0 Maximum H/C 3

Estimate carbon number Generate immediately

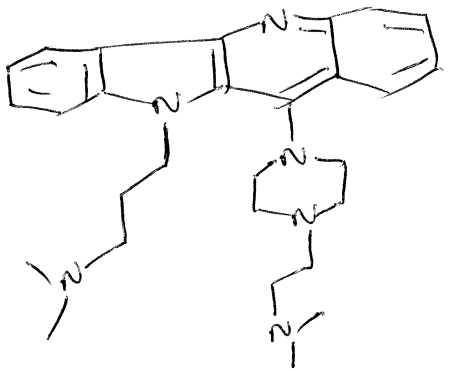
Save for Reporting

Show Pattern

S103

8.511 8.485 8.391 8.362 8.342 8.314 7.603 7.589 7.487 7.461 7.434 7.316 7.291 7.275 7.267 4.847 4.826 4.803 4.008 3.588 3.540 3.471 3.361 3.198 3.131 2.895 2.672 2.652 2.609 2.591 2.480 2.461 2.410 2.388 2.357 2.352 2.248 2.243 2.148 2.137 2.008 1.986 1.964 1.247

VB-GSA-118



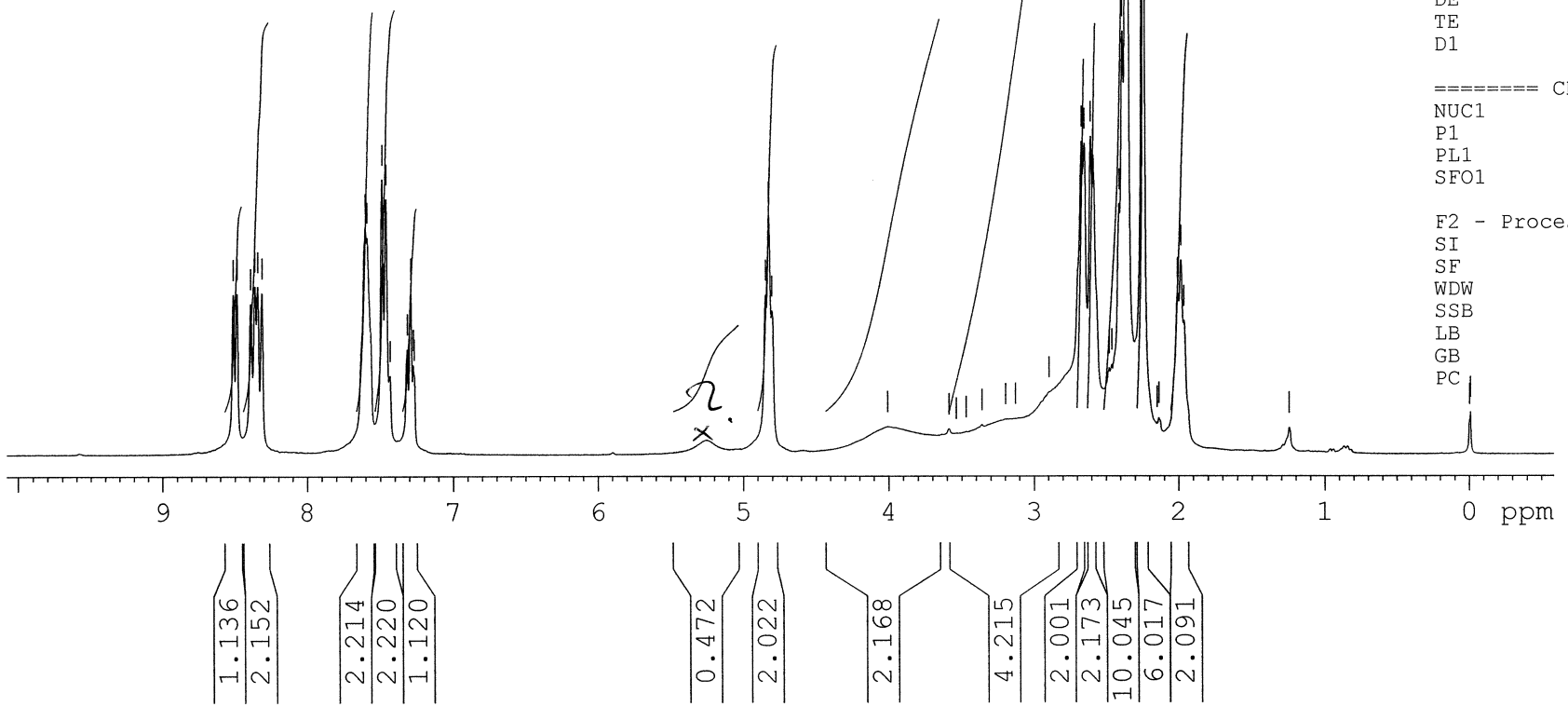
Compound 12

Current Data Parameters
NAME VB-GSA-01-118
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081106
Time 15.16
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 71.8
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 9.25 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

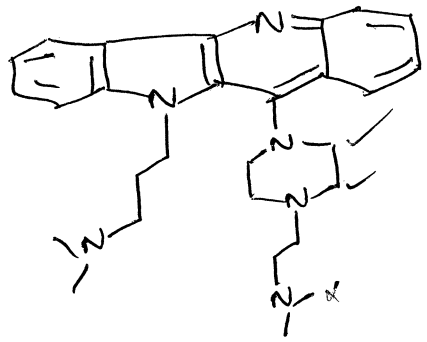


148.714
146.013
145.462
135.920
130.760
130.131
129.972
127.498
126.105
124.473
124.440
122.189
120.124
109.438

77.961
77.537
77.113

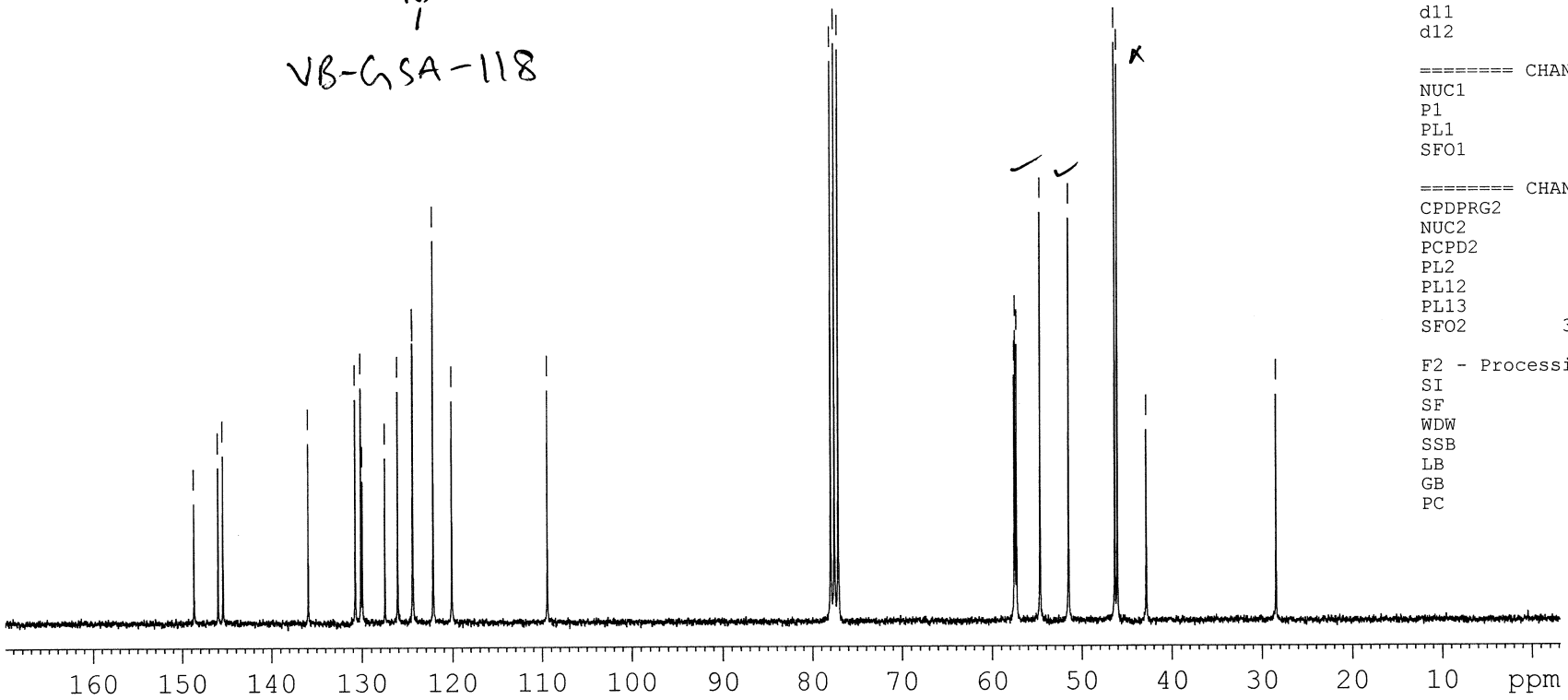
57.519
57.403
57.245
54.638
51.458
46.321
46.030
42.824

28.408



Compound 12

VB-GSA-118



Current Data Parameters
NAME VB-GSA-01-118
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081106
Time 17.09
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1407
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 11585.2
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 2.00 dB
SFO1 75.4752653 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 20.00 dB
PL13 20.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

Data File D:\HPCHEM\1\DATA\MASS1\NOV06_07.D Sample Name: VB-GSA-118

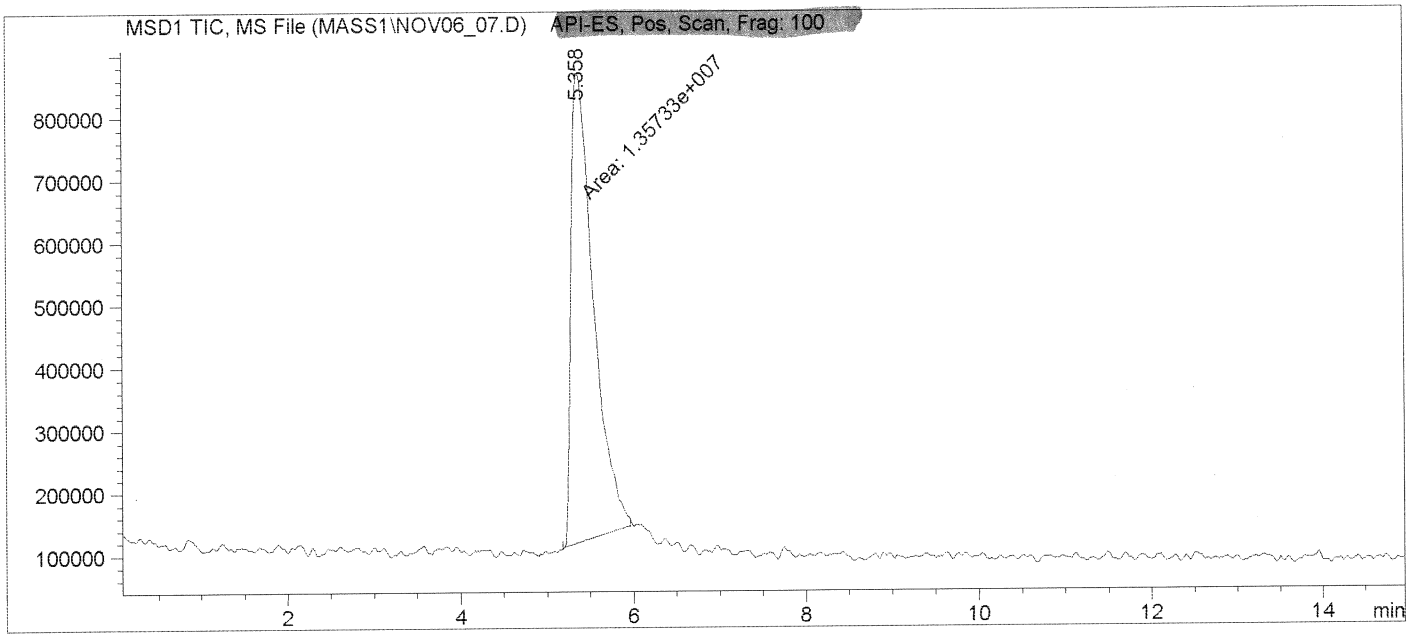
S105

Injection Date : 11/6/2008 11:25:42 AM
Sample Name : VB-GSA-118
Acq. Operator : Karen

Vial : 1
Inj : 1
Inj Volume : 0.1 ul

Method : D:\HPCHEM\1\METHODS\SCOTT_C.M
Last changed : 11/6/2008 11:01:55 AM by Karen
(modified after loading)

Zorbax C18 SB column,3.5u, 4.6 x 150mm, mp=20/80/0.25, MeCN:HOH:HAc (pH2.8); scan 150-550; flow 0.5mL/min; vcap 2500; frag 100; col temp 45



Area Percent Report

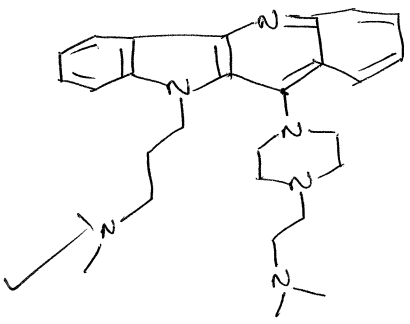
Sorted By : Retention Time
Multiplier : 1.0000
Dilution : 1.0000

Signal 1: MSD1 TIC, MS File

Peak #	RetTime [min]	Sig	Type	Area	Height	Area %
1	5.358	1	MM	1.35733e7	7.55419e5	100.0000

Totals : 1.35733e7 7.55419e5

Compound 12



VB-GSA-118

*** End of Report ***

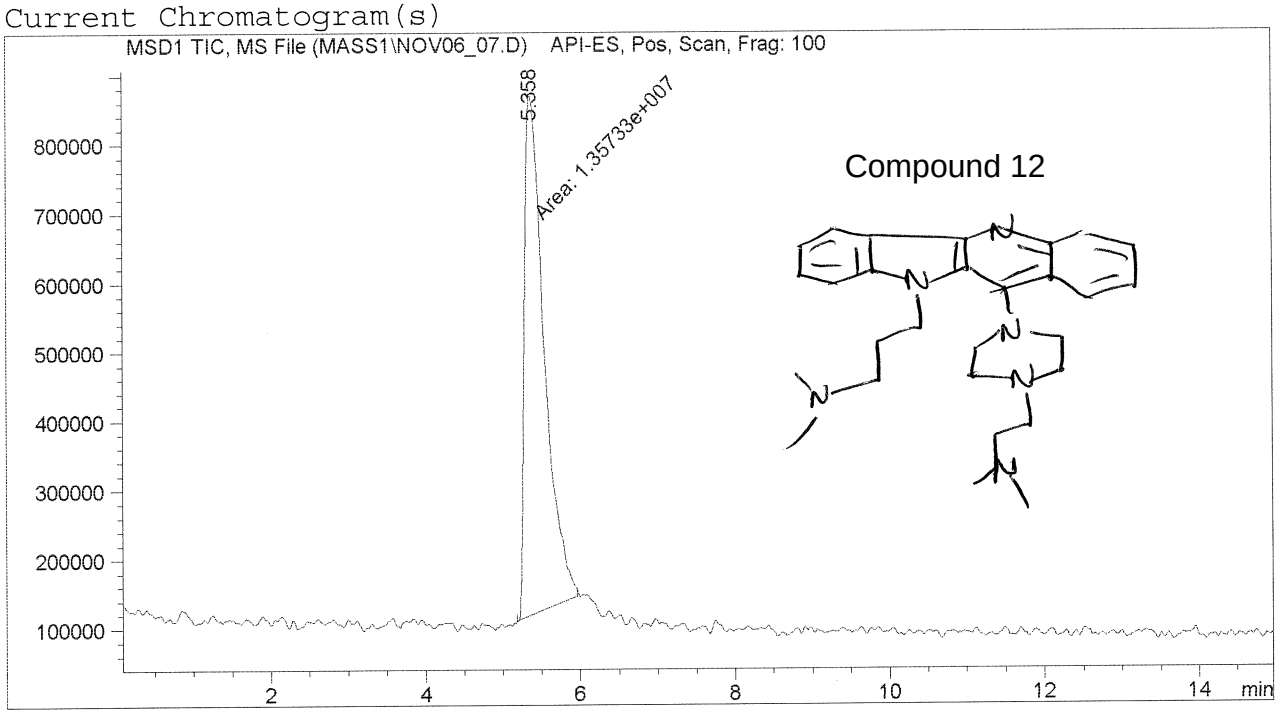
Print of all graphic windows

Injection Date : 11/6/2008 11:25:42 AM
Sample Name : VB-GSA-118 Vial : 1
Acq. Operator : Karen Inj : 1
Inj Volume : 0.1 ul

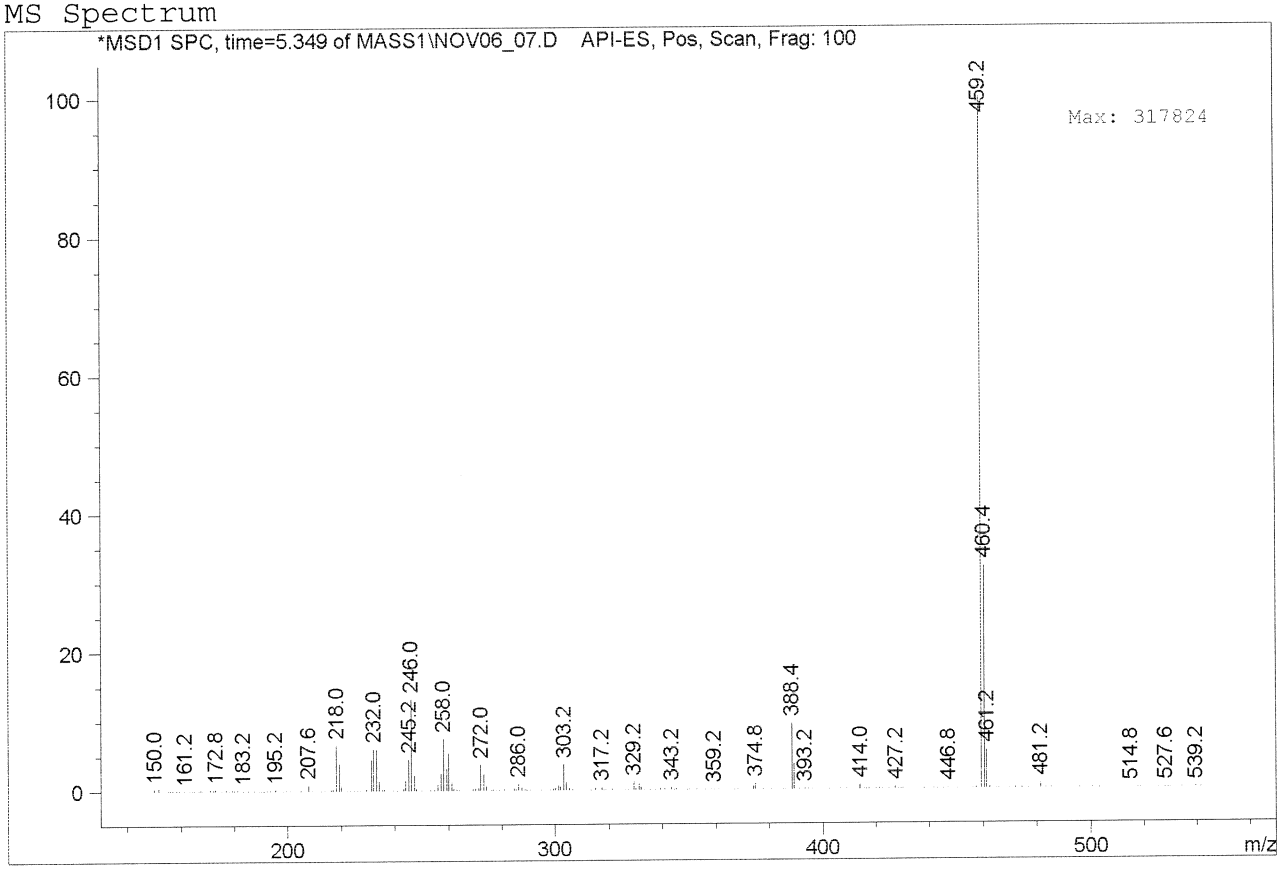
Method : D:\HPCHEM\1\METHODS\SCOTT_C.M
Last changed : 11/6/2008 11:01:55 AM by Karen
(modified after loading)

Zorbax C18 SB column,3.5u, 4.6 x 150mm, mp=20/80/0.25, MeCN:HOH:HAc (pH2.8); scan 150-550; flow 0.5mL/min; vcap 2500; frag 100; col temp 45

Current Chromatogram(s)



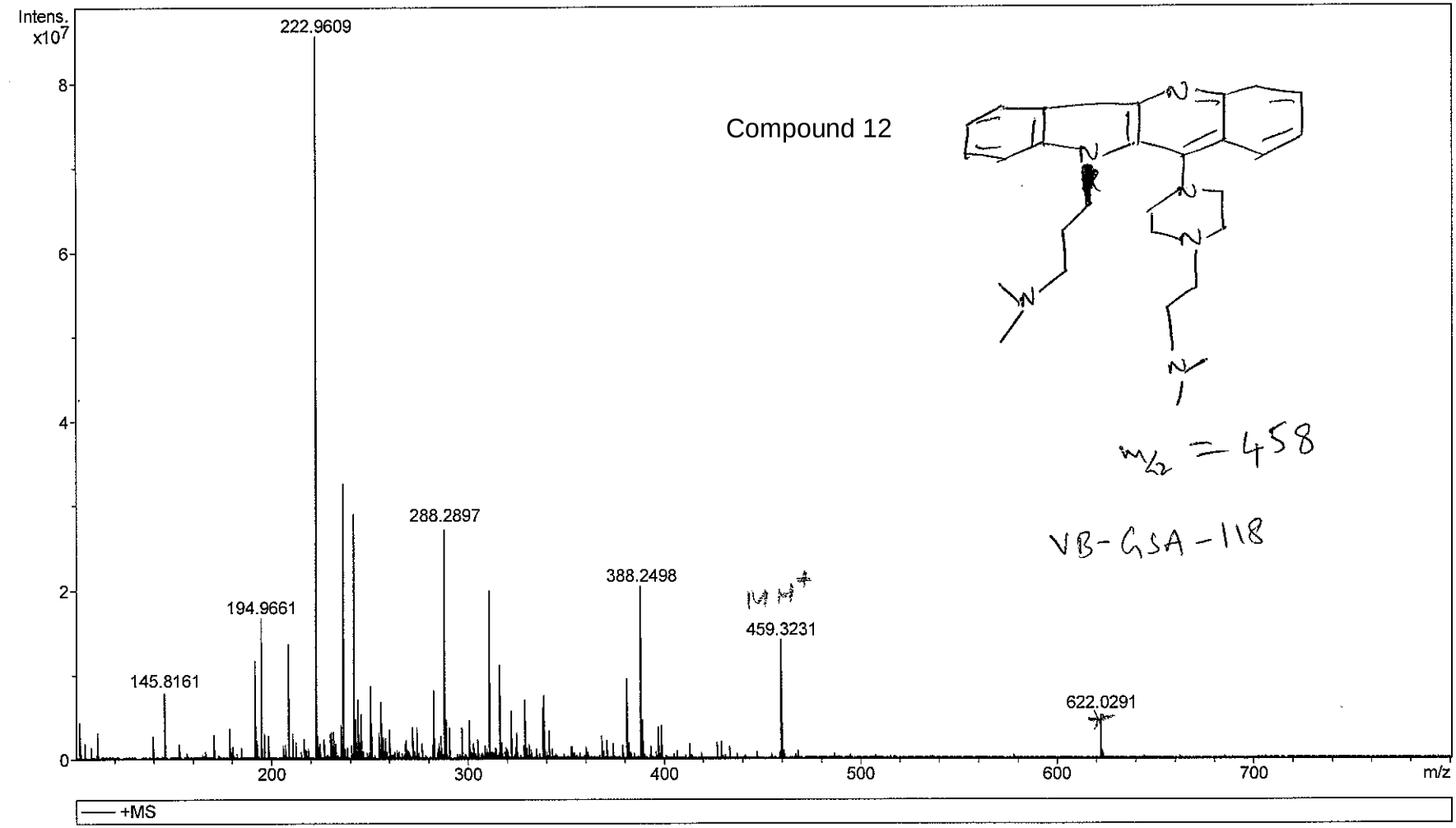
MS Spectrum



Generic Display Report

Analysis Info

Analysis Name	D:\DATA\Facility_Dec-08\VB-GSA-118_000004.d	Acquisition Date	12/19/2008 11:43:44 AM
Method	ESI_101506	Operator	
Sample Name	VB-GSA-118	Instrument	apex-Qe
Comment	Venkat B., MeOH:ACN 1:1		



Compound 12

m/z = 458

VB-GSA-118

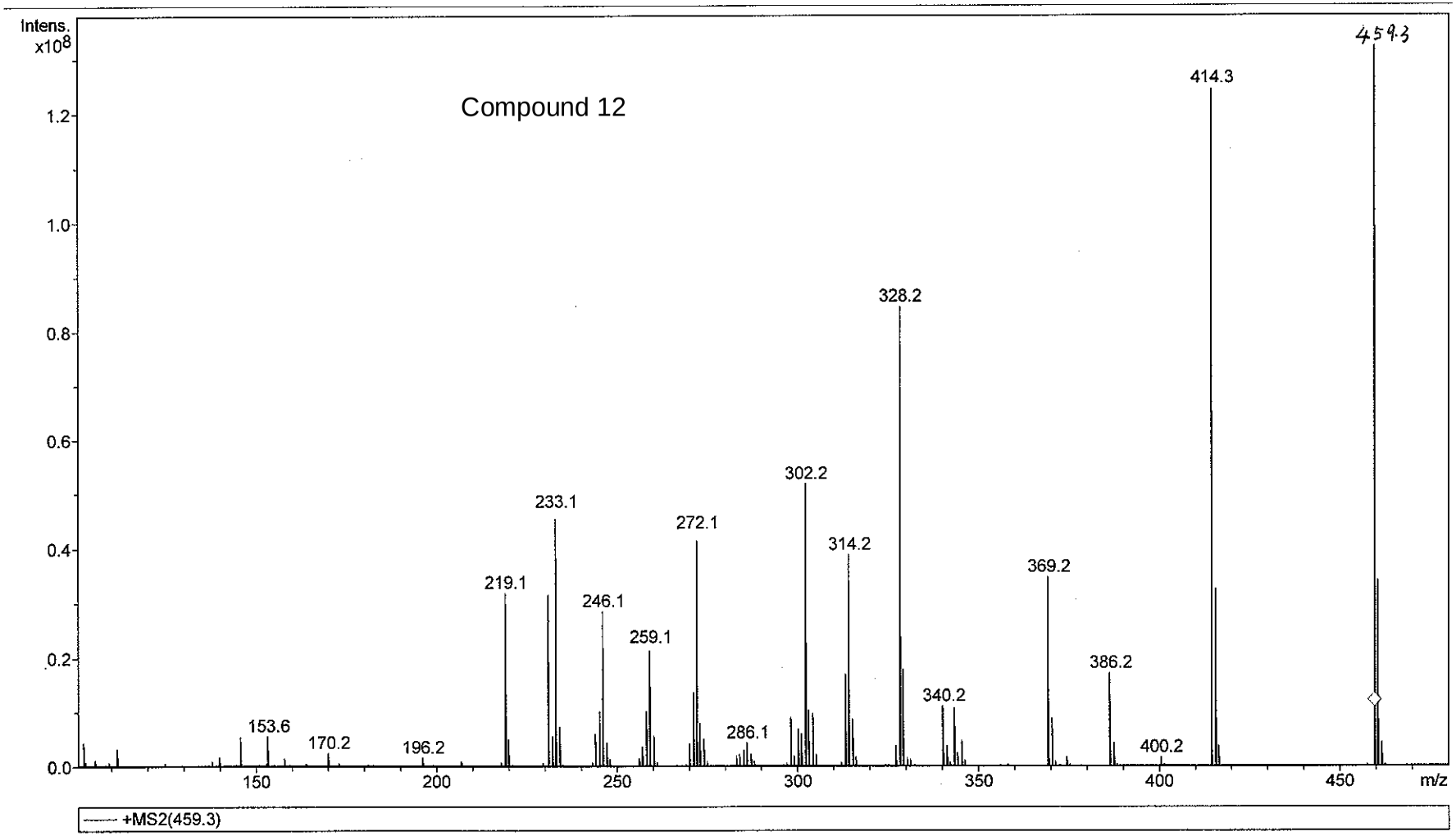
M H+

+ std

Generic Display Report

Analysis Info

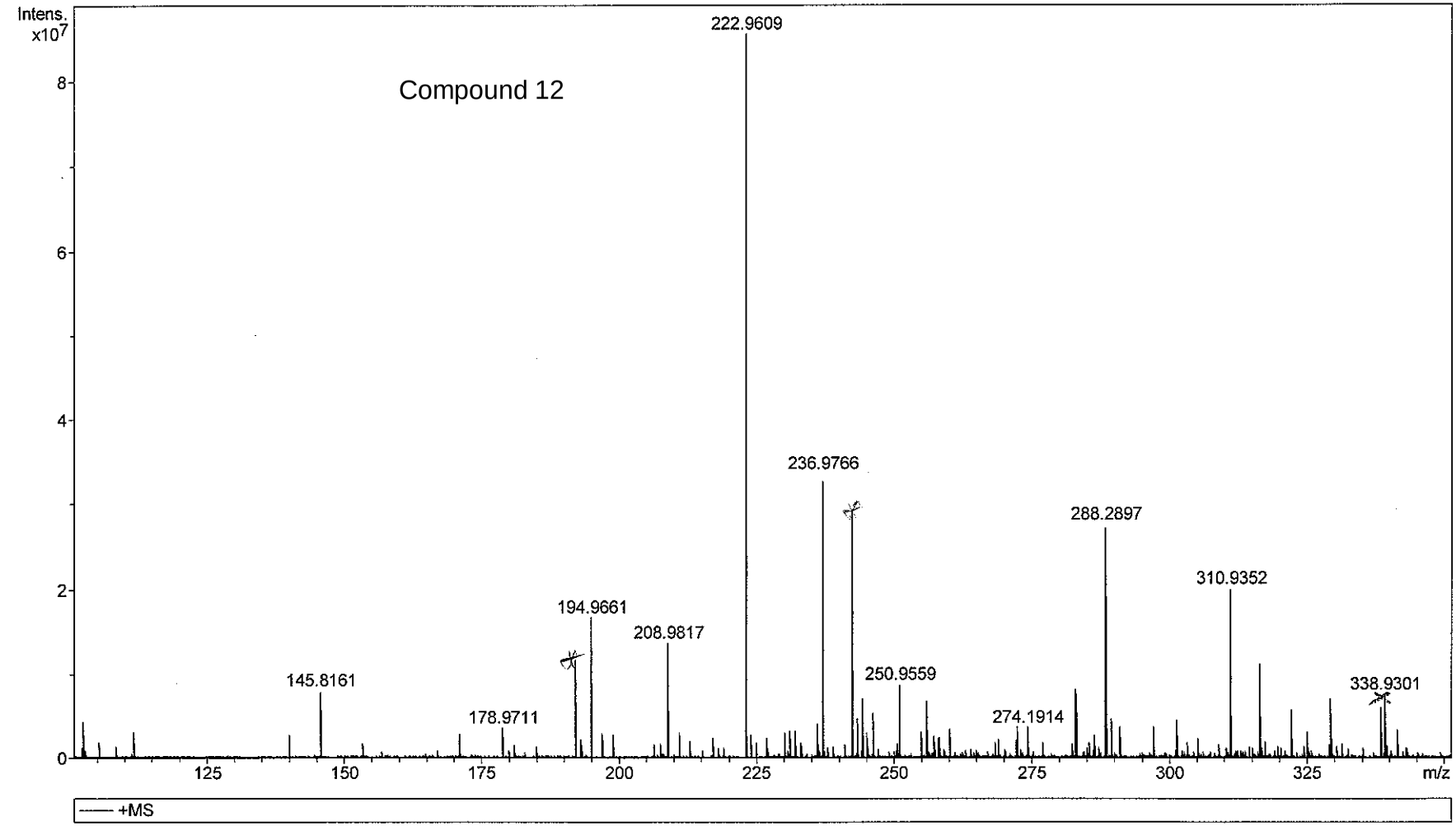
Analysis Name	D:\DATA\Facility_Dec-08\VB-GSA-118-QCID_000001.d	Acquisition Date	12/19/2008 11:20:30 AM
Method	ESI_101506	Operator	
Sample Name	VB-GSA-118	Instrument	apex-Qe
Comment	Venkat B., MeOH:ACN 1:1		



Generic Display Report

Analysis Info

Analysis Name	D:\DATA\Facility_Dec-08\VB-GSA-118_000004.d	Acquisition Date	12/19/2008 11:43:44 AM
Method	ESI_101506	Operator	
Sample Name	VB-GSA-118	Instrument	apex-Qe
Comment	Venkat B., MeOH:ACN 1:1		

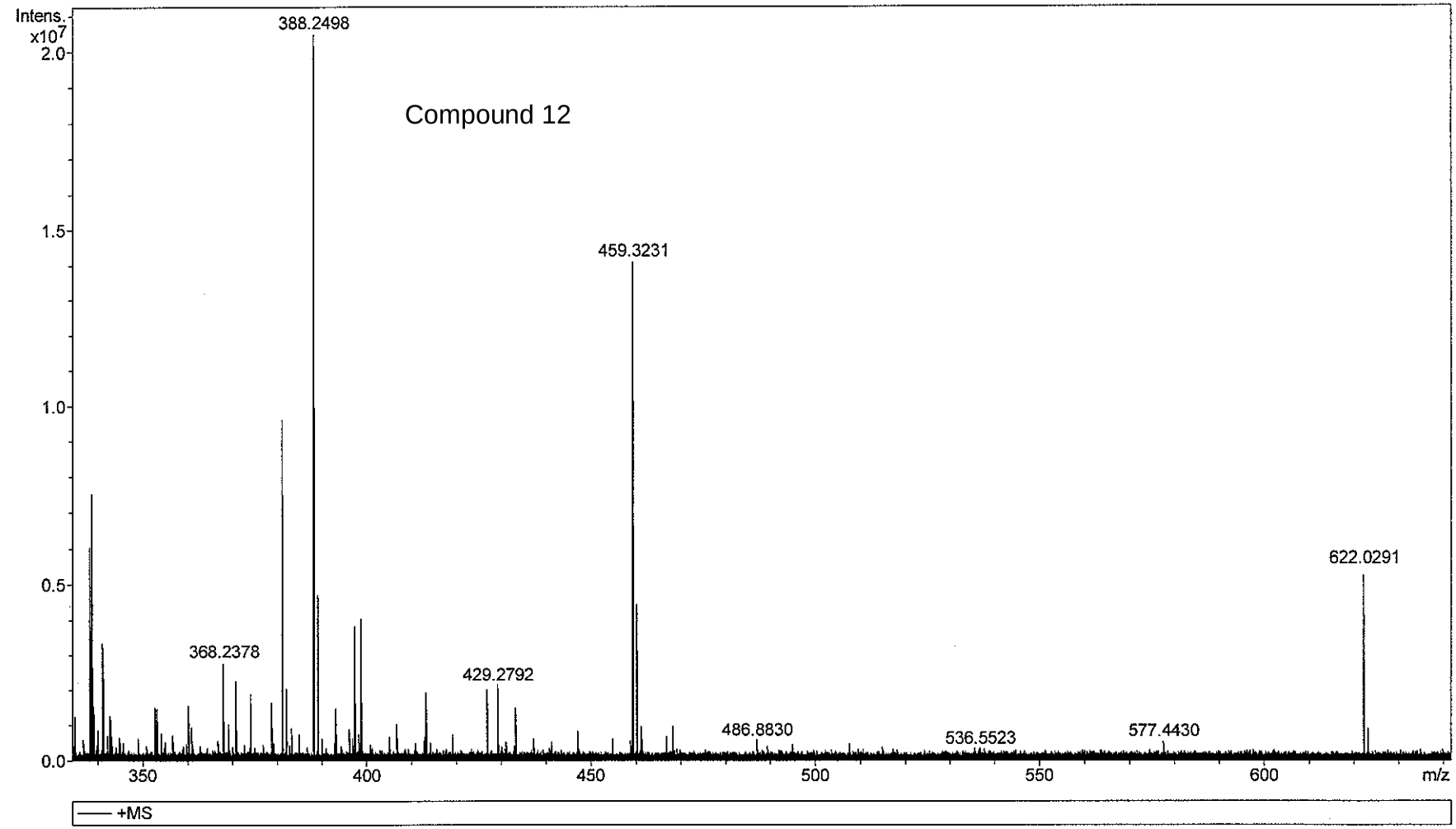


x in background

Generic Display Report

Analysis Info

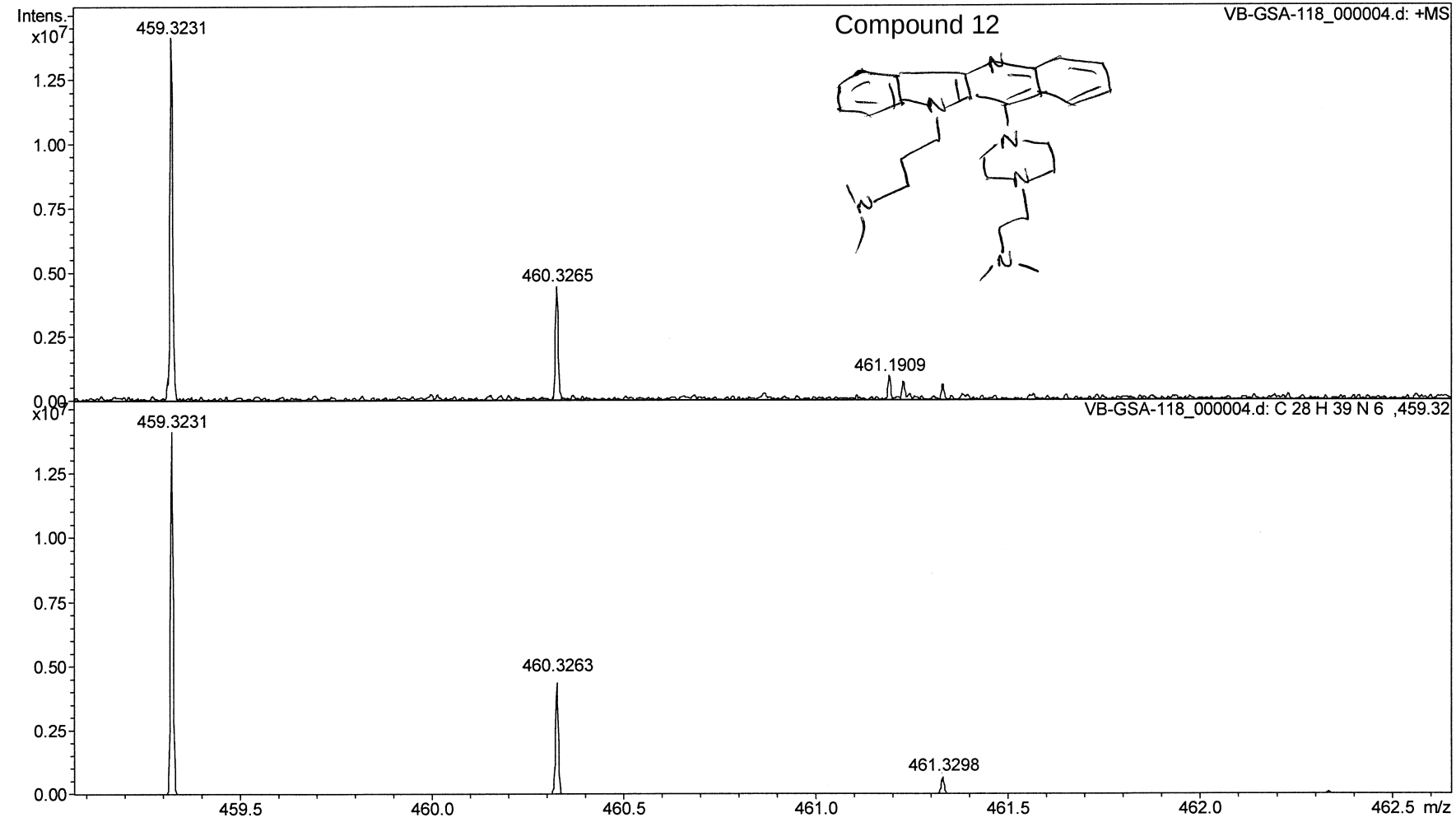
Analysis Name	D:\DATA\Facility_Dec-08\VB-GSA-118_000004.d	Acquisition Date	12/19/2008 11:43:44 AM
Method	ESI_101506	Operator	
Sample Name	VB-GSA-118	Instrument	apex-Qe
Comment	Venkat B., MeOH:ACN 1:1		



Generic Display Report

Analysis Info

Analysis Name	D:\DATA\Facility_Dec-08\VB-GSA-118_000004.d	Acquisition Date	12/19/2008 11:43:44 AM
Method	ESI_101506	Operator	
Sample Name	VB-GSA-118	Instrument	apex-Qe
Comment	Venkat B., MeOH:ACN 1:1		



SmartFormula Manually

Min C_{22}

Max

C 22-n

Generate

Help

Note: for m < 2000 the elements C, H, N, and O are considered implicitly.

Measured m/z 459.3231 Tolerance 2 mDa Charge 1

#	Mol. Formula	m/z	err [mDa]	|err| [ppm]	err [ppm]	mean err [ppm]
1	C 28 H 39 N 6	459.3231	-0.06	0.1	-0.1	-0.2
2	C 27 H 43 N 2 O 4	459.3217	-1.40	3.1	-3.1	-3.1

Automatically locate monoisotopic peak Maximum number of formulas 500

Check rings plus double bonds Minimum -0.5 Maximum 40

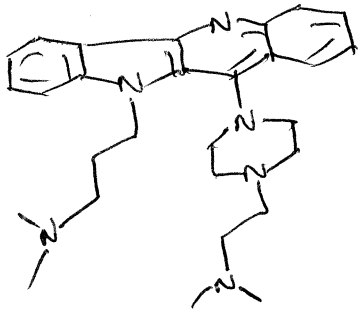
Electron configuration even

Filter H/C element ratio Minimum H/C 0 Maximum H/C 3

Estimate carbon number Generate immediately

Show Pattern

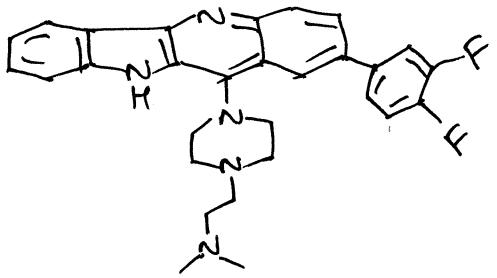
Compound 12



S113

8.517 8.510 8.316 8.291 8.235 8.206 7.965 7.958 7.935 7.928 7.901 7.894 7.886 7.879 7.861 7.669 7.662 7.645 7.637 7.629 7.608 7.605 7.582 7.578 7.296 7.292 7.270 7.247 7.243 3.560 3.220 2.830 2.789 2.765 2.710 2.693 2.509 2.504 2.498 2.440 0.009 -0.002 -0.013

Compound 13



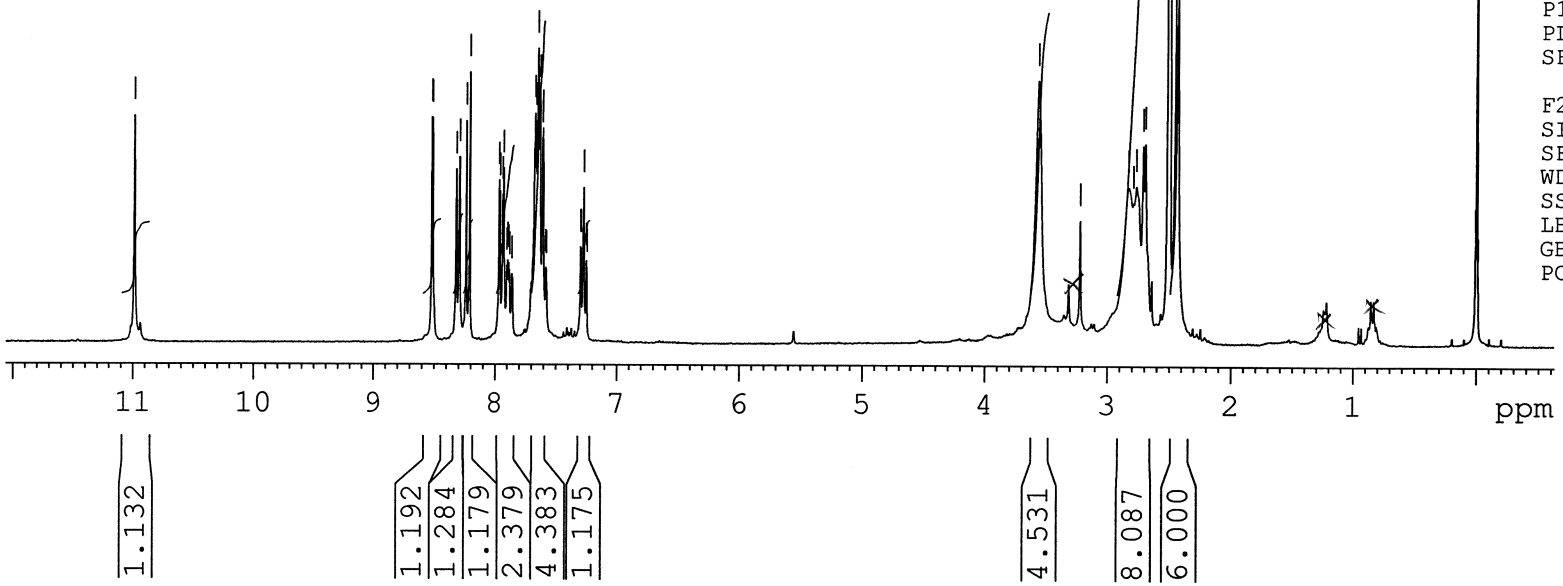
VB-GSA-197 (DMSO-d_6)

Current Data Parameters
NAME VB-GSA-197
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090812
Time 15.28
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 362
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 9.25 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



1.132 1.192 1.284 1.179 2.379 4.383 1.175 4.531 8.087 6.000

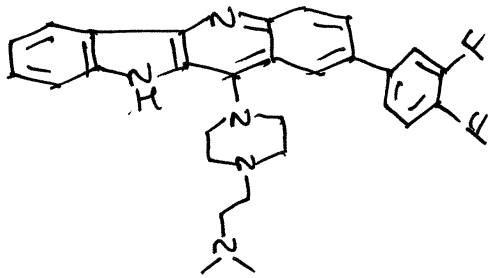
S114

148.440
148.270
145.356
144.937
139.127
137.078
134.524
130.750
130.470
127.553
126.153
124.581
124.221
122.088
121.993
121.938
120.352
119.169
118.942
116.939
116.706
112.991

56.352
55.462
54.589
54.188
51.548
45.446
41.743
41.233
40.956
40.677
40.399
40.121
39.842
39.564

0.962

Compound 13



VB-GSA-197

Current Data Parameters
NAME VB-GSA-197
EXPNO 10
PROCNO 1

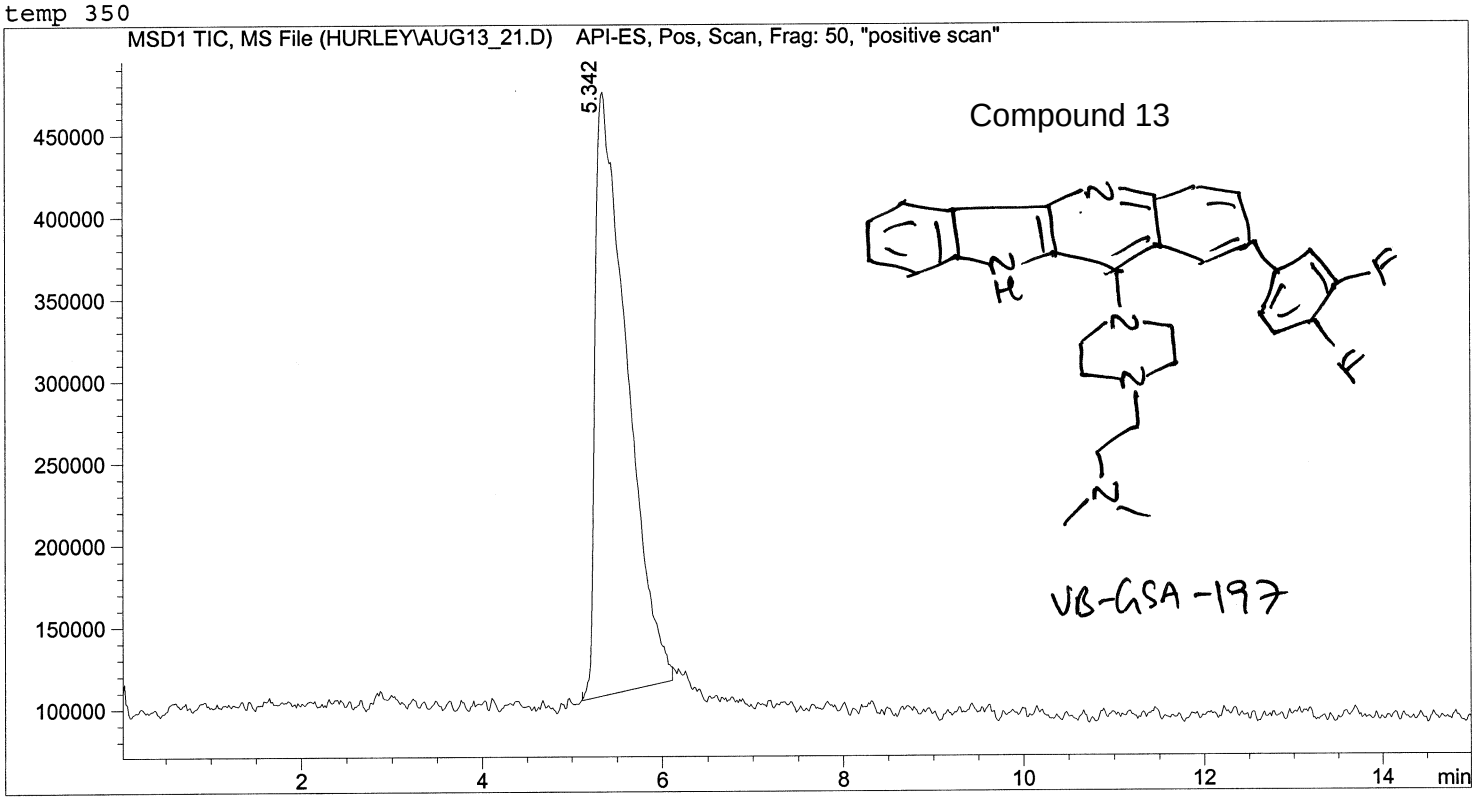
F2 - Acquisition Parameters
Date_ 20090813
Time 8.57
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 15000
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 1448.2
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 2.00 dB
SFO1 75.4752653 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 20.00 dB
PL13 20.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

```
==========================================================================
Injection Date  : 8/13/2009 6:21:56 PM
Sample Name     : VB-GSA-197                        Location : Vial 5
Acq. Operator   : Karen                                Inj :   1
Acq. Instrument : Instrument 1                  Inj Volume : 0.1 µl
Method          : C:\HPCHEM\1\METHODS\LC_MS.M
Last changed    : 8/13/2009 6:37:01 PM by Karen
                  (modified after loading)
Zorbax SB ODS,60:40:0.25; MeOH/water/formicA, POS, 300-550; frag 50; 30C, cap volt 3000, gas
temp 350
```



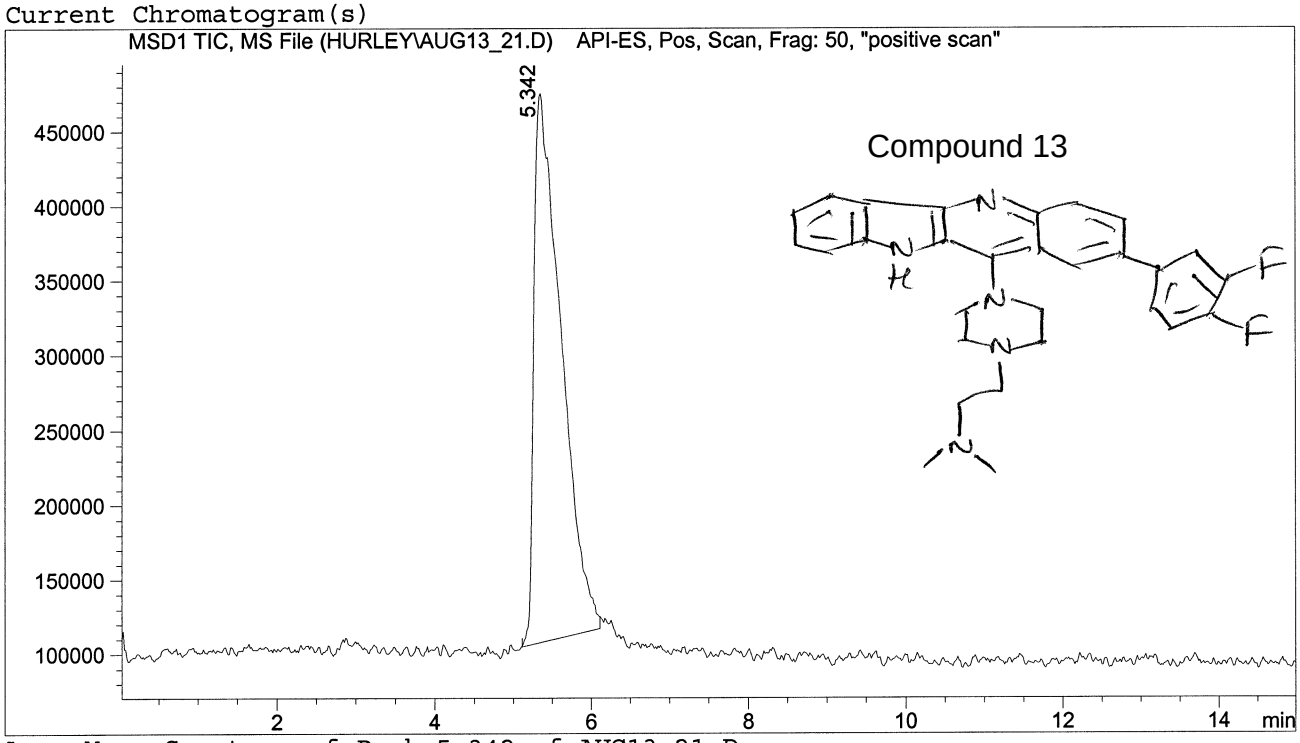

```
==========================================================================
                          Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MSD1 TIC, MS File

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]                          %
----|-------|----|-------|----------|----------|--------|
   1   5.342 BB    0.3207 8.93619e6  3.68294e5  100.0000

Totals :                  8.93619e6  3.68294e5

==========================================================================
                          *** End of Report ***
```

Print of all graphic windows

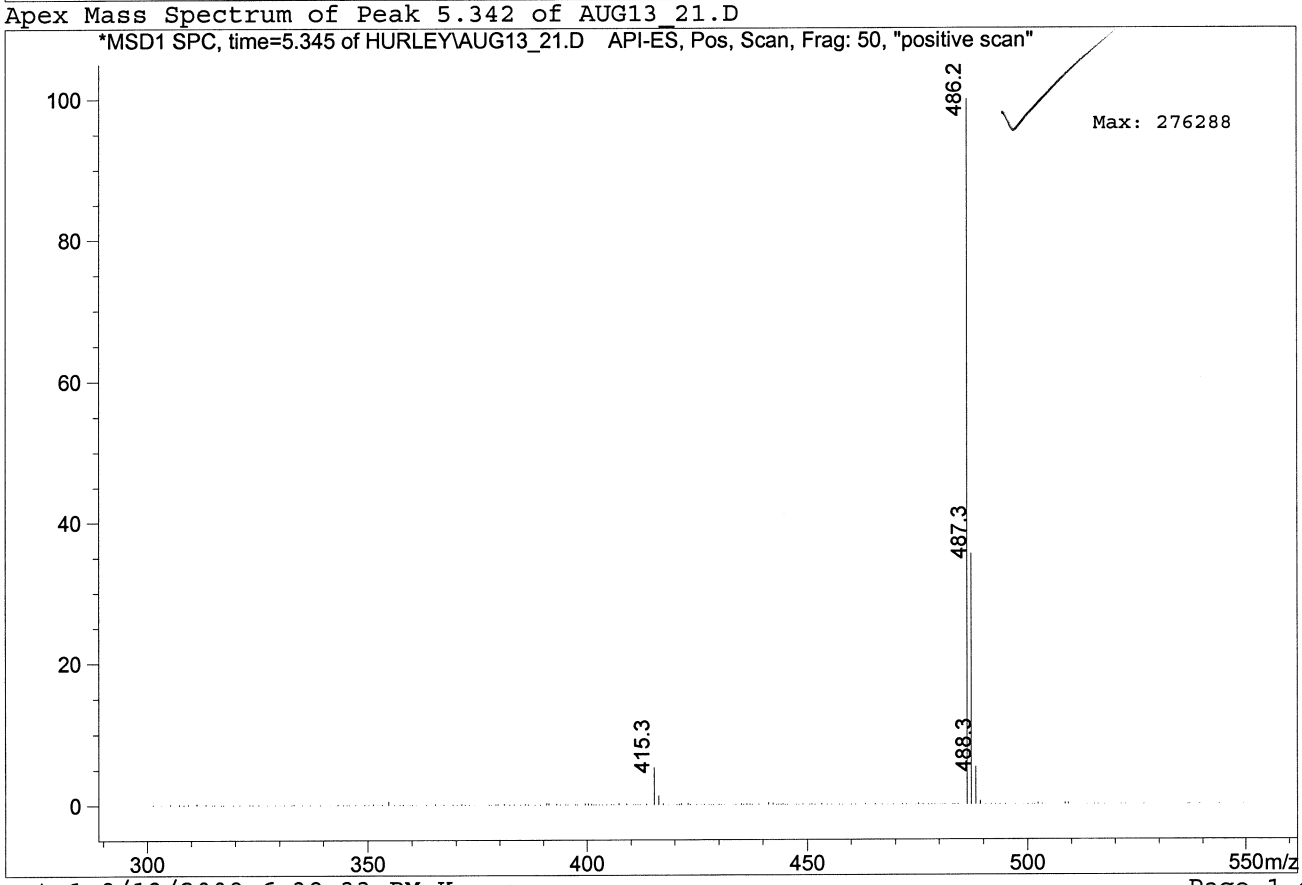
Injection Date : 8/13/2009 6:21:56 PM
Sample Name : VB-GSA-197 Location : Vial 5
Acq. Operator : Karen Inj : 1
Acq. Instrument : Instrument 1 Inj Volume : 0.1 µl
Method : C:\HPCHEM\1\METHODS\LC_MS.M
Last changed : 8/13/2009 6:37:01 PM by Karen
(modified after loading)

Zorbax SB ODS,60:40:0.25; MeOH/water/formicA, POS, 300-550; frag 50; 30C, cap volt 3000, gas temp 350

Current Chromatogram(s)



Apex Mass Spectrum of Peak 5.342 of AUG13_21.D



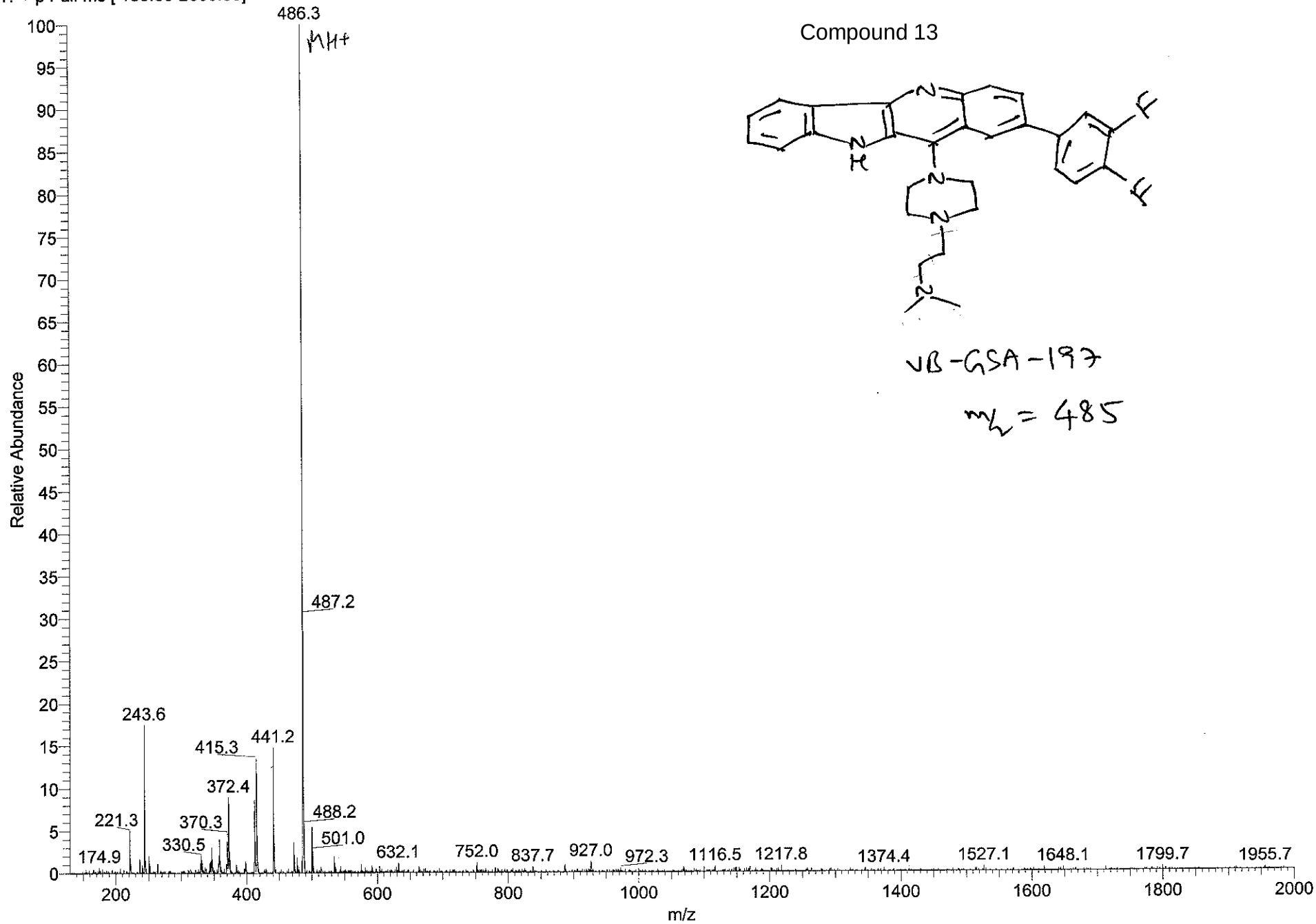
E:\MSLab_LCQ\VB_GSA_197 08/17/2009 03:36:05 PM VB_GSA_197

V. Boddupally, MeOH:ACN 1:1

VB_GSA_197 #31-35 RT: 1.03-1.15 AV: 5 NL: 1.72E7

T: + p Full ms [130.00-2000.00]

S117

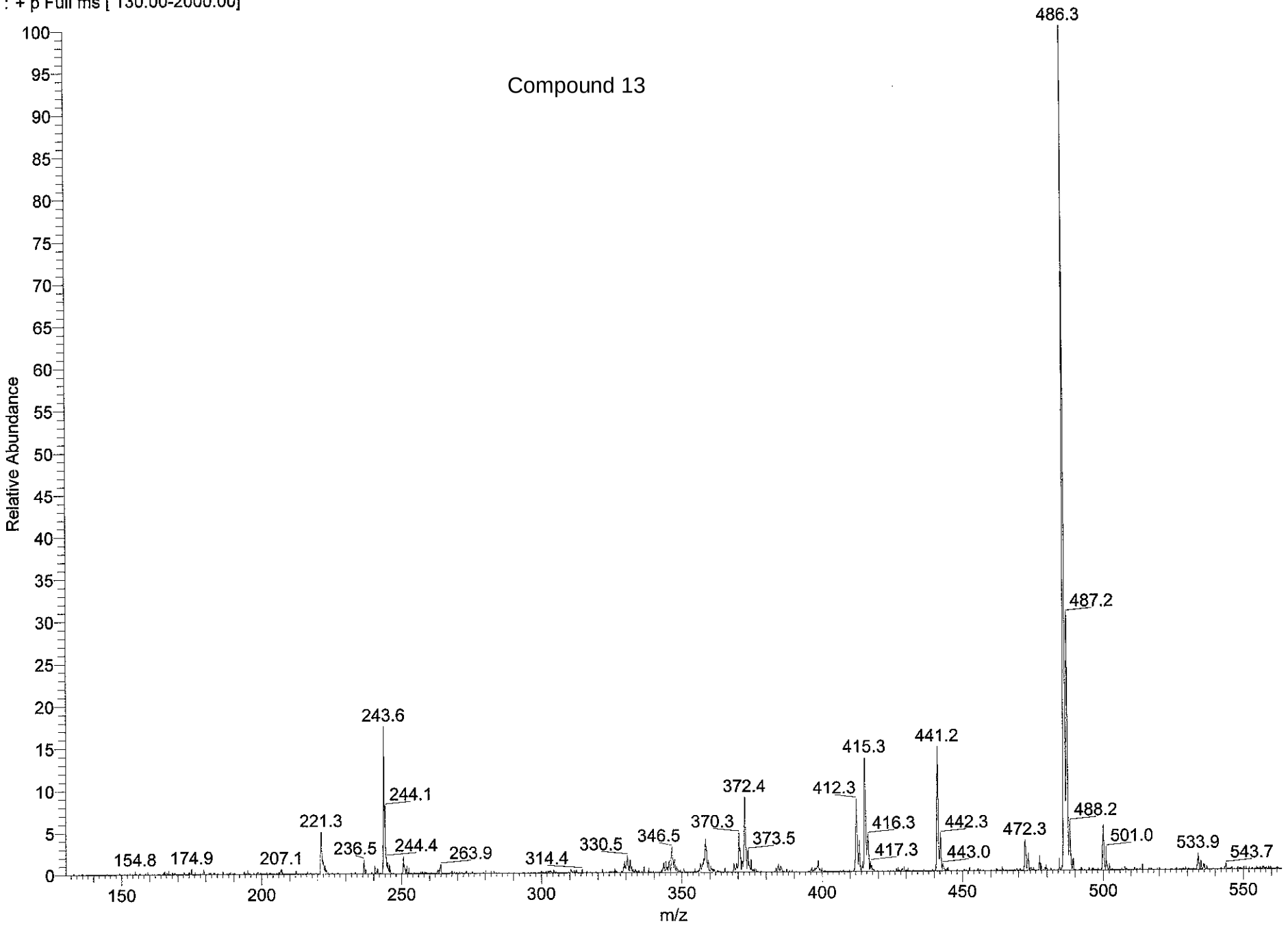


Compound 13

VB-GSA-197

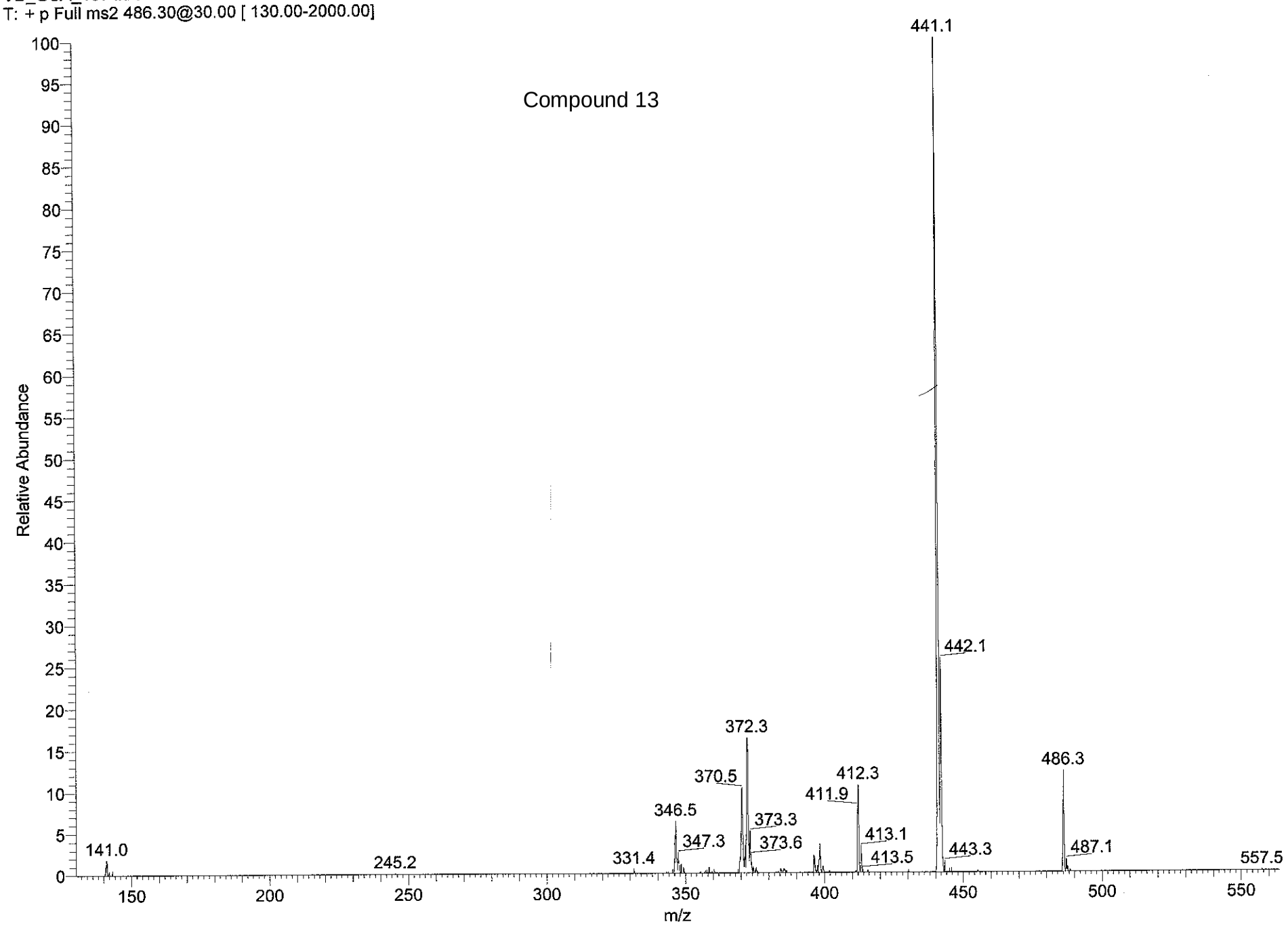
m/z = 485

E:\MSLab_LCQ\VB_GSA_197 08/17/2009 03:36:05 PM VB_GSA_197
V. Boddupally, MeOH:ACN 1:1
VB_GSA_197 #31-35 RT: 1.03-1.15 AV: 5 NL: 1.72E7
T: + p Full ms [130.00-2000.00]
S118



E:\MSLab_LCQ\VB_GSA_197 08/17/2009 03:36:05 PM VB_GSA_197
V. Boddupally, MeOH:ACN 1:1
VB_GSA_197 #25-29 RT: 0.82-0.96 AV: 5 NL: 9.06E6
T: + p Full ms2 486.30@30.00 [130.00-2000.00]

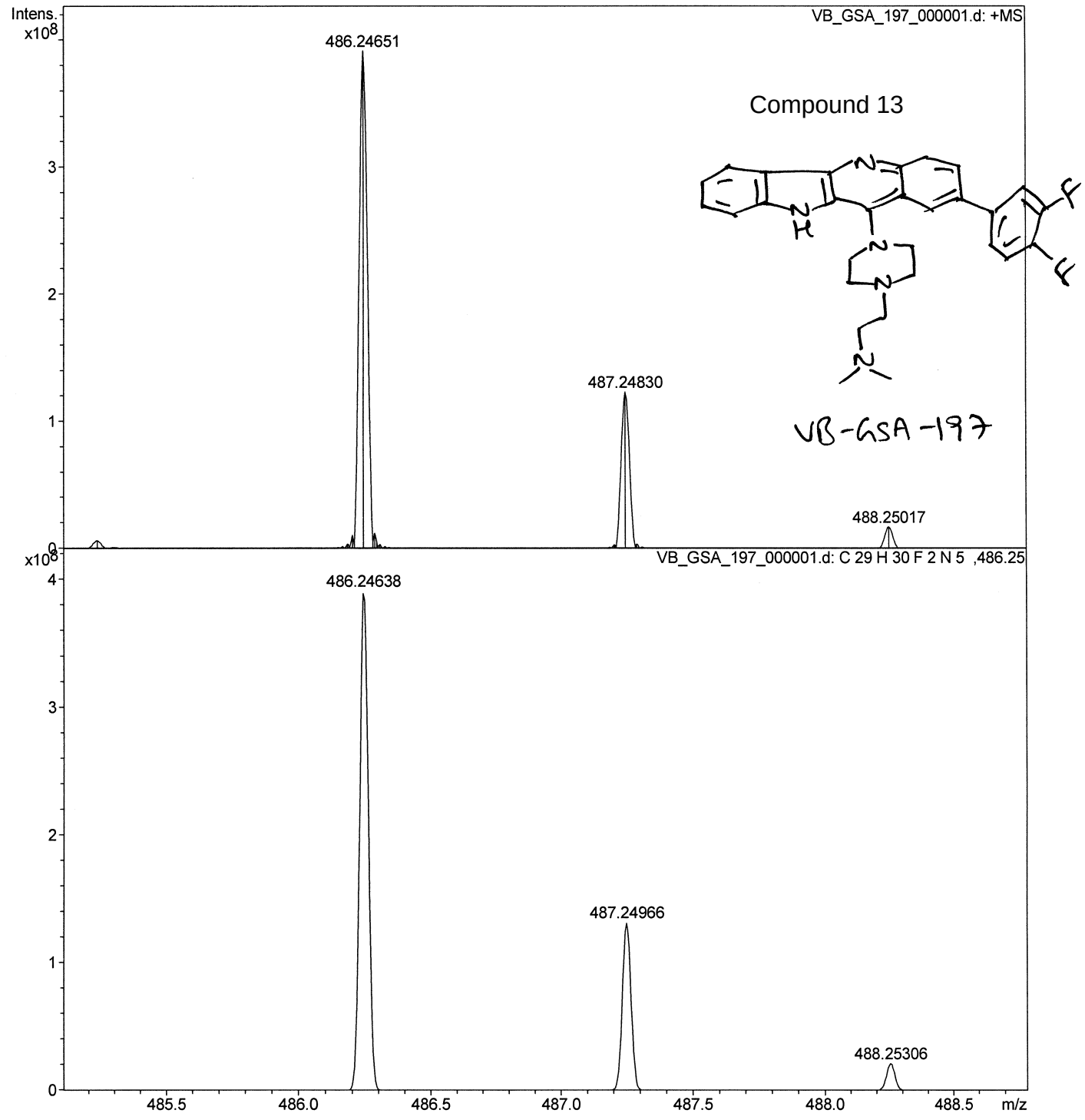
S119



Generic Display Report

Analysis Info

Analysis Name	D:\DATA\Facility_August_09\VB_GSA_197_000001.d	Acquisition Date	8/21/2009 5:04:25 PM
Method	ESI_101506	Operator	
Sample Name	VB_GSA_197	Instrument	apex-Qe
Comment	VB_GSA_197 ACN:H2O 1:1 0.1% FA		



SmartFormula Manually

Min $C_{22}F_2$

Max F_3

C 22-n, F 2-3

Generate

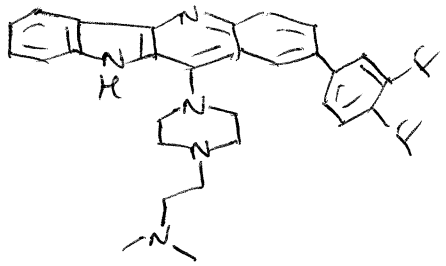
Help

Note: for m < 2000 the elements C, H, N, and O are considered implicitly.

Measured m/z 486.24651 Tolerance 2 mDa Charge 1

#	Mol. Formula	m/z	err [mDa]	|err| [ppm]	err [ppm]	mean err [ppm]	mSigma	Sigma Rank	rdb	N rule	e⁻
1	C 24 H 33 F 3 N 3 O 4	484.24177	1.17	2.4	2.4	5.3	791.4	7	8.5	ok	even
2	C 25 H 35 F 3 N O 5	486.24618	-0.32	0.7	-0.7	0.3	21.0	4	7.5	ok	even
3	C 26 H 31 F 3 N 5 O	486.24752	1.01	2.1	2.1	3.0	6.4	2	12.5	ok	even
4	C 27 H 32 F 2 N 3 O 3	484.24062	0.19	0.4	0.4	3.4	703.2	6	12.5	ok	even
5	C 28 H 34 F 2 N O 4	486.24504	-1.47	3.0	-3.0	-2.1	6.2	1	11.5	ok	even
6	C 29 H 30 F 2 N 5	486.24638	-0.13	0.3	-0.3	0.6	10.2	3	16.5	ok	even
7	C 33 H 32 F 3	485.24506	1.94	4.0	4.0	5.1	600.4	5	16.5	ok	even

Compound 13



☑ Automatically locate monoisotopic peak Maximum number of formulas 500

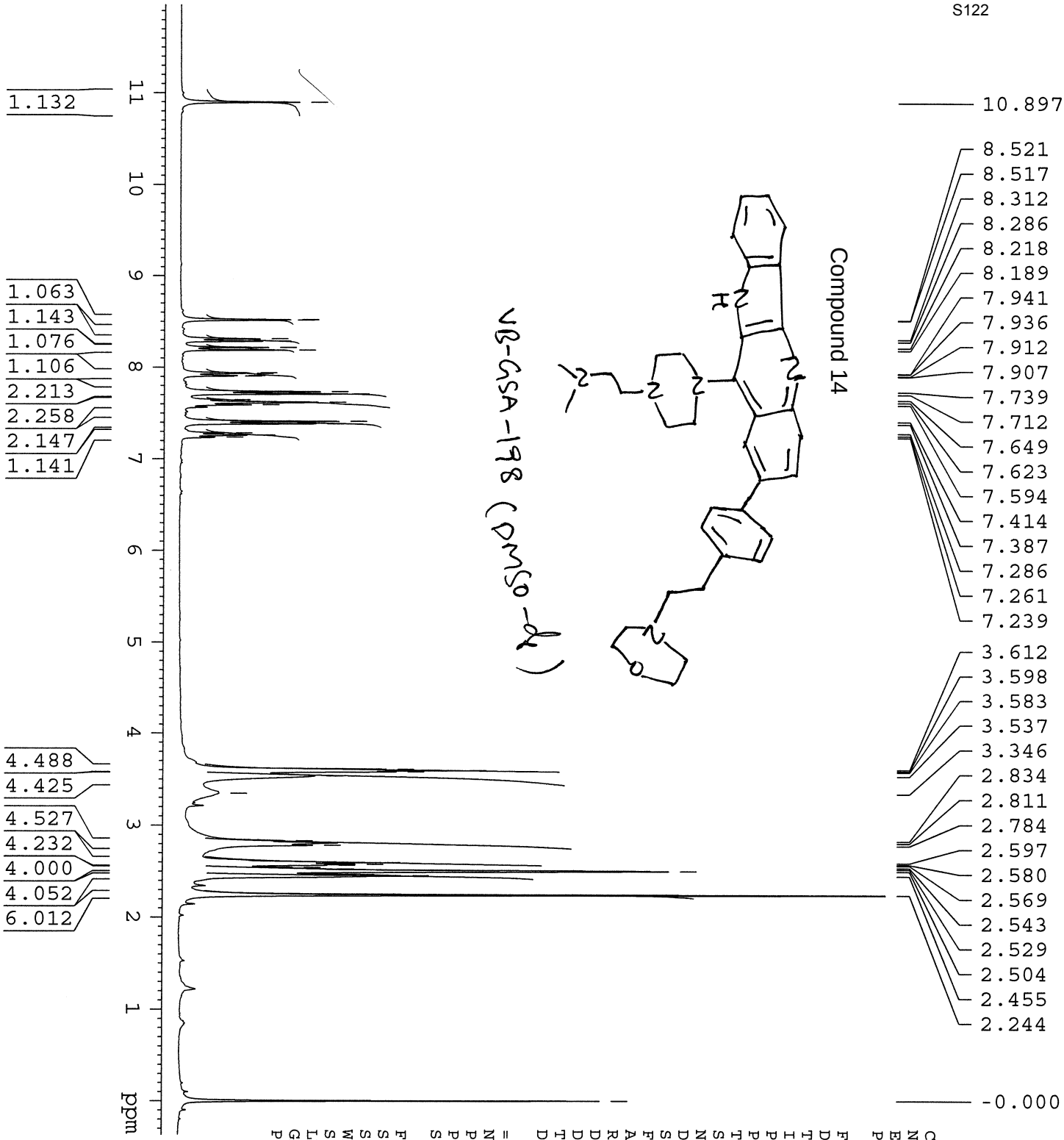
☑ Check rings plus double bonds Minimum -0.5 Maximum 40

Electron configuration even

☑ Filter H/C element ratio Minimum H/C 0 Maximum H/C 3

☑ Estimate carbon number ☑ Generate immediately

Show Pattern




```
Current Data Parameters
NAME                  VB-GSA-198
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_              20090818
Time_                  17.00
INSTRUM                spect
PROBHD     5 mm QNP  1H/1
PULPROG                zg30
TD                    65536
SOLVENT               DMSO
NS                       64
DS                        2
SWH                6172.839 Hz
FIDRES                0.094190 Hz
AQ                    5.3084660 sec
RG                      322.5
DW                     81.000 usec
DE                      6.00 usec
TE                     300.0 K
D1                     1.00000000 sec

========== CHANNEL f1 ========
NUC1                       1H
P1                       9.25 usec
PL1                      0.00 dB
SFO1           300.1318534 MHz

F2 - Processing parameters
SI                        32768
SF             300.1300000 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```

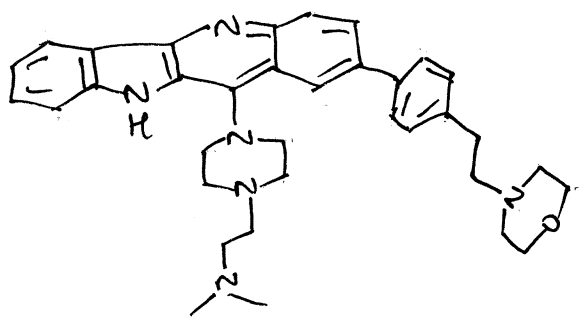
S123

144.854
140.588
138.975
136.871
136.572
130.583
130.360
127.658
127.501
126.264
124.366
122.179
121.923
121.188
120.269
112.936

67.075
60.855
57.436
56.673
54.865
54.156
51.617
46.275
41.236
40.958
40.680
40.401
40.123
39.845
39.567
32.873

0.967

Compound 14



VB-GSA-198

Current Data Parameters
NAME VB-GSA-198
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

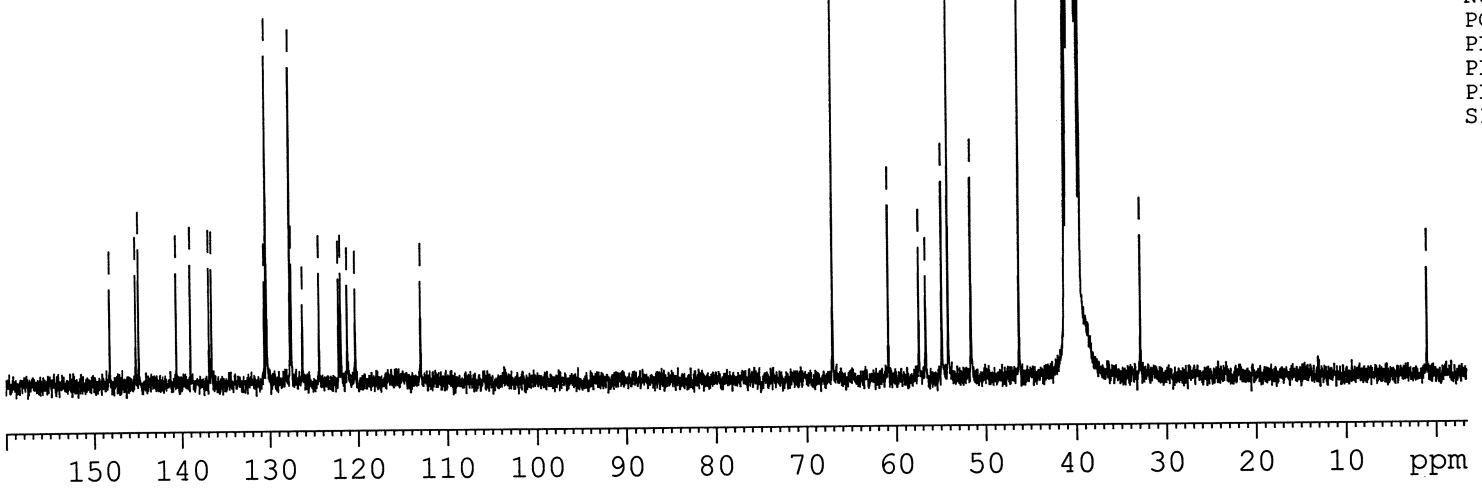
Date_	20090819
Time	9.02
INSTRUM	spect
PROBHD	5 mm QNP 1H/1
PULPROG	zgpg30
TD	65536
SOLVENT	~~cdcl3~~ DMSO-d6
NS	14821
DS	4
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	912.3
DW	27.800 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec
d12	0.00002000 sec

======== CHANNEL f1 ========

NUC1	13C
P1	6.00 usec
PL1	2.00 dB
SFO1	75.4752653 MHz

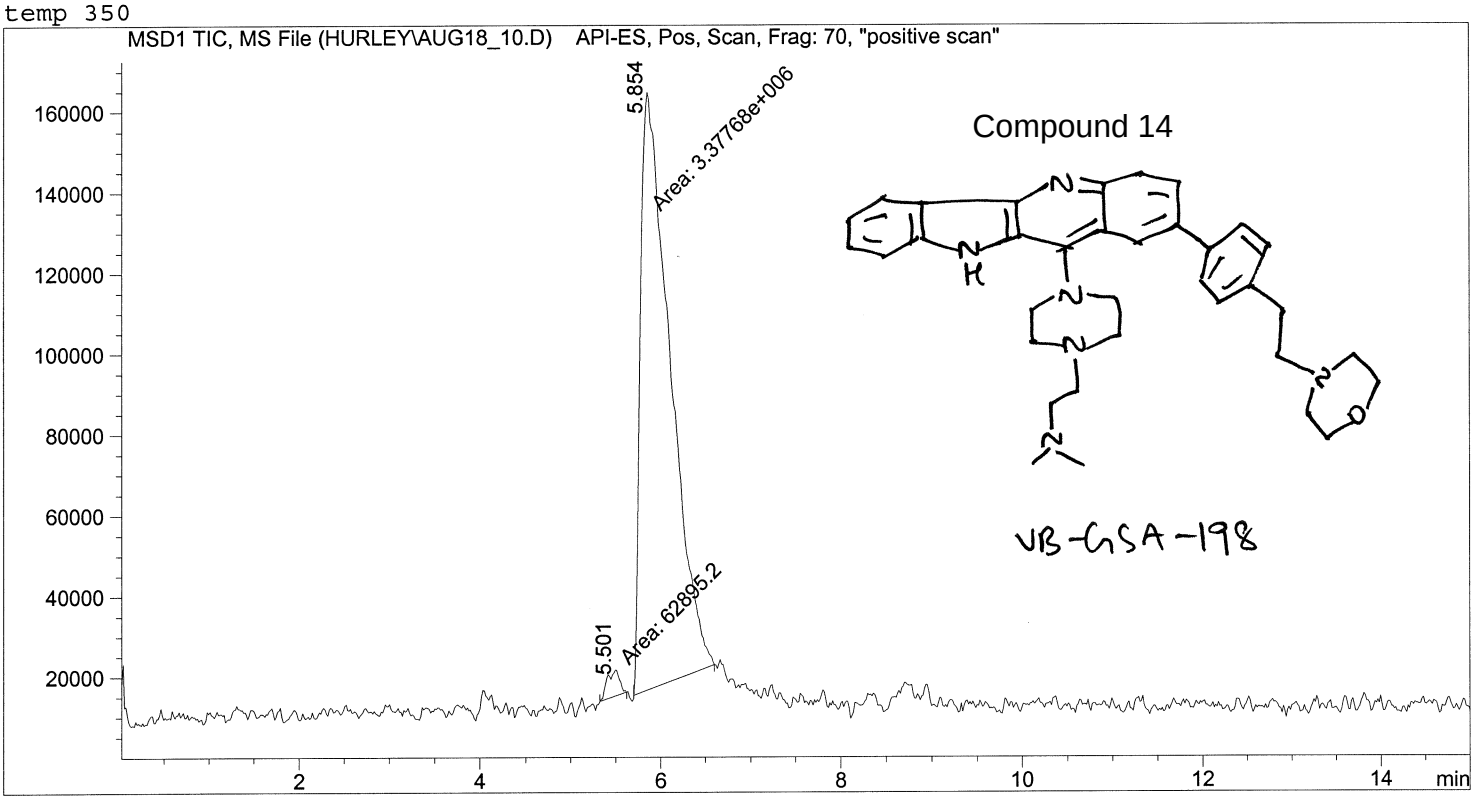
======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	0.00 dB
PL12	20.00 dB
PL13	20.00 dB
SFO2	300.1312005 MHz



S124

```
Injection Date  : 8/18/2009 5:14:55 PM
Sample Name     : VB-GSA-198                    Location : Vial 2
Acq. Operator   : Karen                            Inj :   1
Acq. Instrument : Instrument 1                 Inj Volume : 0.2 µl
Method          : C:\HPCHEM\1\METHODS\LC_MS.M
Last changed    : 8/18/2009 5:13:56 PM by Karen
Zorbax SB ODS,20:80:0.25; MeCN/water/formicA, POS, 350-650; frag 70; 30C, cap volt 3000, gas
temp 350
```

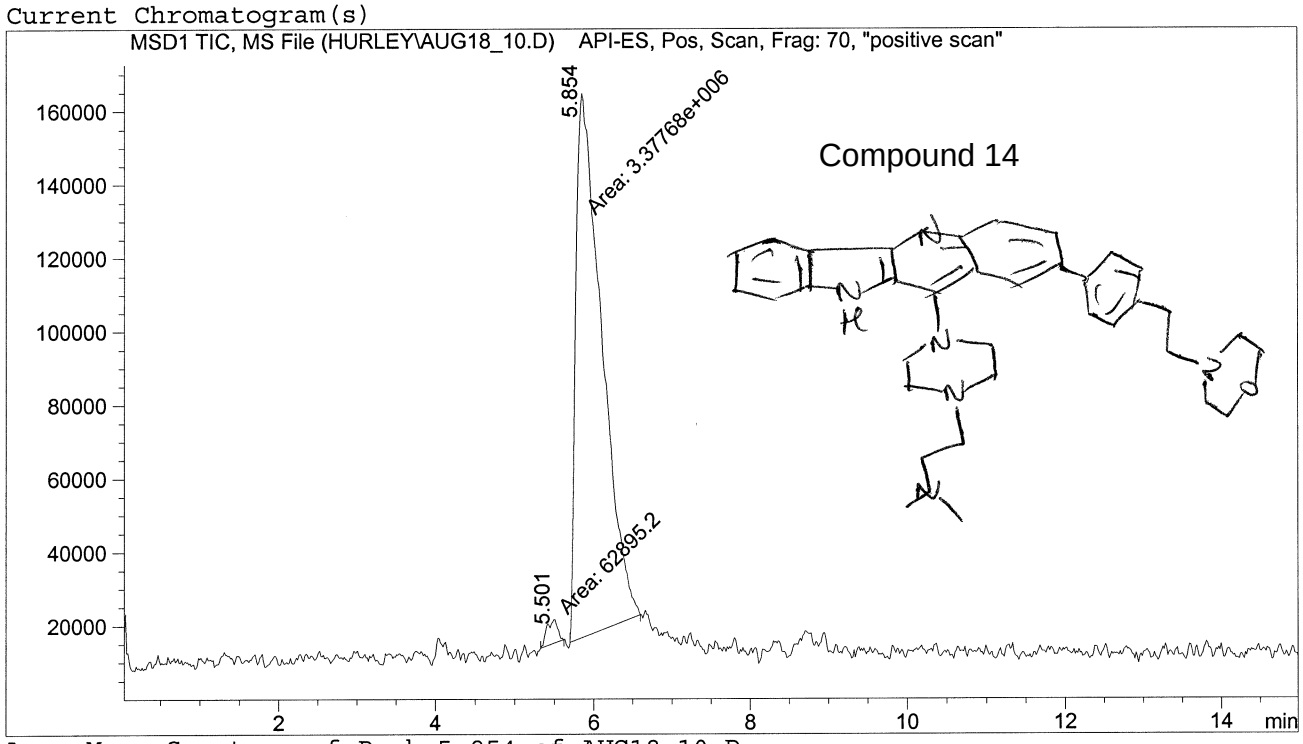



```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MSD1 TIC, MS File

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]                          %
----|-------|----|-------|----------|----------|--------|
   1   5.501 MM    0.1576 6.28952e4  6652.23193   1.8280
   2   5.854 MM    0.3792 3.37768e6  1.48440e5   98.1720

Totals :                  3.44057e6  1.55092e5

=====================================================================
                        *** End of Report ***
```

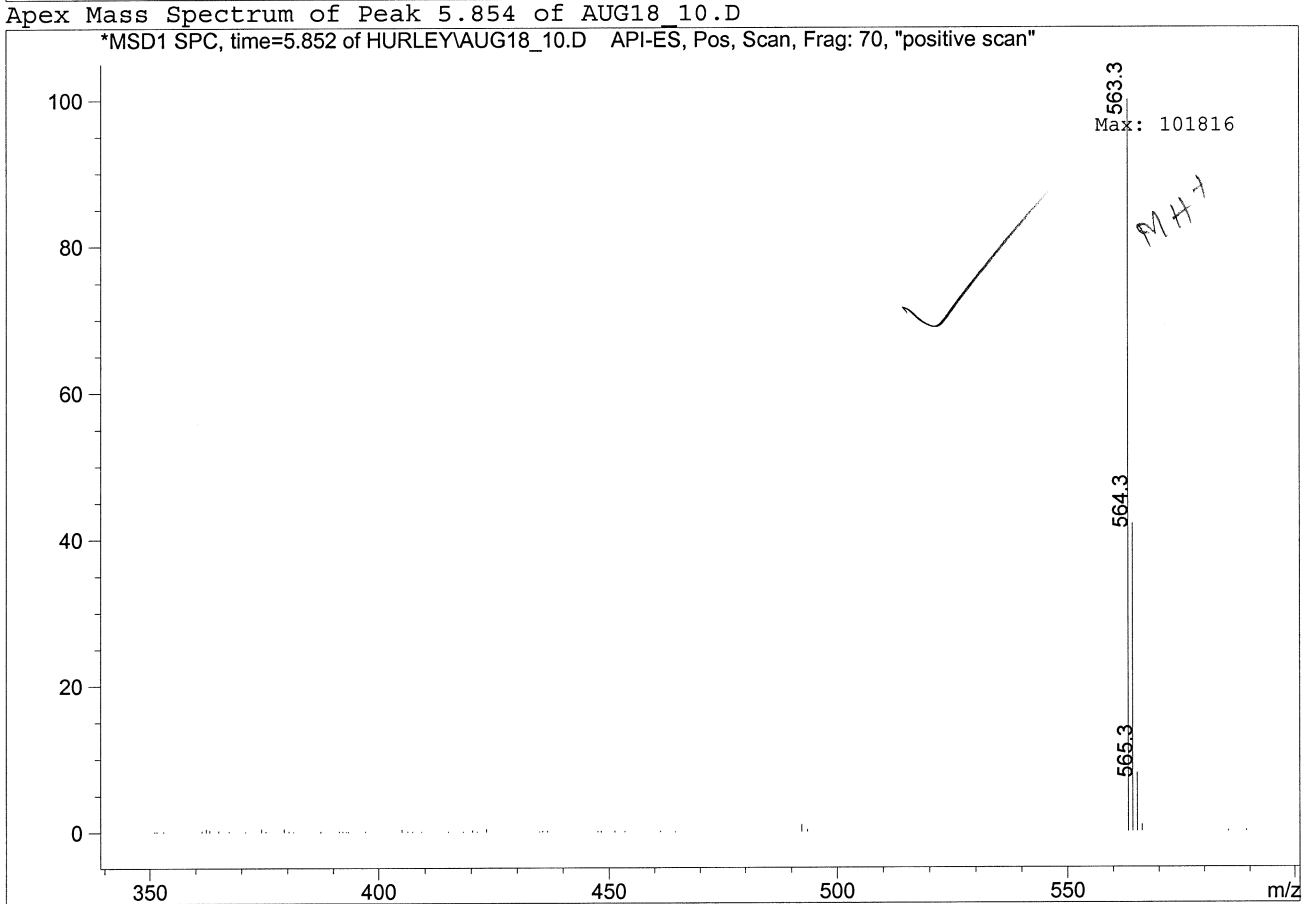
Print of all graphic windows

```
==========================================================================
Injection Date  : 8/18/2009 5:14:55 PM
Sample Name     : VB-GSA-198                        Location : Vial 2
Acq. Operator   : Karen                                Inj :   1
Acq. Instrument : Instrument 1                  Inj Volume : 0.2 µl
Method          : C:\HPCHEM\1\METHODS\LC_MS.M
Last changed    : 8/18/2009 5:13:56 PM by Karen
Zorbax SB ODS,20:80:0.25; MeCN/water/formicA, POS, 350-650; frag 70; 30C, cap volt 3000,
gas temp 350
```

Current Chromatogram(s)



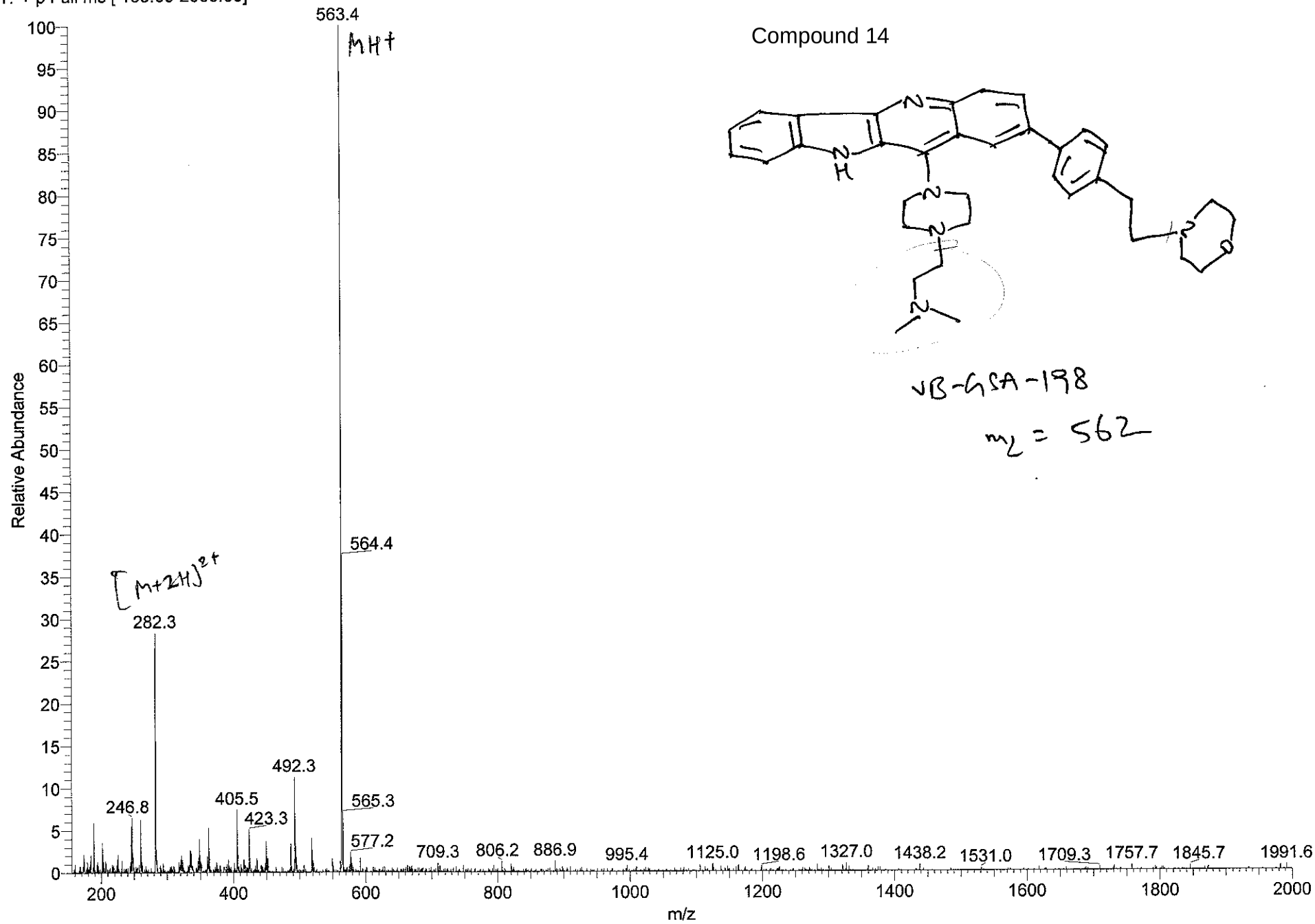
Apex Mass Spectrum of Peak 5.854 of AUG18_10.D



E:\MSLab_LCQ\VB_GSA_198 08/17/2009 03:46:31 PM VB_GSA_198
V. Boddupally, MeOH:ACN 1:1

VB_GSA_198 #16-19 RT: 0.52-0.62 AV: 4 NL: 1.28E7
T: + p Full ms [155.00-2000.00]

S126

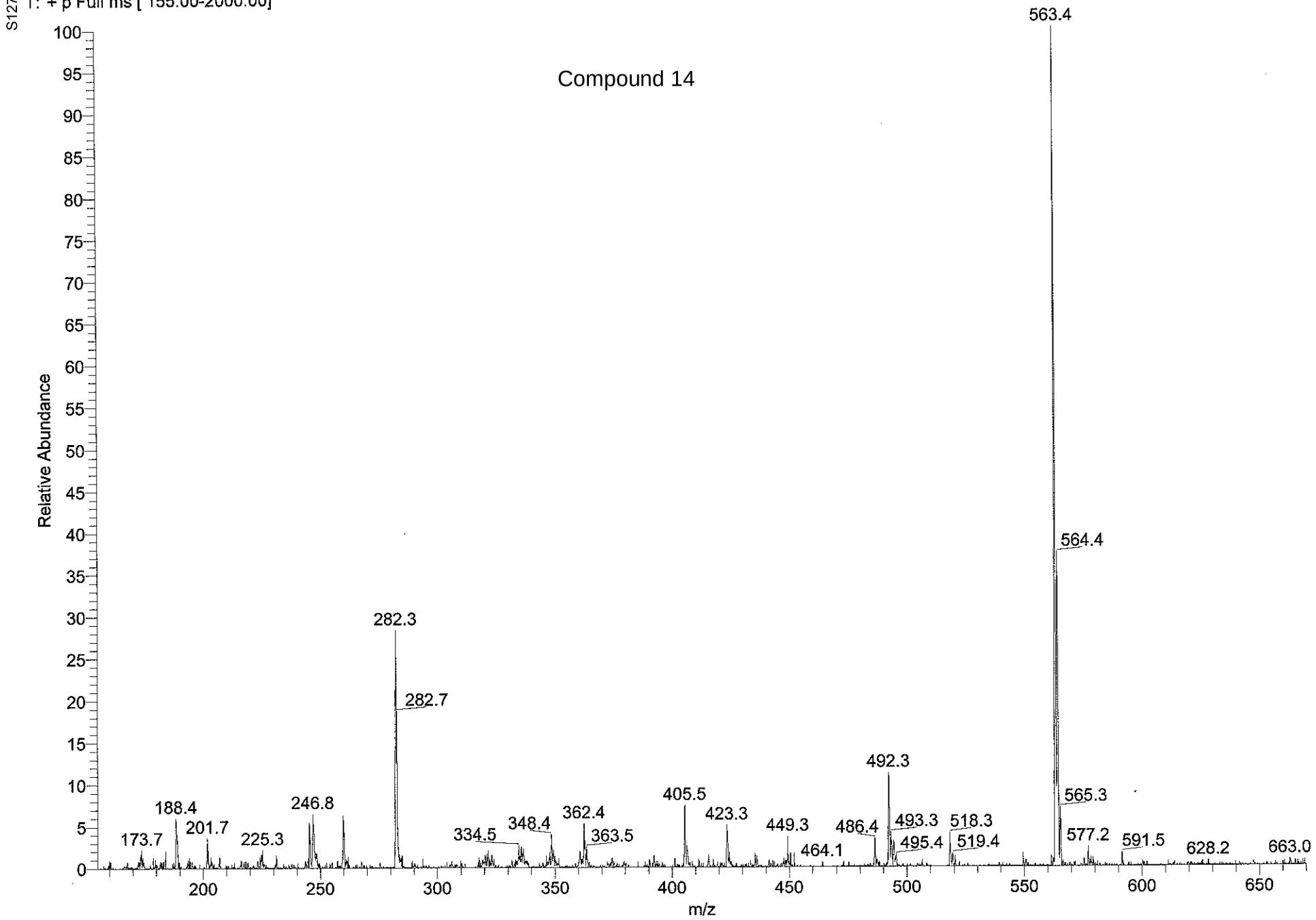


Compound 14

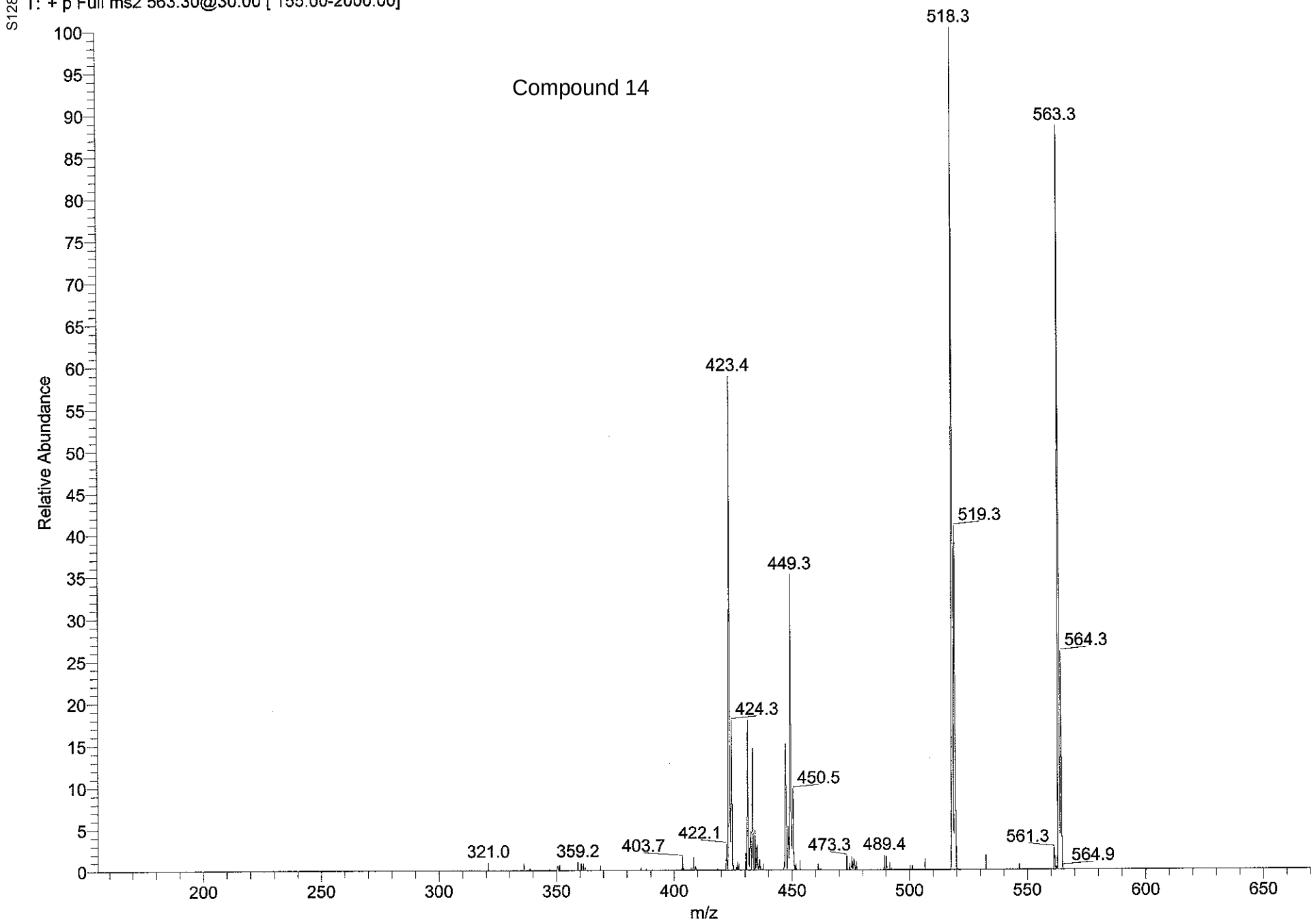
VB-GSA-198

$m_2 = 562$

E:\MSLab_LCQ\VB_GSA_198 08/17/2009 03:46:31 PM VB_GSA_198
V. Boddupally, MeOH:ACN 1:1
VB_GSA_198 #16-19 RT: 0.52-0.62 AV: 4 NL: 1.28E7
T: + p Full ms [155.00-2000.00]



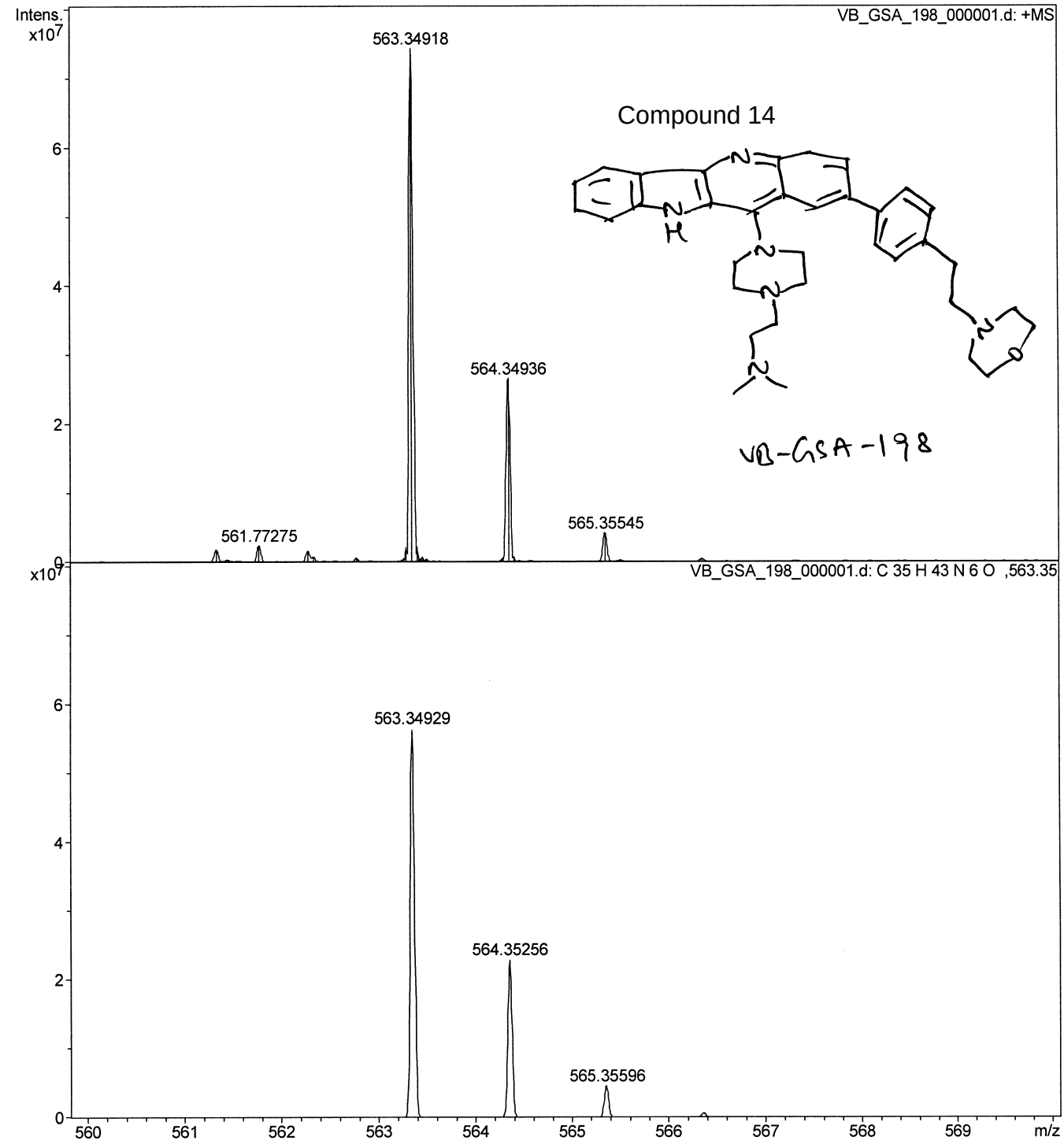
E:\MSLab_LCQ\VB_GSA_198 08/17/2009 03:46:31 PM VB_GSA_198
V. Boddupally, MeOH:ACN 1:1
VB_GSA_198 #9-13 RT: 0.29-0.42 AV: 5 NL: 4.07E6
T: + p Full ms2 563.30@30.00 [155.00-2000.00]



Generic Display Report

Analysis Info

Analysis Name	D:\DATA\Facility_August_09\VB_GSA_198_000001.d	Acquisition Date	8/21/2009 5:13:46 PM
Method	ESI_101506	Operator	
Sample Name	VB_GSA_198	Instrument	apex-Qe
Comment	VB_GSA_198 ACN:H2O 1:1 0.1% FA		



SmartFormula Manually

Min C_{25}

Max

C 25-n

Generate

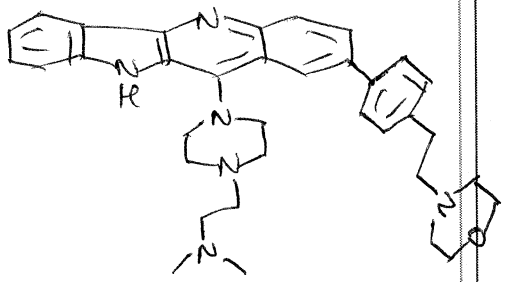
Help

Note: for m < 2000 the elements C, H, N, and O are considered implicitly.

Measured m/z 563.34918 Tolerance 2 mDa Charge 1

#	Mol. Formula	m/z	err [mDa]	|err| [ppm]	err [ppm]	mean err [ppm]	mSigma	Sigma Rank	rdb	N rule	e⁻
1	C 25 H 48 N 5 O 9	562.34465	-1.50	2.7	-2.7	-0.8	626.3	5	4.5	ok	even
2	C 26 H 44 N 9 O 5	562.34599	-0.44	0.8	-0.8	1.7	714.6	7	9.5	ok	even
3	C 27 H 40 N 13 O	562.34733	0.66	1.2	1.2	4.0	612.9	4	14.5	ok	even
4	C 32 H 49 O 8	561.34219	-0.71	1.3	-1.3	1.4	714.1	6	8.5	ok	even
5	C 33 H 45 N 4 O 4	561.34353	0.43	0.8	0.8	3.8	717.1	8	13.5	ok	even
6	C 34 H 41 N 8	561.34487	1.52	2.7	2.7	6.1	720.2	9	18.5	ok	even
7	C 34 H 47 N 2 O 5	563.34795	-1.23	2.2	-2.2	-0.7	16.8	1	12.5	ok	even
8	C 35 H 43 N 6 O	563.34929	0.10	0.2	0.2	1.6	26.9	2	17.5	ok	even
9	C 36 H 42 N 5 O	560.33839	-1.64	2.9	-2.9	-0.6	730.5	10	18.5	ok	even
10	C 42 H 44 N	562.34683	0.98	1.7	1.7	3.4	577.5	3	21.5	ok	even

Compound 14



☑ Automatically locate monoisotopic peak Maximum number of formulas 500

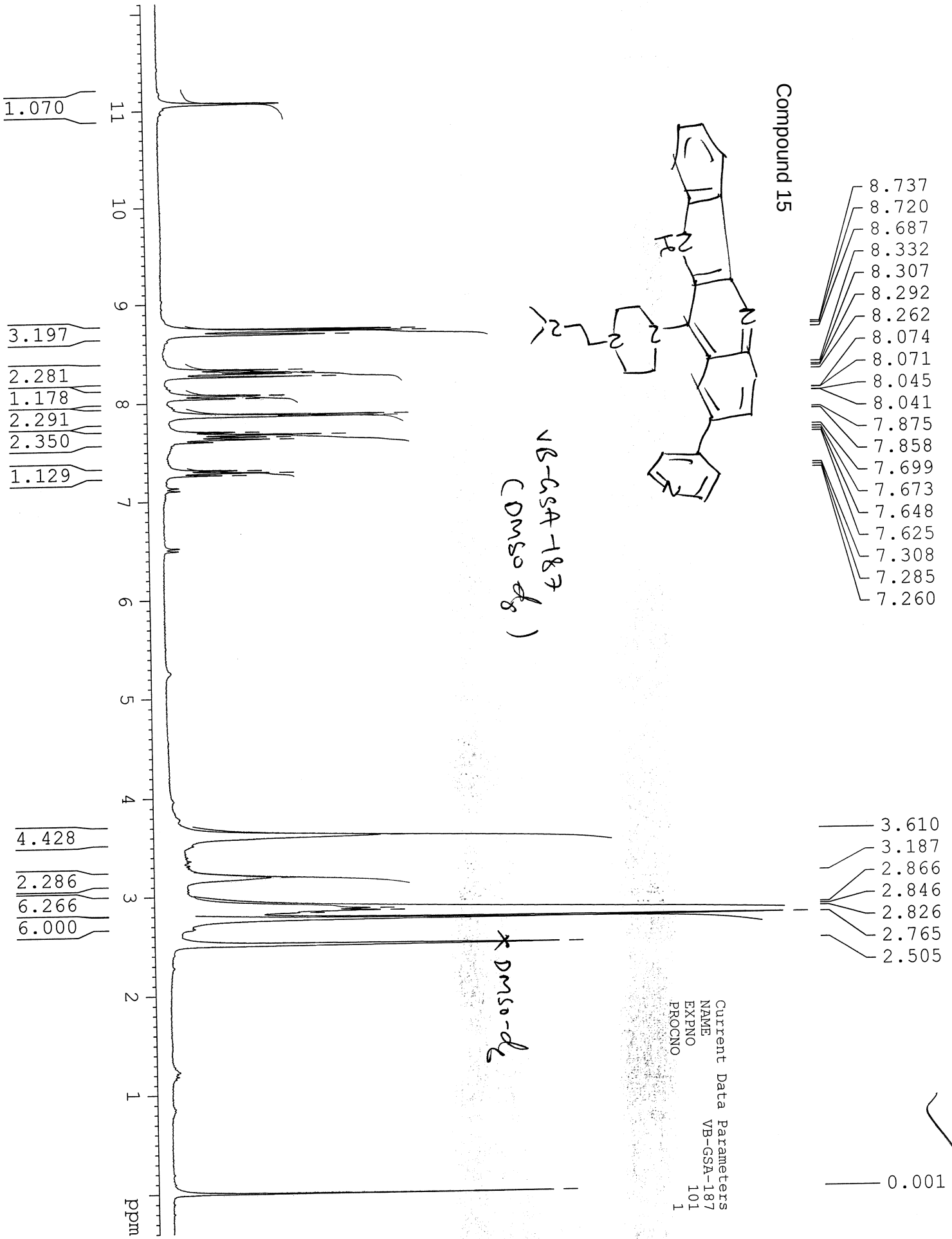
☑ Check rings plus double bonds Minimum -0.5 Maximum 40

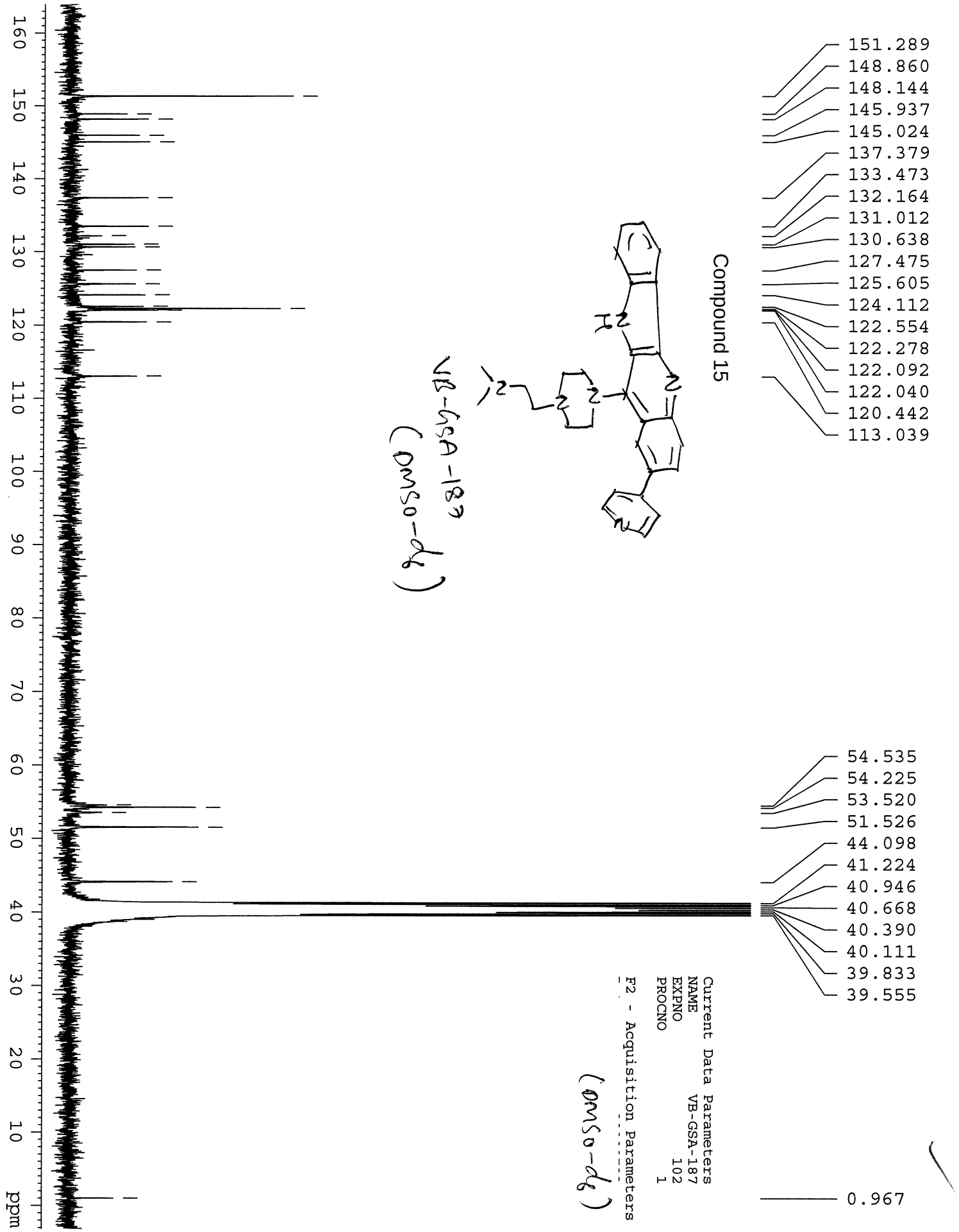
Electron configuration even

☑ Filter H/C element ratio Minimum H/C 0 Maximum H/C 3

☑ Estimate carbon number ☑ Generate immediately

Show Pattern


Compound 15
VB-GSA-187
(DMSO d_6)
DMSO-d_6
Current Data Parameters
NAME VB-GSA-187
EXPNO 101
PROCNO 1
ppm
1.070
3.197
2.281
1.178
2.291
2.350
1.129
4.428
2.286
6.266
6.000
8.737
8.720
8.687
8.332
8.307
8.292
8.262
8.074
8.071
8.045
8.041
7.875
7.858
7.699
7.673
7.648
7.625
7.308
7.285
7.260
3.610
3.187
2.866
2.846
2.826
2.765
2.505
0.001


Compound 15
VB-GSA-187
(DMSO-d6)
151.289
148.860
148.144
145.937
145.024
137.379
133.473
132.164
131.012
130.638
127.475
125.605
124.112
122.554
122.278
122.092
122.040
120.442
113.039
54.535
54.225
53.520
51.526
44.098
41.224
40.946
40.668
40.390
40.111
39.833
39.555
0.967
Current Data Parameters
NAME VB-GSA-187
EXPNO 102
PROCNO 1
F2 - Acquisition Parameters
(DMSO-d6)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

Empower software

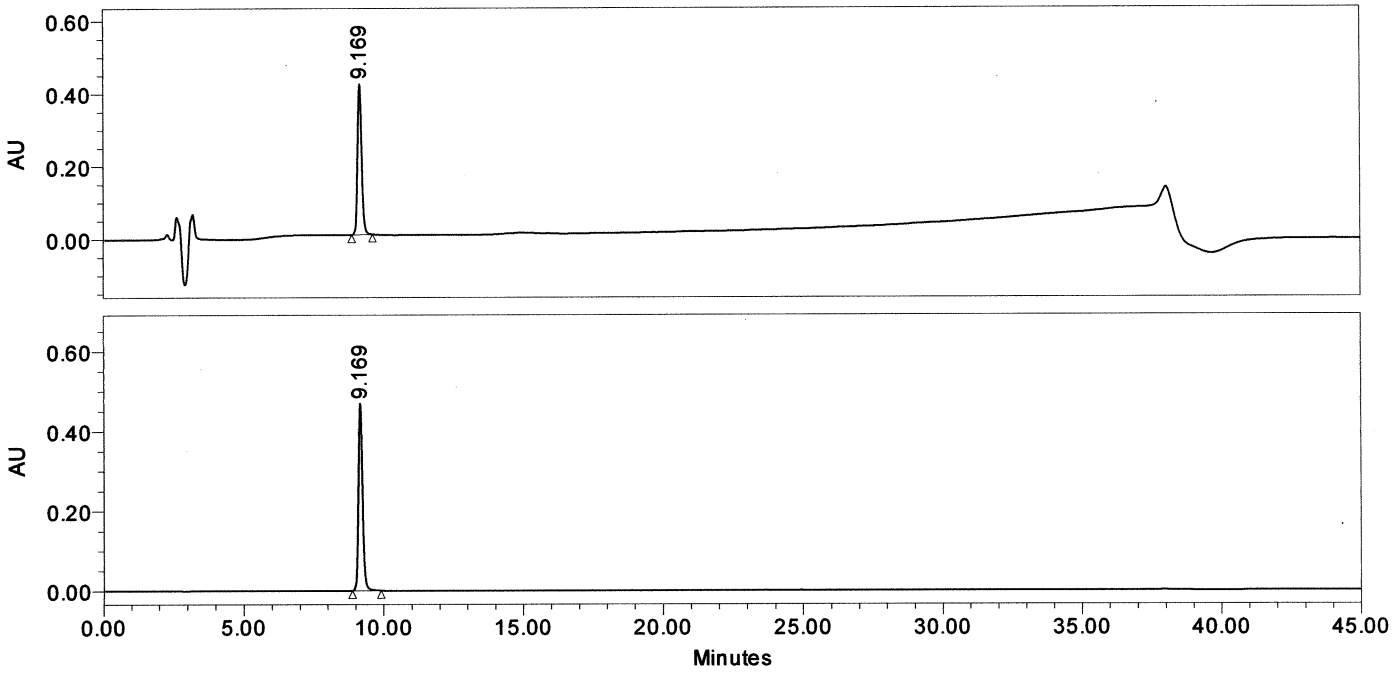
Dual Channel Summary

Reported by User: Jatinder J. (Jatinder)

Project Name: BIO5_HPLC1

SAMPLE INFORMATION

Sample Name:	vb-187 prep	Acquired By:	Jatinder
Sample Type:	Unknown	Date Acquired:	9/28/2009 4:07:06 PM
Vial:	57	Acq. Method Set:	10_90B_in
Injection #:	1	Date Processed:	9/29/2009 8:48:11 AM, 9/29/2009
Injection Volume:	10.00 ul	Processing Method	Peptide_general
Run Time:	45.0 Minutes	Channel Name:	2487Channel 1, 2487Channel 2
Sample Set Name	Prime_Run	Proc. Chnl. Descr.:	220nm, 280nm



Channel 220 nm
Channel: 2487Channel 1

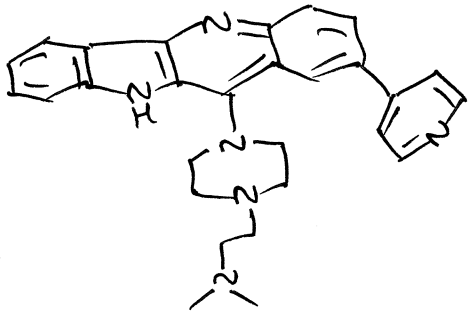
	RT	Area (µV*sec)	% Area	Channel
1	9.169	4.35e+006	100.00	2487Channel 1

Channel 280 nm
Channel: 2487Channel 2

	RT	Area (µV*sec)	% Area	Channel
1	9.169	5.01e+006	100.00	2487Channel 2

NOTES:

Compound 15



VB-GSA-187

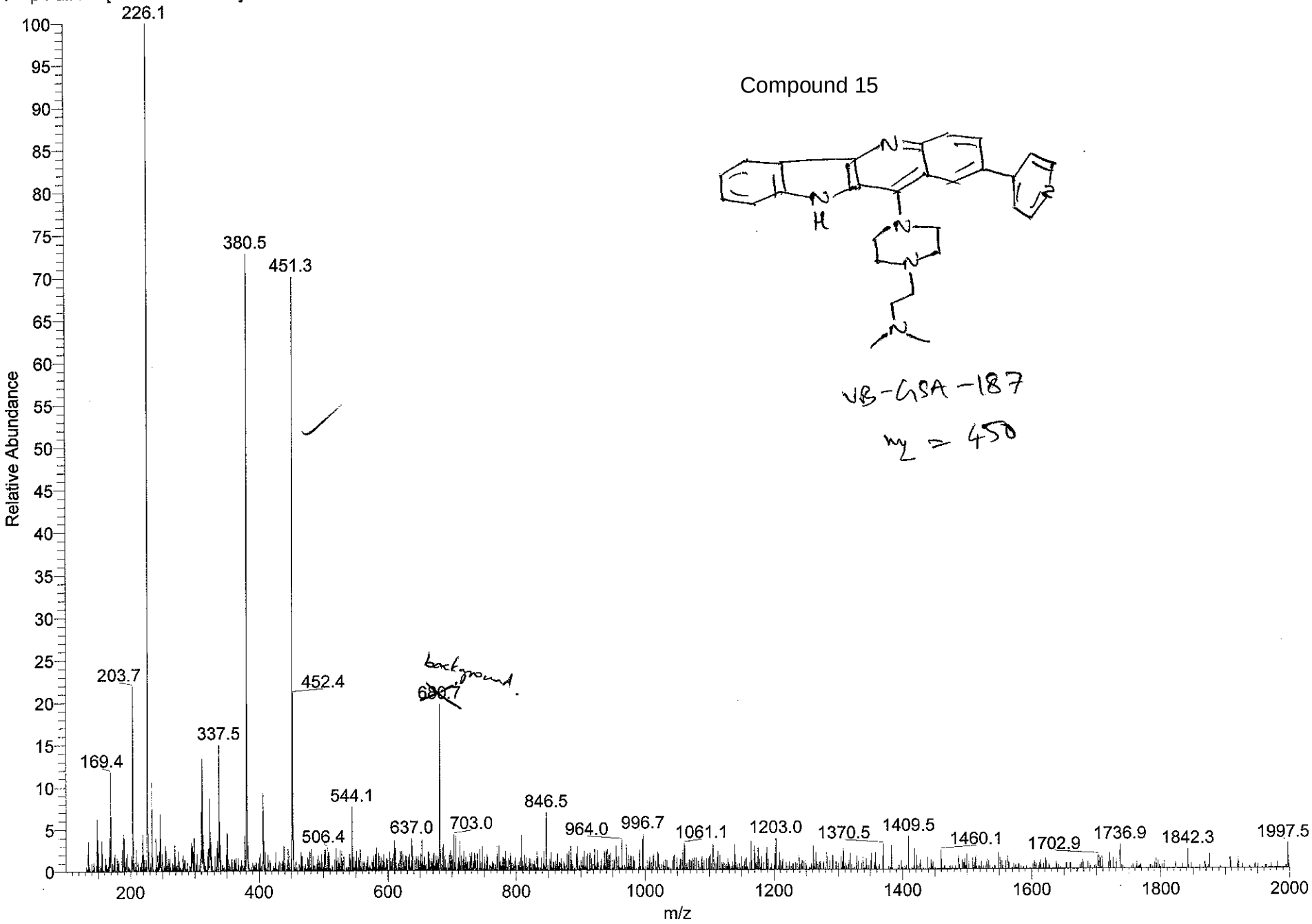
E:\MSLab_LCQ\VB-187
Venkat Boddupally, MeOH:H2O 1:1

11/12/2009 04:12:02 PM

VB-187

VB-187 #26-27 RT: 0.93-0.96 AV: 2 NL: 6.64E5
T: + p Full ms [100.00-2000.00]

S134

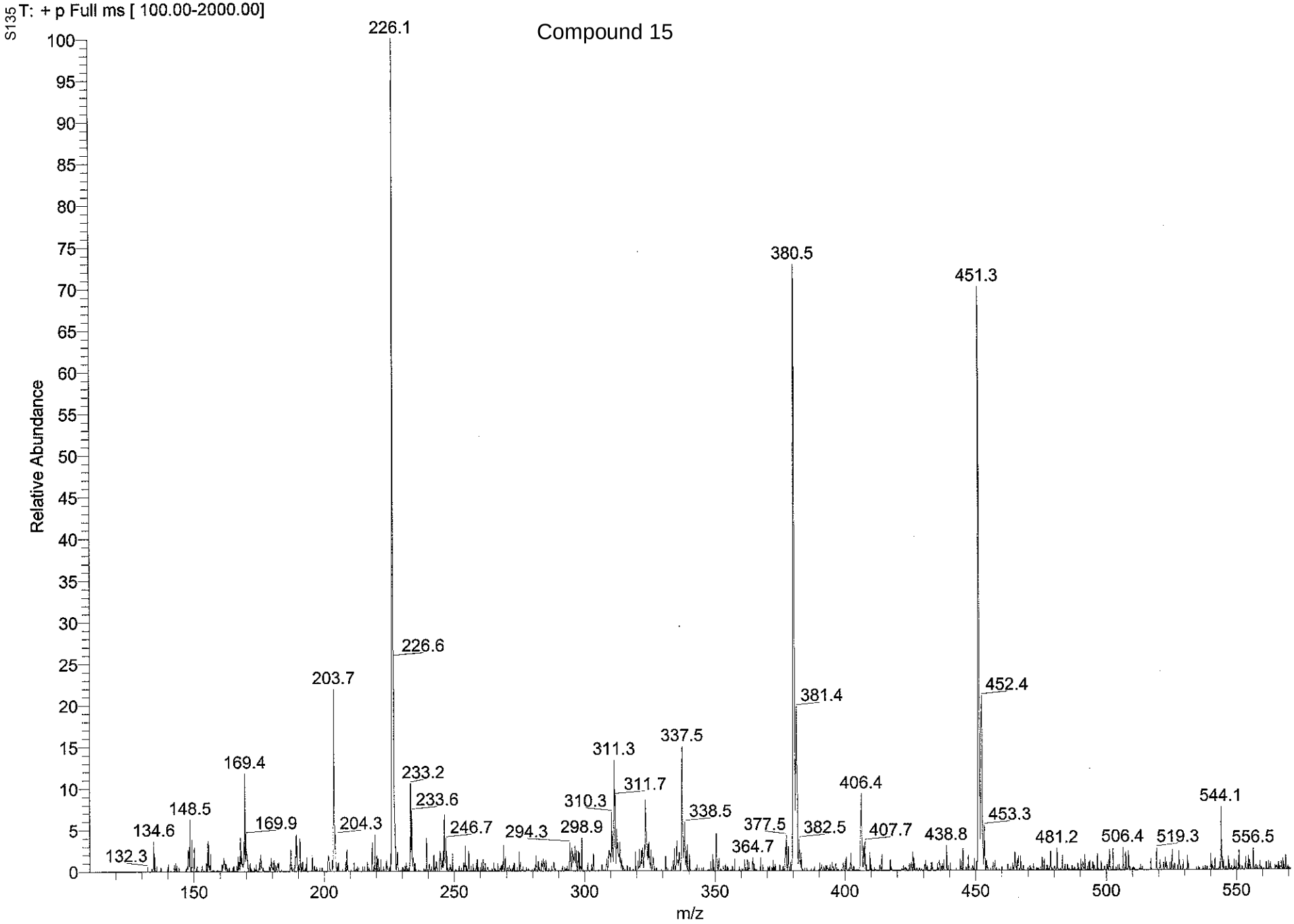


Compound 15

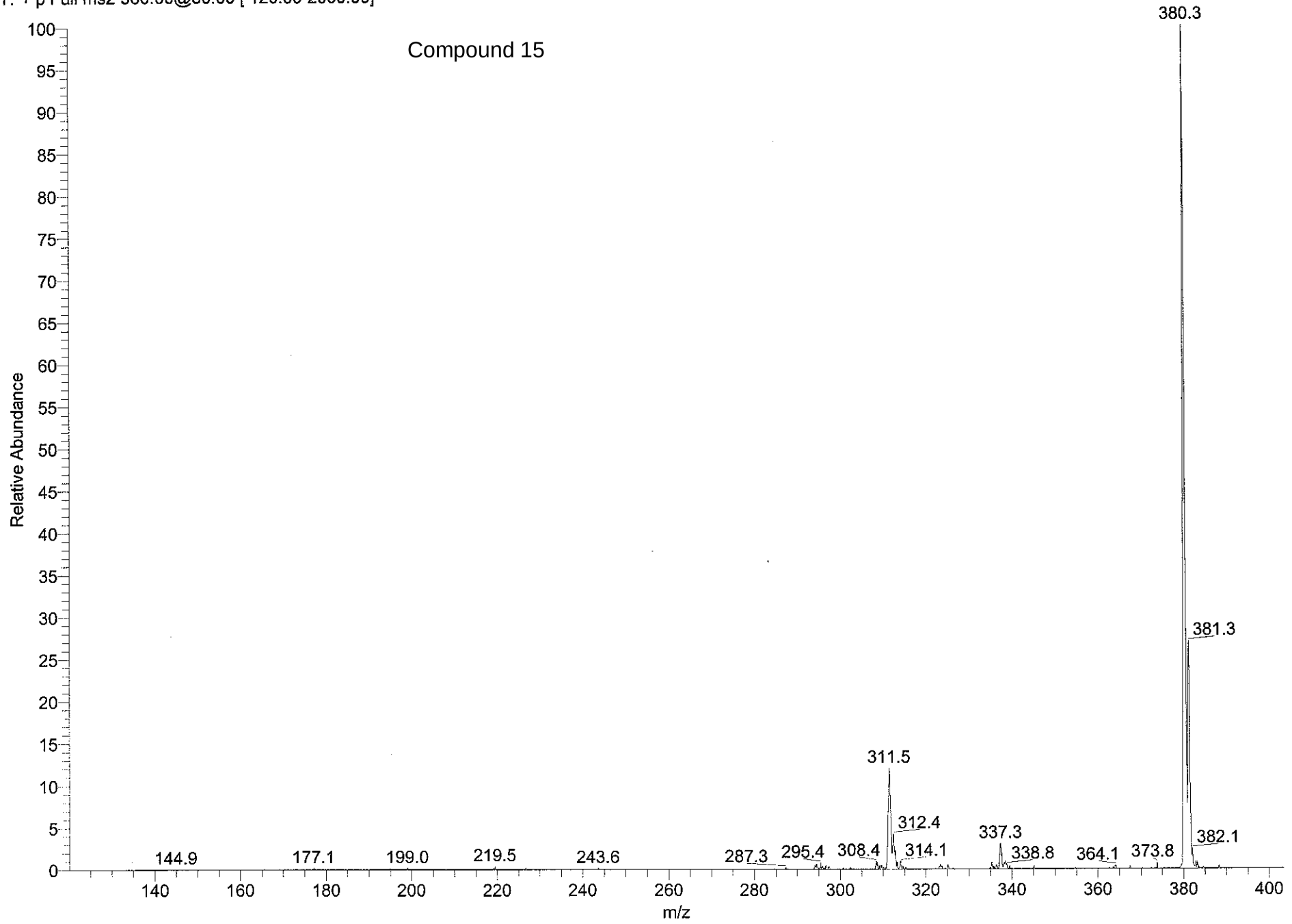
VB-GSA-187

m/z = 450

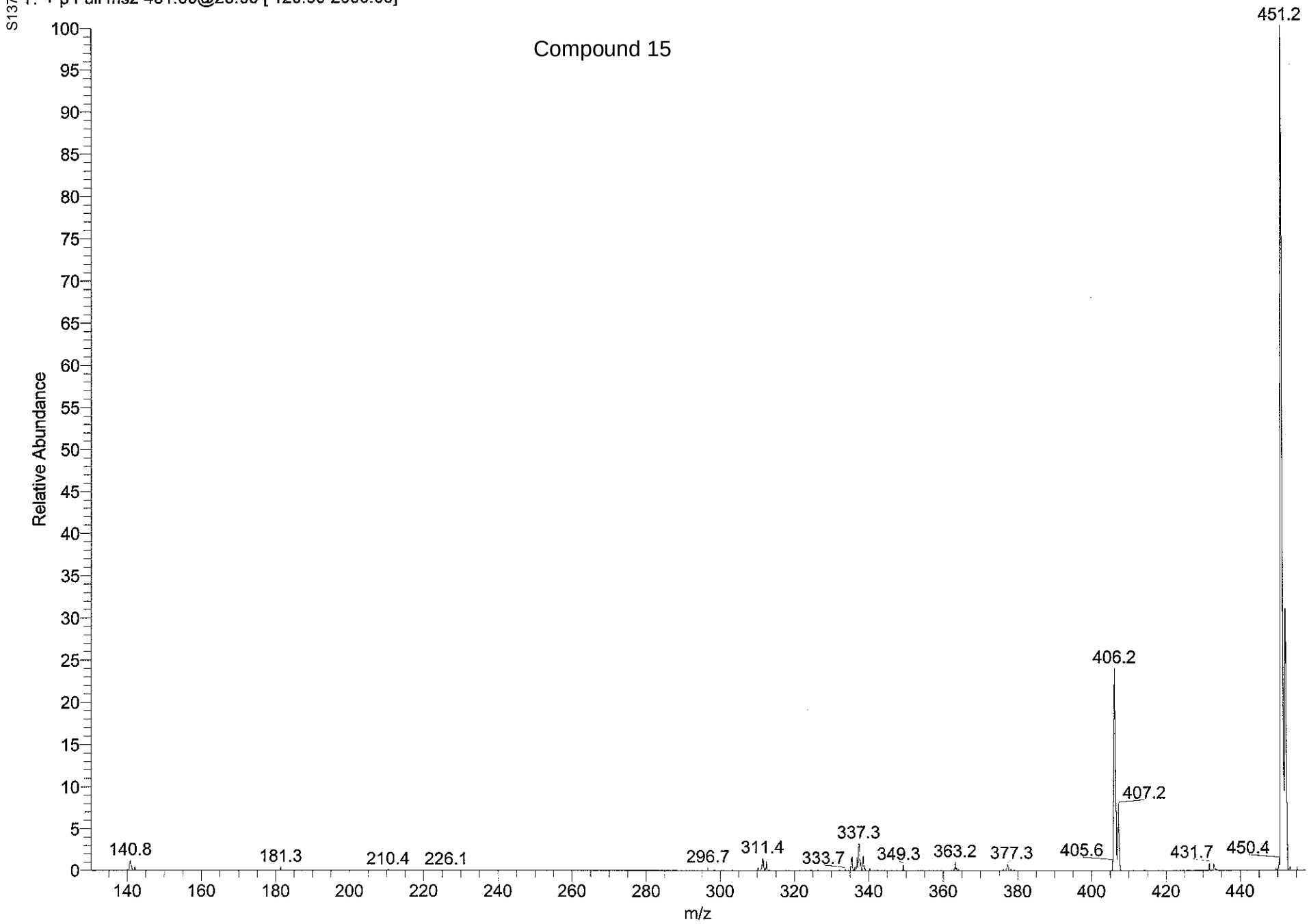
E:\MSLab_LCQ\VB-187 11/12/2009 04:12:02 PM VB-187
Venkat Boddupally, MeOH:H2O 1:1
VB-187 #26-27 RT: 0.93-0.96 AV: 2 NL: 6.64E5
T: + p Full ms [100.00-2000.00]
S135



E:\MSLab_LCQ\VB-187 11/12/2009 04:12:02 PM VB-187
Venkat Boddupally, MeOH:H2O 1:1
VB-187 #23-24 RT: 0.82-0.86 AV: 2 NL: 4.26E5
T: + p Full ms2 380.00@30.00 [120.00-2000.00]
S136



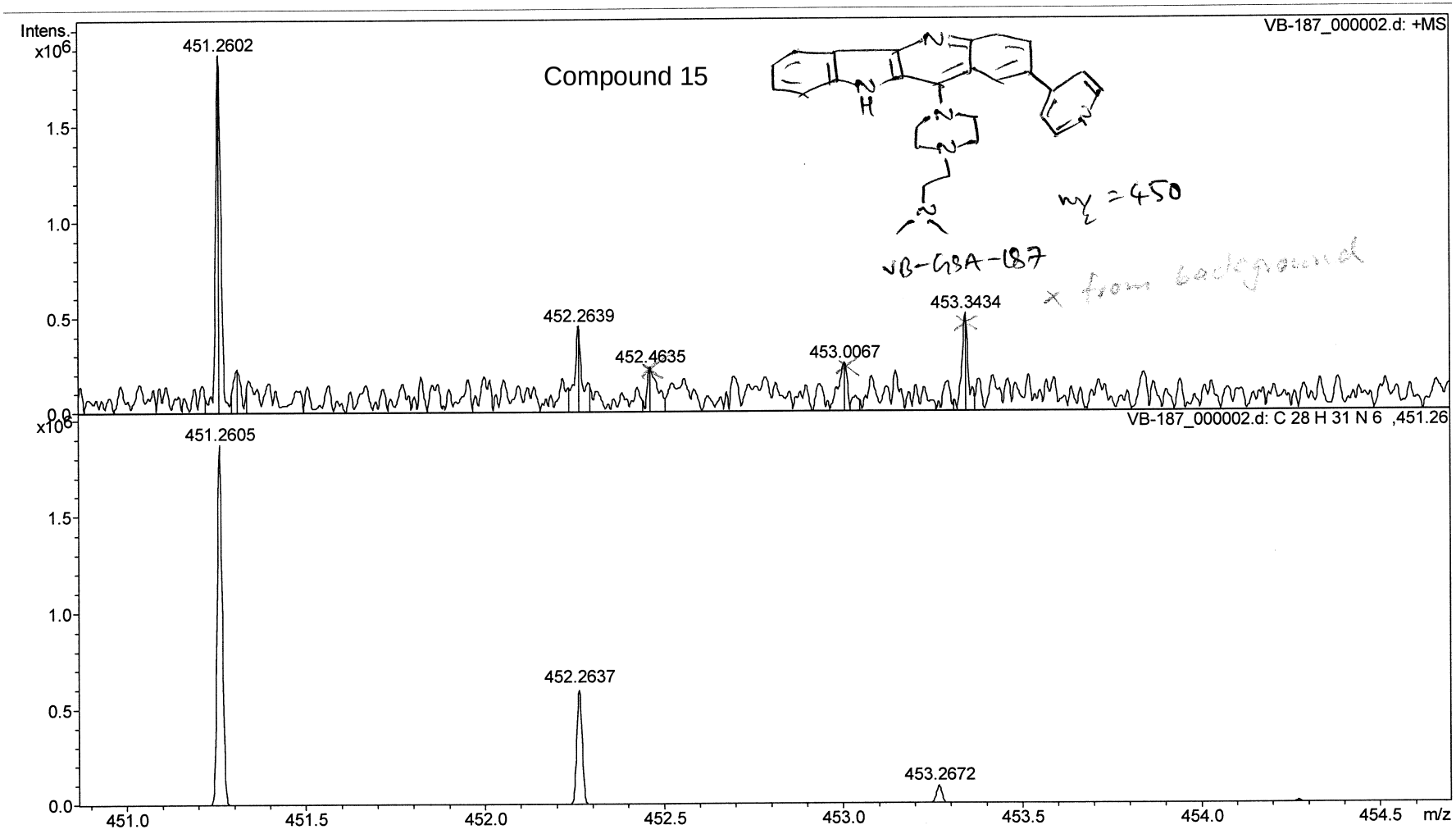
E:\MSLab_LCQ\VB-187 11/12/2009 04:12:02 PM VB-187
Venkat Boddupally, MeOH:H2O 1:1
VB-187 #9-10 RT: 0.29-0.33 AV: 2 NL: 4.64E5
T: + p Full ms2 451.00@25.00 [120.00-2000.00]



Generic Display Report

Analysis Info

Analysis Name	D:\DATA\Facility_Nov_09\VB-187_000002.d	Acquisition Date	11/13/2009 10:48:56 AM
Method	ESI_101506	Operator	
Sample Name	VB-187	Instrument	apex-Qe
Comment	Venkat B., ACN:H2O 1:1:0.1%FA		



SmartFormula Manually

Min C_{16}

Max

C 16-n

Generate

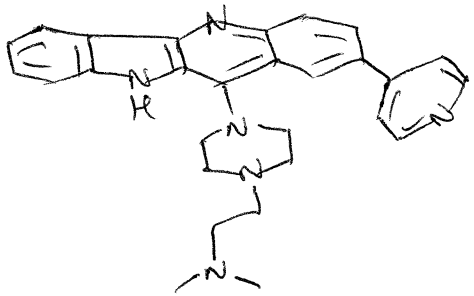
Help

Note: for m < 2000 the elements C, H, N, and O are considered implicitly.

Measured m/z 451.2602 Tolerance 2 mDa Charge 1

#	Mol. Formula	m/z	err [mDa]	|err| [ppm]	err [ppm]	mean err [ppm]	mSigma	Sigma Rank	rdb	N rule	e⁻
1	C 27 H 35 N 2 O 4	451.2591	-1.03	2.3	-2.3	-2.5	40.3	1	11.5	ok	even
2	C 28 H 31 N 6	451.2605	0.31	0.7	0.7	0.5	50.3	2	16.5	ok	even

Compound 15



☐ Automatically locate monoisotopic peak Maximum number of formulas 500

☑ Check rings plus double bonds Minimum -0.5 Maximum 40

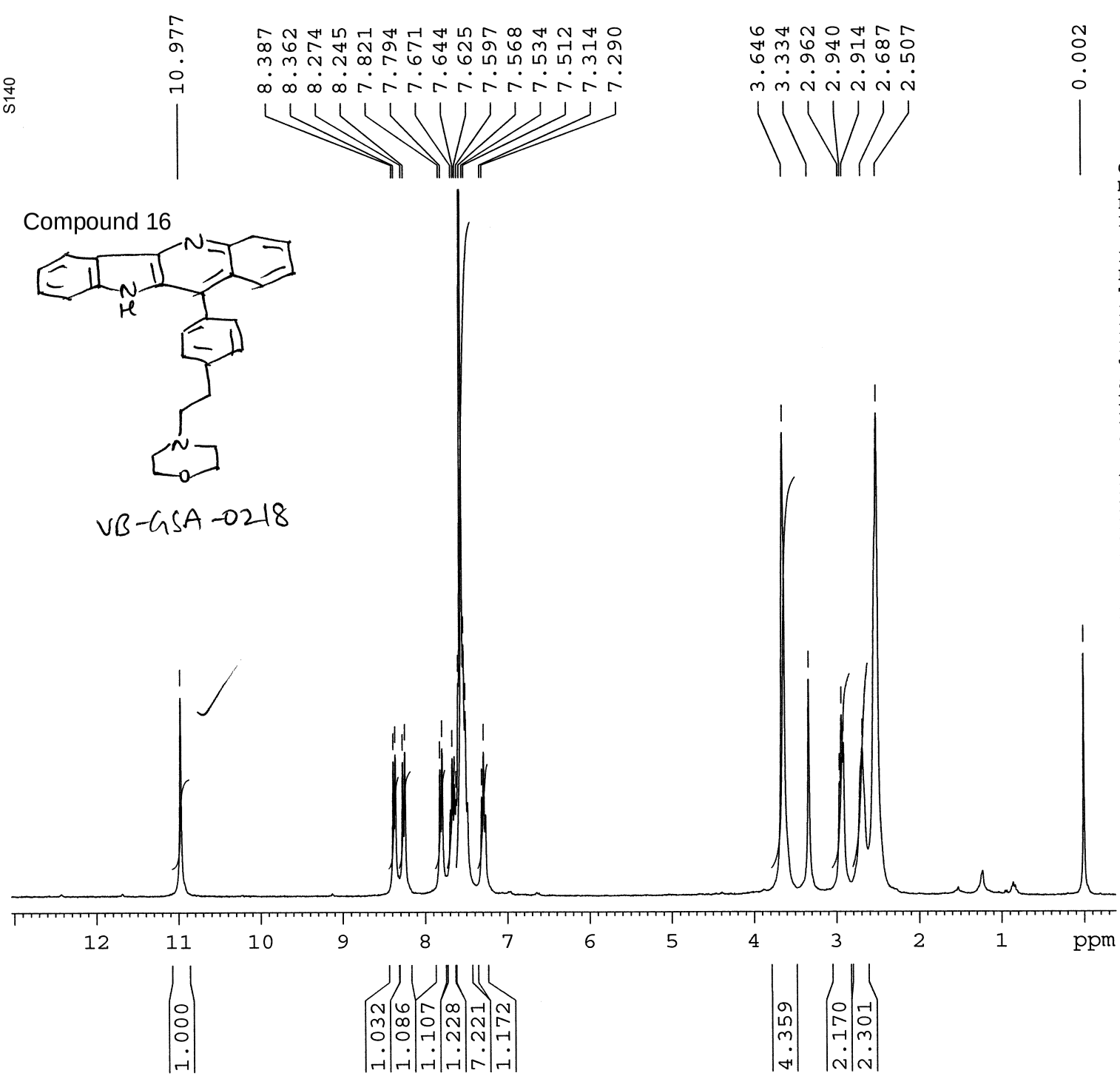
Electron configuration even

☑ Filter H/C element ratio Minimum H/C 0 Maximum H/C 3

☑ Estimate carbon number ☑ Generate immediately

Show Pattern

S140

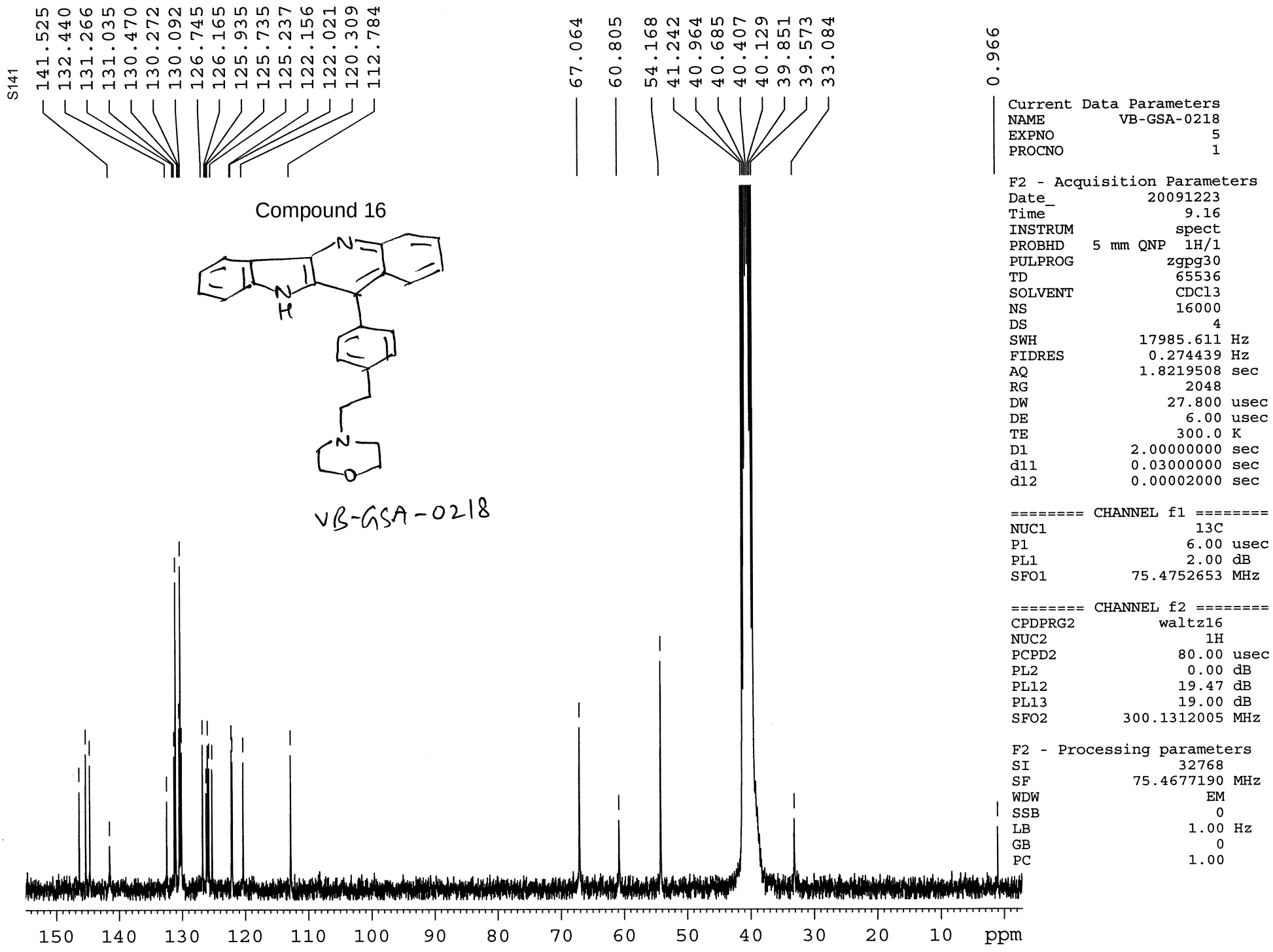


Current Data Parameters
NAME VB-GSA-0218
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20091222
Time 15.56
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 128
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 512
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 8.50 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

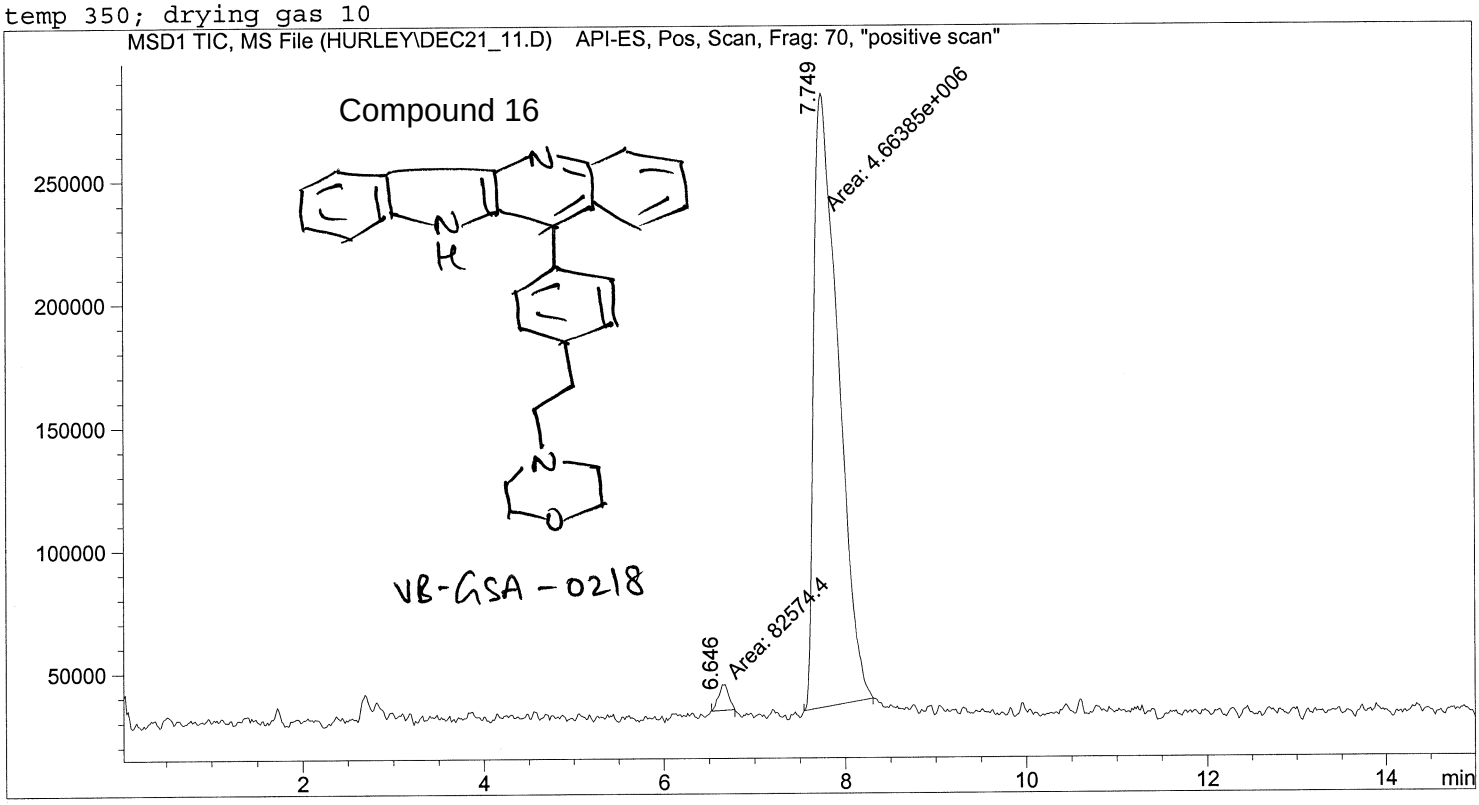
F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


S141
141.525
132.440
131.266
131.035
130.470
130.272
130.092
126.745
126.165
125.935
125.735
125.237
122.156
122.021
120.309
112.784
67.064
60.805
54.168
41.242
40.964
40.685
40.407
40.129
39.851
39.573
33.084
0.966
Compound 16
VB-GSA-0218
Current Data Parameters
NAME VB-GSA-0218
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20091223
Time 9.16
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16000
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2048
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 2.00 dB
SFO1 75.4752653 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 19.47 dB
PL13 19.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

run w/ acid

```
==========================================================================
Injection Date  : 12/21/2009 5:11:44 PM
Sample Name     : VB0218                          Location : Vial 6
Acq. Operator   : Karen                              Inj :   1
Acq. Instrument : Instrument 1                   Inj Volume : 0.2 µl
Method          : C:\HPCHEM\1\METHODS\LC_MS.M
Last changed    : 12/21/2009 5:06:35 PM by Karen
                  (modified after loading)
```

Zorbax SB ODS,45:55:0.25; MeOH/water/formicA, POS, 300-500; frag 70; 25C, cap volt 2500, gas temp 350; drying gas 10




```
==========================================================================
                          Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MSD1 TIC, MS File

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]                          %
----|-------|----|-------|----------|----------|--------|
   1   6.646 MM    0.1278 8.25744e4  1.07671e4    1.7397
   2   7.749 MM    0.3111 4.66384e6  2.49868e5   98.2603

Totals :                  4.74642e6  2.60635e5

==========================================================================
                          *** End of Report ***
```

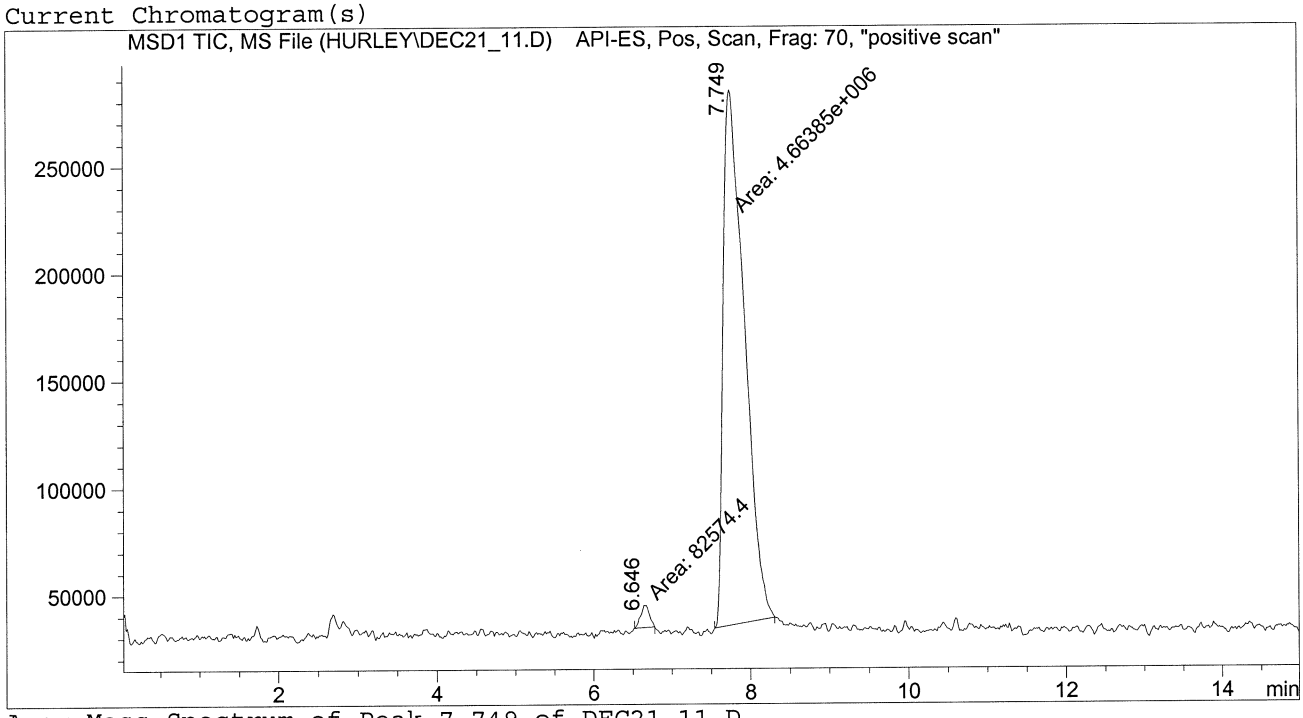
Print of all graphic windows
run w/ acid

==========

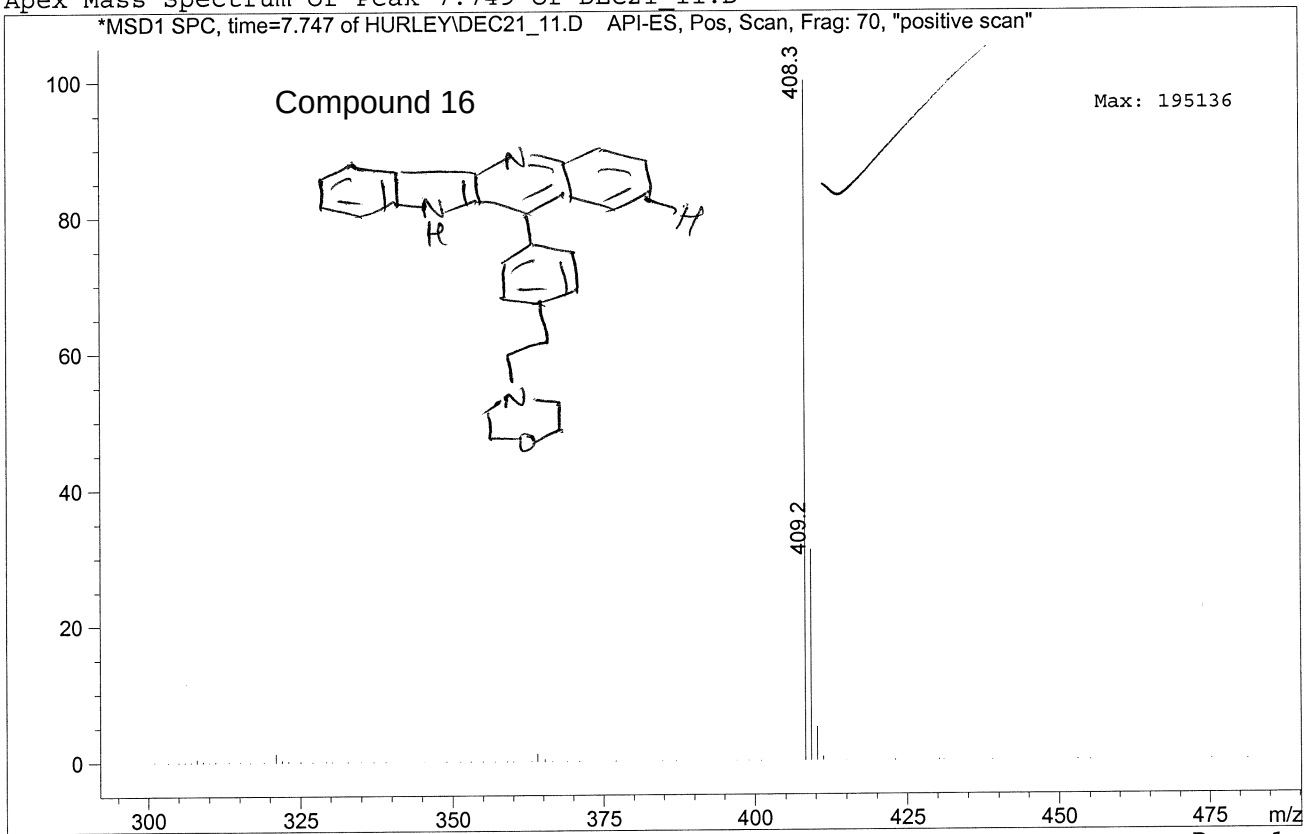
Injection Date : 12/21/2009 5:11:44 PM
Sample Name : VB0218 Location : Vial 6
Acq. Operator : Karen Inj : 1
Acq. Instrument : Instrument 1 Inj Volume : 0.2 µl
Method : C:\HPCHEM\1\METHODS\LC_MS.M
Last changed : 12/21/2009 5:06:35 PM by Karen
(modified after loading)

Zorbax SB ODS,45:55:0.25; MeOH/water/formicA, POS, 300-500; frag 70; 25C, cap volt 2500, gas temp 350; drying gas 10

Current Chromatogram(s)

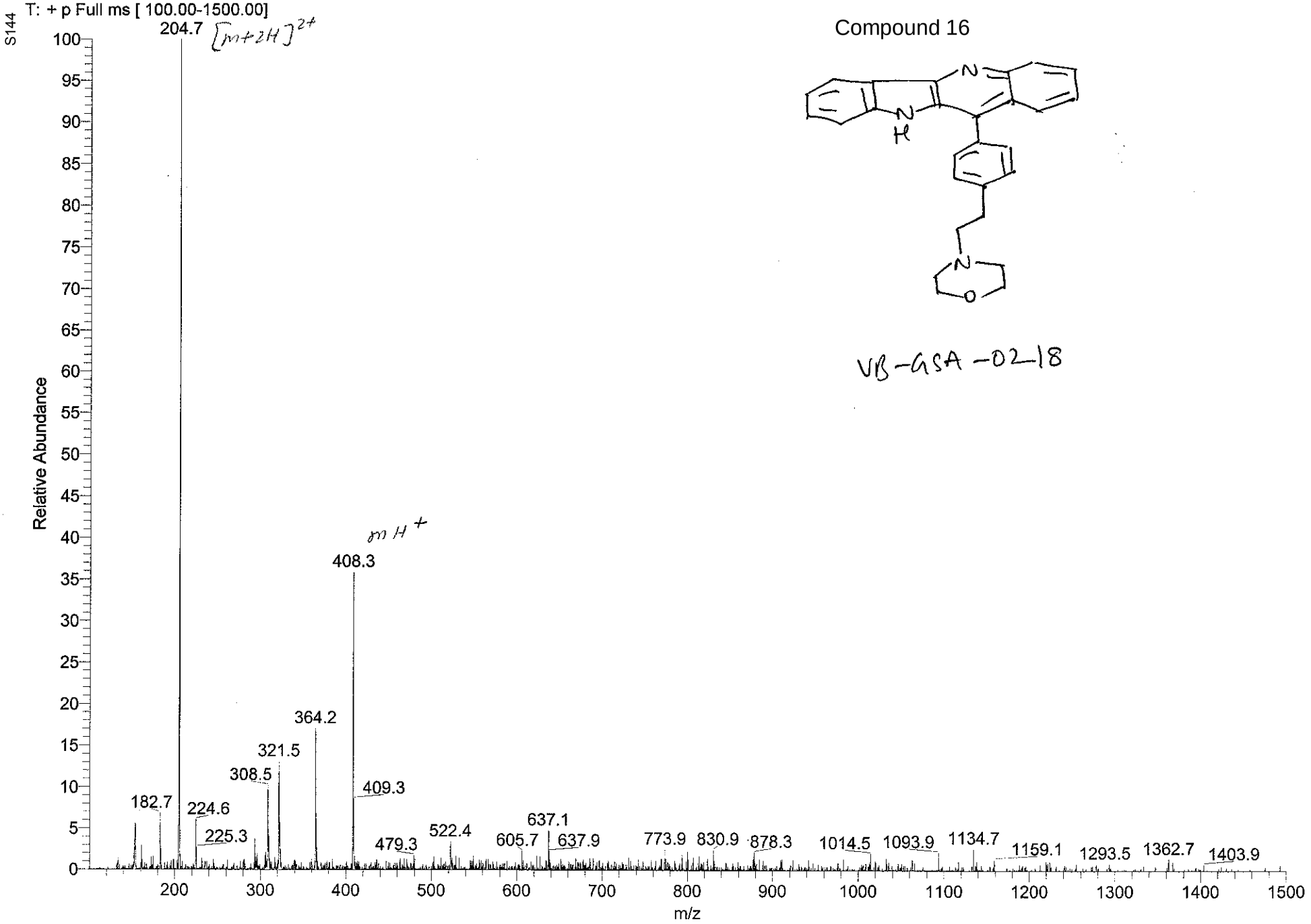


Apex Mass Spectrum of Peak 7.749 of DEC21_11.D



E:\MSLab_LCQ\VB-GSA-0218 12/22/2009 11:52:18 AM VB-GSA-0218
Venkat B., ACN:H2O 1:1:0.1%FA
VB-GSA-0218 #38-41 RT: 1.11-1.18 AV: 4 NL: 3.32E6
T: + p Full ms [100.00-1500.00]

S144

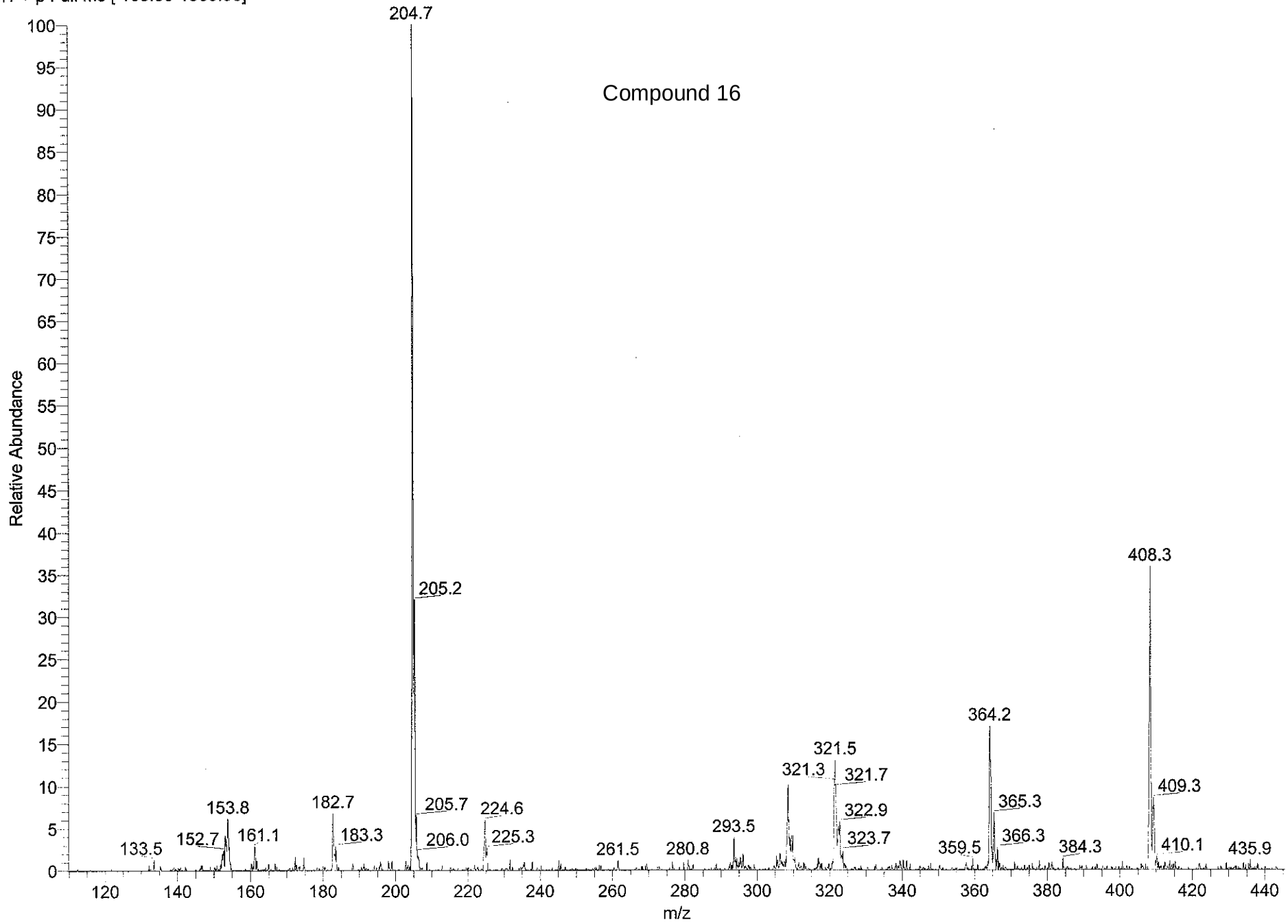


Compound 16

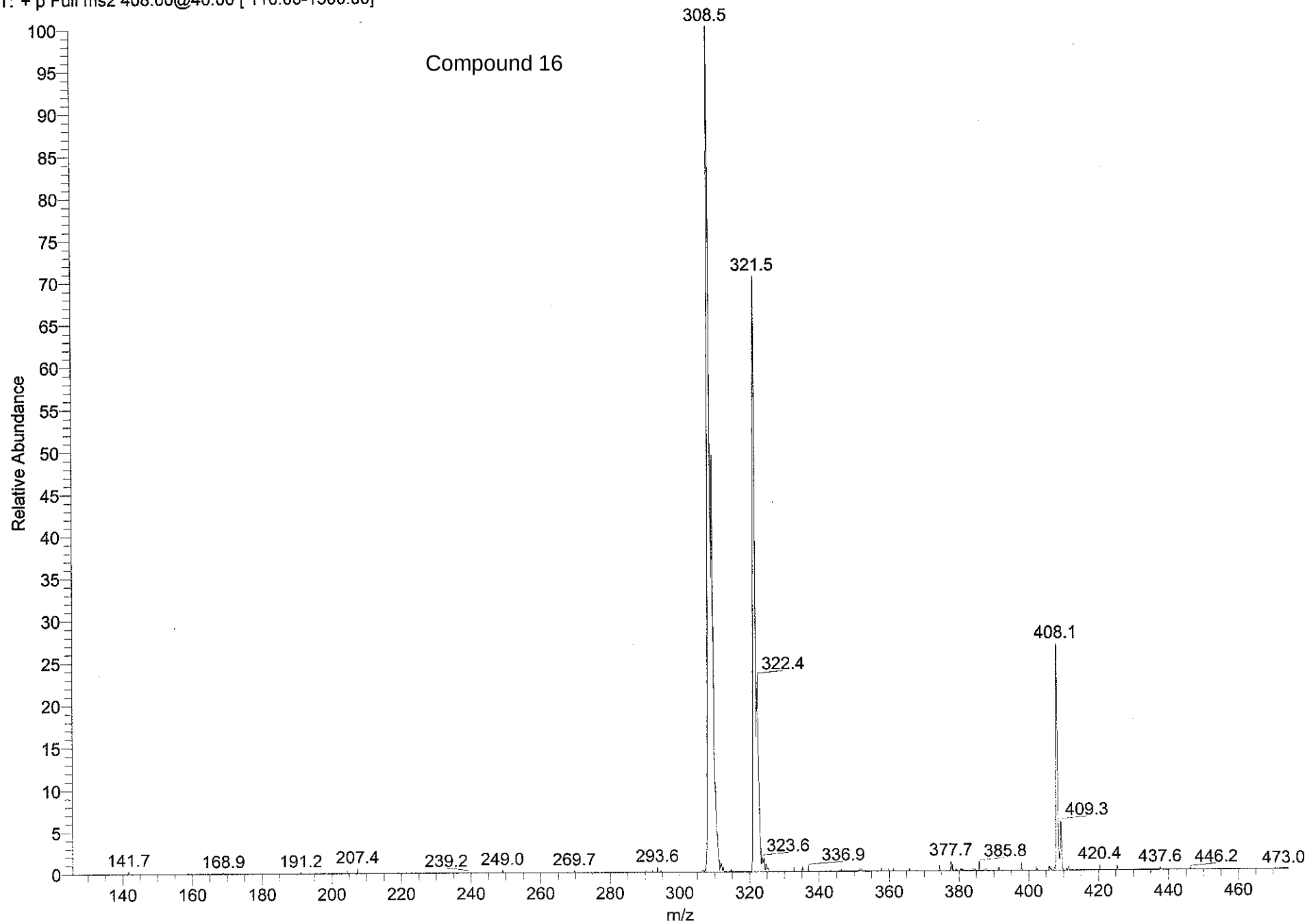
VB-GSA-0218

E:\MSLab_LCQ\VB-GSA-0218 12/22/2009 11:52:18 AM VB-GSA-0218
Venkat B., ACN:H2O 1:1:0.1%FA
VB-GSA-0218 #38-41 RT: 1.11-1.18 AV: 4 NL: 3.32E6
T: + p Full ms [100.00-1500.00]

S145



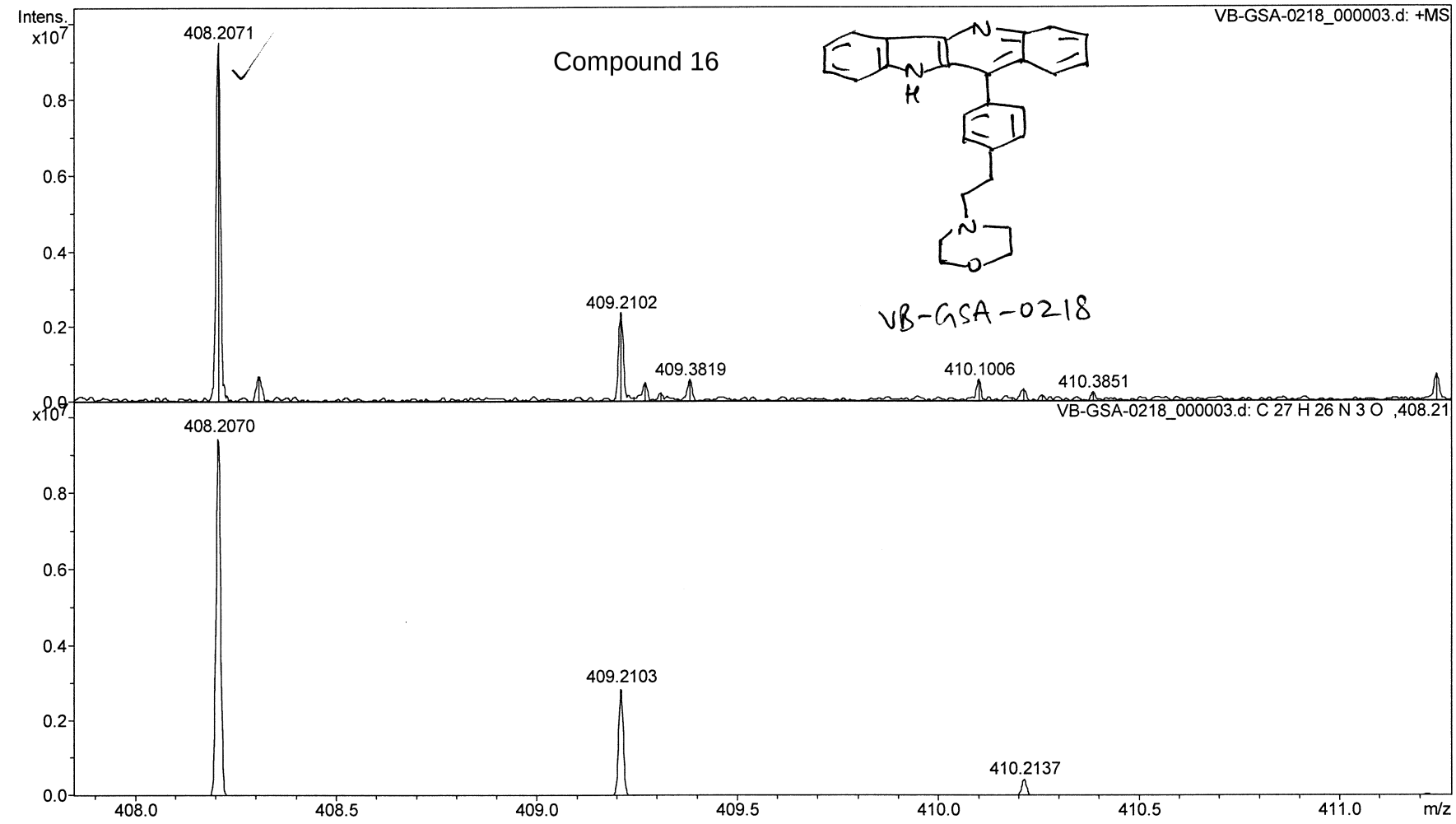
E:\MSLab_LCQ\VB-GSA-0218 12/22/2009 11:52:18 AM VB-GSA-0218
Venkat B., ACN:H2O 1:1:0.1%FA
VB-GSA-0218 #32-35 RT: 0.93-1.02 AV: 4 NL: 3.66E5
T: + p Full ms2 408.00@40.00 [110.00-1500.00]
S146



Generic Display Report

Analysis Info

Analysis Name	D:\DATA\Facility_Dec_09\VB-GSA-0218_000003.d	Acquisition Date	12/22/2009 1:44:30 PM
Method	ESI_101506	Operator	
Sample Name	VB-GSA-0218	Instrument	apex-Qe
Comment	Venkat B., ACN:H2O 1:1:0.1%FA		



SmartFormula Manually

Min C_{16}

Max

C 16-n

Generate

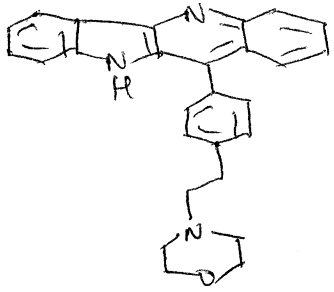
Help

Note: for m < 2000 the elements C, H, N, and O are considered implicitly.

Measured m/z 408.2071 Tolerance 2 mDa Charge 1

#	Mol. Formula	m/z	err [mDa]	|err| [ppm]	err [ppm]	mean err [ppm]	mSigma	Sigma Rank	rdb	N rule	e^-
1	C 27 H 26 N 3 O	408.2070	-0.05	0.1	-0.1	0.1	27.0	1	16.5	ok	even

Compound 16



Automatically locate monoisotopic peak Maximum number of formulas 500

Check rings plus double bonds Minimum -0.5 Maximum 40

Electron configuration even

Filter H/C element ratio Minimum H/C 0 Maximum H/C 3

Estimate carbon number Generate immediately

Show Pattern