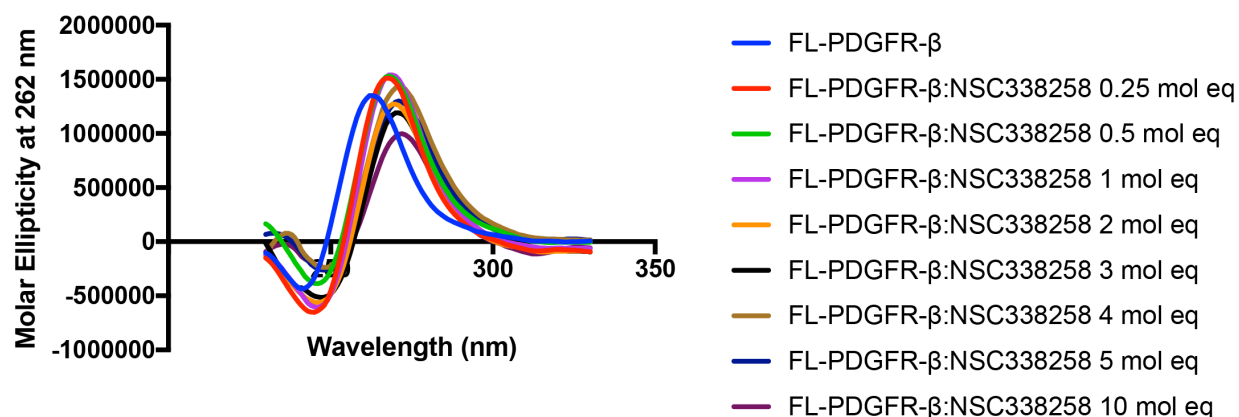
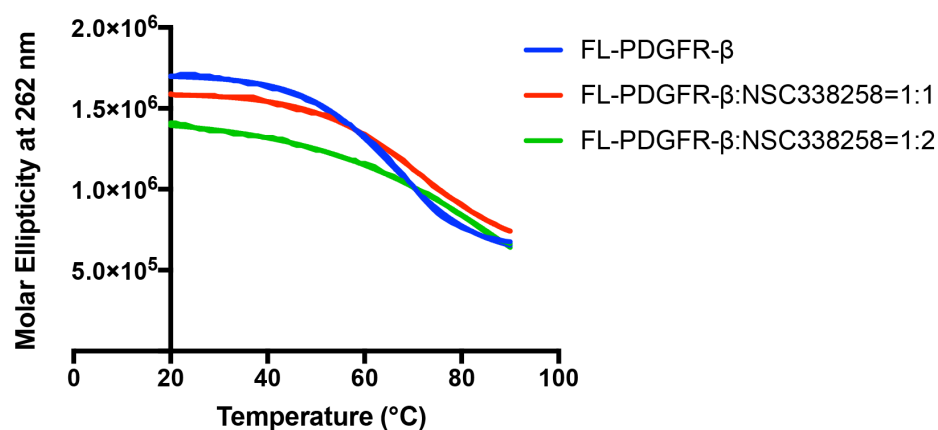


The Consequences of Overlapping G-Quadruplexes and i-Motifs in the Platelet-Derived Growth Factor Receptor β Core Promoter Nuclease Hypersensitive Element Can Explain the Unexpected Effects of Mutations and Provide Opportunities for Selective Targeting of Both Structures by Small Molecules to Downregulate Gene Expression

Robert V. Brown, Ting Wang, Venkateshwar Reddy Chappeta, Guanhui Wu, Buket Onel, Reena Chawla, Hector Quijada, Sara M. Camp, Eddie T. Chiang, Quinea R. Lassiter, Carmen Lee, Shivani Phanse, Megan A. Turnidge, Ping Zhou, Joe G. N. Garcia, Vijay Gokhale, Danzhou Yang, Laurence H. Hurley

A**B**

	FL-PDGFR-β:NSC338258	FL-PDGFR-β:NSC338258 1 mol. equiv.	FL-PDGFR-β:NSC338258 2 mol. equiv.
T_m (°C)	75	86	86
ΔT_m	—	11	11

Figure S1. (A) CD of the titration of the FL 41 mer with NSC338258 and (B) increase in the thermal stability of the WT 41-mer (red and green) relative to the no drug control (WT, green). NSC338258 stabilizes the WT 41-mer by 11 °C.

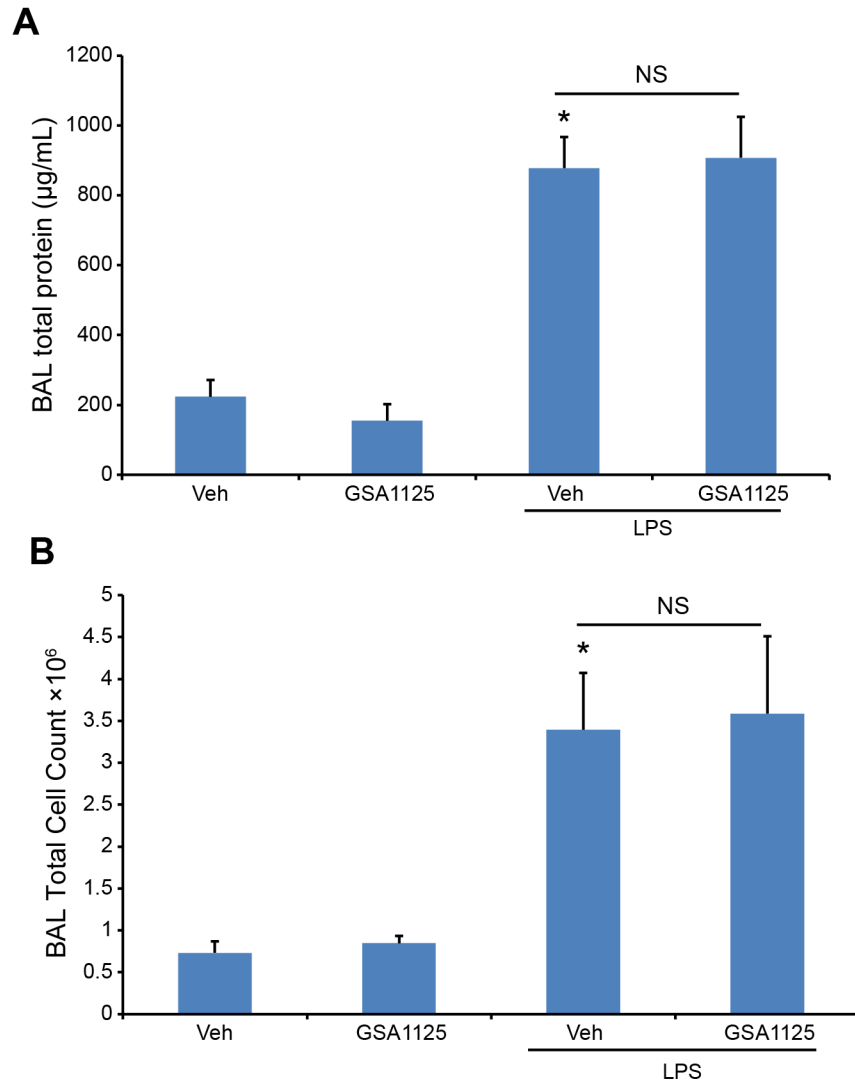


Figure S2. GSA1125 does not protect against LPS-induced lung injury. C57/B6 mice were challenged with an intratracheal administration of LPS solution (1.0 mg/kg) and GSA1125 (10 mg/kg) simultaneously. The animals were allowed to recover for 18 h, and BAL fluids were extracted for analysis. (A) BAL total protein. (B) BAL total cell counts were elevated by LPS challenge, but not affected by GSA1125 treatment. *, $p < 0.05$ compared to vehicle control. NS, not statistically significant.

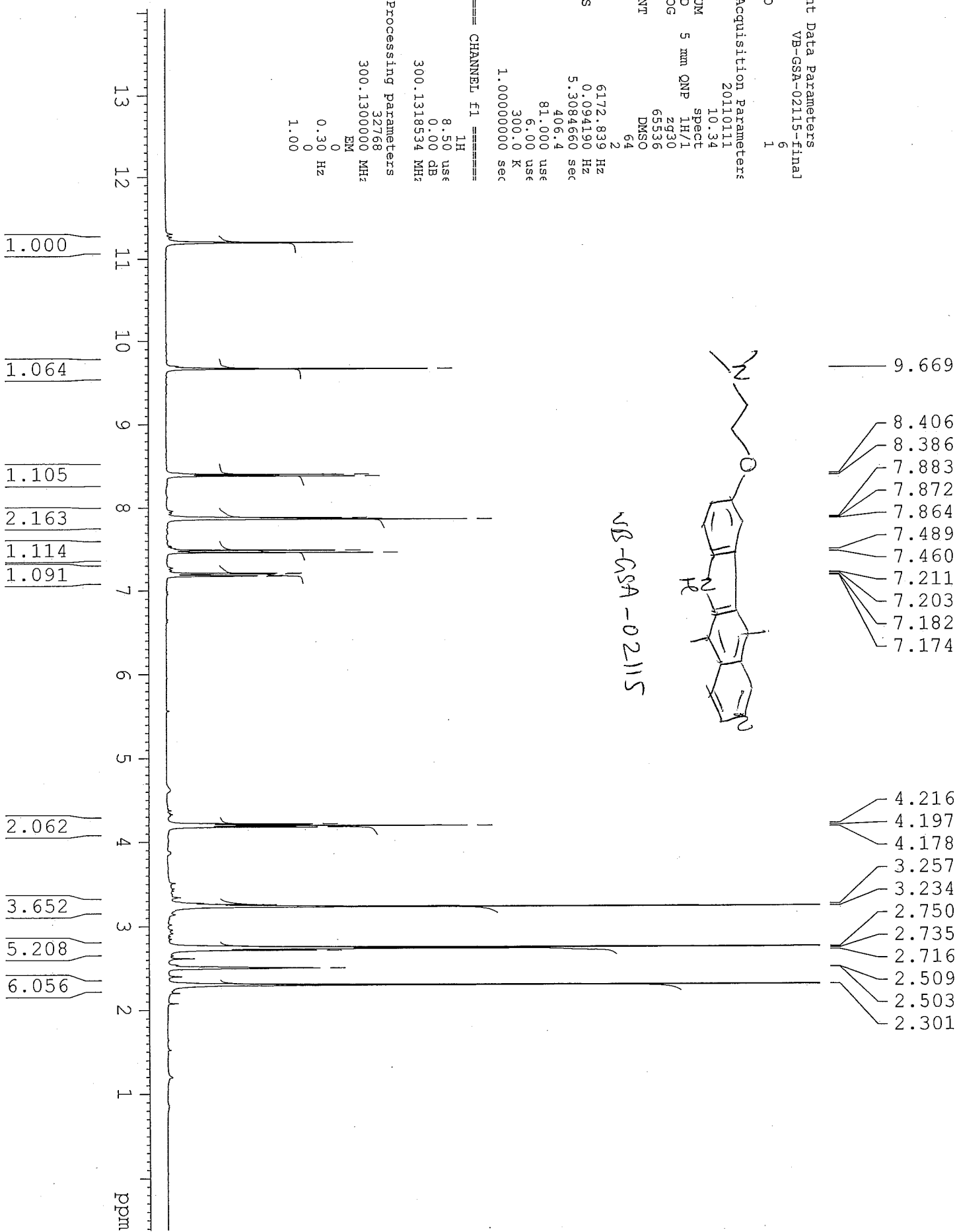
Current Data Parameters
 NAME VB-GSA-02115-final
 EXPNO 6
 PROCNO 1

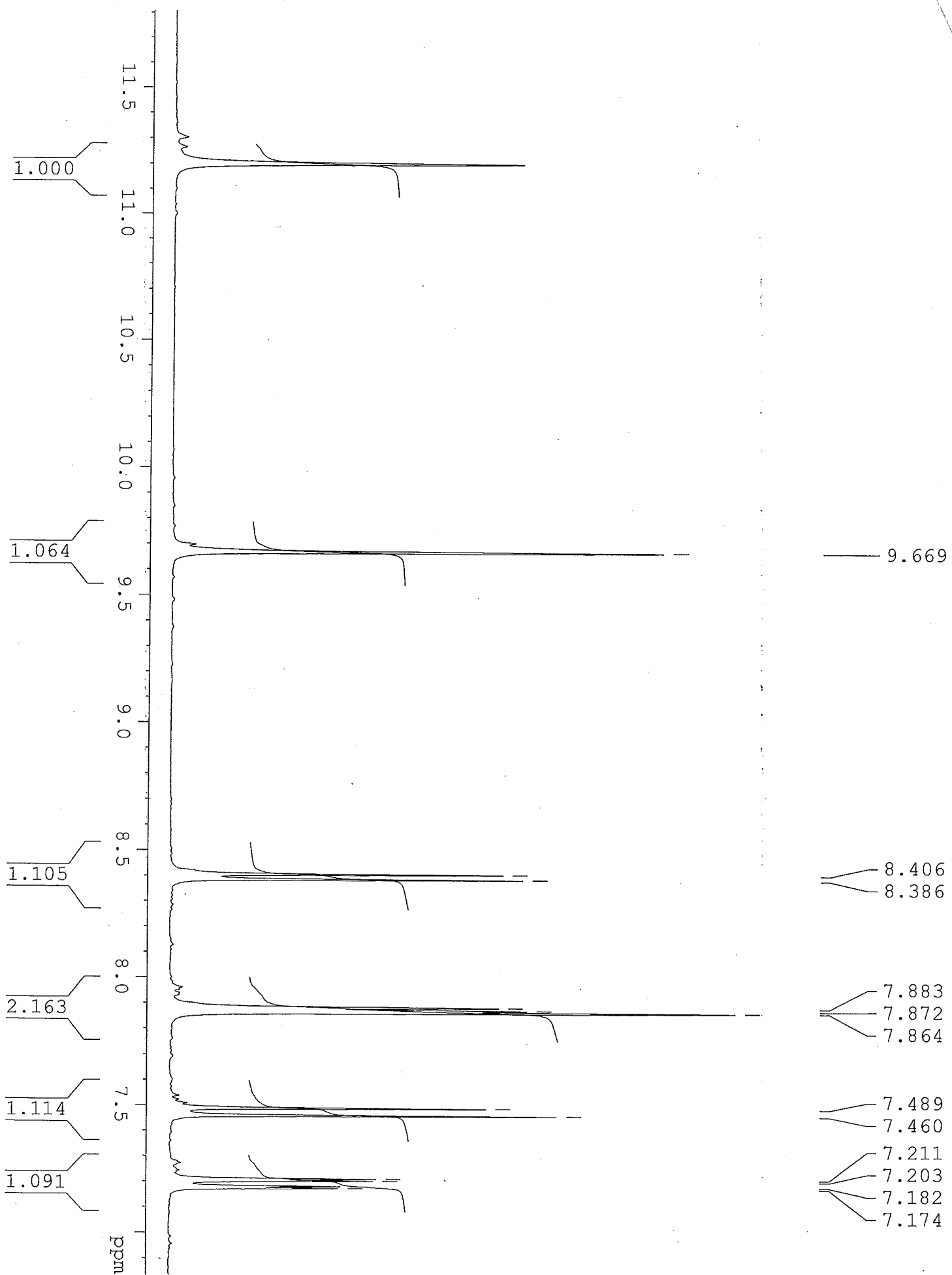
F2 - Acquisition Parameters
 Date_ 20110111
 Time 10.34
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 64
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 406.4
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

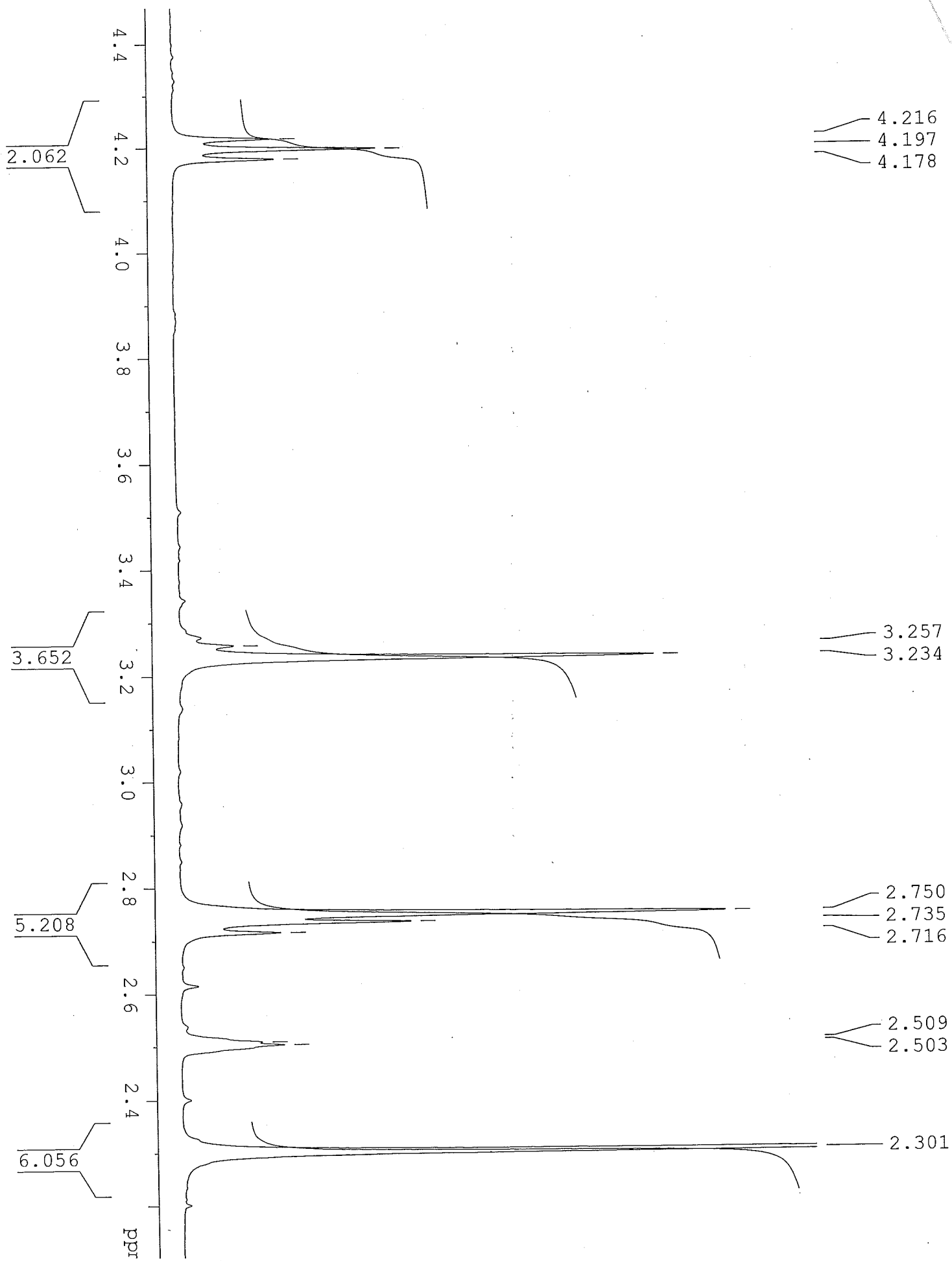
===== CHANNEL f1 =====
 NUC1 1H
 P1 8.50 usec
 PL1 0.00 dB
 SFO1 300.1318534 MHz
 F2 - Processing parameters
 SI 32768
 SF 300.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



VB-GSA-02115







Current Data Parameters
 NAME VB-GSA-02115-13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters:
 Date_ 20110113
 Time 10.45
 INSTRUM spect
 PROBD 5 mm QNP 1H/1
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 18650
 DS 4
 SWH 17985.611 H:
 FIDRES 0.274439 H:
 AQ 1.8219508 s:
 RG 3251
 DW 27.800 u:
 DE 6.00 u:
 TE 300.0 K
 D1 2.00000000 s:
 d11 0.03000000 s:
 d12 0.00002000 s:

CHANNEL F1
 NUC1 13C
 P1 6.00 u:
 PL1 2.00 d:
 SFO1 75.4752653 M

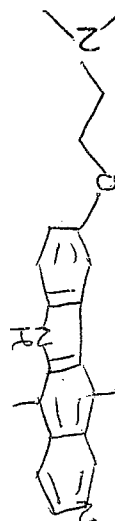
CHANNEL F2
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 u:
 PL2 0.00 d:
 PL12 19.47 d:
 PL13 19.00 d:
 SFO2 300.1312005 M

F2 - Processing parameters:
 SI 32768
 SF 75.4677190 M
 WDW EM
 SSB 0
 LB 1.00 H:
 GB 0
 PC 1.00

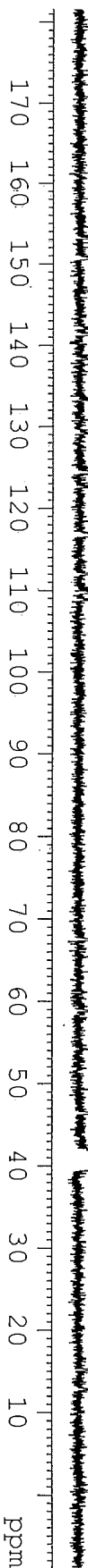
153.093
 150.586
 142.061
 141.240
 138.258
 133.180
 129.056
 124.417
 124.242
 122.531
 116.647
 111.977
 109.654
 108.726

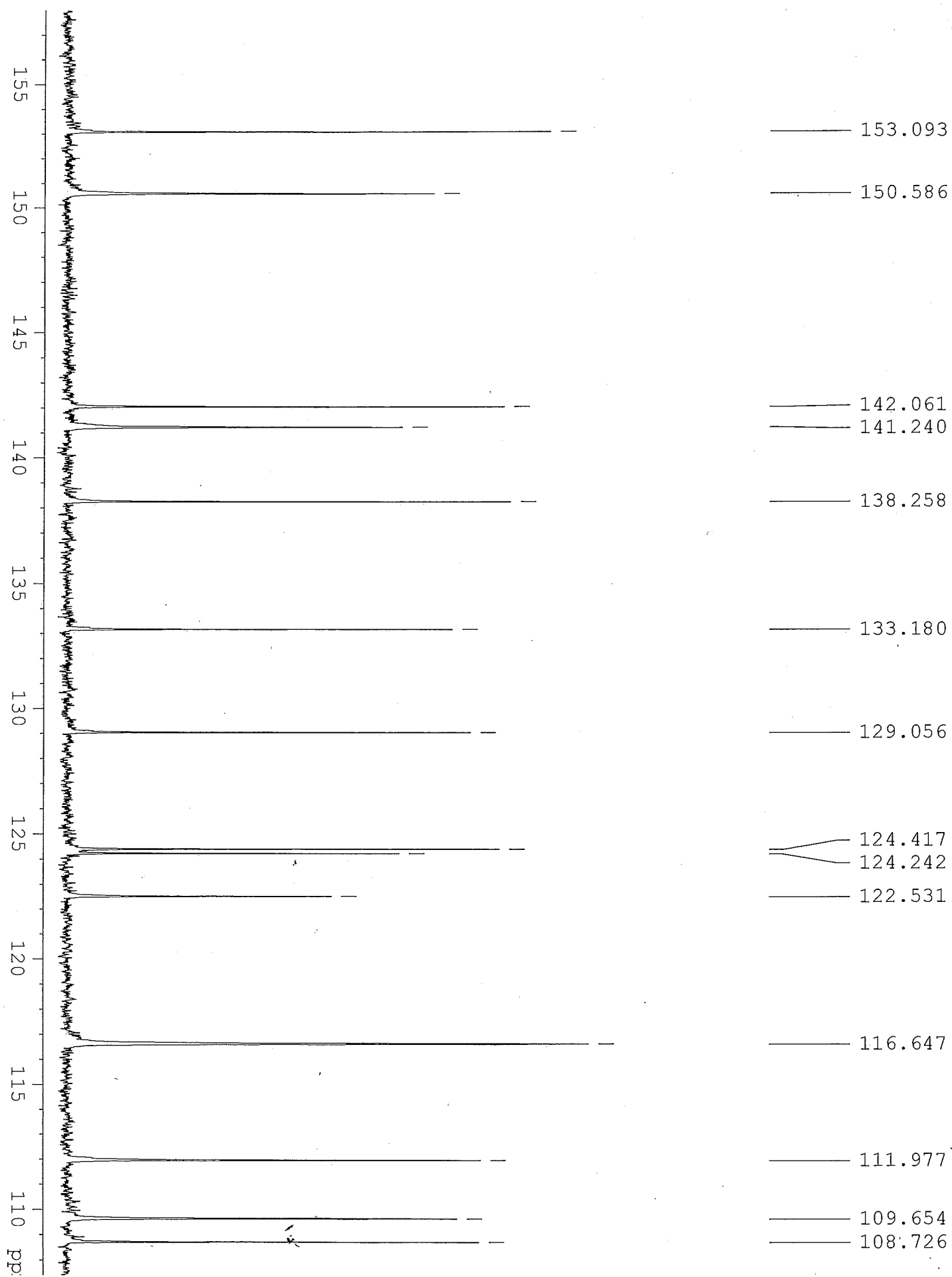
67.451
 58.782
 46.392
 41.222
 40.944
 40.665
 40.387
 40.108
 39.830
 39.552

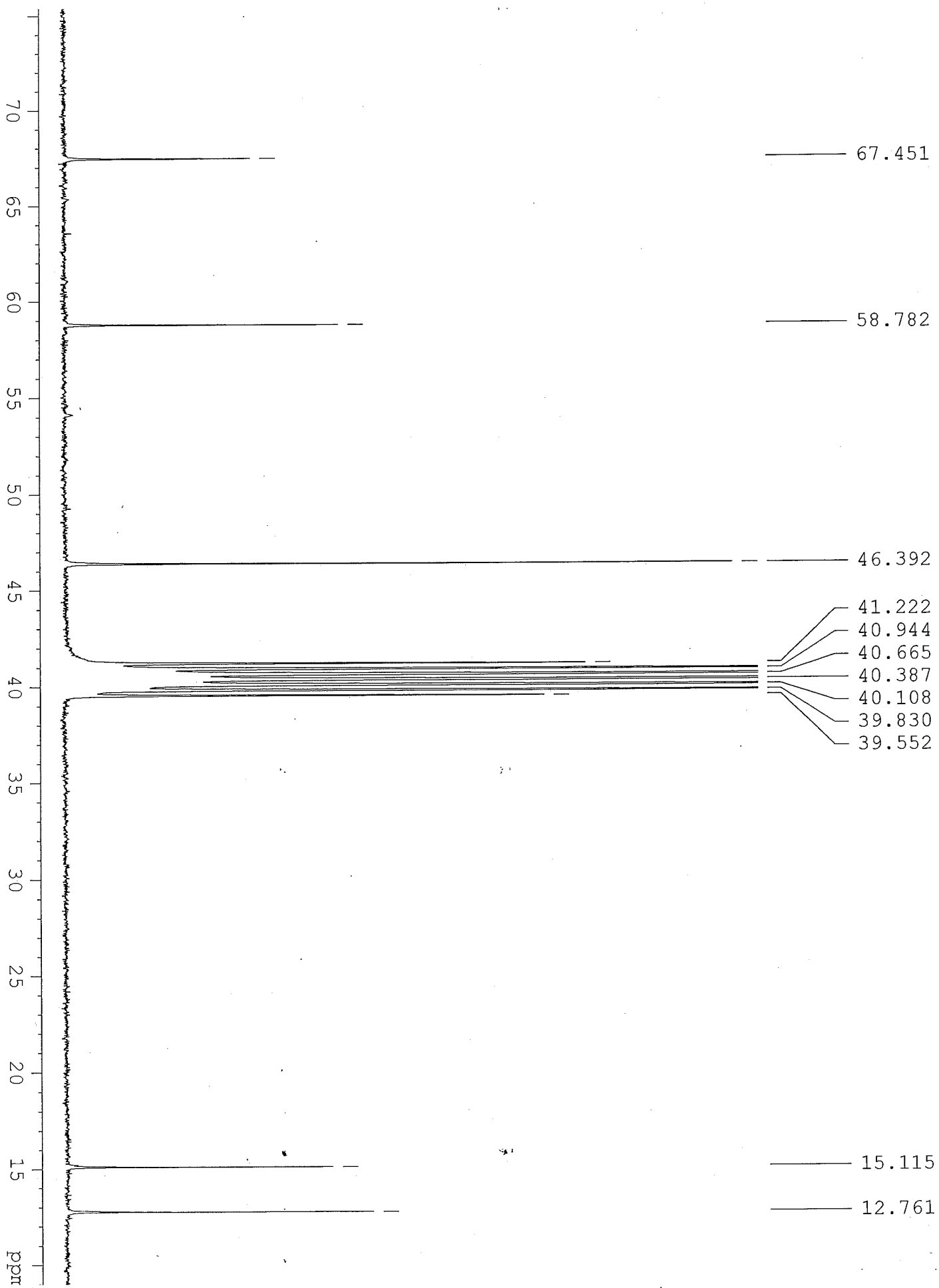
15.115
 12.761



VB-GSA-02115







Injection Date : 1/11/2011 5:22:07 PM

Sample Name : VB-GSA-02-115

Location : Vial 2

Acq. Operator : Karen

Inj : 1

Acq. Instrument : Instrument 1

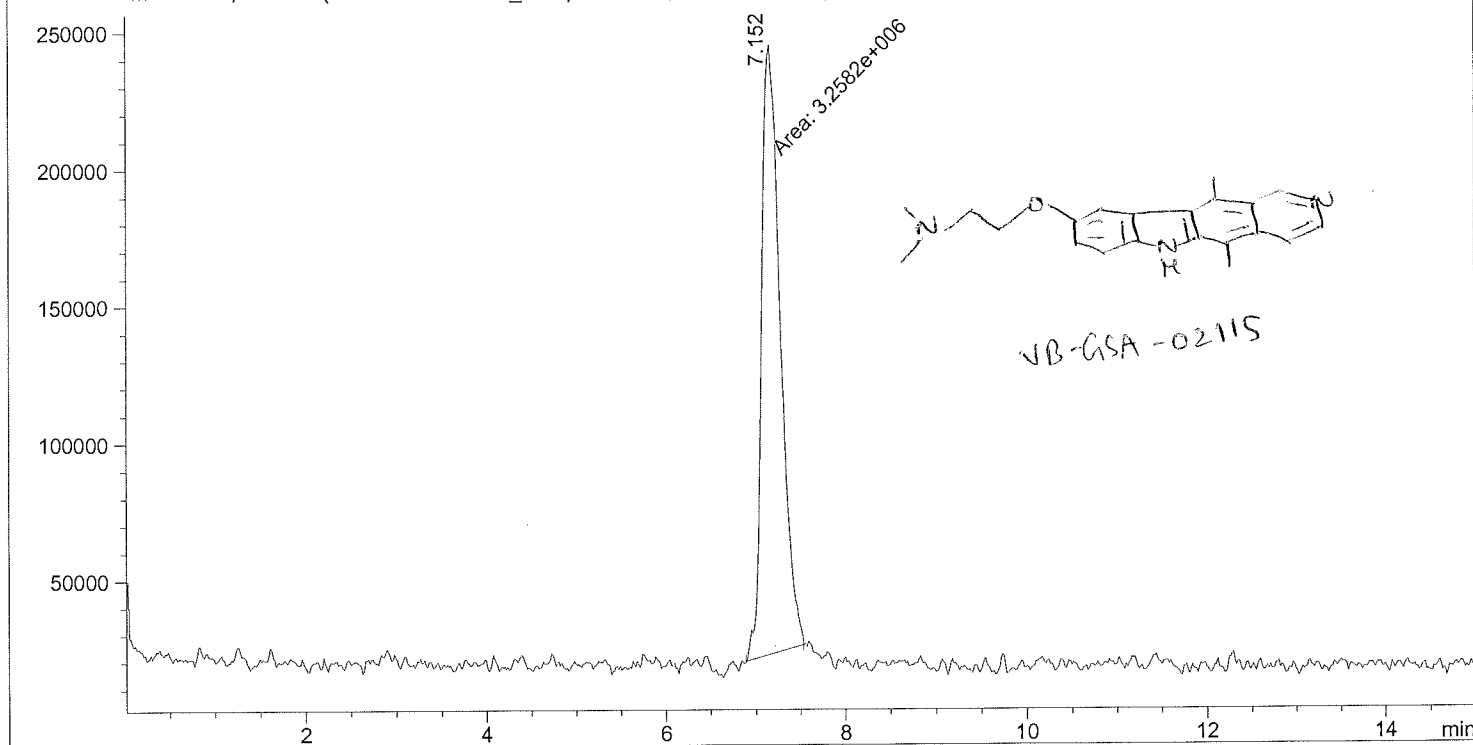
Inj Volume : 0.1 µl

Method : C:\HPCHEM\1\METHODS\LC_MS_UV.M

Last changed : 1/11/2011 5:19:55 PM by Karen

Zorbax SB C18, 150 x 4.6, 3.5µ, 30/70/0.25, MeOH/water/formic, POS, 150-550; frag 70; 40C, cap
volt 2500, gas temp 325; drying gas 10

MSD1 TIC, MS File (HURLEY10\JAN11_09.D) API-ES, Pos, Scan, Frag: 70, "positive scan"



Area Percent Report

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

Signal 1: MSD1 TIC, MS File

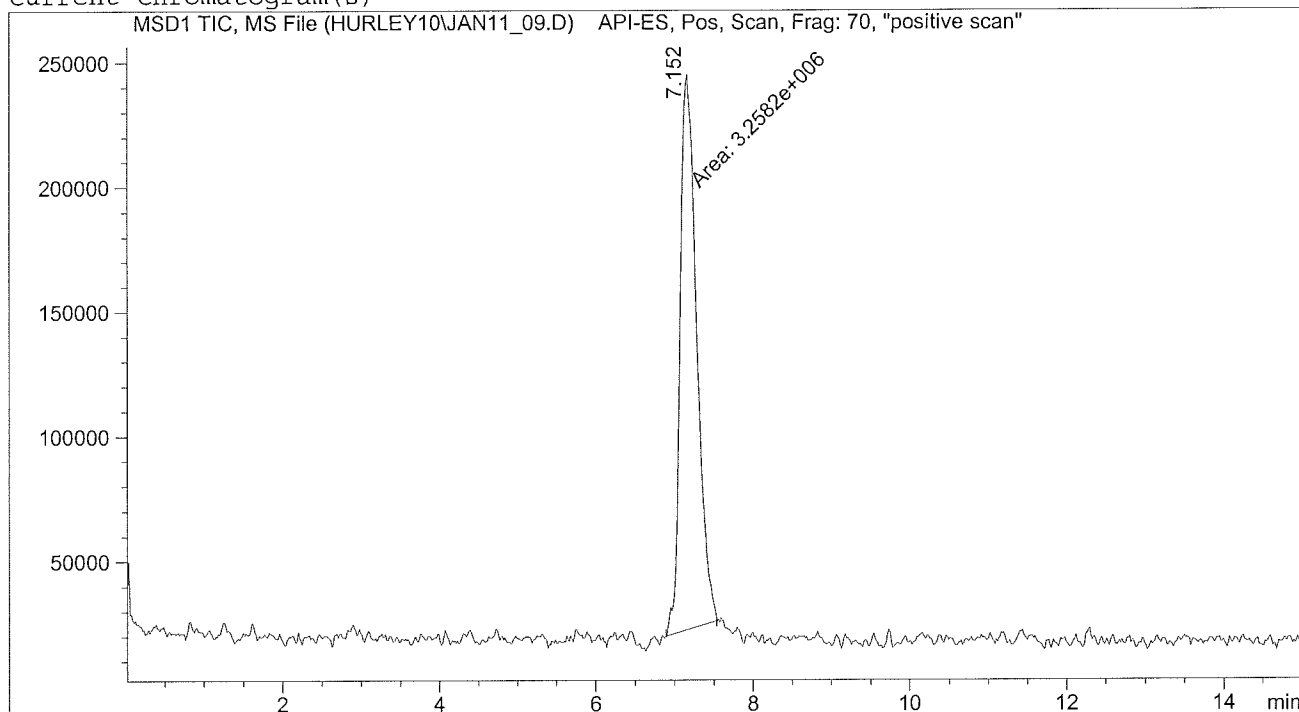
Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	7.152	MM	0.2431	3.25820e6	2.23333e5	100.0000

Totals : 3.25820e6 2.23333e5

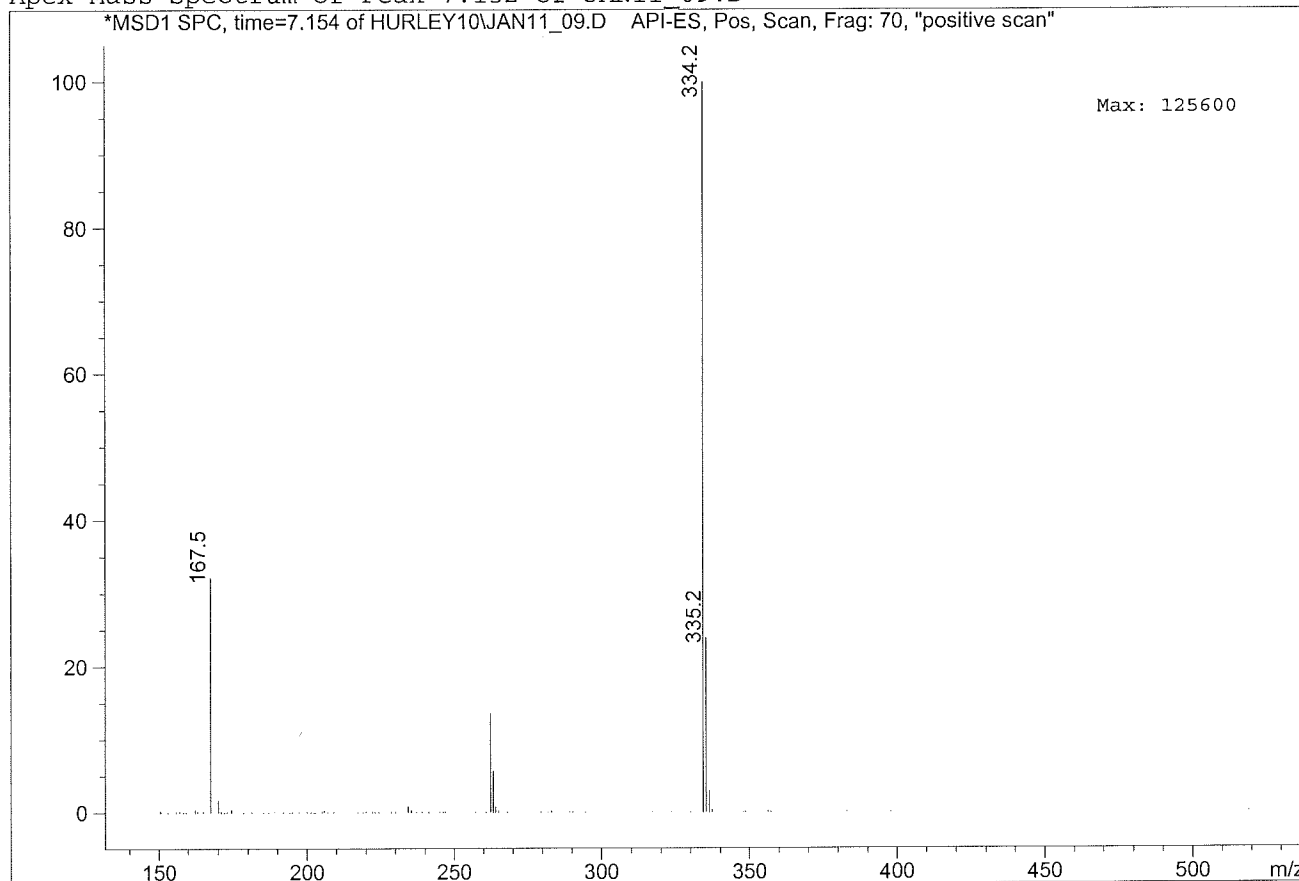
*** End of Report ***

```
=====
Injection Date   : 1/11/2011 5:22:07 PM
Sample Name      : VB-GSA-02-115
Acq. Operator    : Karen
Acq. Instrument  : Instrument 1
Method           : C:\HPCHEM\1\METHODS\LC_MS_UV.M
Last changed     : 1/11/2011 5:19:55 PM by Karen
Zorbax SB C18, 150 x 4.6, 3.5u,30/70/0.25,MeOH/water/formic, POS, 150-550; frag 70; 40C, cap
volt 2500, gas temp 325; drying gas 10
=====
```

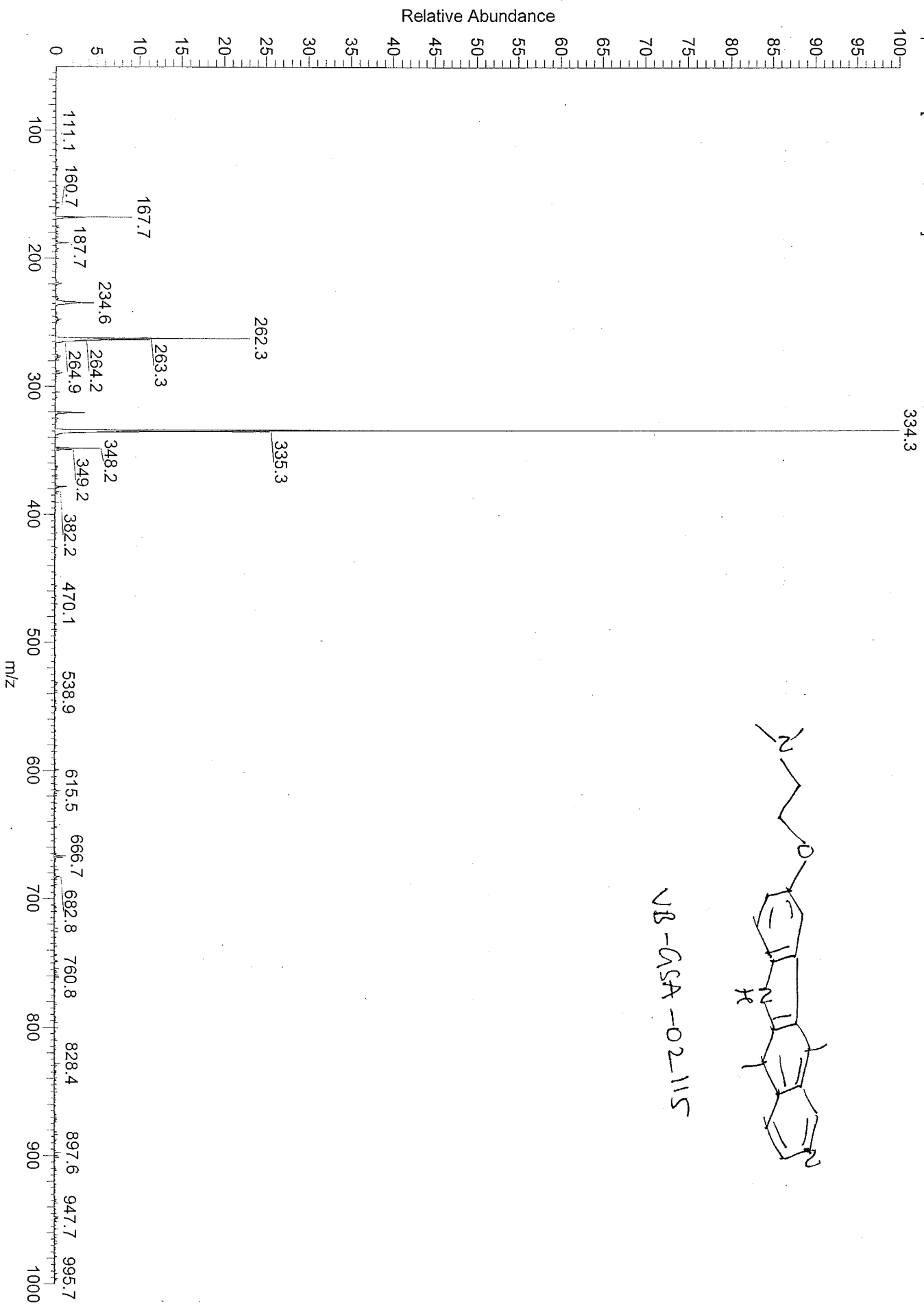
Current Chromatogram(s)



Apex Mass Spectrum of Peak 7.152 of JAN11_09.D



VB-02115 #59-63 RT: 1.40-1.47 AV: 5 NL: 1.62E7
T: + p Full ms [50.00-1000.00]



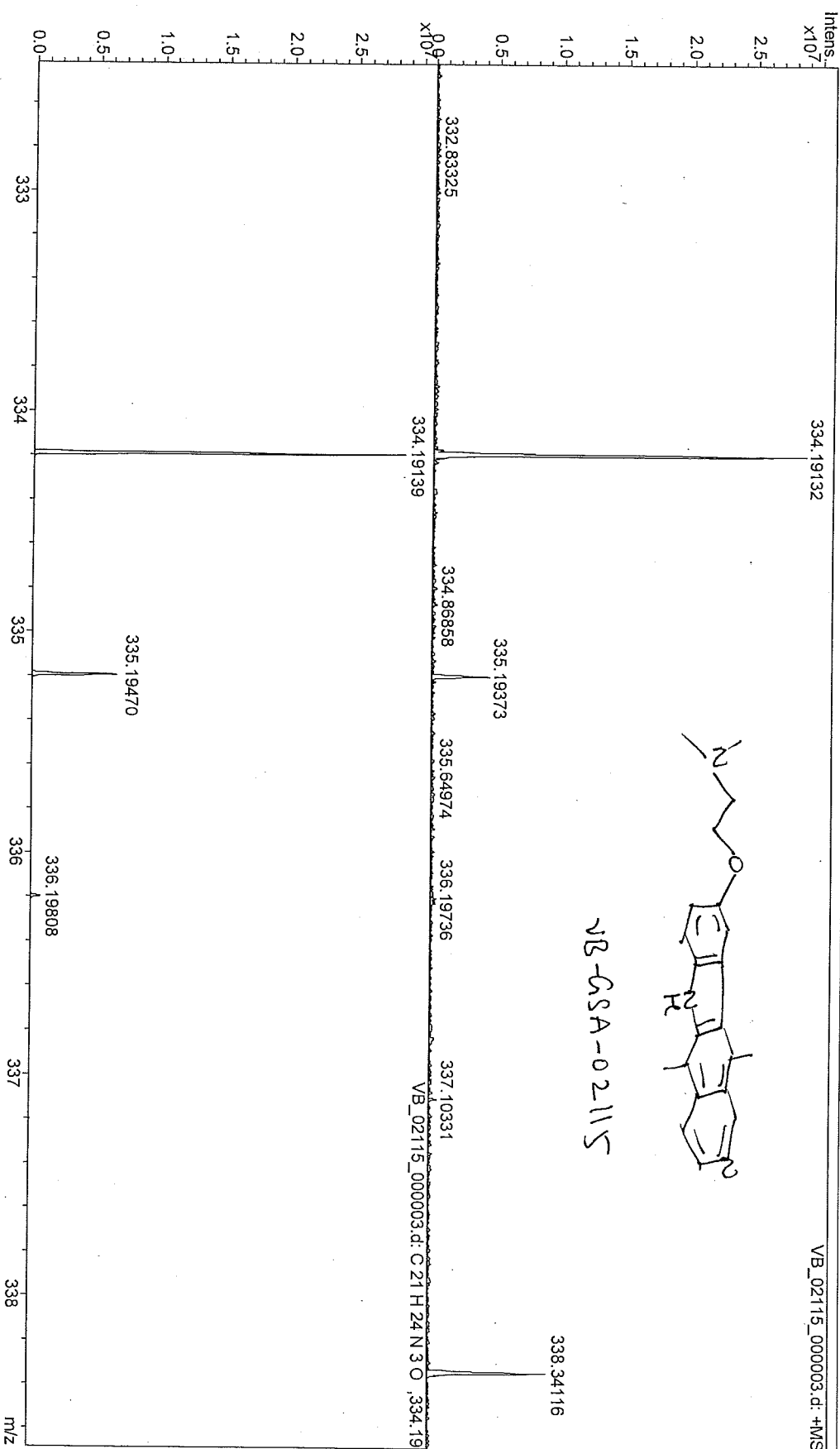
Generic Display Report

Analysis Info

Analysis Name D:\DATA\Facility_Jan_11\VB_02115_000003.d
Method ESI_101506
Sample Name VB_02115
Comment Venkat B., ACN:H2O 1:1.0.1%FA

Acquisition Date 1/18/2011 4:14:22 PM

Operator
Instrument apex-Ultra



SmartFormula Manually



Min

Max

Generate

Help

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

Measured m/z Tolerance mDa Charge

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdB	e ⁻ Conf	N-Rule
334.19132	1	C ₂₁ H ₂₄ N ₃ O	100.00	334.19139	0.1	0.2	46.8	11.5	even	ok

☐ Automatically locate monoisotopic peak Maximum number of formulas

☒ Check rings plus double bonds Minimum Maximum

☒ Filter H/C element ratio Minimum H/C Maximum H/C

☒ Estimate carbon number Electron configuration

☒ Generate immediately

Show Pattern

Current Data Parameters
 NAME ascs02-66-2
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100920
 Time 13.48
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 16
 DS 4
 SWH 6248.749 Hz
 FIDRES 0.190697 Hz
 AQ 2.6220949 sec
 RG 256
 DW 80.016 usec
 DE 6.00 usec
 TE 298.0 K
 D1 0.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 12.50 usec
 PL1 -2.00 dB
 SFO1 499.3829460 MHz

F2 - Processing parameters
 SI 32768
 SF 499.3800000 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00



9.934

8.397
 8.391
 7.888
 7.618
 7.601
 7.312
 7.307
 7.294
 7.290

3.941
 3.891
 3.376
 3.307
 2.837
 2.522
 2.518
 2.515

1.000

2.079

0.995

0.992

0.989

3.165

3.091

3.008

12 11 10 9 8 7 6 5 4 3 2 1 pp

Current Data Parameters
 NAME ascs02-66-2
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100920
 Time 13.48
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 16
 DS 4
 SWH 6248.749 Hz
 FIDRES 0.190697 Hz
 AQ 2.6220949 sec
 RG 256
 DW 80.016 usec
 DE 6.00 usec
 TE 298.0 K
 D1 0.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 12.50 usec
 PL1 -2.00 dB
 SFO1 499.3829460 MHz

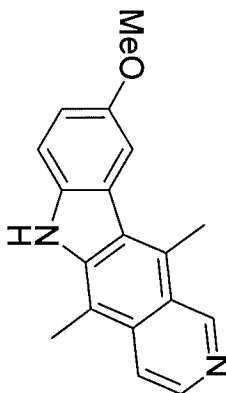
F2 - Processing parameters
 SI 32768
 SF 499.3800000 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00



- 9.934
- 8.397
- 8.391
- 7.888
- 7.618
- 7.601
- 7.312
- 7.307
- 7.294
- 7.290
- 3.941
- 3.891
- 3.376
- 3.307
- 2.837
- 2.522
- 2.518
- 2.515



154.587
145.055
143.642
137.731
133.934
133.840
127.654
126.018
123.100
119.810
117.187
112.698
110.401
108.168



Current Data Parameters
NAME asgsa02-66-C
EXPNO 5
PROCNO 1

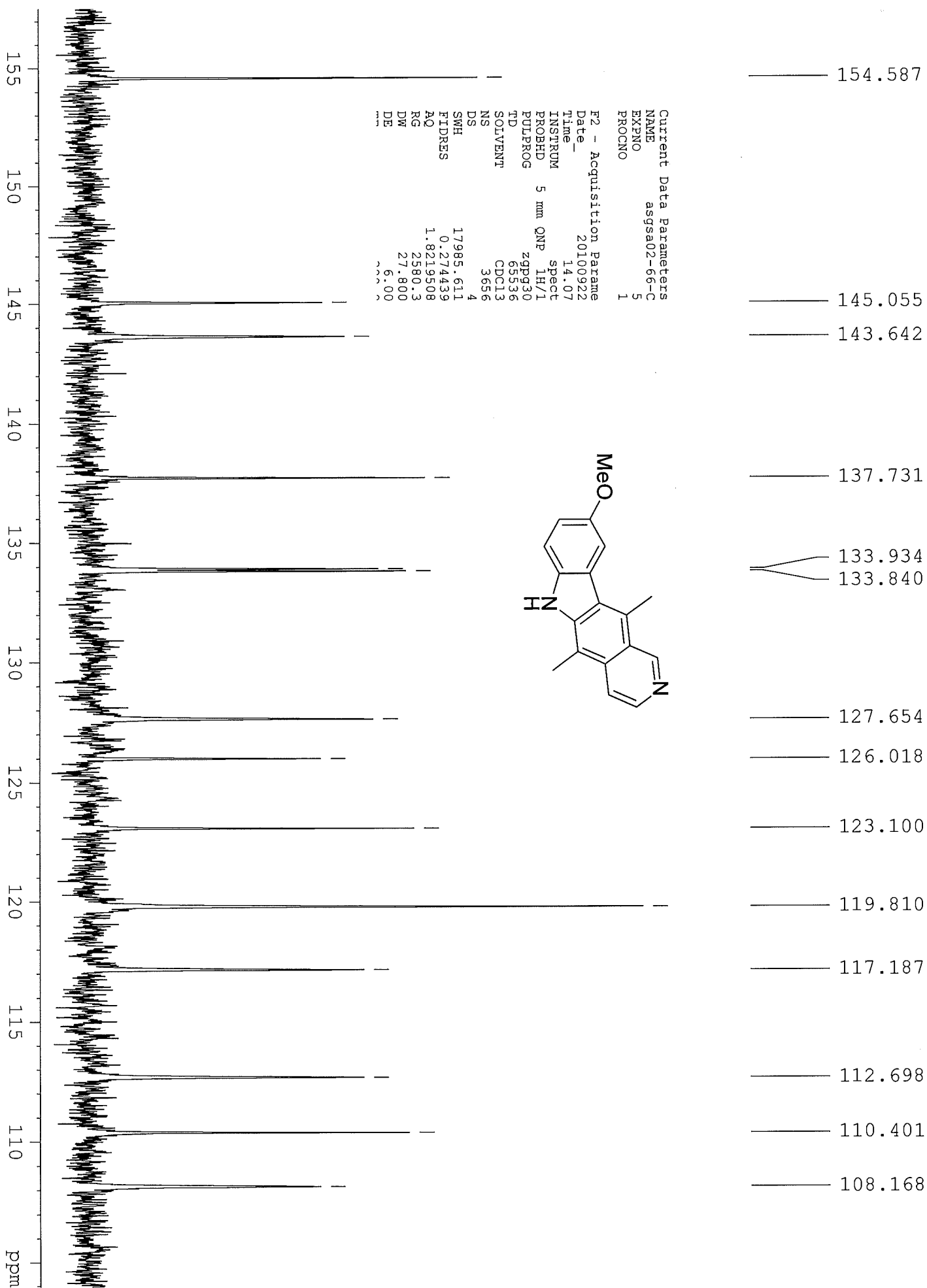
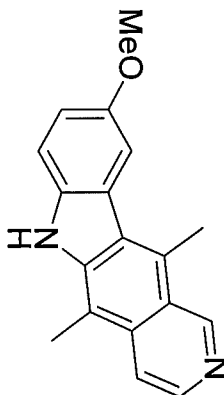
F2 - Acquisition Parameters
Date_ 20100922
Time_ 14.07
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3656
DS 4
SWH 17985.611
FIDRES 0.274439
AQ 1.8219508
RG 2580.3
DW 27.800
DE 6.00

56.460
41.241
40.962
40.684
40.406
40.128
39.849
39.571

160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

Current Data Parameters
NAME asgsa02-66-C
EXPNO 5
PROCNO 1

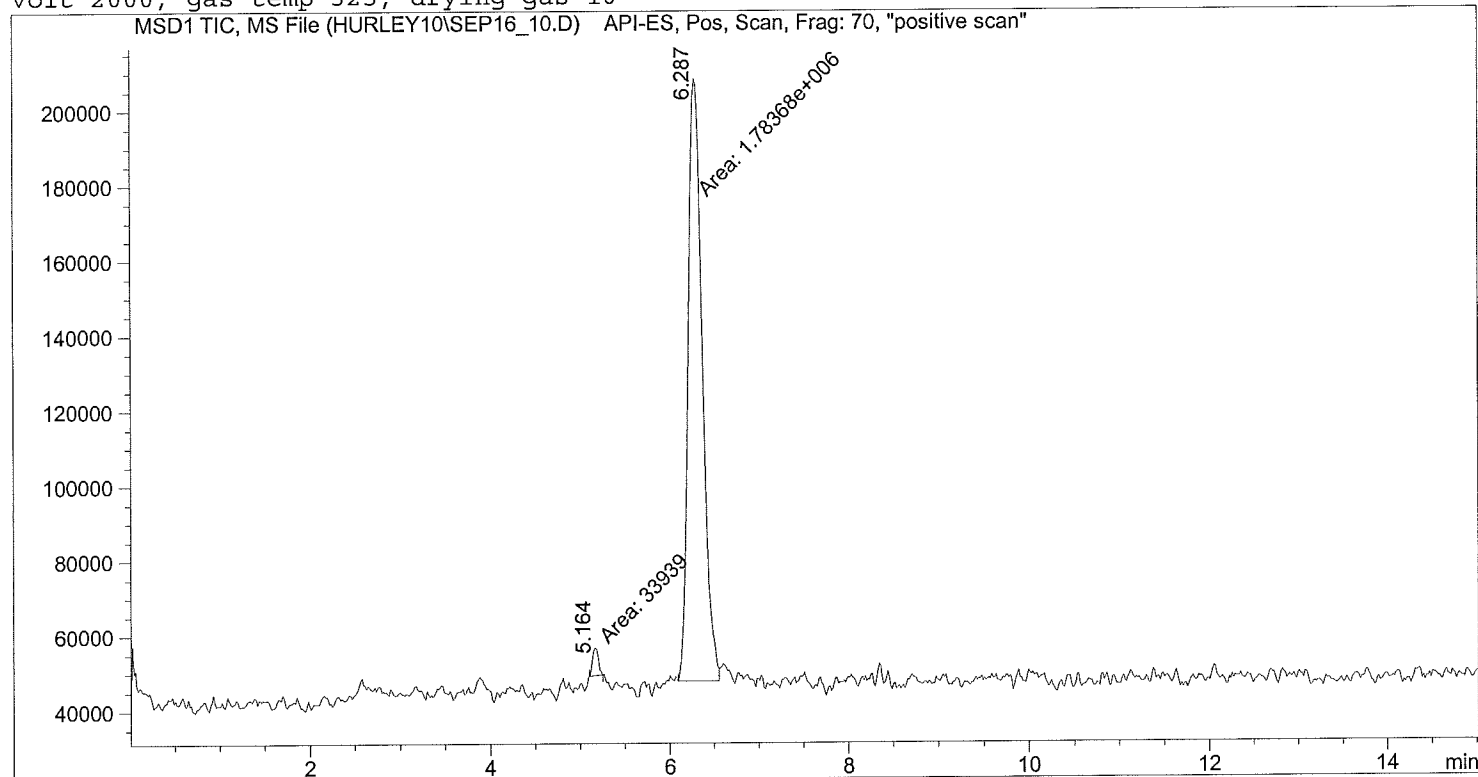
F2 - Acquisition Parameters
Date_ 20100922
Time_ 14.07
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3656
DS 4
SWH 17985.611
FIDRES 0.274439
AQ 1.8219508
RG 2580.3
DW 27.800
DE 6.00



=====

Injection Date : 9/16/2010 4:06:49 PM
Sample Name : AS-02/66-i Location : Vial 6
Acq. Operator : Karen Inj : 1
Acq. Instrument : Instrument 1 Inj Volume : 0.1 µl
Method : C:\HPCHEM\1\METHODS\LC_MS.M
Last changed : 9/16/2010 4:05:11 PM by Karen
(modified after loading)

Zorbax SB C18, 150 x 4.6, 3.5µ, 60:40:0.25, MeOH/H2O/formic, POS, 150-400; frag 70; 25C, cap
volt 2000, 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

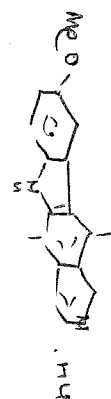
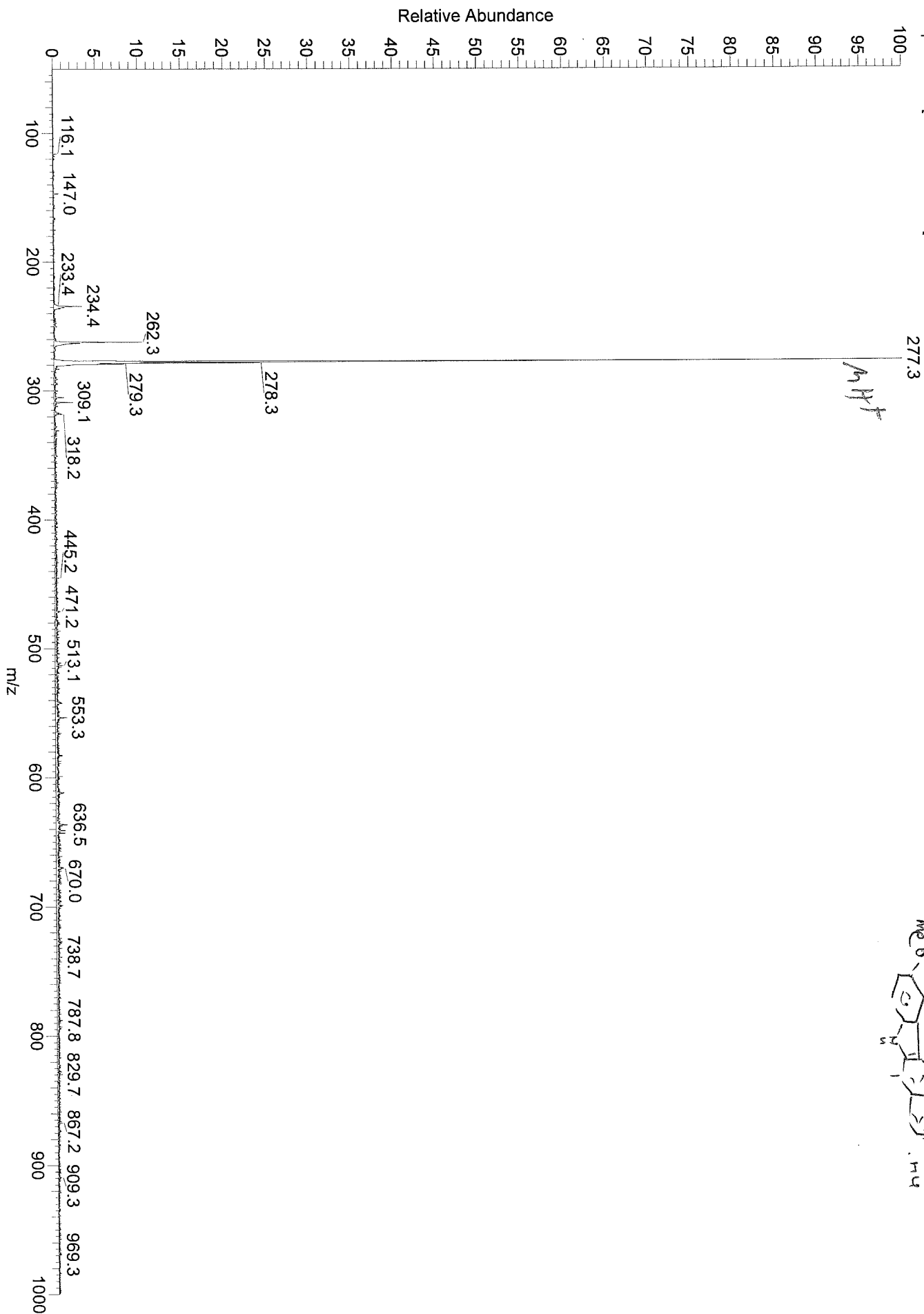
Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	5.164	MM	0.0763	3.39390e4	7411.62695	1.8672
2	6.287	MM	0.1845	1.78368e6	1.61115e5	98.1328

Totals : 1.81762e6 1.68527e5

=====

*** End of Report ***

CHO2_66 #3-12 RT: 0.04-0.22 AV: 10 NL: 4.12E6
T: + p Full ms [50.00-1000.00]



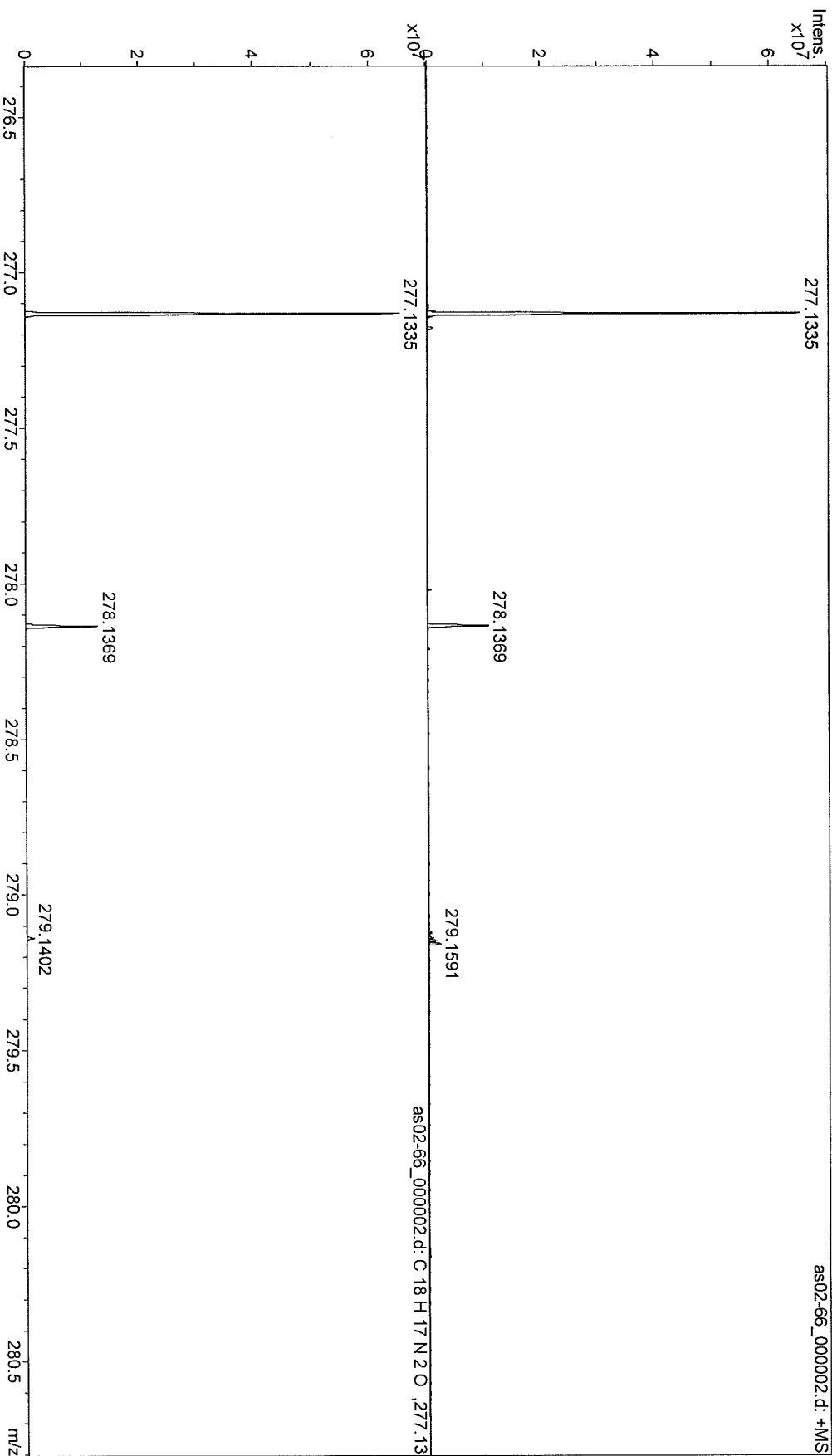
Generic Display Report

Analysis Info

Analysis Name D:\DATA\Facility_Sept_10\as02-66_0000002.d
Method ESL_101506
Sample Name as02-66
Comment Anuj S., positive mode, ACN:H2O 1:1:0.1%FA

Acquisition Date 9/17/2010 4:10:40 PM

Operator
Instrument apex-Ultra



SmartFormula Manually



Min

C₉

Generate

Max

C 9-n

Help

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

Measured m/z

277.1335

Tolerance

2

mDa

Charge

1

Meas. m/z

#

Formula

Score

m/z

err [mDa]

err [ppm]

mSigma

rdb

e_Conf

N-Rule

277.1335

1

C18H17N2O

100.00

277.1335

-0.0

-0.0

20.4

11.5

even

ok

☐ Automatically locate monoisotopic peak

Maximum number of formulas

500

☒ Check rings plus double bonds

Minimum

-0.5

Maximum

40

Electron configuration

☒ Filter H/C element ratio

Minimum H/C

0

Maximum H/C

3

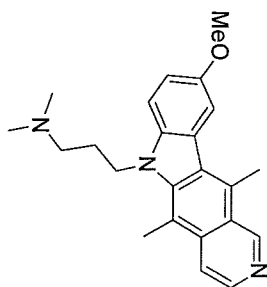
☒ Estimate carbon number

☒ Generate immediately

Show Pattern

9.695
8.511
8.490
7.918
7.902
7.895
7.434
7.405
7.281
7.229
7.220
7.199
7.191

4.607
4.582
4.557
3.983
3.248
2.992
2.366
2.343
2.320
2.259
2.058
2.035
2.010
1.985



C₂₃H₂₇N₃O
Exact Mass: 361.22

1.003

1.020

2.024

1.090

1.035

2.021

3.177

3.027

3.020

2.084

6.110

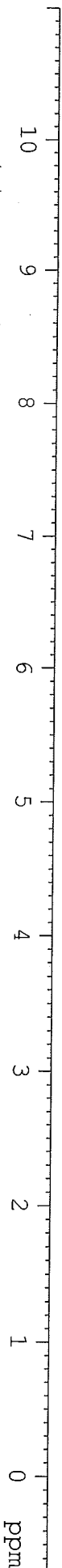
2.279

Current Data Parameters
NAME CV-GSA-02110
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110412
Time_ 16.31
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 256
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

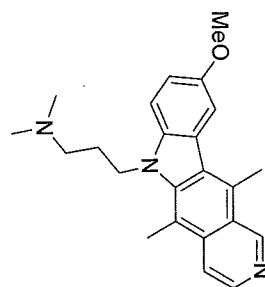


9.695

8.511
8.490

7.918
7.902
7.895

7.434
7.405
7.281
7.229
7.220
7.199
7.191



$C_{23}H_{27}N_3O$
Exact Mass: 361.22

1.003

1.020

2.024

1.090

1.035

ppm

Current Data Parameters
NAME CV-GSA-02110
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110412
Time 16.31
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 5.308460 sec
RG 256
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

4.607
4.582
4.557

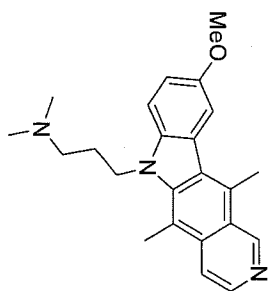
3.983

3.248

2.992

2.366
2.343
2.320
2.259

2.058
2.035
2.010
1.985



$C_{23}H_{27}N_3O$
Exact Mass: 361.22

2.021

3.177

3.027

3.020

2.084

6.110

2.279

ppm

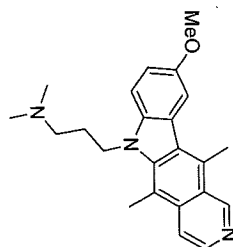
Current Data Parameters
NAME CV-GSA-02110
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110412
Time_ 16.31
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 65536
FIDRES 0.094190 Hz
AQ 5.308460 sec
RG 256
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 300.130000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

154.261
150.154
141.909
141.350
139.876
134.772
129.398
125.346
124.696
122.894
116.295
114.854
109.734
109.296
108.823



$C_{23}H_{17}N_3O$
Exact Mass: 361.22

77.856
77.637
77.433
77.010

57.026
56.685

45.852
44.359

28.483

15.110
13.960

Current Data Parameters
NAME CV-GSA-02110
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110413
Time 8.39

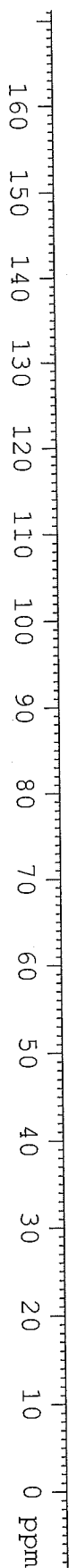
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 15000
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec

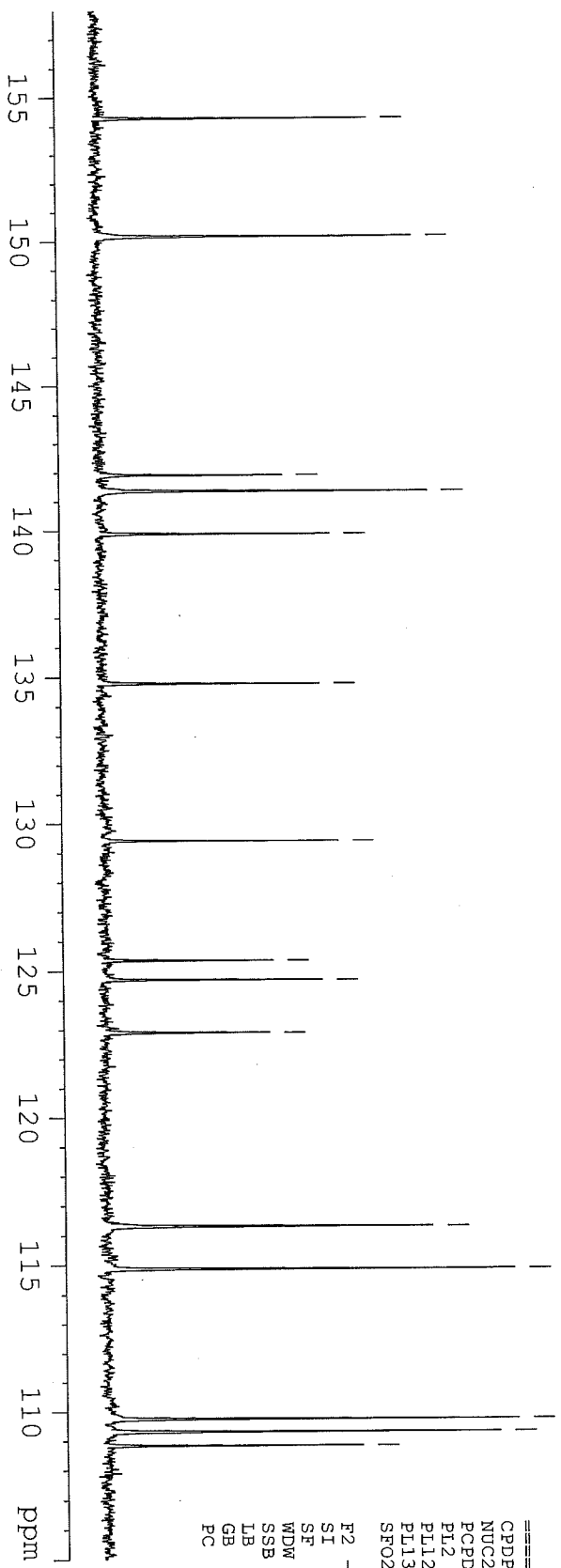
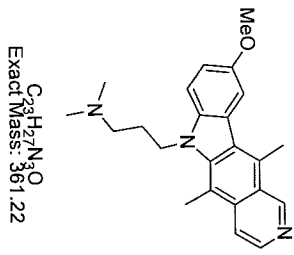
RG 7298.2
DM 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00020000 sec

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





154.261
150.154
141.909
141.350
139.876
134.772
129.398
125.346
124.696
122.894
116.295
114.854
109.734
109.296
108.823

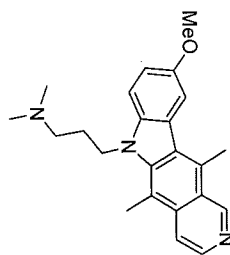
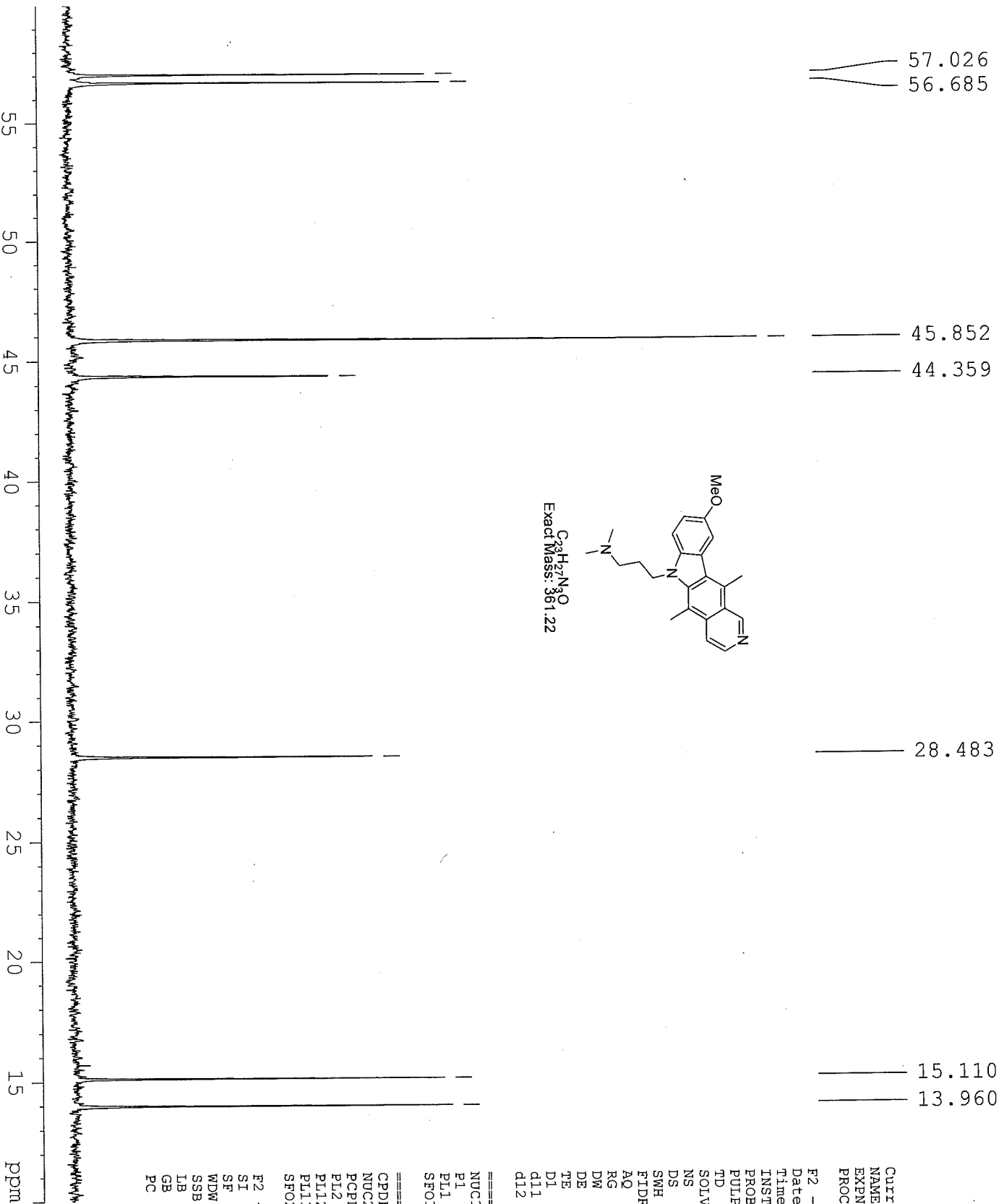
Current Data Parameters
 NAME CV-GSA-02110
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110413
 Time 8.39
 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 7298.2
 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 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



C₁₇H₁₇N₂O
Exact Mass: 361.22

Current Data Parameters
NAME CV-GSA-02110
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110413
Time 8.39

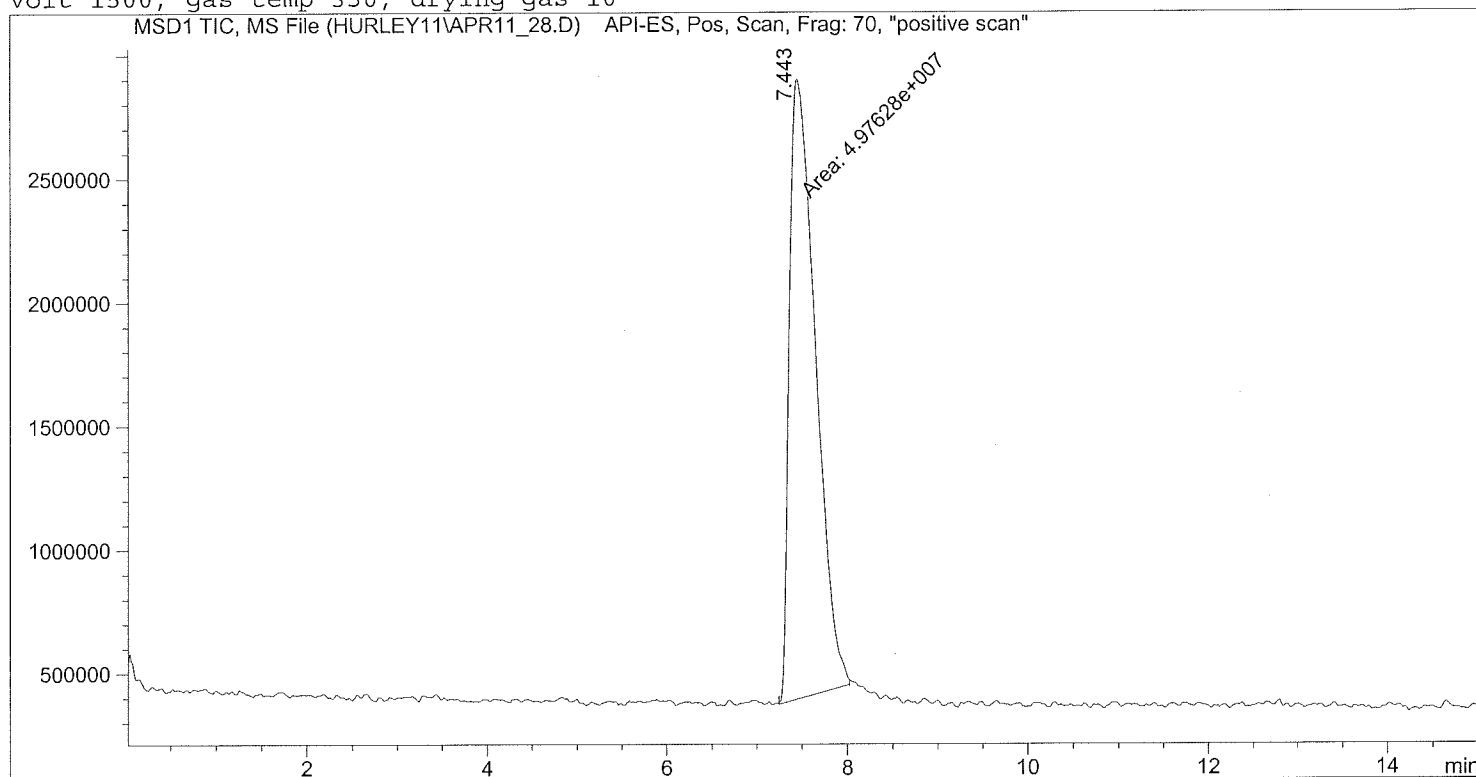
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 15000
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 7298.2
DM 27.800
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

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

=====
Injection Date : 4/11/2011 5:23:21 PM
Sample Name : CV-GSA-02110
Acq. Operator : Karen
Acq. Instrument : Instrument 1
Method : C:\HPCHEM\1\METHODS\LC_MS_UV.M
Last changed : 4/11/2011 5:21:21 PM by Karen
Zorbax SB C18, 150 x 4.6, 3.5u,35/65/0.25,MeOH/water/formic, POS, 150-500; frag 70; 35C, cap
volt 1500, gas temp 350; drying gas 10
Location : Vial 19
Inj : 1
Inj Volume : 0.1 µl



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

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

Signal 1: MSD1 TIC, MS File

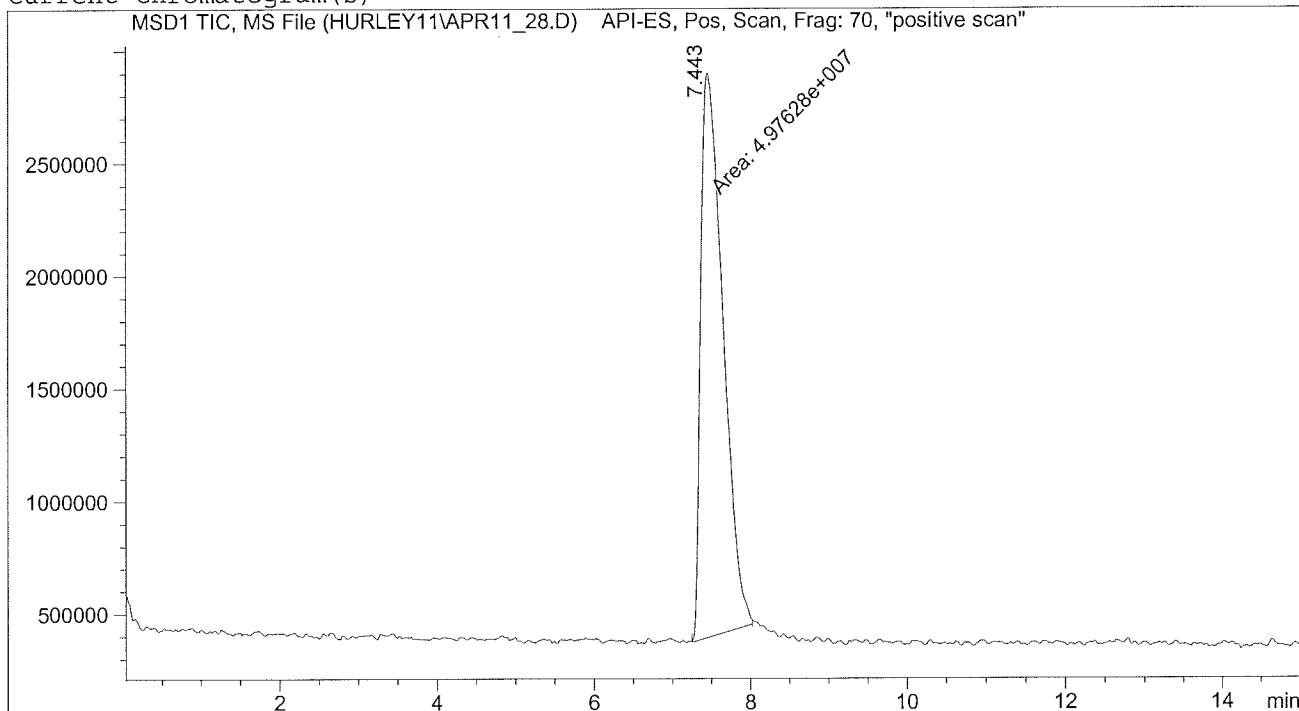
Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	7.443	MM	0.3303	4.97628e7	2.51123e6	100.0000

Totals : 4.97628e7 2.51123e6

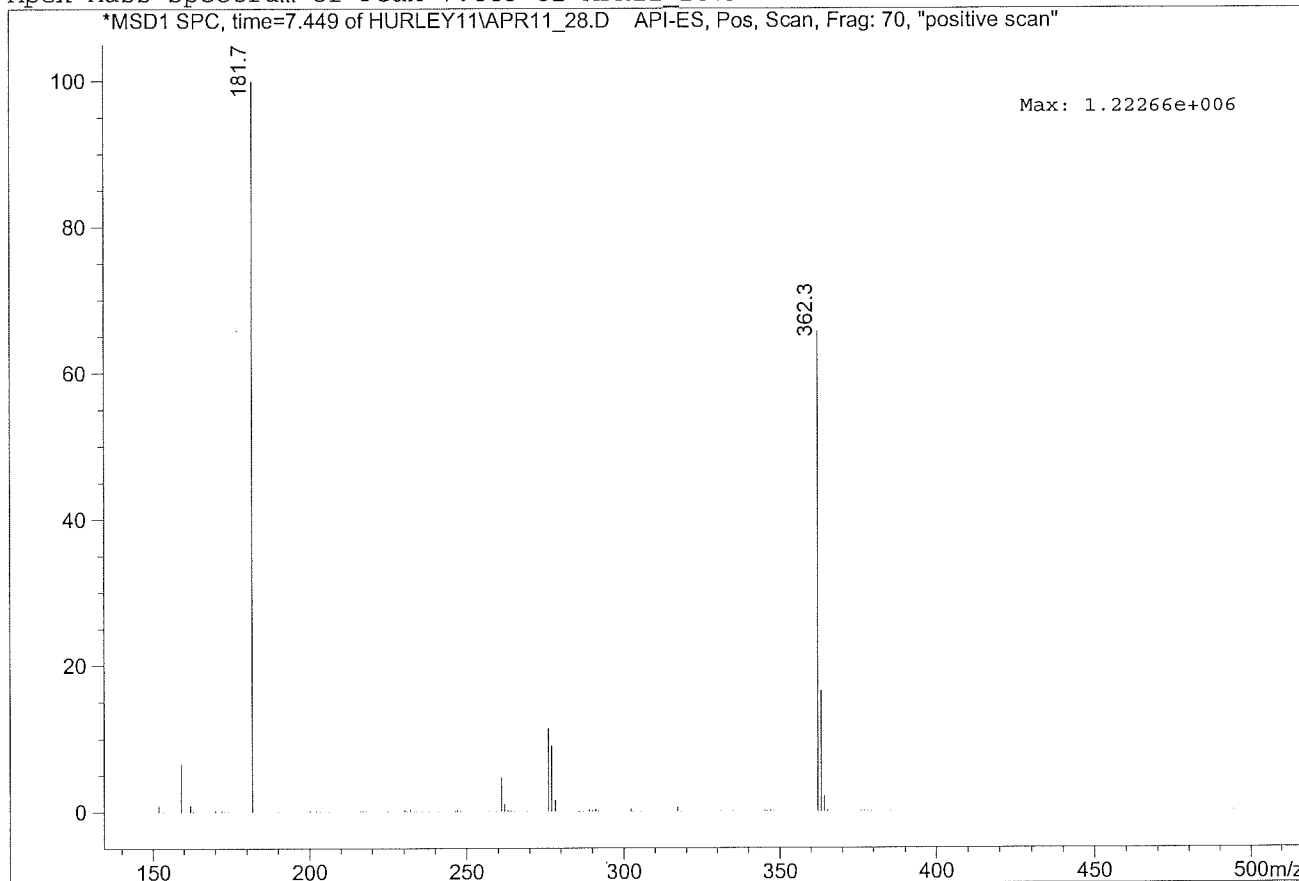
=====
*** End of Report ***

```
=====
Injection Date   : 4/11/2011 5:23:21 PM
Sample Name      : CV-GSA-02110
Acq. Operator    : Karen
Acq. Instrument  : Instrument 1
Method           : C:\HPCHEM\1\METHODS\LC_MS_UV.M
Last changed     : 4/11/2011 5:21:21 PM by Karen
Zorbax SB C18, 150 x 4.6, 3.5u,35/65/0.25,MeOH/water/formic, POS, 150-500; frag 70; 35C, cap
volt 1500, gas temp 350; drying gas 10
=====
```

Current Chromatogram(s)



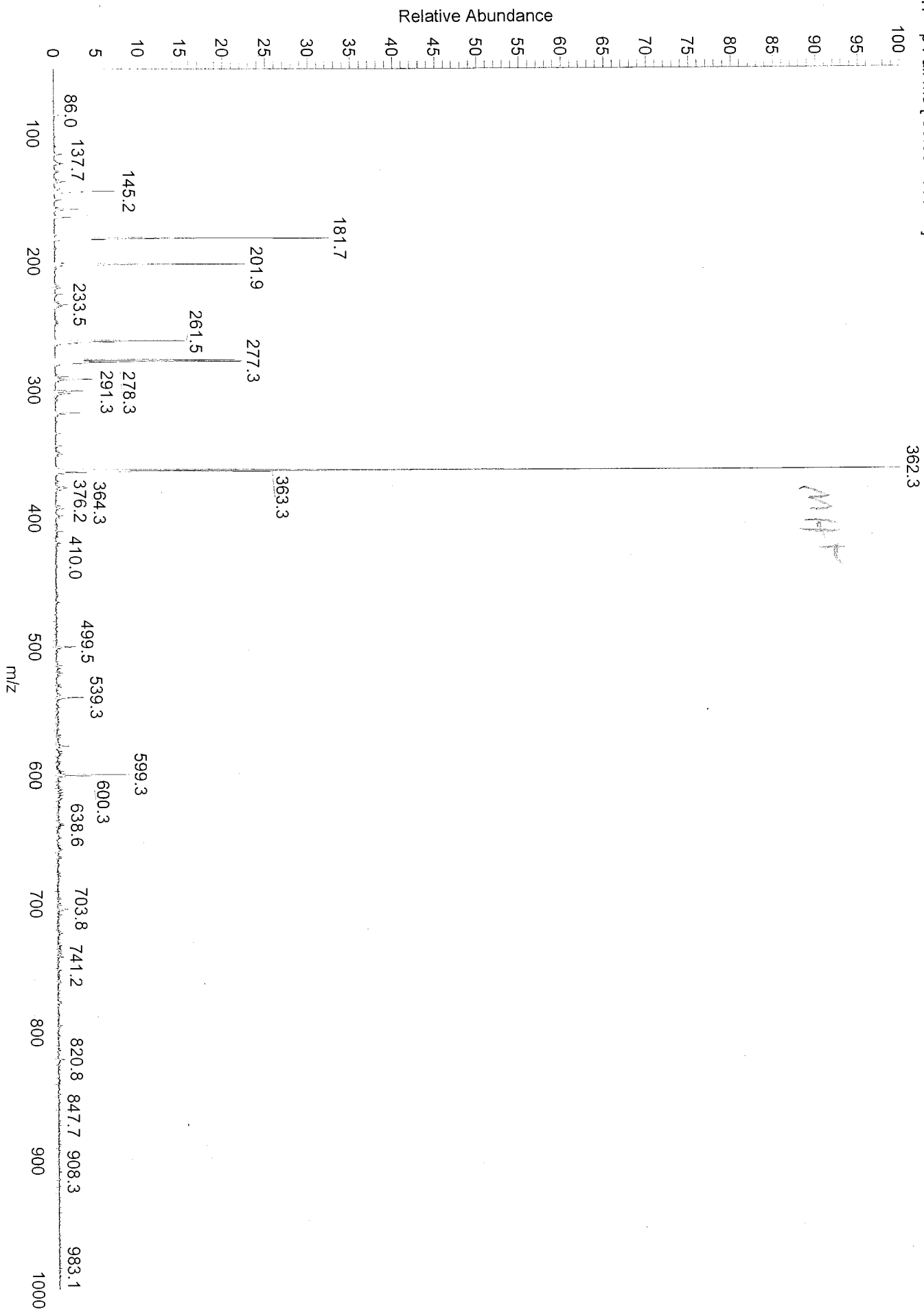
Apex Mass Spectrum of Peak 7.443 of APR11_28.D



E:\MSLab_LCQ\CV_GSA_02110
V. R. Chappeta, MeOH:ACN
CV_GSA_02110 #54-57 RT: 1.10-1.16 AV: 4 NL: 3.52E6
T: + p Full ms [50.00-1000.00]

04/11/2011 05:21:29 PM

CV_GSA_02110



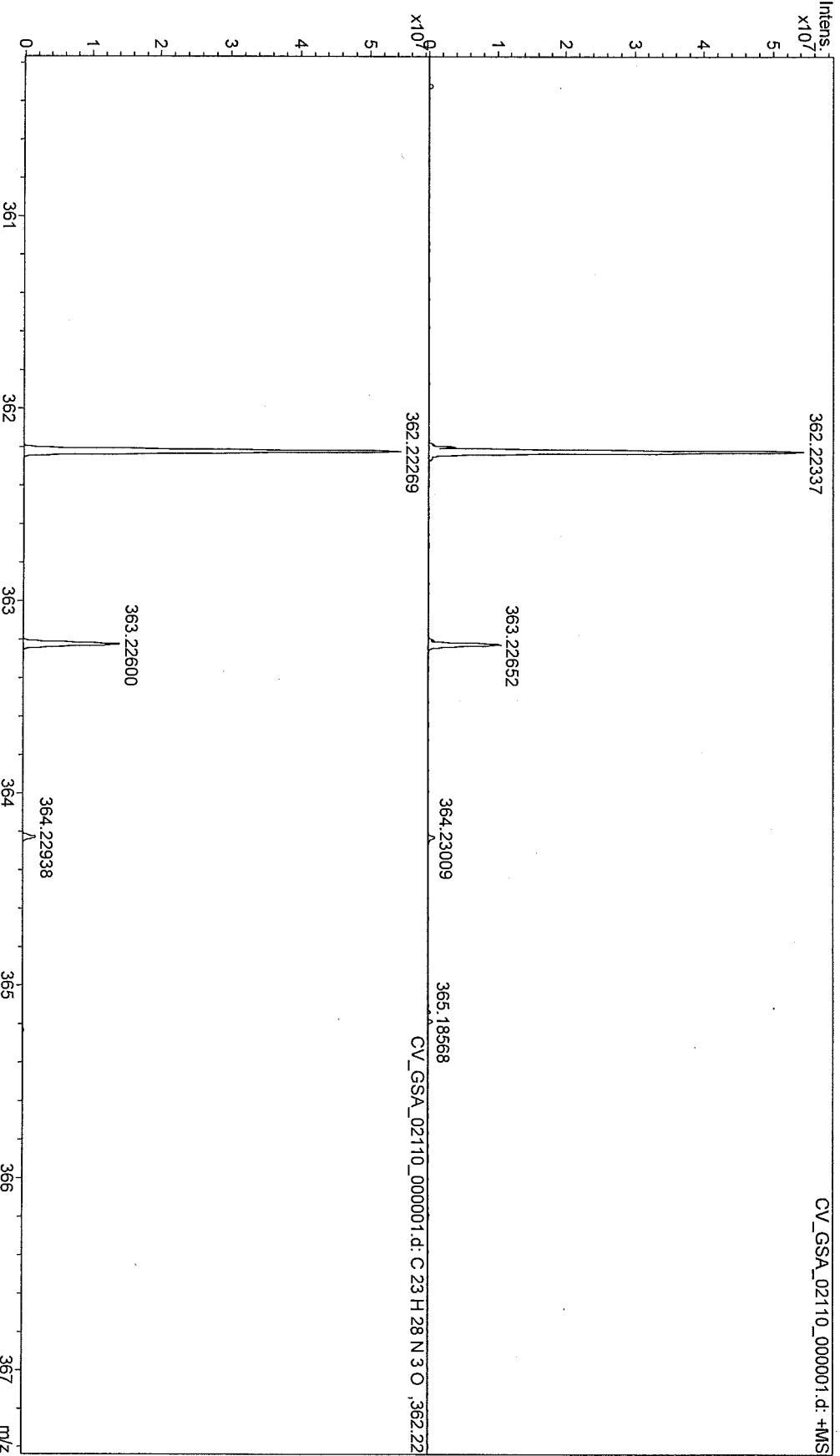
Generic Display Report

Analysis Info

Analysis Name D:\DATA\Facility_Apr_11\CV_GSA_02110_000001.d
Method ESI_101506
Sample Name CV_GSA_02110
Comment V. Chappetta, positive mode, ACN:H2O

Acquisition Date 4/12/2011 10:49:42 AM

Operator
Instrument apex-Ultra



SmartFormula Manually



Min

C₁₂

Generate

Max

C 12-n

Help

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

Measured m/z

362.22337

Tolerance

2

mDa

Charge

1

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
362.22337	1	C 23 H 28 N 3 O	100.00	362.22269	-0.7	-1.9	36.8	11.5	even	ok

☐ 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

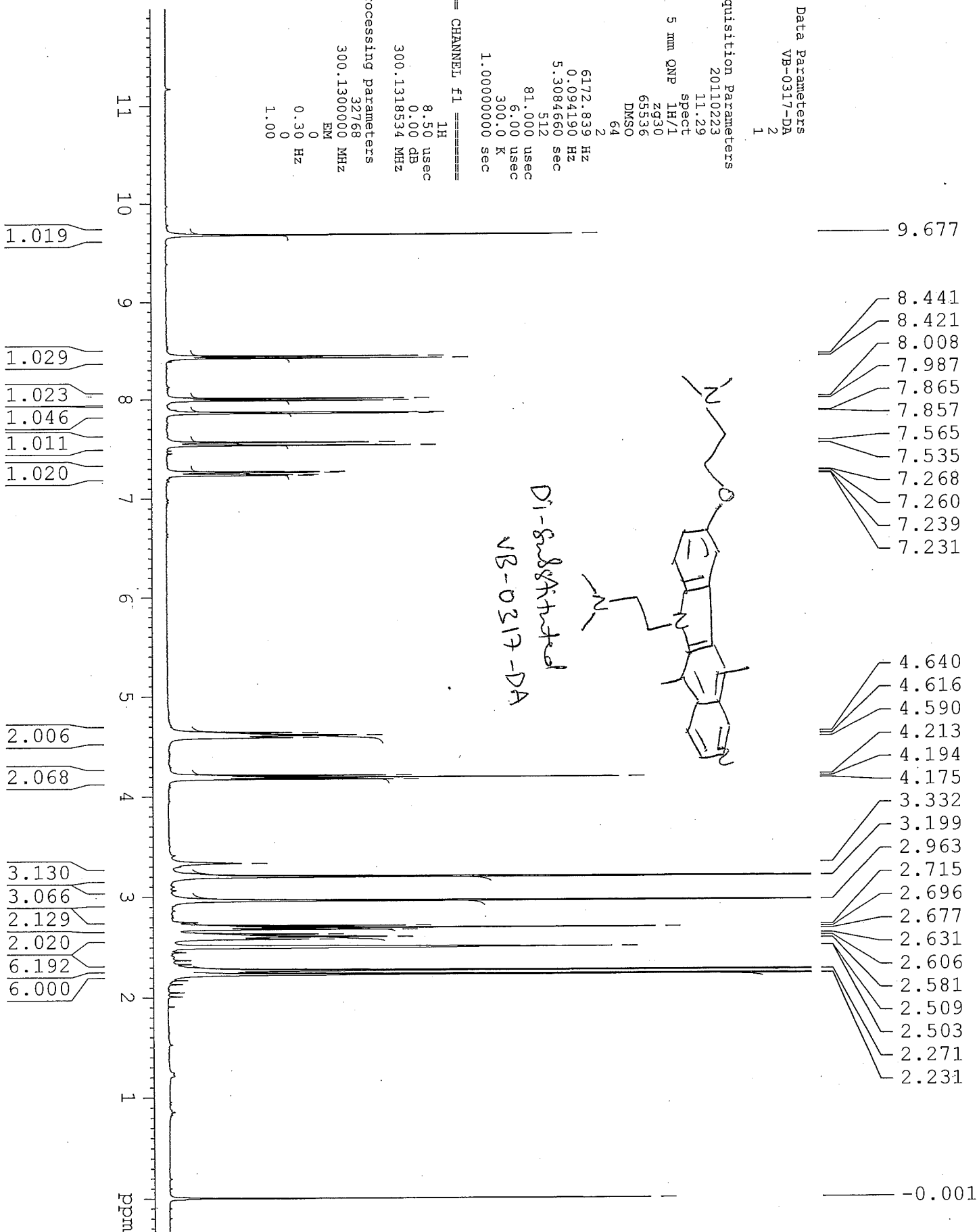
Current Data Parameters
 NAME VB-0317-DA
 EXPNO 2
 PROCNO 1

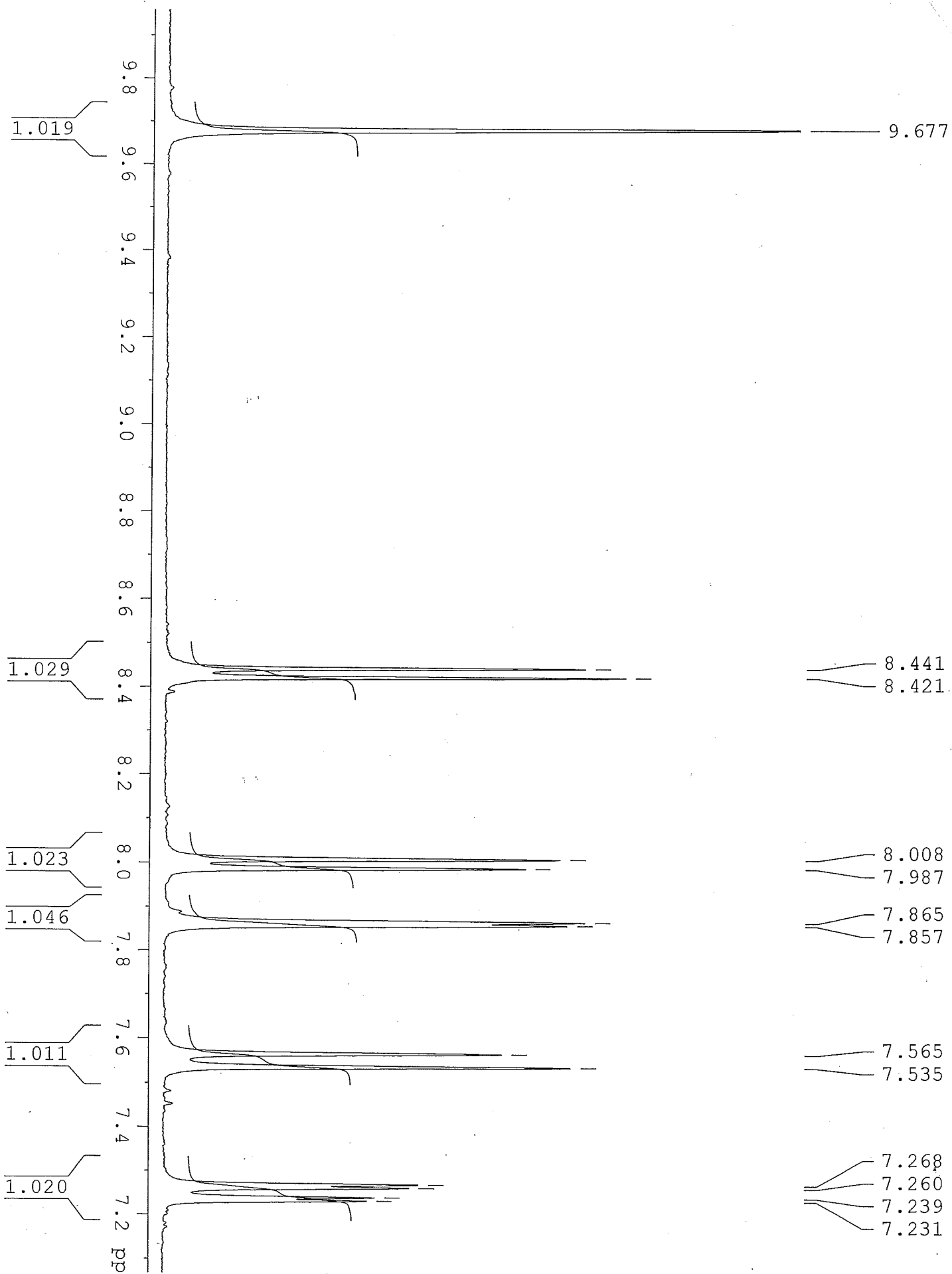
F2 - Acquisition Parameters
 Date_ 20110223
 Time_ 11.29

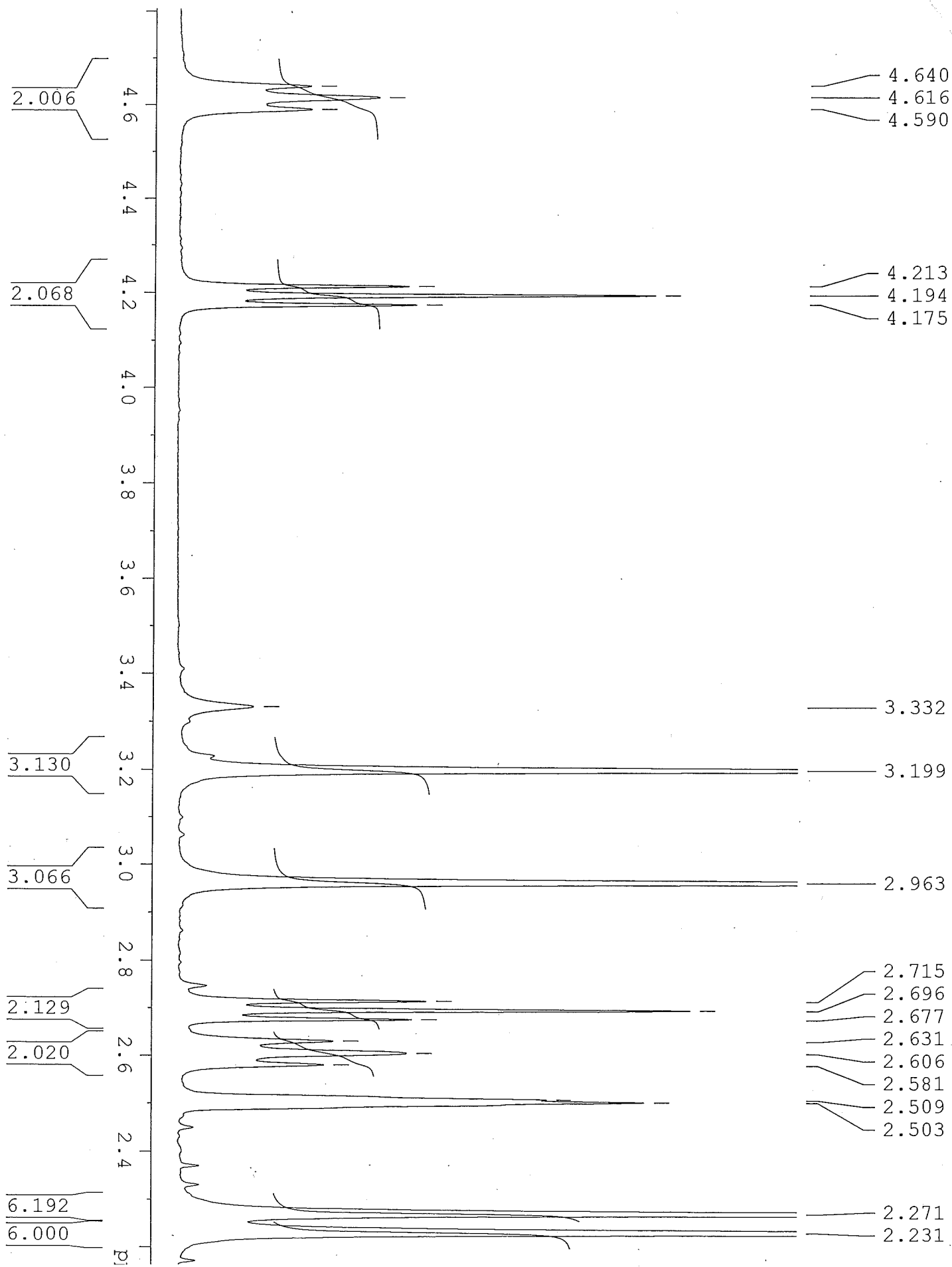
INSTRUM spect
 PROBD 5 mm QNP 1H/1
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 64
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.308460 sec
 RG 512
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.0000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 8.50 usec
 PL 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-0317-DA
 EXENO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110223
 Time 13.28

INSTRUM spect
 PROBD 5 mm QNP 1H/1
 PULPROG zgpg30

TD 65536
 SOLVENT CDCl3
 NS 18000

DS 4
 SMH 17985.611 Hz
 FIDRES 0.274439 Hz

RG 1.8219508 sec
 DW 812.7
 DE 27.800 usec

TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec

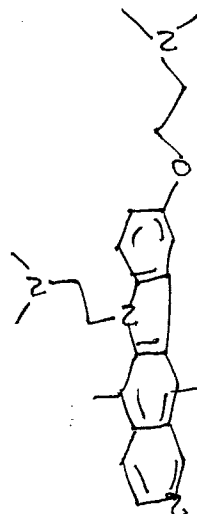
===== CHANNEL f1 =====
 NUC1 13C
 P1 6.00 usec
 PL1 2.00 dB
 SFO1 75.4752653 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCDP2 80.00 usec
 PL2 0.00 dB
 PL12 19.47 dB
 PL13 19.00 dB
 SFO2 300.1312005 MHz

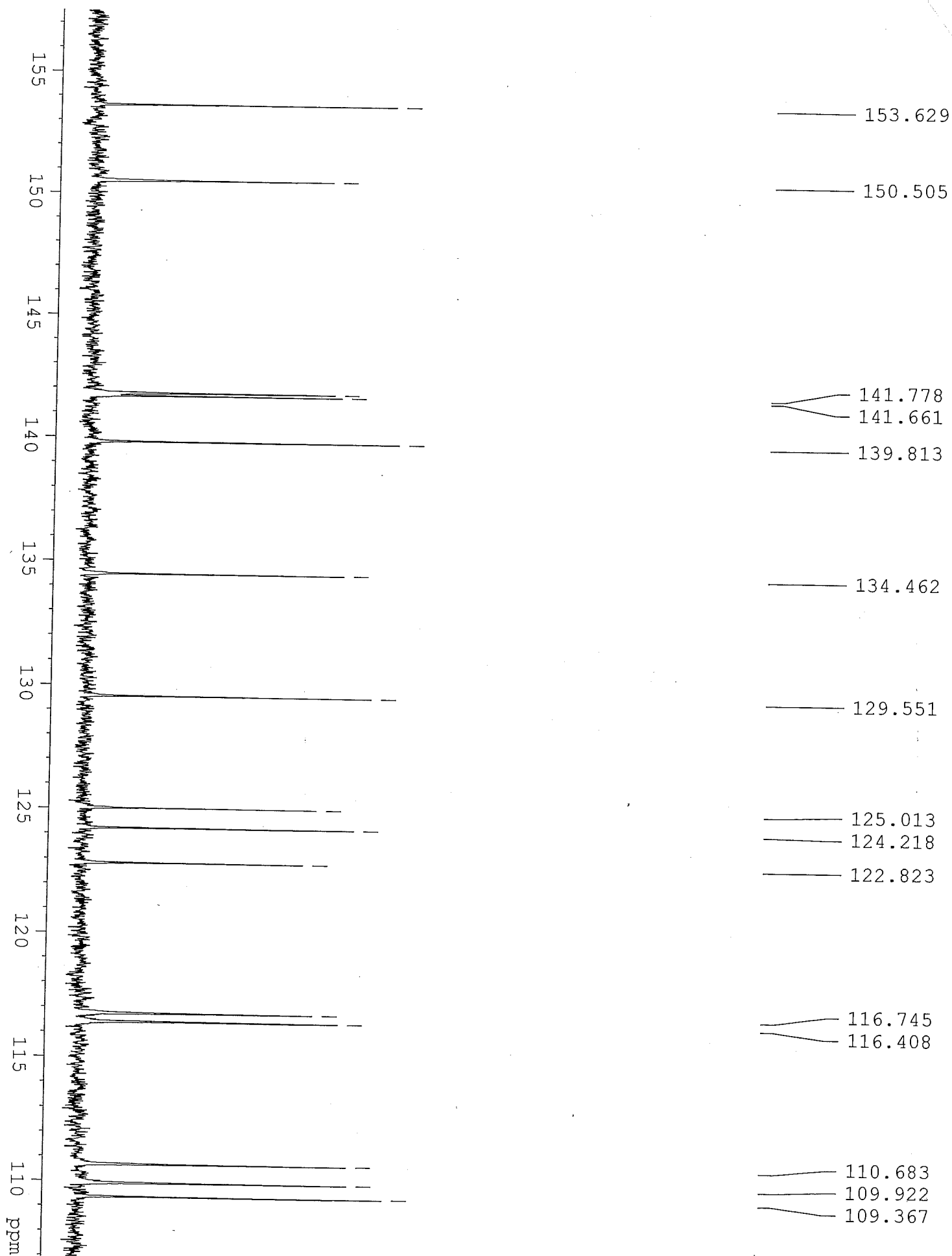
F2 - Processing parameters
 SI 32768
 SF 75.4677190 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

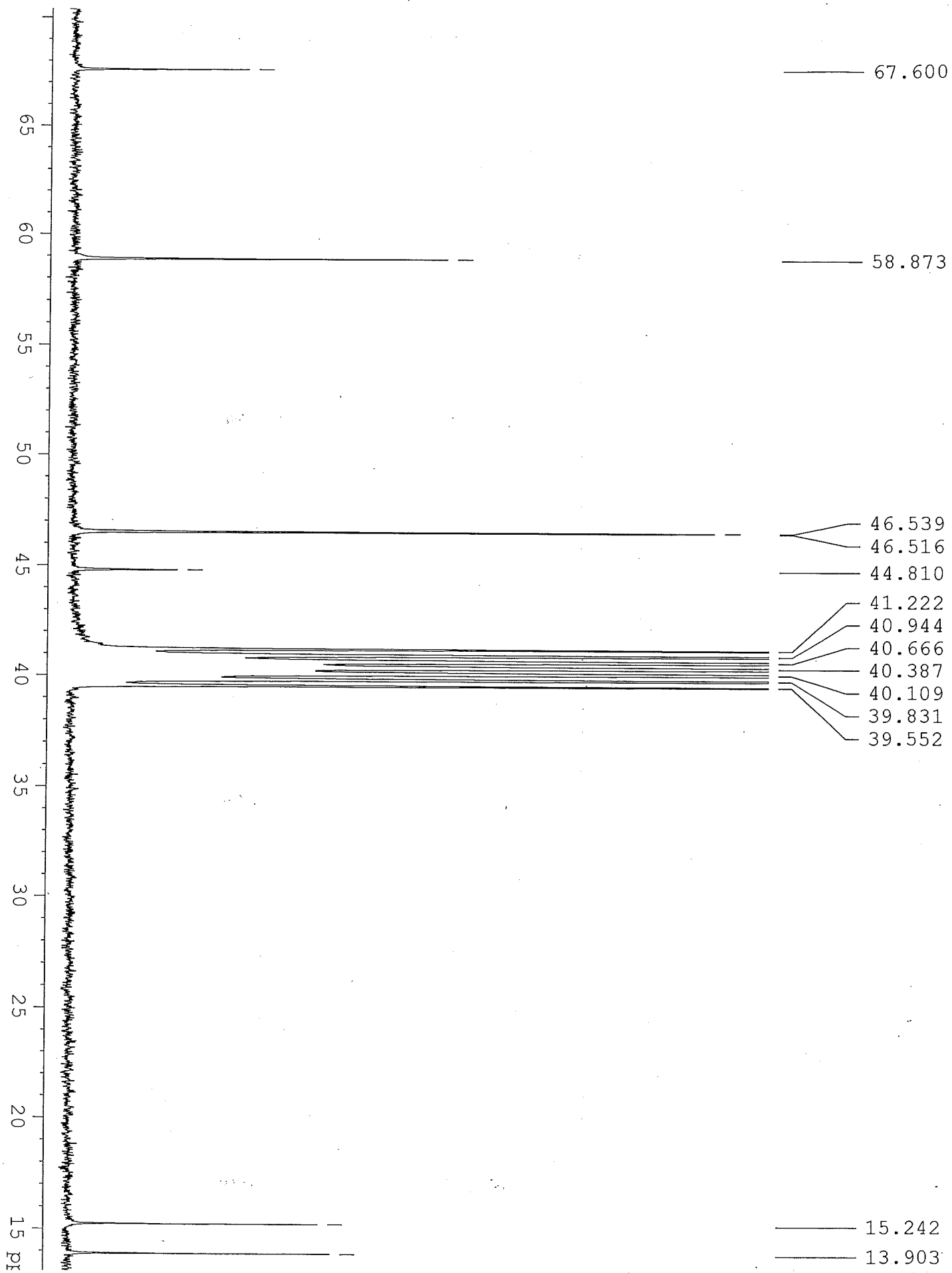
153.629
 150.505
 141.778
 141.661
 139.813
 134.462
 129.551
 125.013
 124.218
 122.823
 116.745
 116.408
 110.683
 109.922
 109.367

67.600
 58.873
 46.539
 46.516
 44.810
 41.222
 40.944
 40.666
 40.387
 40.109
 39.831
 39.552
 15.242
 13.903
 0.966

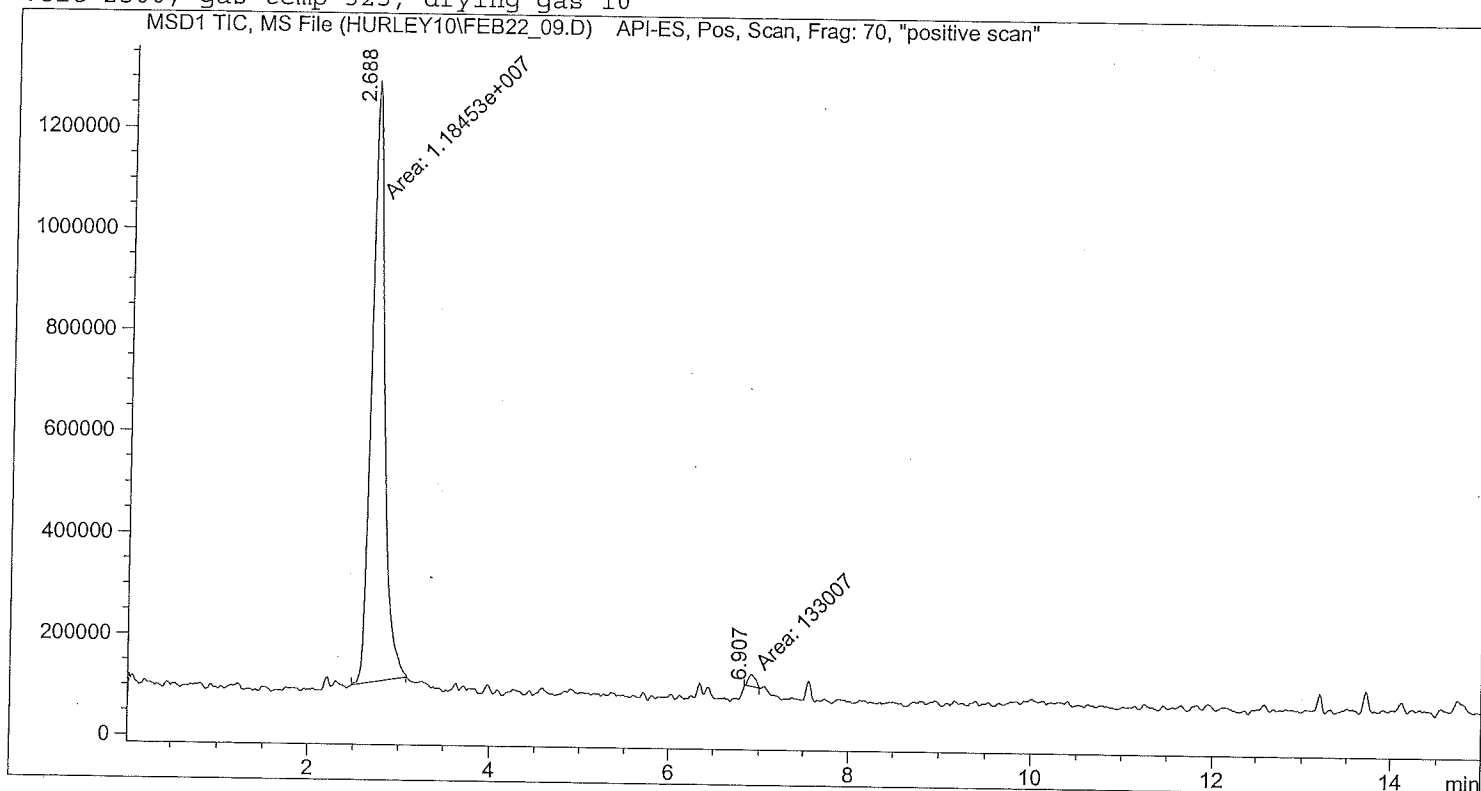


170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm





=====
Injection Date : 2/22/2011 3:39:59 PM
Sample Name : VB-GSA0316-DA-Y2 Location : Vial 6
Acq. Operator : Karen Inj : 1
Acq. Instrument : Instrument 1 Inj Volume : 0.1 µl
Method : C:\HPCHEM\1\METHODS\LC_MS_UV.M
Last changed : 2/22/2011 2:45:41 PM by Karen
Zorbax SB C18, 150 x 4.6, 3.5µ, 17/83/0.25, MeOH/water/formic, POS, 150-500; frag 70; 35C, cap
volt 2500, gas temp 325; drying gas 10
=====



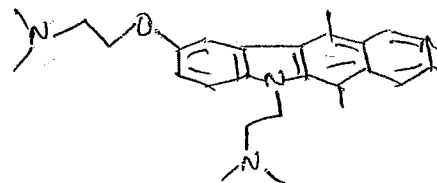
=====
Area Percent Report
=====

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

Signal 1: MSD1 TIC, MS File

Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	2.688	MM	0.1654	1.18453e7	1.19327e6	98.8896
2	6.907	MM	0.0928	1.33007e5	2.38938e4	1.1104

Totals : 1.19783e7 1.21717e6



VB-0317-DA

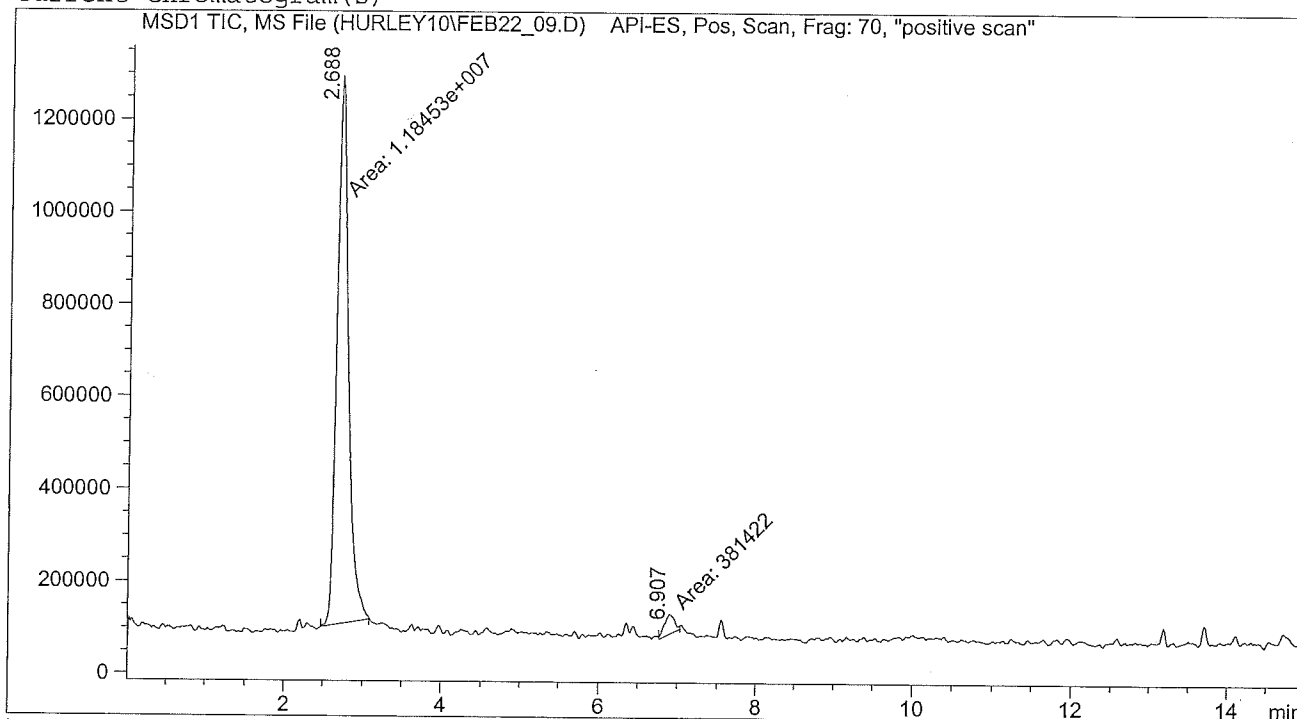
Di-substituted

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

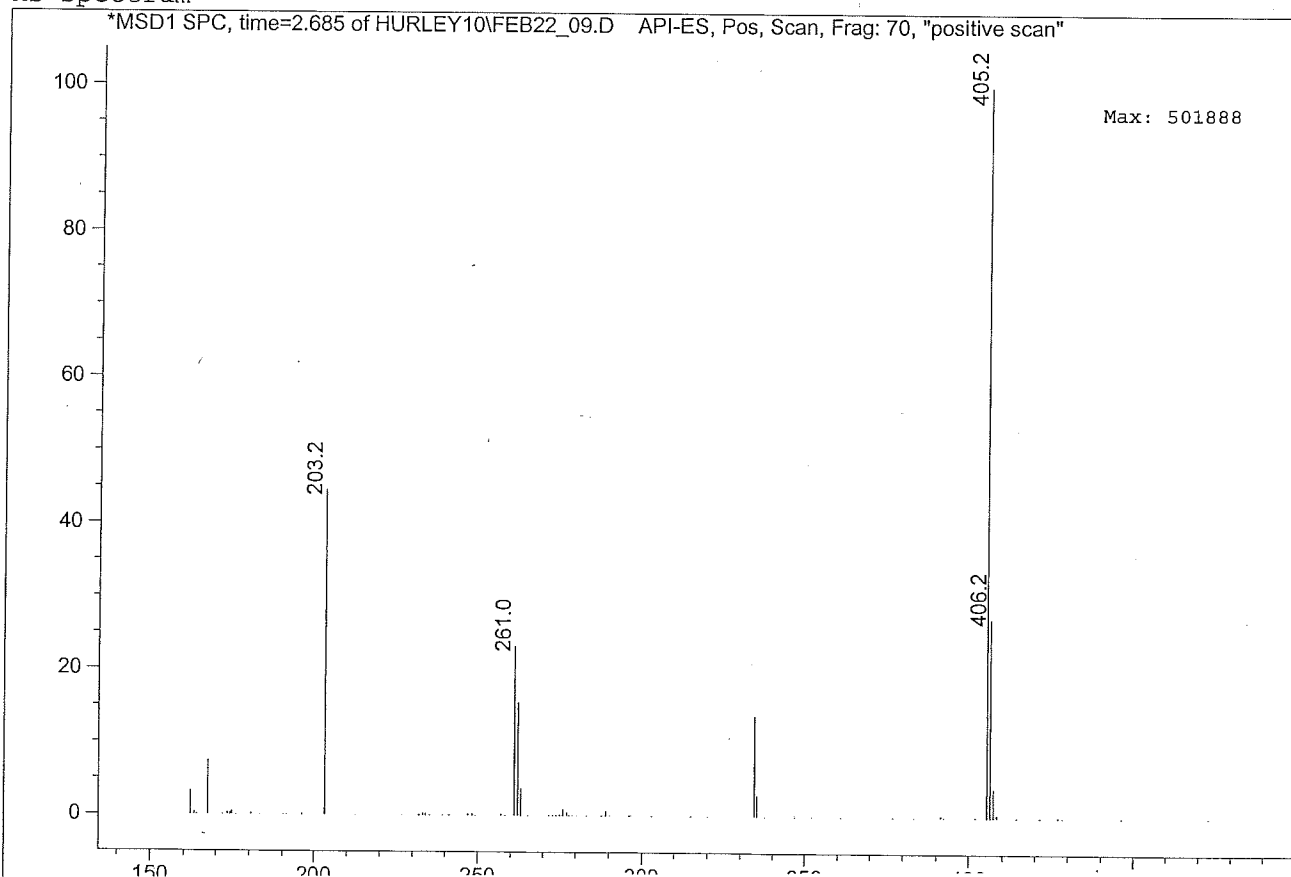
all graphic windows

=====
ion Date : 2/22/2011 3:39:59 PM
e Name : VB-GSA0316-DA-Y2 Location : Vial 6
Operator : Karen Inj : 1
Instrument : Instrument 1 Inj Volume : 0.1 μ l
Method : C:\HPCHEM\1\METHODS\LC_MS_UV.M
Last changed : 2/22/2011 2:45:41 PM by Karen
Agilent 1100B, Agilent SB C18, 150 x 4.6, 3.5 μ m, 17/83/0.25, MeOH/water/formic, POS, 150-500; frag 70; 35C, cap
voltage 2500, gas temp 325; drying gas 10

Current Chromatogram(s)



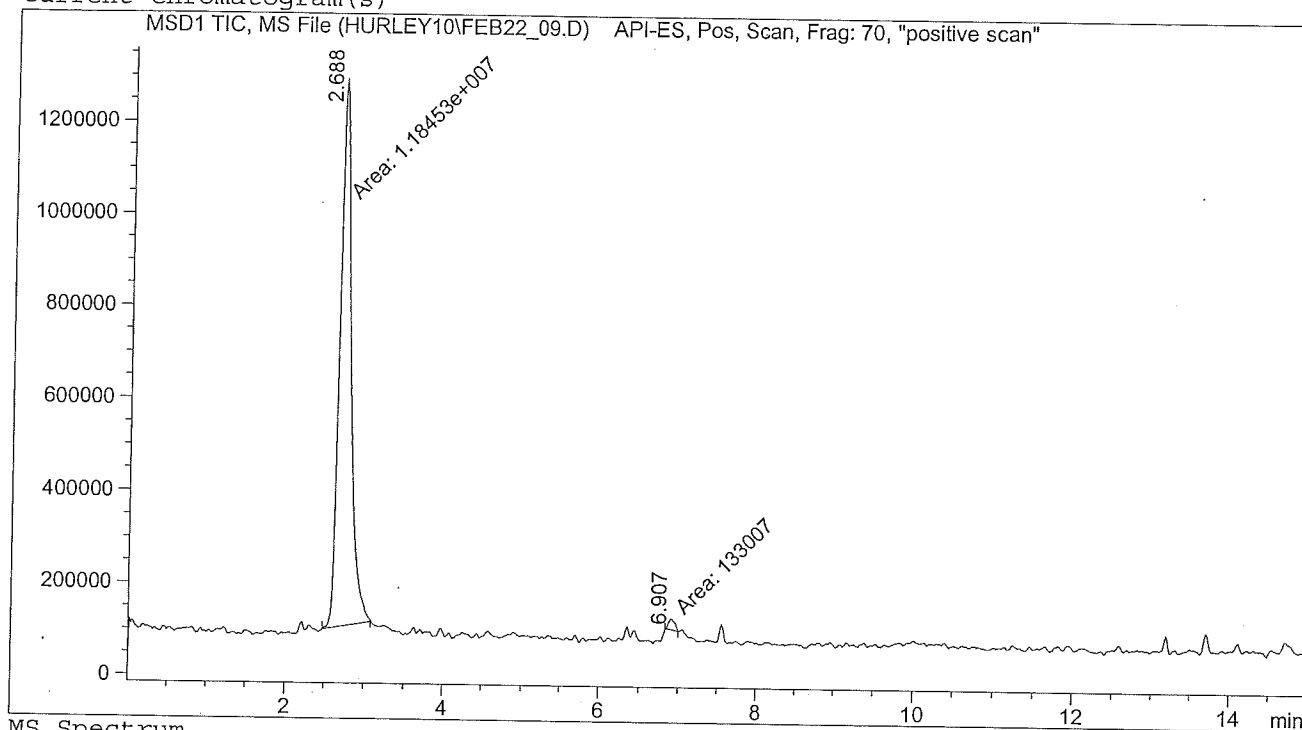
MS Spectrum



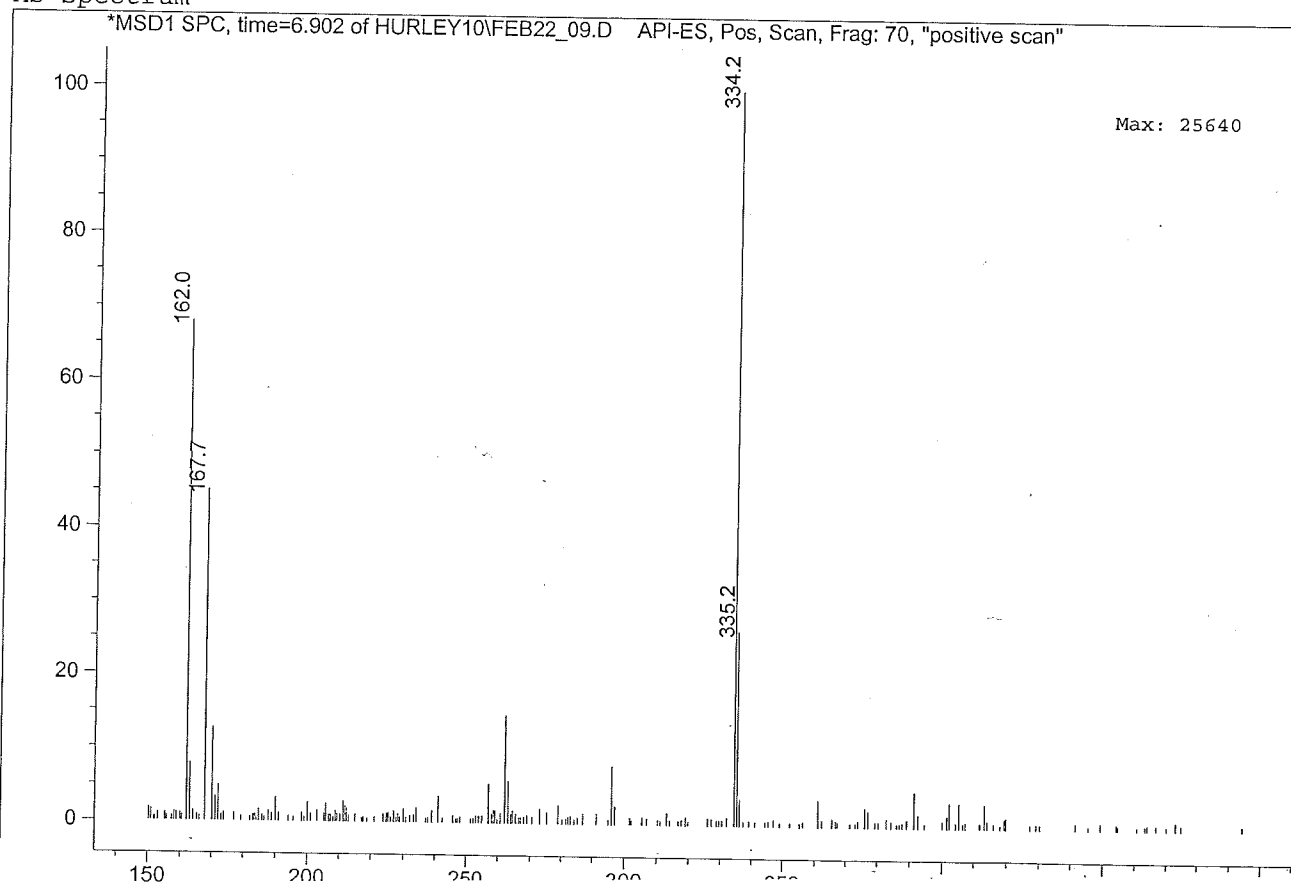
all graphic windows

=====
ion Date : 2/22/2011 3:39:59 PM
Sample Name : VB-GSA0316-DA-Y2 Location : Vial 6
Operator : Karen Inj : 1
Instrument : Instrument 1 Inj Volume : 0.1 μ l
Method : C:\HPCHEM\1\METHODS\LC_MS_UV.M
Last changed : 2/22/2011 2:45:41 PM by Karen
Corbax SB C18, 150 x 4.6, 3.5u, 17/83/0.25, MeOH/water/formic, POS, 150-500; frag 70; 35C,
cap volt 2500, gas temp 325; drying gas 10

Current Chromatogram(s)



MS Spectrum



Generic Display Report

Analysis Info

Analysis Name
Method
Sample Name
Comment

D:\DATA\Facility_Feb_11\VB_0317_DA_000001.d
ESL_101506
VB_0317_DA
Venkat B., positive mode, ACN:MeOH

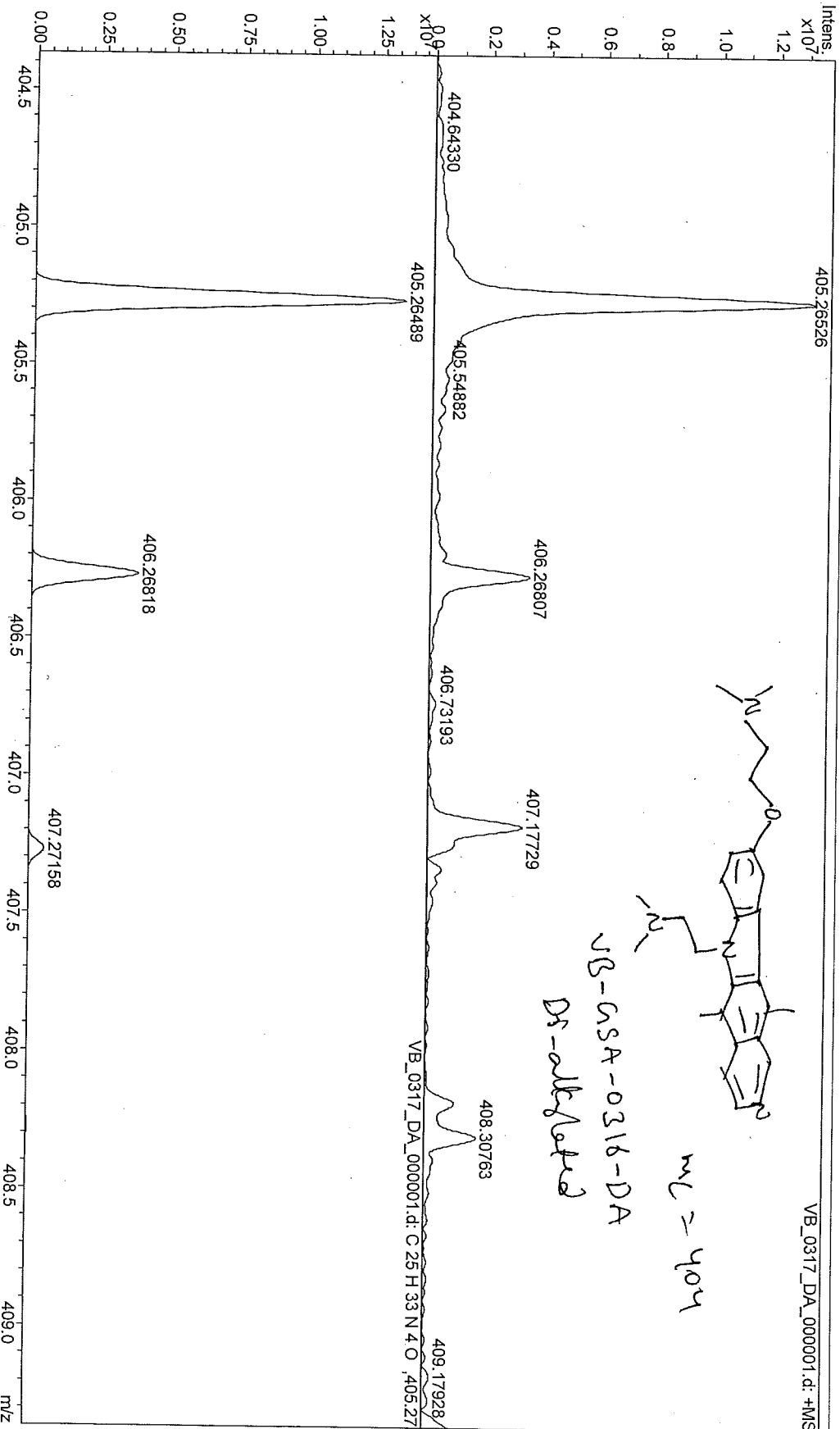
Acquisition Date

2/25/2011 10:08:14 AM

Operator

Instrument

apex-Ultra



SmartFormula Manually



Min

C₁₇H₃₀N₃O₁

Generate

Max

C 17-n, H 30-n, N 3-n, O 1-n

Help

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

Measured m/z 405.26526

Tolerance 5

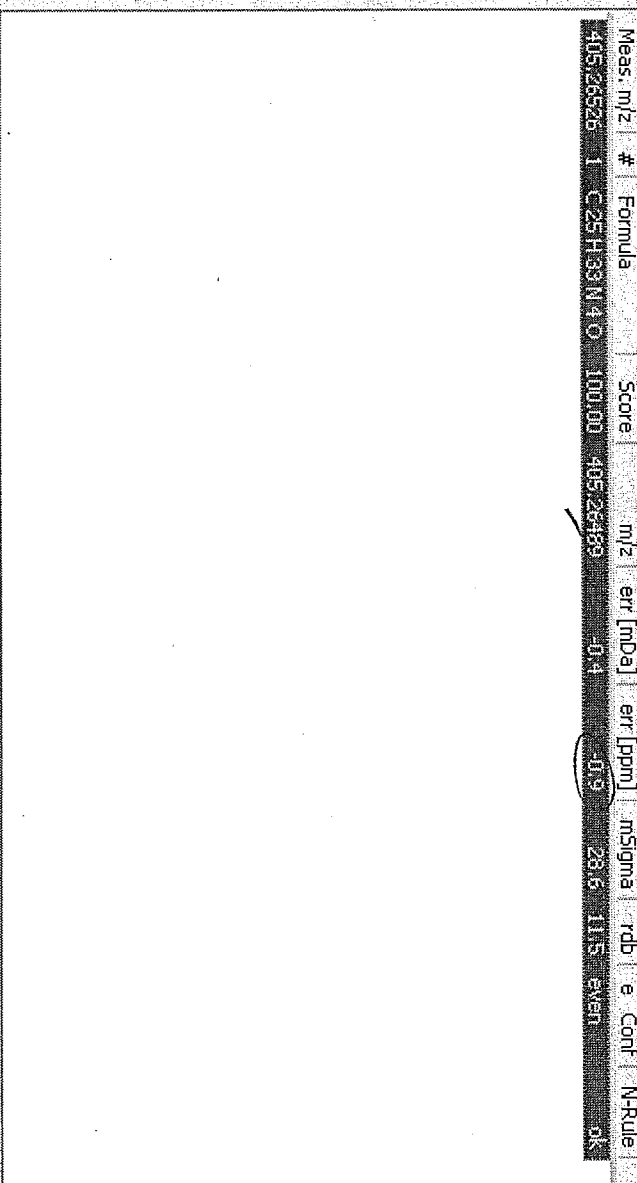
ppm

Charge

1



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdB	e ⁻ Conf	N-Rule
405.26526	1	C ₂₅ H ₃₃ N ₄ O	100.00	405.26489	-0.4	-0.9	28.6	11.5	even	ok



☐ 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

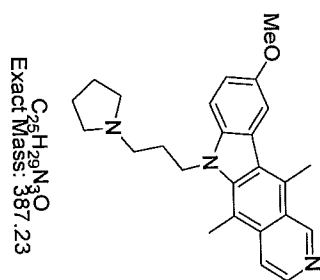
Show Pattern

9.696

8.512
8.492
7.911
7.899
7.435
7.405
7.281
7.221
7.214
7.191
7.185

4.630
4.607
4.582
4.065
3.982

3.248
2.988
2.553
2.531
2.507
2.140
2.116
2.093
2.068
2.044
1.825



1.000

1.065

2.174

1.174

1.063

2.167

3.226

3.369

3.241

6.426

2.326

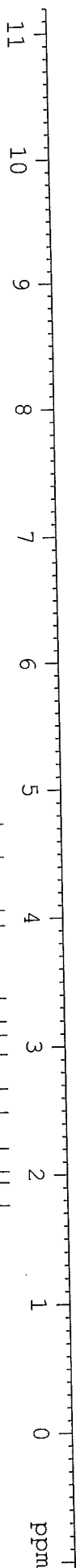
4.265

Current Data Parameters
 NAME CV-GSA-02112
 EXPNO 1
 PROCNO 1

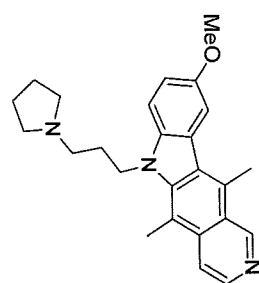
F2 - Acquisition Parameters
 Date_ 20110422
 Time 16.38
 INSTRUM spect
 PROBD 5 mm QNP 1H/1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 456.1
 DE 81.000 usec
 TE 300.0 K
 D1 1.00000000 sec

===== 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



9.696



C₂₅H₂₈N₃O
Exact Mass: 387.23

8.512
8.492

7.911
7.899

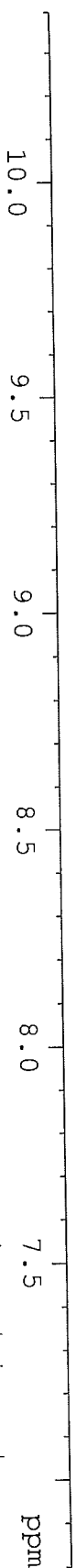
7.435
7.405
7.281
7.221
7.214
7.191
7.185

Current Data Parameters
NAME CV-GSA-02112
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110422
Time 16.38
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 456.1
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.0000000 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



4.630
4.607
4.582

4.065
3.982

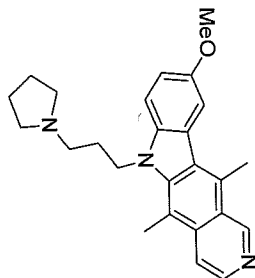
3.248

2.988

2.553
2.531
2.507

2.140
2.116
2.093
2.068
2.044

1.825



$C_{26}H_{29}N_3O$
Exact Mass: 387.23

Current Data Parameters
NAME CV-GSA-02112
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110422
Time 16.38
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 456.1
DE 81.000 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

2.167

3.226

3.369

3.241

6.426

2.326

4.265

ppm

154.264
150.195
141.914
141.438
139.881
134.776
129.368
125.329
124.723
122.926
116.281
114.811
109.787
109.311
108.858

77.855
77.431
77.008

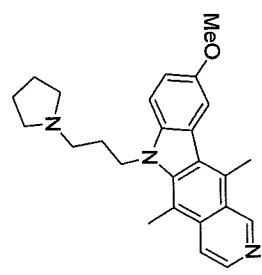
56.687
54.533
53.614

44.406

29.593

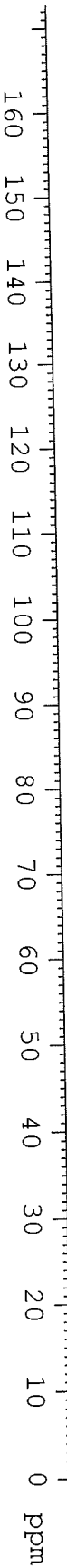
23.895

15.109
13.993



$C_{20}H_{20}N_2O$
Exact Mass: 387.23

CDCl₃



Current Data Parameters
NAME CV-GSA-02112
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110423
Time_ 8.41

INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 8192
DE 27.800 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.0002000 sec

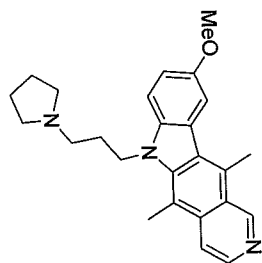
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec

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

CHANNEL f1
=====

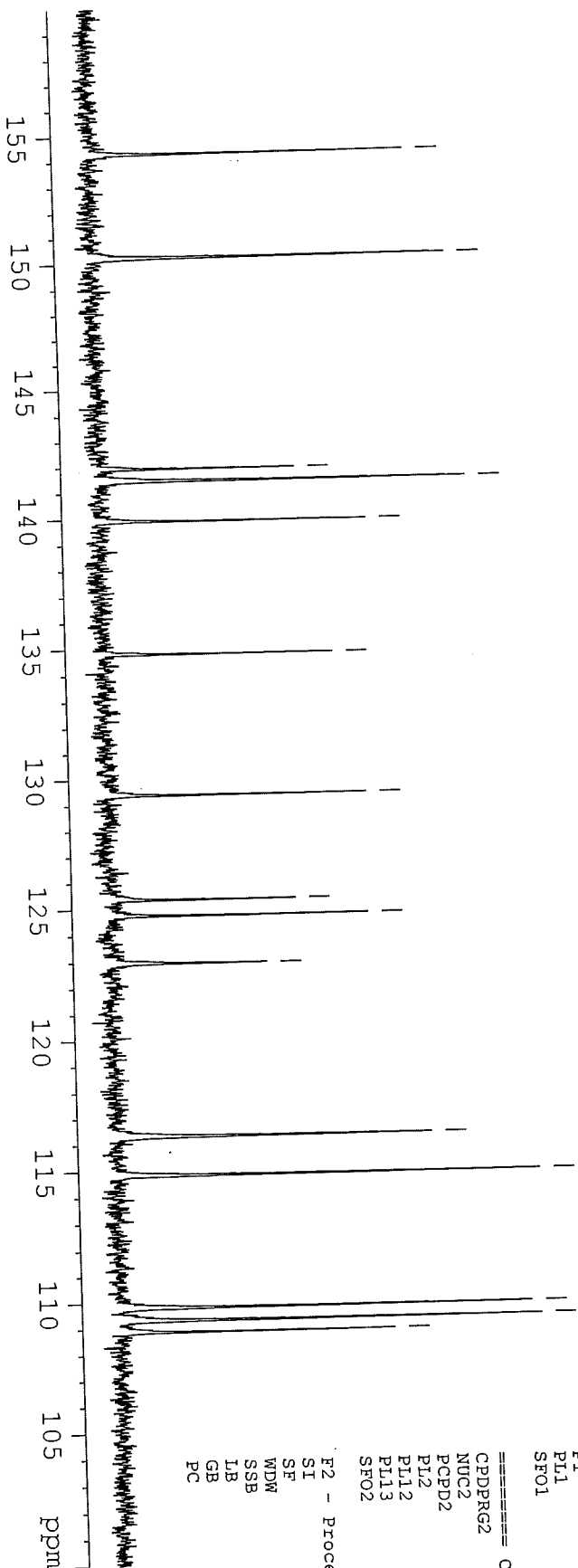
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 19.47 dB
PL13 19.00 dB
SFO2 300.1312005 MHz

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



$C_{25}H_{26}N_2O$
Exact Mass: 387.23

154.264
150.195
141.914
141.438
139.881
134.776
129.368
125.329
124.723
122.926
116.281
114.811
109.787
109.311
108.858



Current Data Parameters
NAME CV-GSA-02112
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20110423
Time_ 8.41
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 8192
DE 27.800 usec
TE 6.00 usec
D1 300.0 K
d11 2.00000000 sec
d12 0.03000000 sec
d13 0.0002000 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

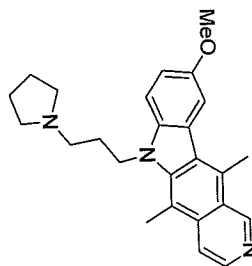
56.687
54.533
53.614

44.406

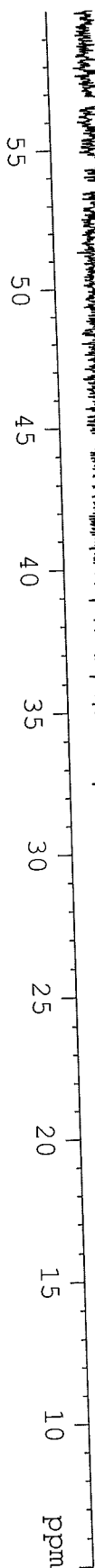
29.593

23.895

15.109
13.993



$C_{25}H_{29}N_3O$
Exact Mass: 387.23



Current Data Parameters
NAME CV-GSA-02112
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20110423
Time 8.41

INSTRUM spect
PROBHD 5 mm QNP 1H/1

PULPROG zgpg30
TD 65536

CDCL3
SOLVENT 15000

DS 4
SWH 17985.611 Hz

FIDRES 0.274439 Hz
AQ 1.8219508 sec

RG 8192
DW 27.800 usec

DE 6.00 usec
TE 300.0 K

D1 2.0000000 sec
d11 0.0300000 sec

d12 0.0002000 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

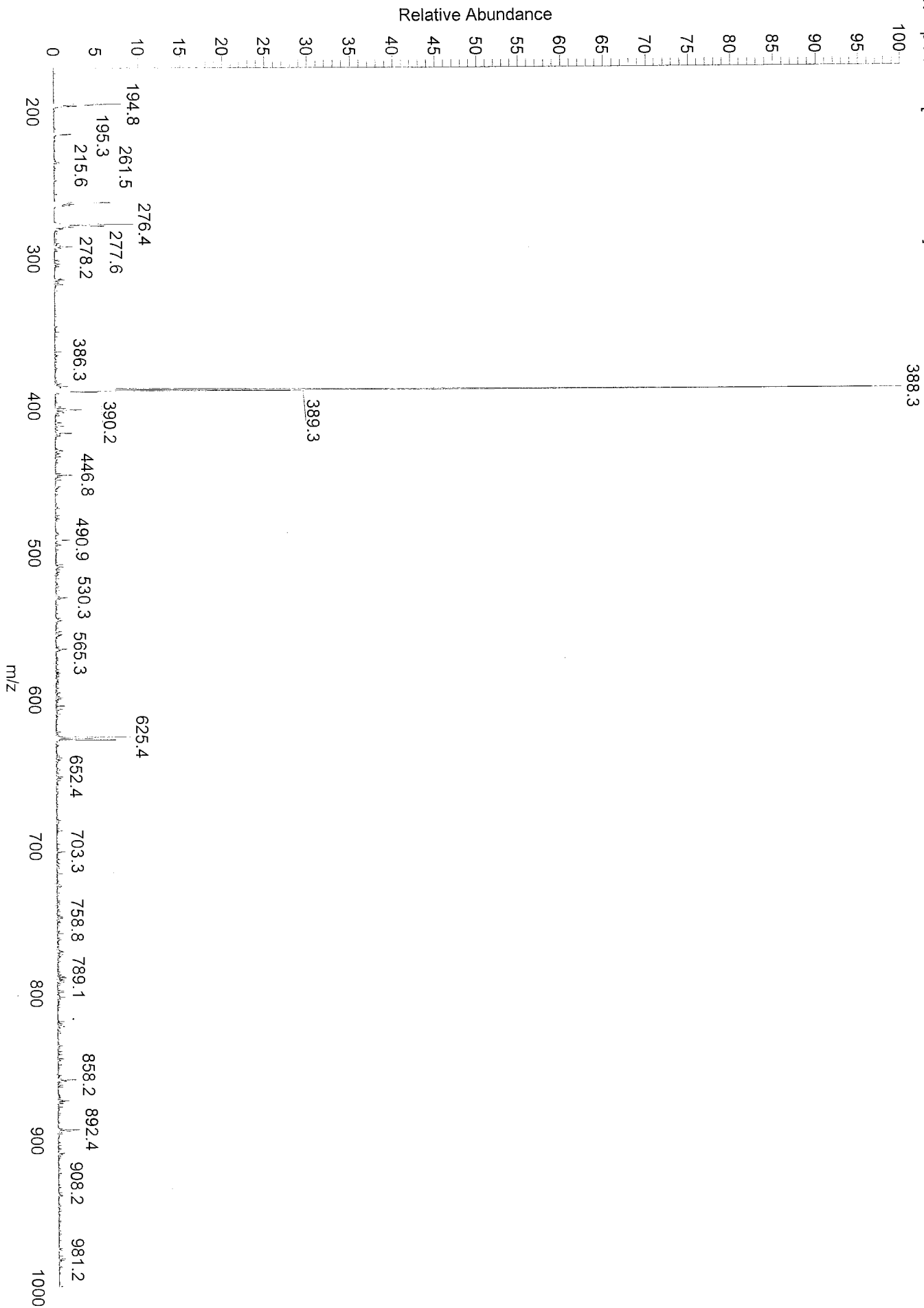
SSB 0
LB 1.00 Hz

GB 0
PC 1.00

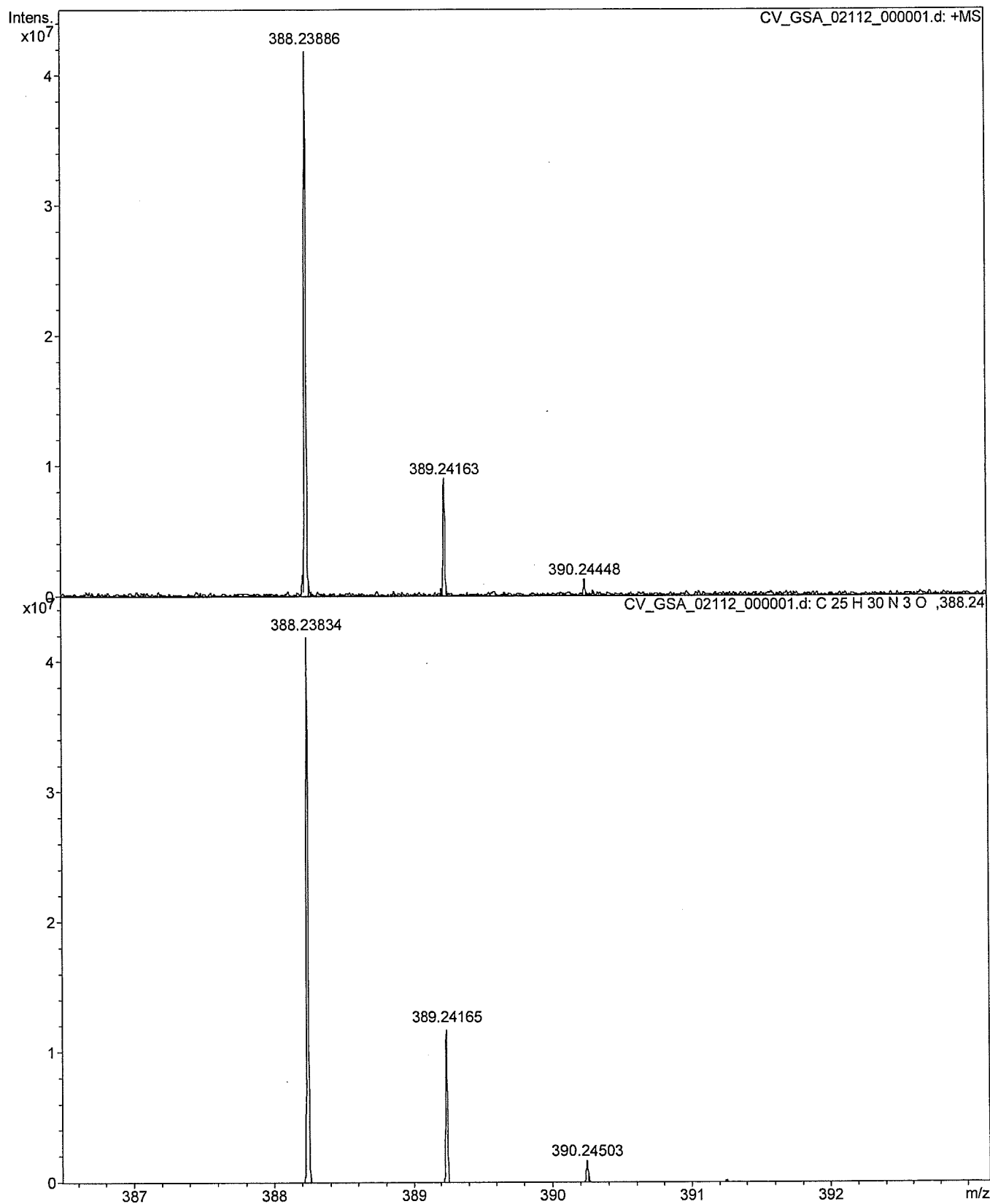
V. Chappeta, ACN:MeOH 1:1

CV_GSA_02122 #51-58 RT: 1.01-1.13 AV: 8 NL: 2.72E7

T: + p Full ms [170.00-1000.00]



Generic Display Report (all)



Min

Max

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

Measured m/z Tolerance mDa Charge

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
388.23886	1	C 13 H 34 N 5 O 8	78.04	388.24019	1.3	3.4	30.3	-0.5	even	ok
	2	C 25 H 30 N 6 O	100.00	388.23884	-0.5	-1.3	38.3	12.5	even	ok

☐ Automatically locate monoisotopic peak Maximum number of formulas

☒ Check rings plus double bonds Minimum Maximum

Electron configuration

☒ Filter H/C element ratio Minimum H/C Maximum H/C

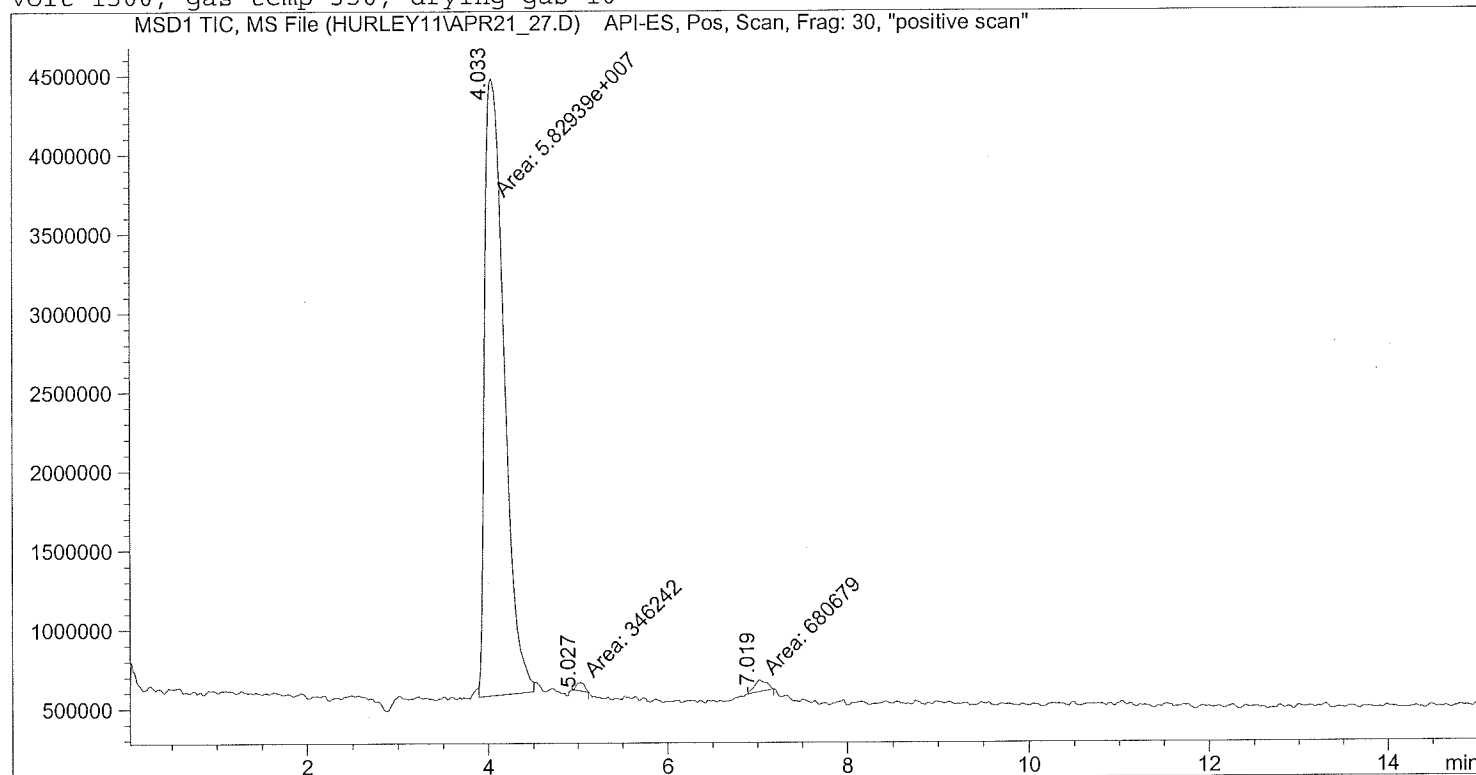
☒ Estimate carbon number ☒ Generate immediately

```

=====
Injection Date   : 4/21/2011 5:04:20 PM
Sample Name      : CV-GSA-02112
Acq. Operator    : Karen
Acq. Instrument  : Instrument 1
Acq. Method      : C:\HPCHEM\1\METHODS\LC_MS_UV.M
Last changed     : 4/21/2011 5:00:29 PM by Karen
Analysis Method  : C:\HPCHEM\1\METHODS\LC_MS_UV.M
Last changed     : 4/21/2011 5:18:10 PM by Karen
                  (modified after loading)

```

Zorbax SB C18, 150 x 4.6, 3.5u, 45/55/0.25, MeOH/water/formic, POS, 150-500; frag 30; 30C, cap
voltage 1500, 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 [min]	Type	Width [min]	Area	Height	Area %
1	4.033	MF	0.2490	5.82939e7	3.90198e6	98.2689
2	5.027	MM	0.1013	3.46242e5	5.69697e4	0.5837
3	7.019	MM	0.1483	6.80679e4	7.64851e4	1.1475

Totals : 5.93208e7 4.03543e6

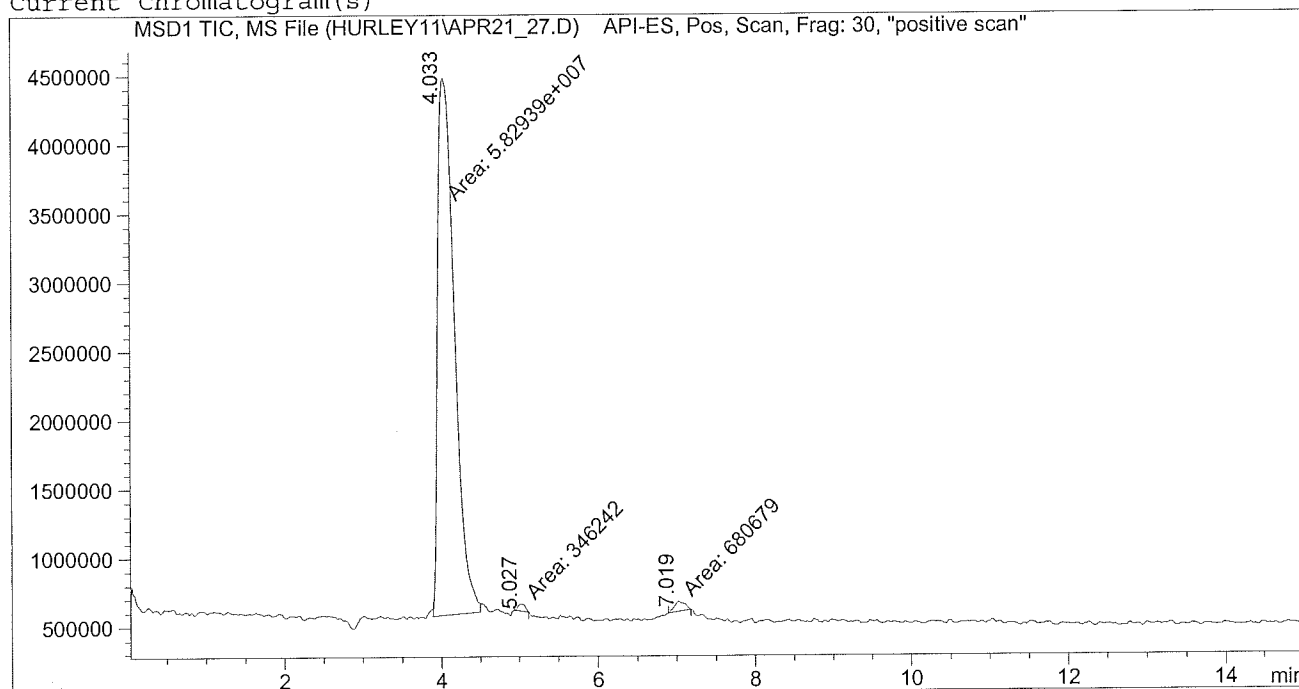
=====
*** End of Report ***

```

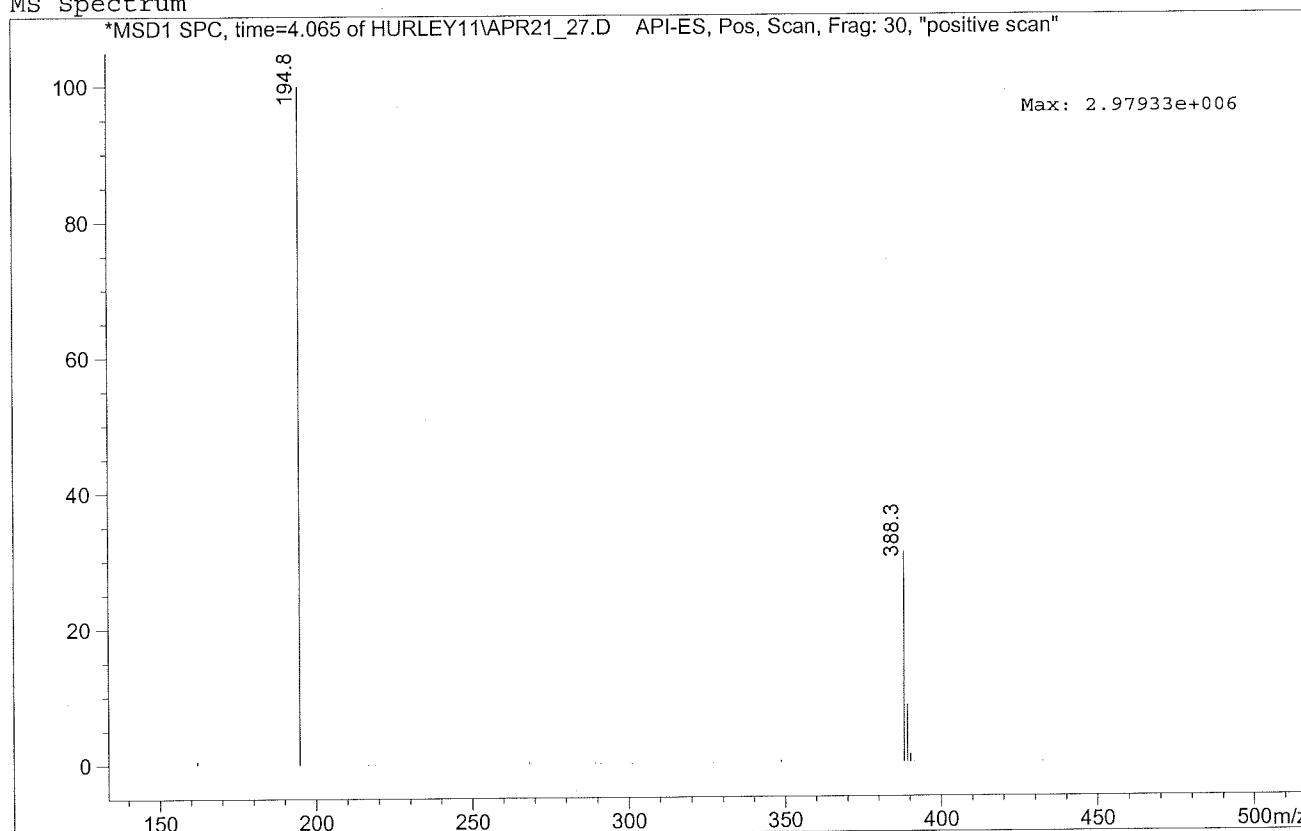
=====
Injection Date   : 4/21/2011 5:04:20 PM
Sample Name      : CV-GSA-02112
Acq. Operator    : Karen
Acq. Instrument  : Instrument 1
Acq. Method      : C:\HPCHEM\1\METHODS\LC_MS_UV.M
Last changed     : 4/21/2011 5:00:29 PM by Karen
Analysis Method  : C:\HPCHEM\1\METHODS\LC_MS_UV.M
Last changed     : 4/21/2011 5:18:10 PM by Karen
                  (modified after loading)
  
```

Zorbax SB C18, 150 x 4.6, 3.5u, 45/55/0.25, MeOH/water/formic, POS, 150-500; frag 30; 30C, cap volt 1500, gas temp 350; drying gas 10

Current Chromatogram(s)



MS Spectrum



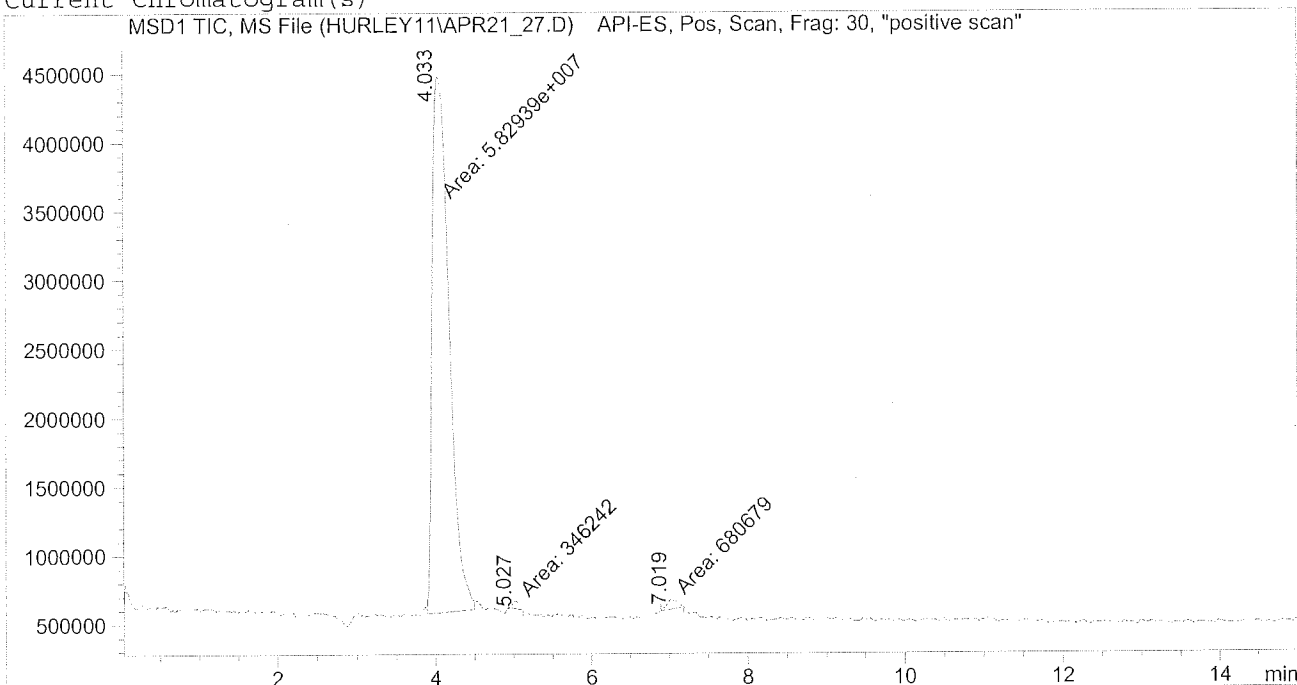
=====

Injection Date	: 4/21/2011 5:04:20 PM	Location	: Vial 121
Sample Name	: CV-GSA-02112	Inj	: 1
Acq. Operator	: Karen	Inj Volume	: 0.1 µl
Acq. Instrument	: Instrument 1		
Acq. Method	: C:\HPCHEM\1\METHODS\LC_MS_UV.M		
Last changed	: 4/21/2011 5:00:29 PM by Karen		
Analysis Method	: C:\HPCHEM\1\METHODS\LC_MS_UV.M		
Last changed	: 4/21/2011 5:18:10 PM by Karen		

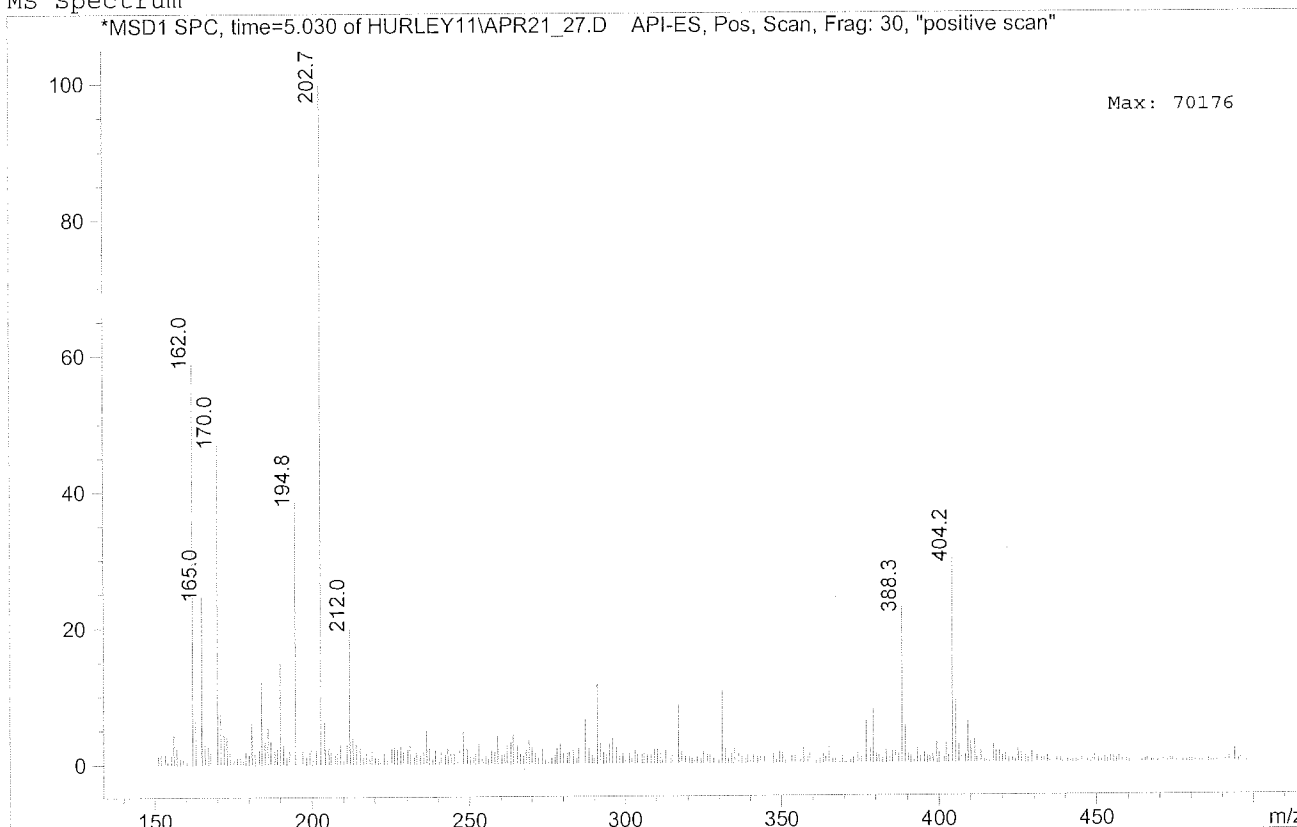
(modified after loading)

Zorbax SB C18, 150 x 4.6, 3.5µ, 45/55/0.25, MeOH/water/formic, POS, 150-500; frag 30; 30C, cap volt 1500, gas temp 350; drying gas 10

Current Chromatogram(s)



MS Spectrum

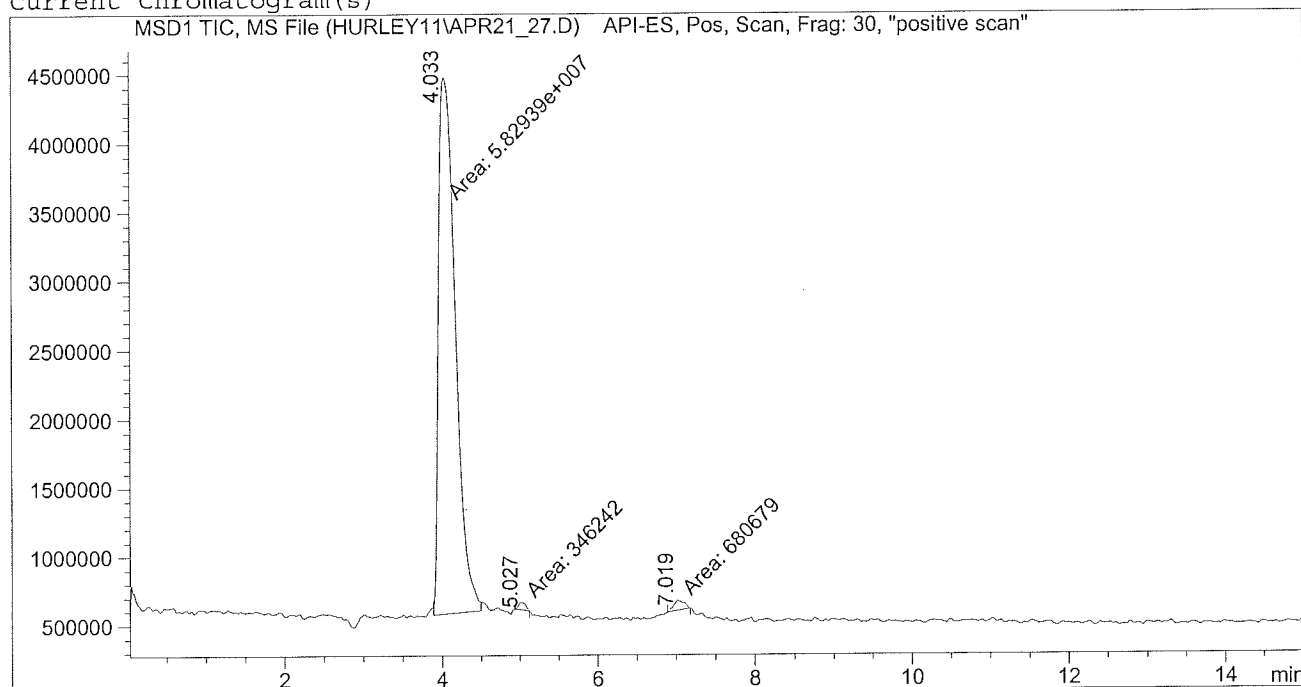



```

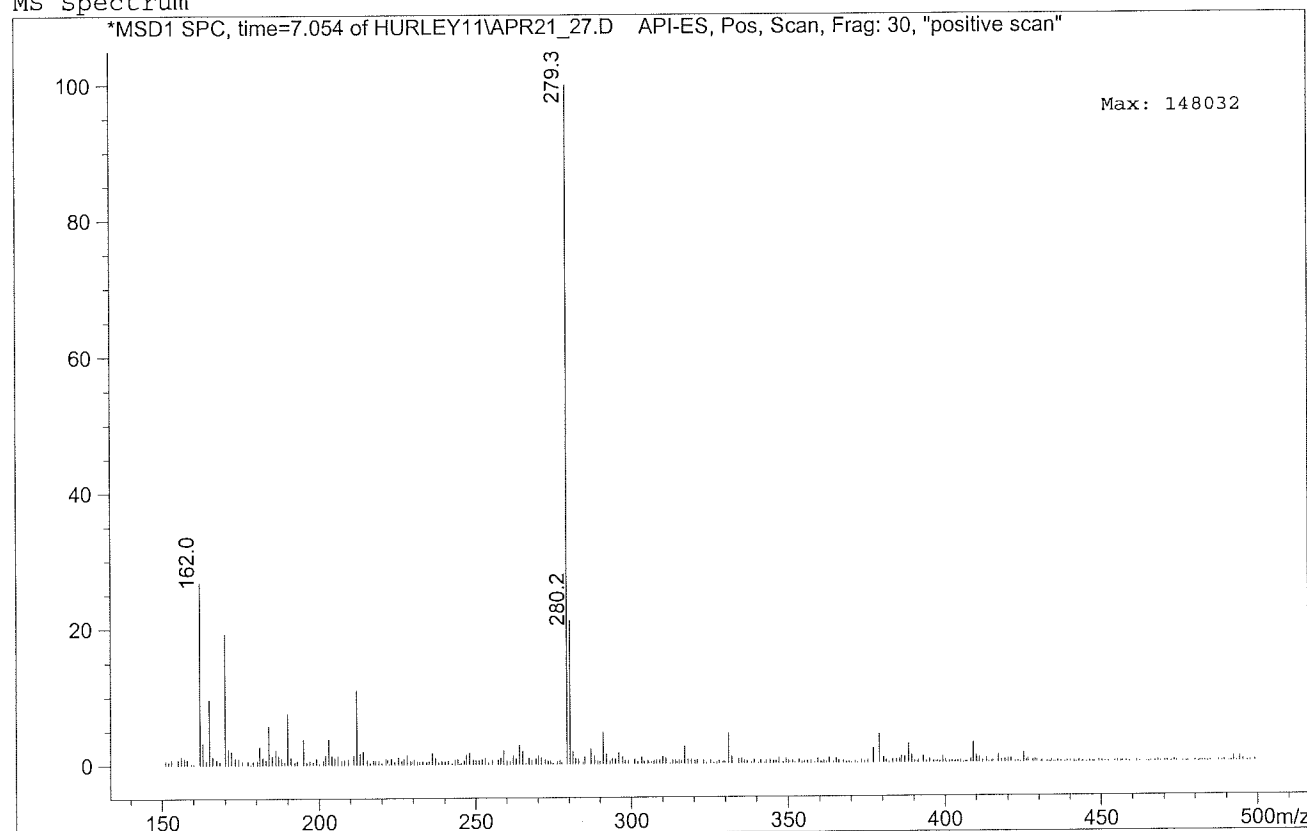
=====
Injection Date   : 4/21/2011 5:04:20 PM
Sample Name      : CV-GSA-02112
Location         : Vial 121
Acq. Operator    : Karen
Inj              : 1
Acq. Instrument  : Instrument 1
Inj Volume       : 0.1 µl
Acq. Method      : C:\HPCHEM\1\METHODS\LC_MS_UV.M
Last changed     : 4/21/2011 5:00:29 PM by Karen
Analysis Method  : C:\HPCHEM\1\METHODS\LC_MS_UV.M
Last changed     : 4/21/2011 5:18:10 PM by Karen
                  (modified after loading)
  
```

Zorbax SB C18, 150 x 4.6, 3.5µ, 45/55/0.25, MeOH/water/formic, POS, 150-500; frag 30; 30C, cap volt 1500, gas temp 350; drying gas 10

Current Chromatogram(s)



MS Spectrum



9.697

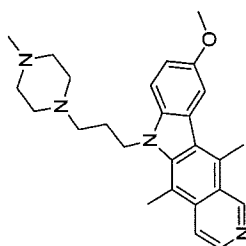
8.514
8.493
7.919
7.900
7.894
7.438
7.409
7.281
7.215
7.207
7.185
7.177

5.313

4.612
4.588
4.563

3.984

3.254
2.995
2.462
2.355
2.328
2.311
2.043
2.021
1.997
1.973



$C_{26}H_{32}N_4O$
Exact Mass: 416.2576

Current Data Parameters
NAME CV-GSA-02119
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110527
Time 14.31
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 456.1
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

1.000

1.017

2.119

1.115

1.005

2.173

3.055

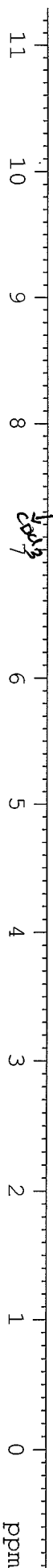
3.156

3.217

8.124

5.318

2.260

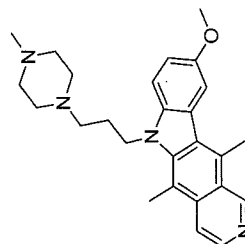


9.697

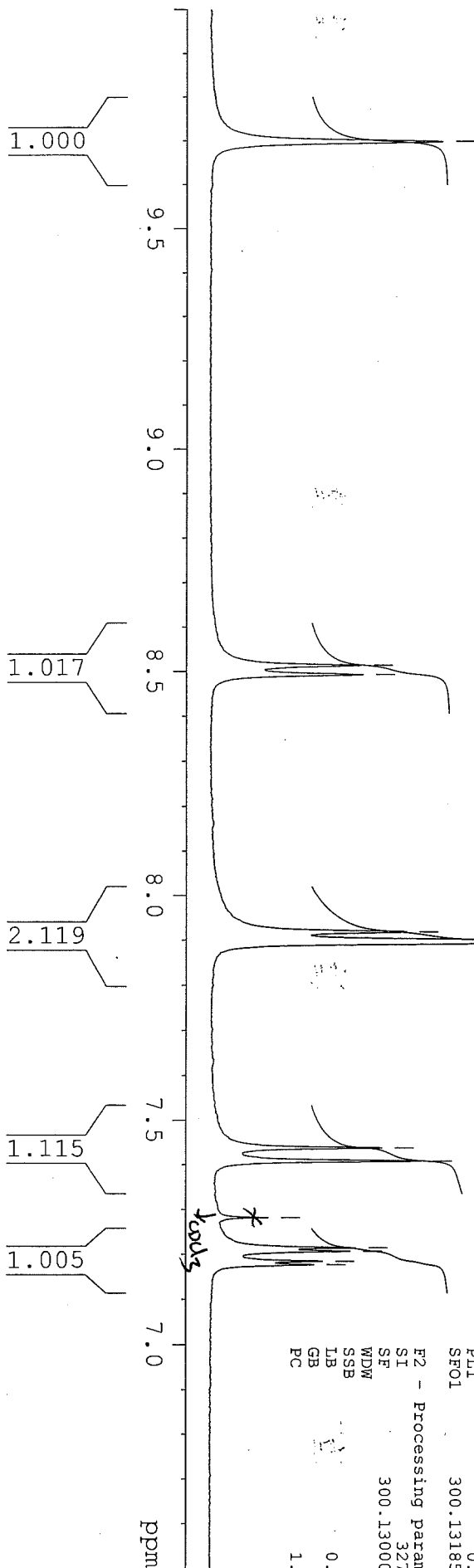
8.514
8.493

7.919
7.900
7.894

7.438
7.409
7.281
7.215
7.207
7.185
7.177



$C_{26}H_{32}N_4O$
Exact Mass: 416.2576



Current Data Parameters
NAME CV-GSA-02119
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110527
Time 14.31
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 456.1
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

4.612
4.588
4.563

3.984

3.254

2.995

2.462

2.355

2.328

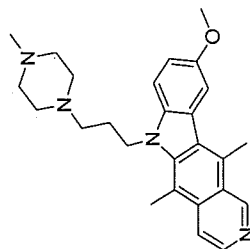
2.311

2.043

2.021

1.997

1.973



C₂₆H₃₂N₄O
Exact Mass: 416.2576

Current Data Parameters
NAME CV-GSA-02119
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110527
Time 14.31
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 2930
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 456.1
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

2.173

3.055

3.156

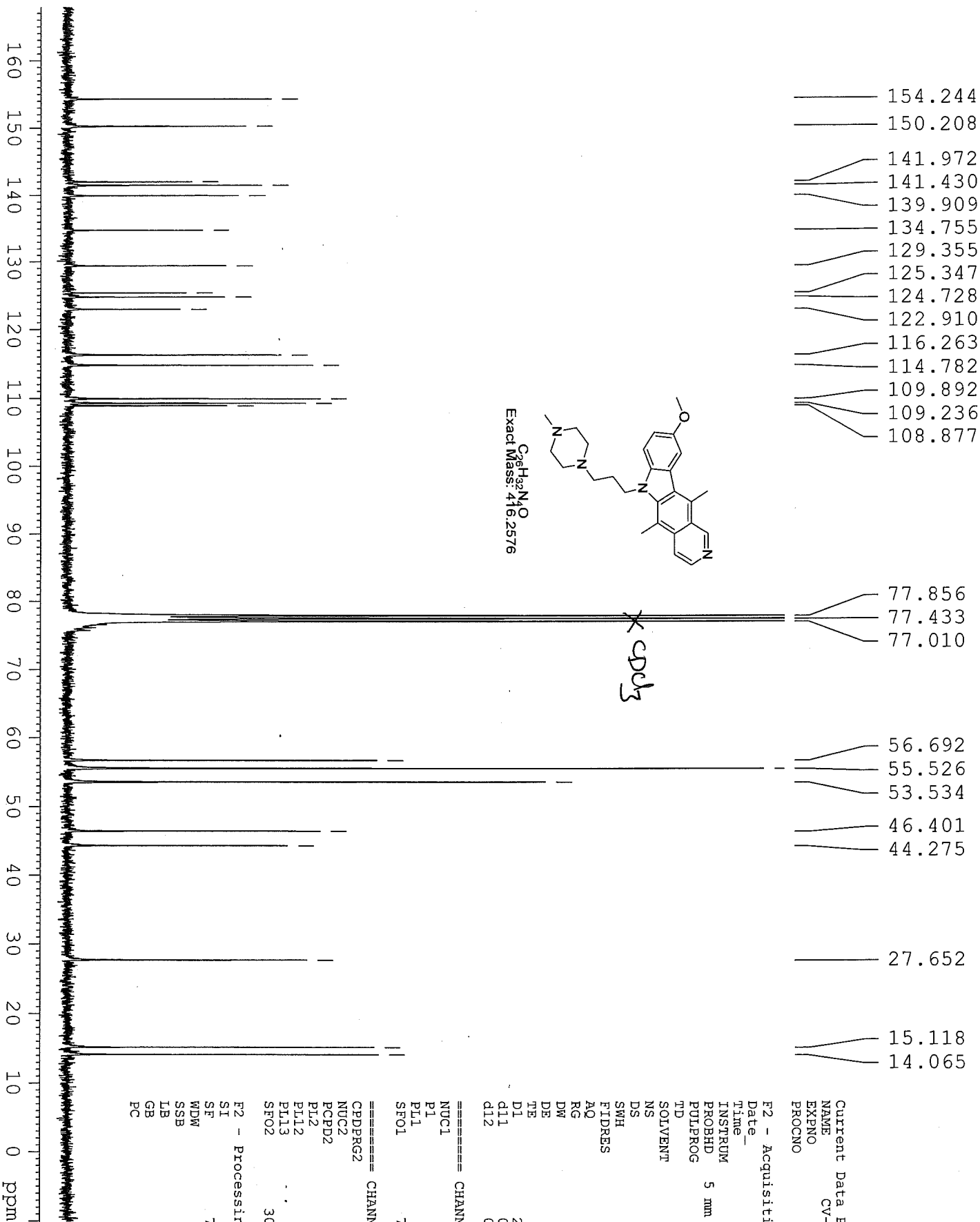
3.217

8.124

5.318

2.260

ppm



Current Data Parameters
NAME CV-GSA-02119
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110528
Time 6.34

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

RG 1.8219508 sec
DE 10321.3
DW 27.800 usec

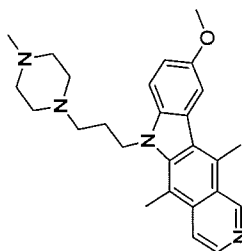
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 6.00 usec
PL1 2.00 dB
SF01 75.4752653 MHz

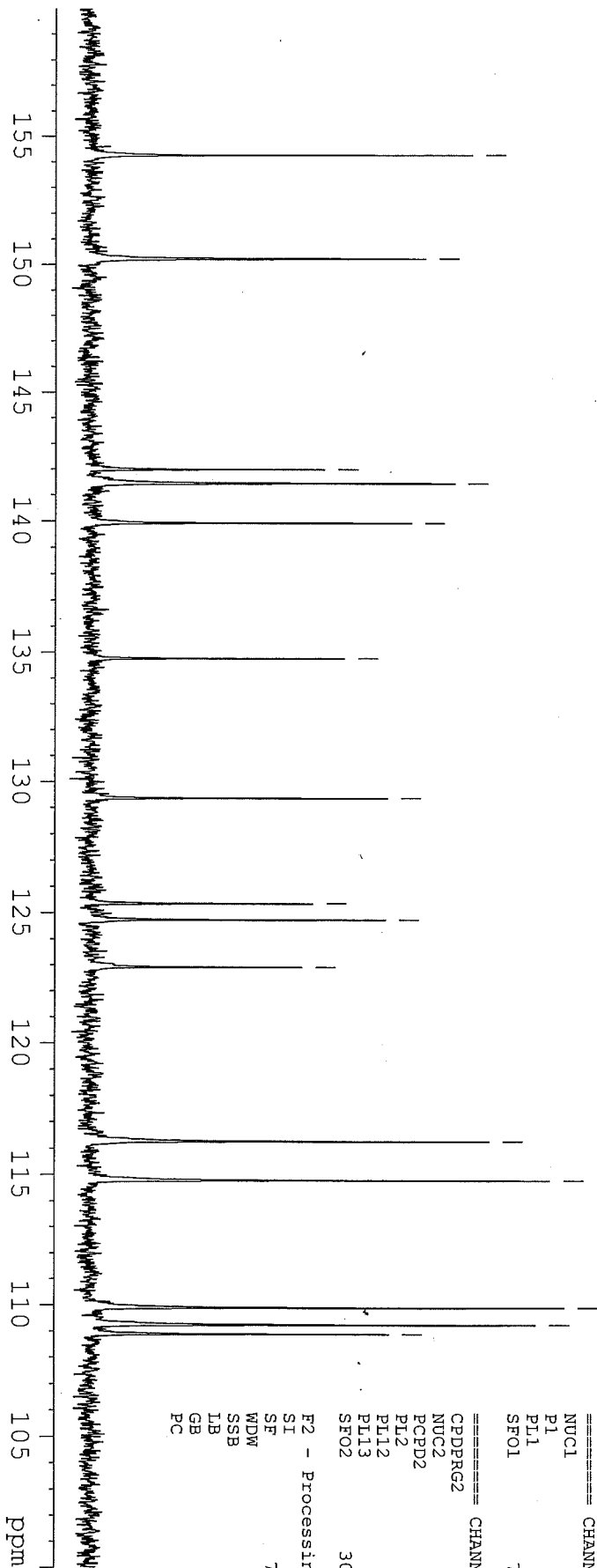
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 19.47 dB
PL13 19.00 dB
SFO2 300.1312005 MHz

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

154.244
150.208
141.972
141.430
139.909
134.755
129.355
125.347
124.728
122.910
116.263
114.782
109.892
109.236
108.877



$C_{26}H_{32}N_4O$
Exact Mass: 416.2576



Current Data Parameters
NAME CV-GSA-02119
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20110528
Time 6.34
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 10321.3
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 80.00 usec
PL2 0.00 dB
PL12 19.47 dB
PL13 19.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters

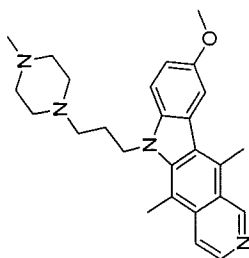
SI 32768
SF 75.4677190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

56.692
55.526
53.534

46.401
44.275

27.652

15.118
14.065



C₂₆H₃₂N₄O
Exact Mass: 416.2576

Current Data Parameters
NAME CV-GSA-02119
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110528
Time 6.34

INSTRUM 5 mm QNP spect
PROBHD 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 10321.3
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

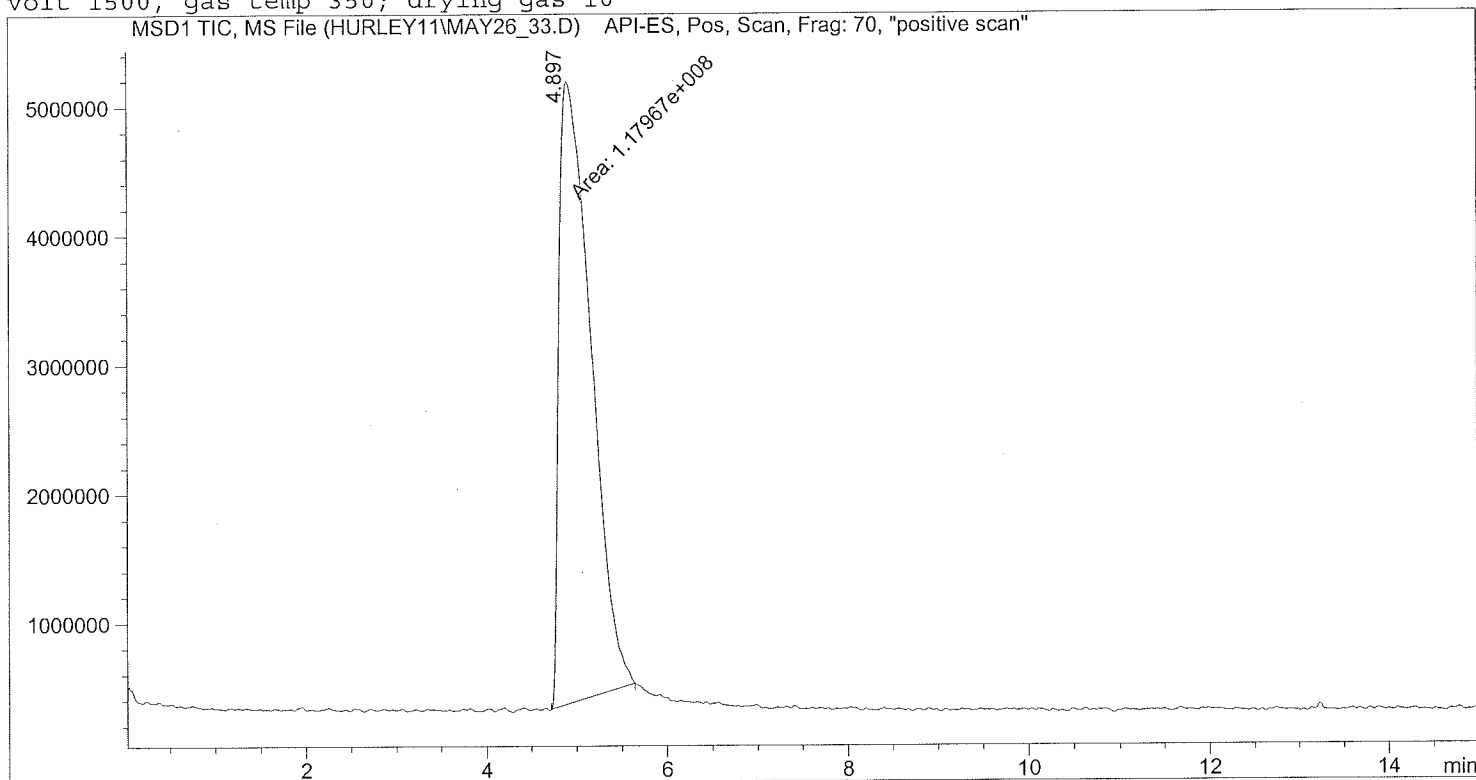
===== CHANNEL f1 =====
NUC1 13C
P1 6.00 usec
PL1 2.00 dB
SFO1 75.4752653 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 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



=====
Injection Date : 5/26/2011 6:46:51 PM
Sample Name : CV-GSA-02119 Location : Vial 120
Acq. Operator : Karen Inj : 1
Acq. Instrument : Instrument 1 Inj Volume : 0.1 µl
Method : C:\HPCHEM\1\METHODS\LC_MS_UV.M
Last changed : 5/26/2011 6:43:10 PM by Karen
Zorbax SB C18, 150 x 4.6, 3.5µ, 45/55/0.25, MeOH/water/formic, POS, 150-550; frag 70; 25C, cap
volt 1500, 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

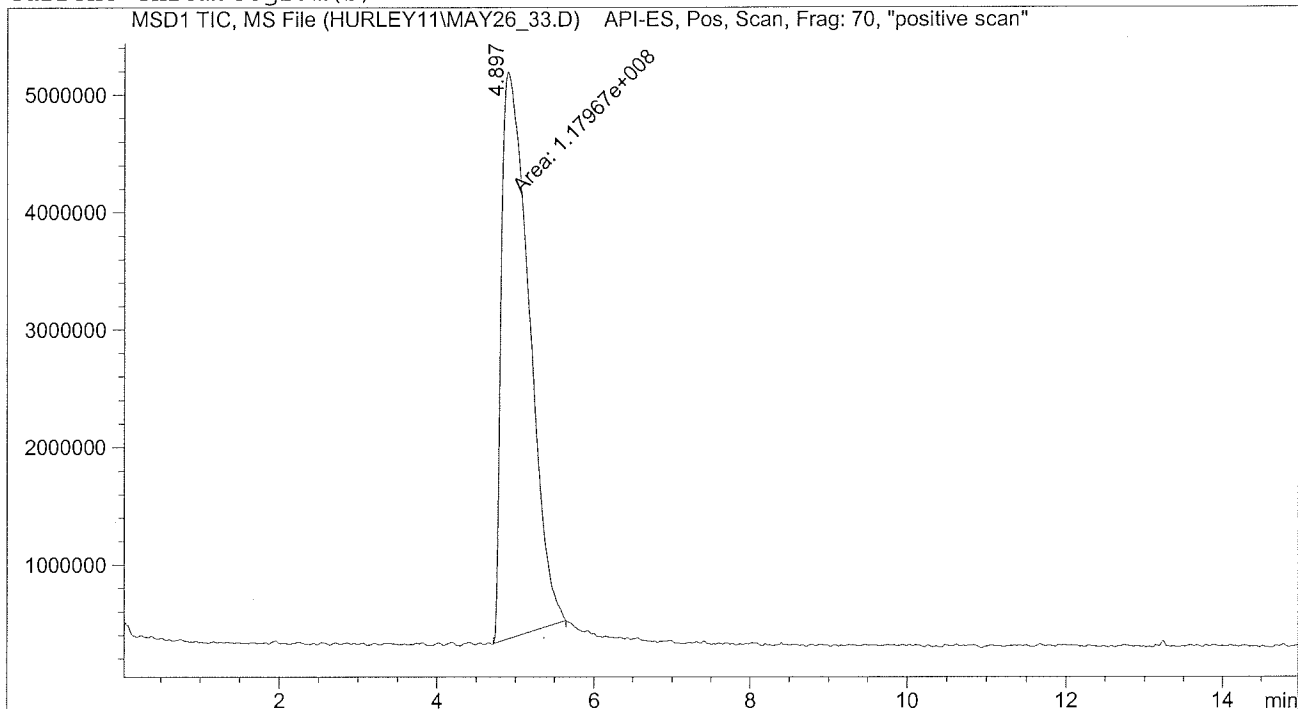
Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	4.897	MM	0.4071	1.17967e8	4.82939e6	100.0000

Totals : 1.17967e8 4.82939e6

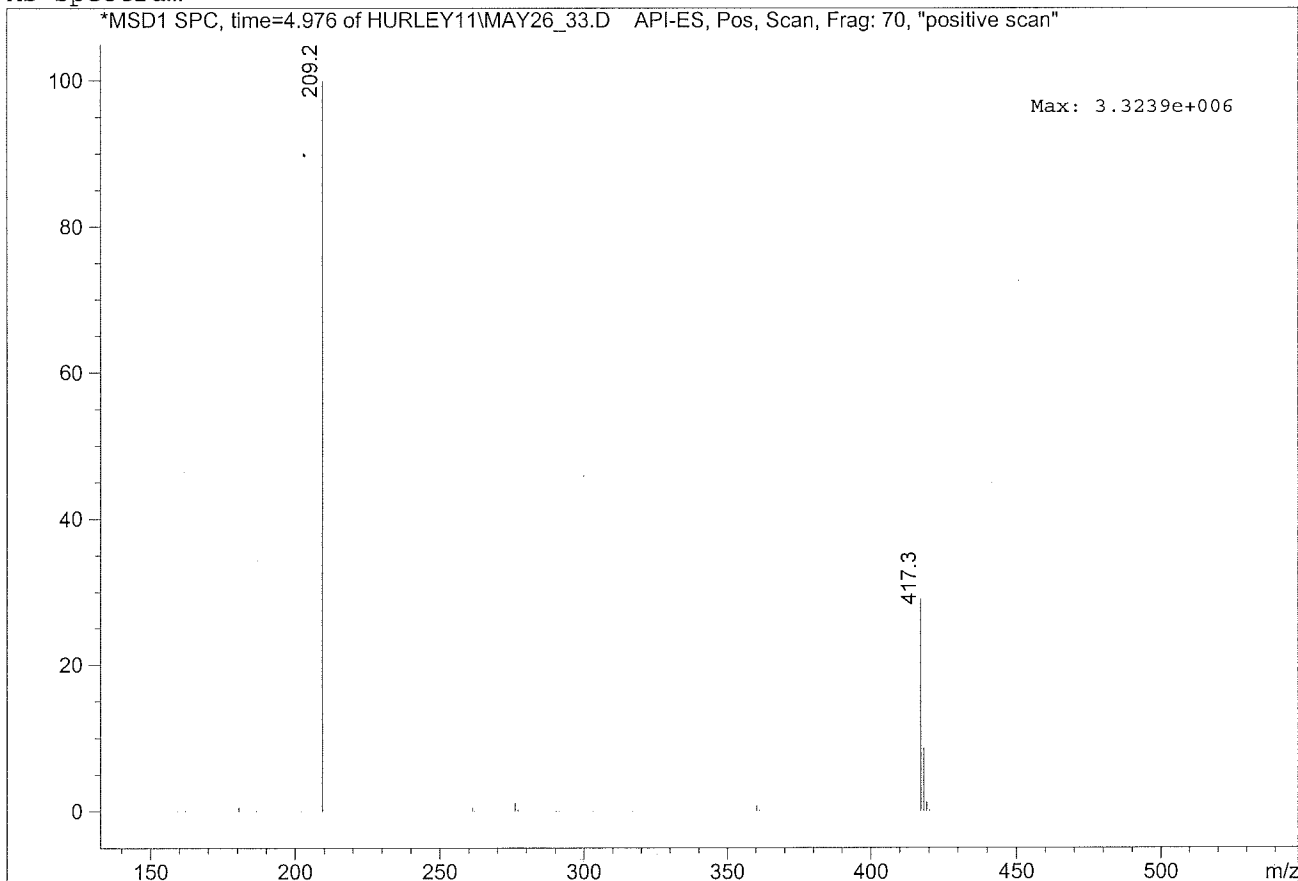
=====
*** End of Report ***


```
=====
Injection Date   : 5/26/2011 6:46:51 PM
Sample Name      : CV-GSA-02119
Acq. Operator    : Karen
Acq. Instrument  : Instrument 1
Method           : C:\HPCHEM\1\METHODS\LC_MS_UV.M
Last changed     : 5/26/2011 6:43:10 PM by Karen
Zorbax SB C18, 150 x 4.6, 3.5u,45/55/0.25,MeOH/water/formic, POS, 150-550; frag 70; 25C,
cap volt 1500, gas temp 350; drying gas 10
=====
```

Current Chromatogram(s)



MS Spectrum



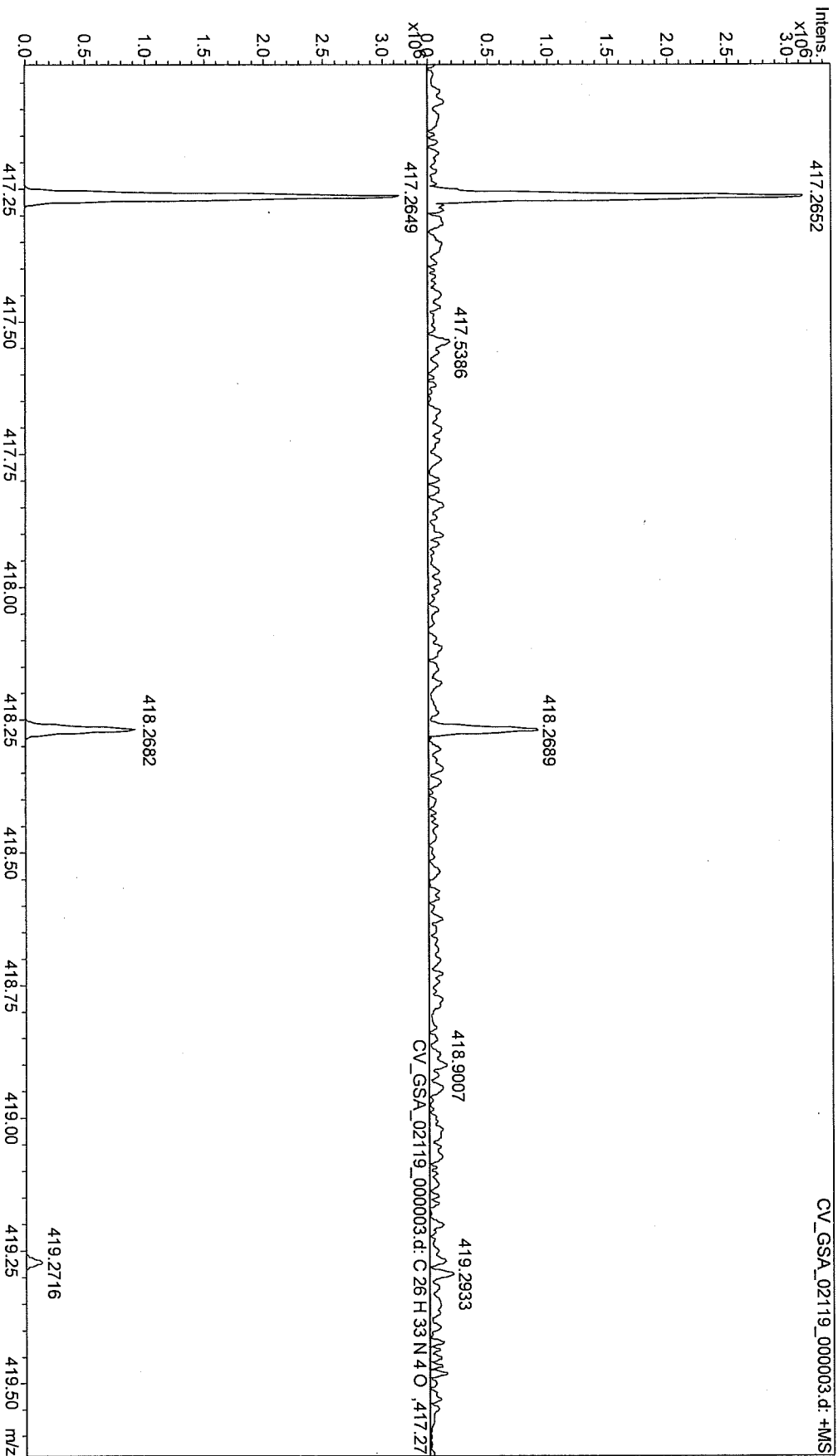
Generic Display Report

Analysis Info

Analysis Name D:\DATA\Facility_May_11\CV_GSA_02119_000003.d
Method Scott_tune
Sample Name CV_GSA_02119
Comment V. R. Chappeta, ACN:H2O 1:1:0.1%FA

Acquisition Date 5/27/2011 10:32:51 AM

Operator
Instrument apex-Ultra



SmartFormula Manually



Min

C₂₀

Generate

Max

C 20-n

Help

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

Measured m/z 417.2652

Tolerance 2

mDa

Charge 1

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdB	e ₋ Conf	N-Rule
417.2852	1	C ₂₆ H ₃₈ N ₄ O	100.00	417.2649	-0.4	-0.8	25.3	12.5	even	ok
2	C ₂₅ H ₃₇ O ₅		42.59	417.2636	-1.7	-4.0	28.9	7.5	even	ok

☐ Automatically locate monoisotopic peak Maximum number of formulas 500

☒ Check rings plus double bonds Minimum -0.5 Maximum 40

Electron configuration

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

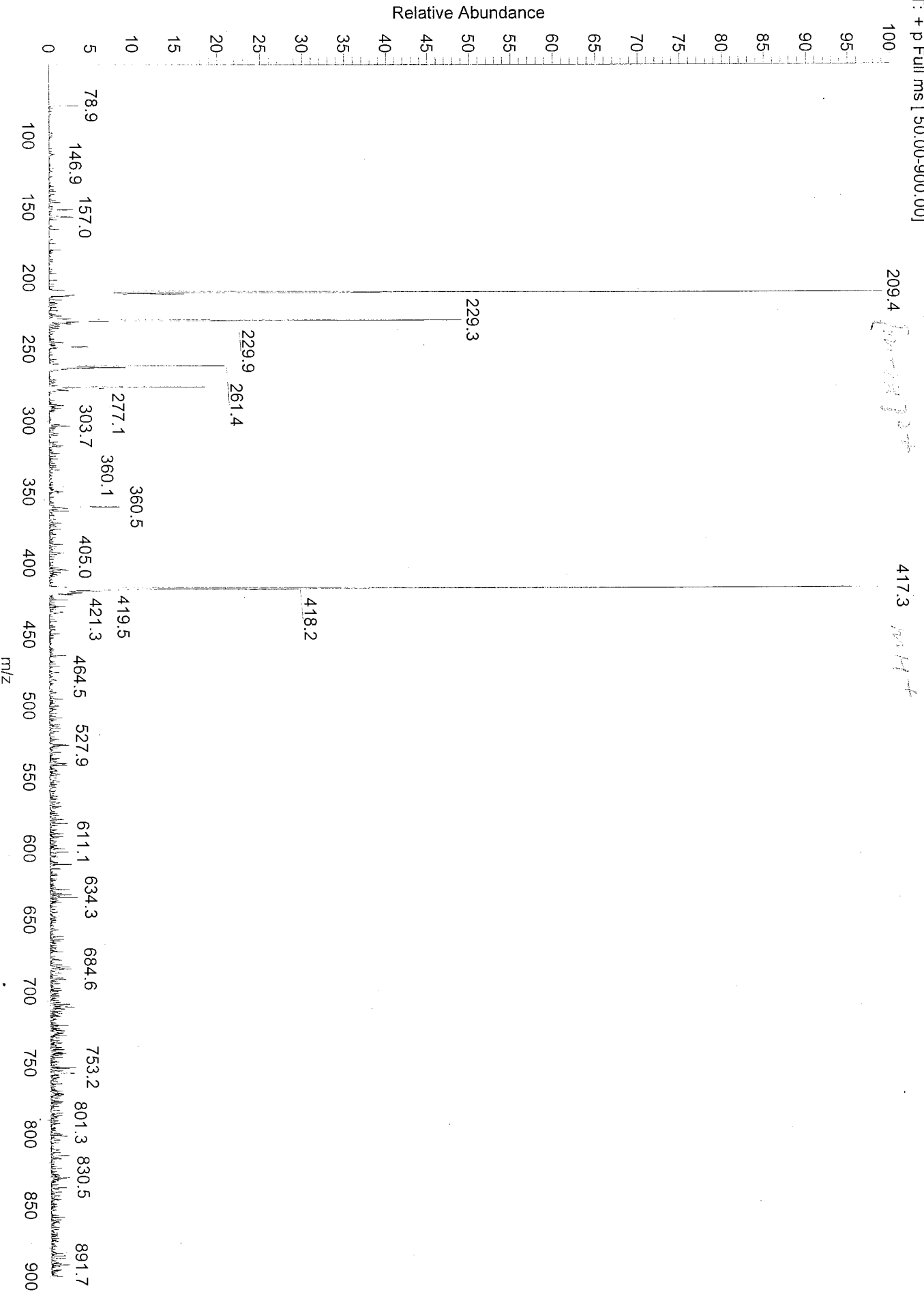
☒ Estimate carbon number ☒ Generate immediately

Show Pattern

E:\MSLab_LC\CV-GSA-02119
V. R. Chappeta, ACN:H2O 1:1:0.1%FA
CV-GSA-02119 #43-44 RT: 0.85-0.87 AV: 2 NL: 4.10E6
T: + p Full ms [50.00-900.00]

05/26/2011 04:01:35 PM

CV-GSA-02119



Current Data Parameters
NAME KS-GSA-01-166 1H NMR
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date 20110622
Time 9.20
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 65536
SOLVENT CDCl3
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 8.50 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters

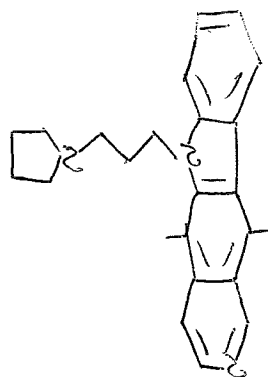
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

9.698
8.464
8.459
8.444
8.439
8.400
8.374
8.041
8.039
8.021
7.722
7.695
7.619
7.593
7.567
7.338
7.312
7.287

4.690
4.665
4.641

3.242
3.236
3.217
2.984
2.950
2.775
2.645
2.507
2.501
2.030
2.007
1.985
1.740
1.207

-0.001
-0.006



8.464
8.459
8.444
8.439
8.400
8.374

Current Data Parameters
NAME KS-GSA-01-166 1H NMR
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20110622
Time 9.20
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 65536
SOLVENT CDCl3
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 8.50 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters

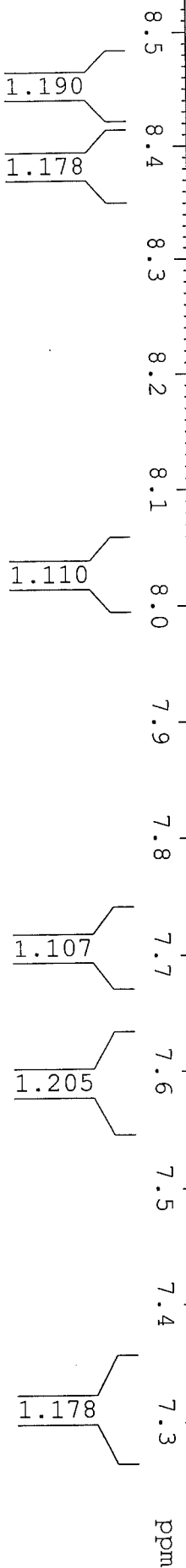
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

8.041
8.039
8.021

7.722
7.695

7.619
7.593
7.567

7.338
7.312
7.287



Current Data Parameters
NAME RS-GSA-01-166 1H NMR
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110622
Time 9.20

INSTRUM 5 mm QNP 1H/1
PROBHD zg30
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 2
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.308460 sec
RG 436.1
RG 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
GB 0
PC 1.00

4.690
4.665
4.641

3.242
3.236
3.217

2.984
2.950

2.775

2.645

2.507
2.501

2.030
2.007
1.985

1.740

1.207

2.171

3.508

3.331

6.000

2.331

4.302

* DMSO



Current Data Parameters
NAME KS-GSA-01-166.13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

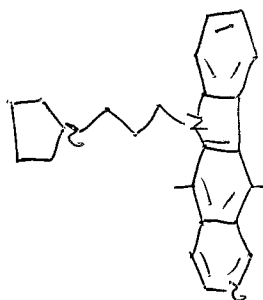
Date_ 20110622
Time_ 8.54
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 16000
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 645.1
RW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

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

150.435
144.959
141.806
140.947
134.542
129.287
128.101
125.079
124.723
123.692
123.054
120.666
116.810
110.253
109.573



Current Data Parameters
NAME KS-GSA-01-166 13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date 20110622
Time 8.54
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 645.1
RG 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.0000000 sec
d11 0.0300000 sec
d12 0.0002000 sec

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

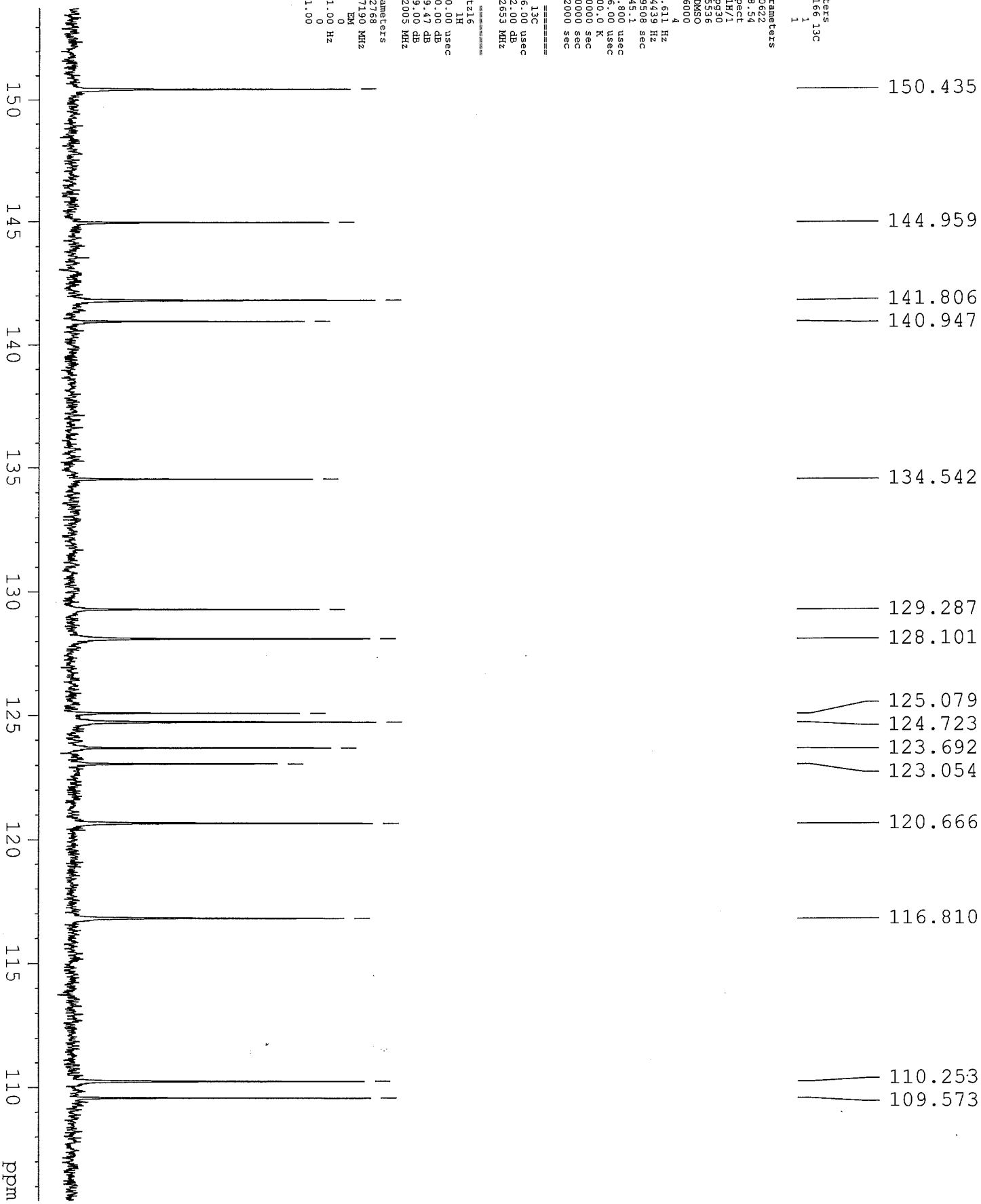
NUC1 13C
P1 6.00 usec
PL1 2.00 dB
SFO1 75.4752653 MHz

===== 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

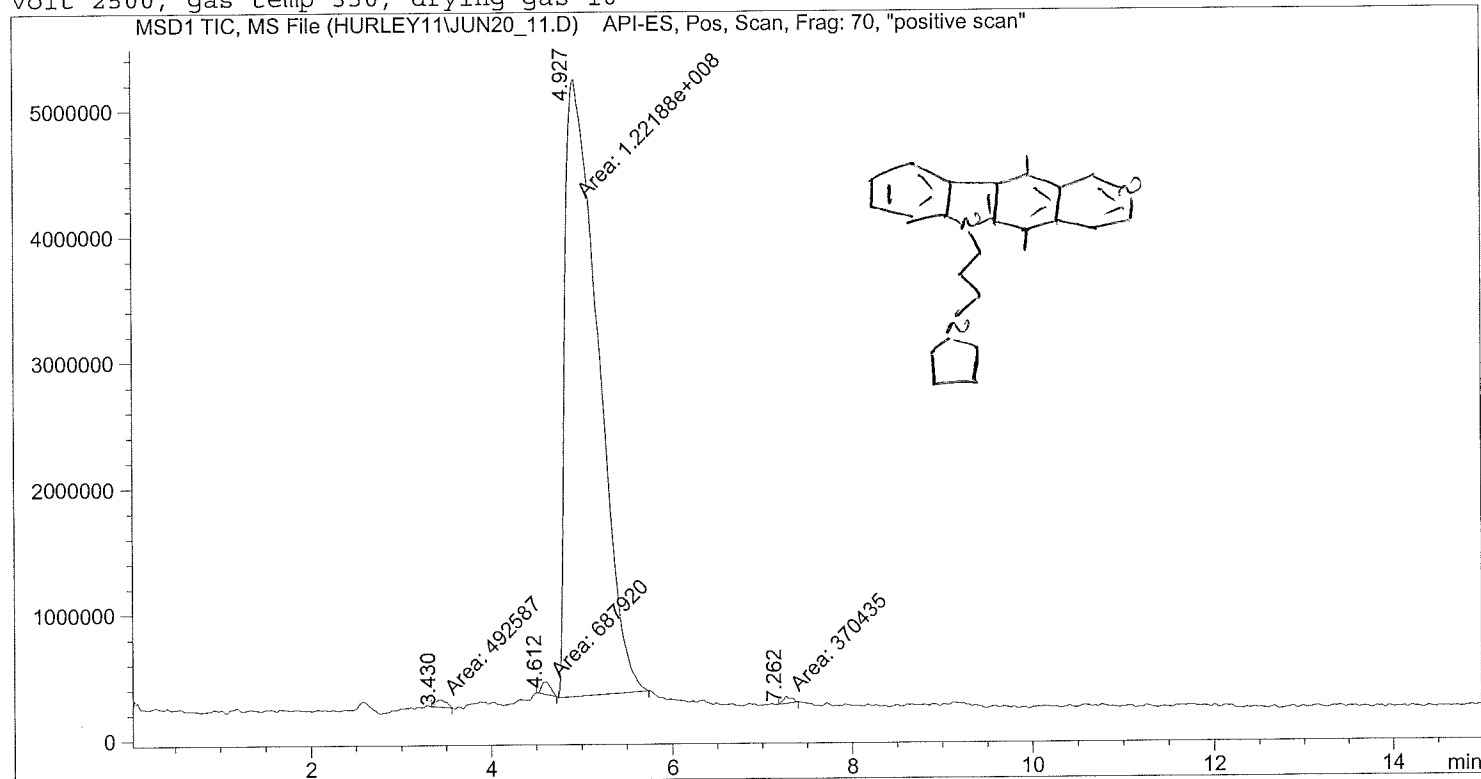
F2 - Processing Parameters

SF 52768
SE 75.4677190 MHz
WDR 0
SSB 0
GB 1.00 Hz
PC 1.00



=====
Injection Date : 6/20/2011 4:58:56 PM
Sample Name : KS-GSA-01-166 Location : Vial 105
Acq. Operator : Karen Inj : 1
Acq. Instrument : Instrument 1 Inj Volume : 0.1 µl
Method : C:\HPCHEM\1\METHODS\LC_MS_UV.M
Last changed : 6/20/2011 5:09:49 PM by Karen
(modified after loading)

Zorbax SB C18, 150 x 4.6, 3.5µ, 40/60/0.25, MeOH/water/formic, POS, 150-600; 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

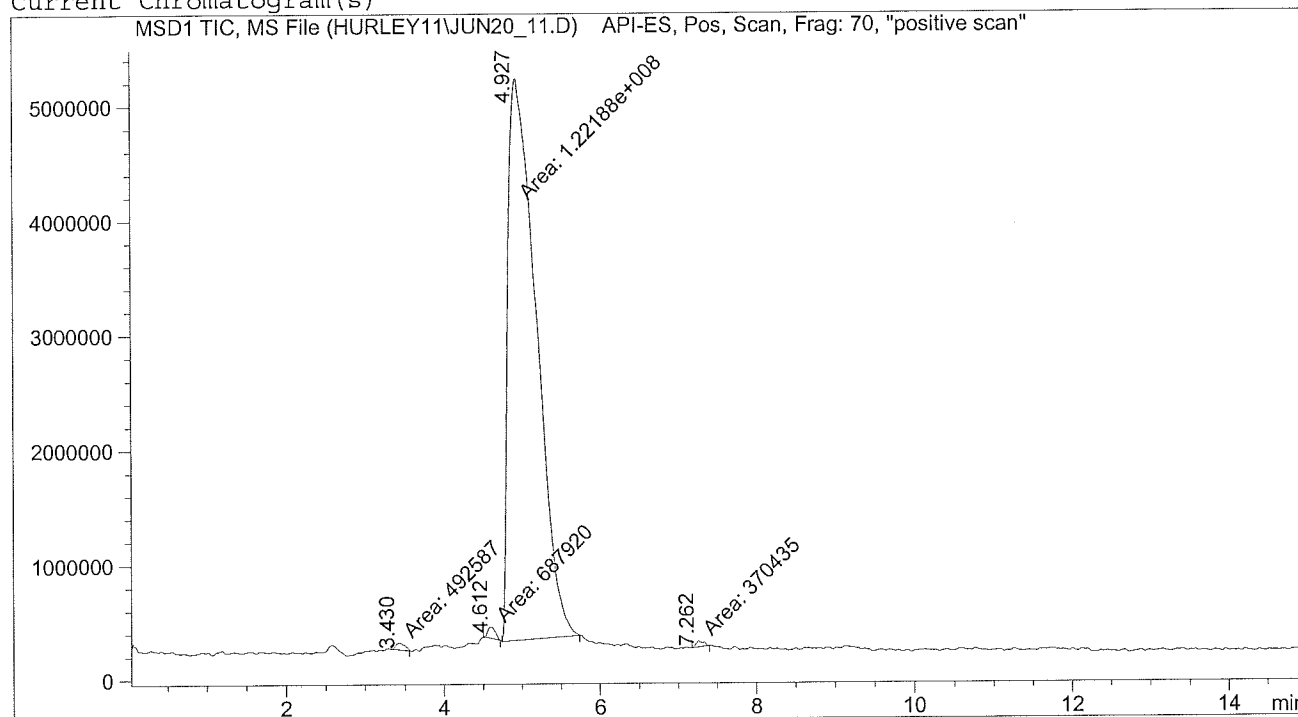
Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	3.430	MM	0.1352	4.92587e5	6.07403e4	0.3981
2	4.612	MM	0.1131	6.87920e5	1.01330e5	0.5559
3	4.927	MM	0.4146	1.22188e8	4.91153e6	98.7466
4	7.262	MM	0.1048	3.70435e5	5.89016e4	0.2994

Totals : 1.23739e8 5.13250e6

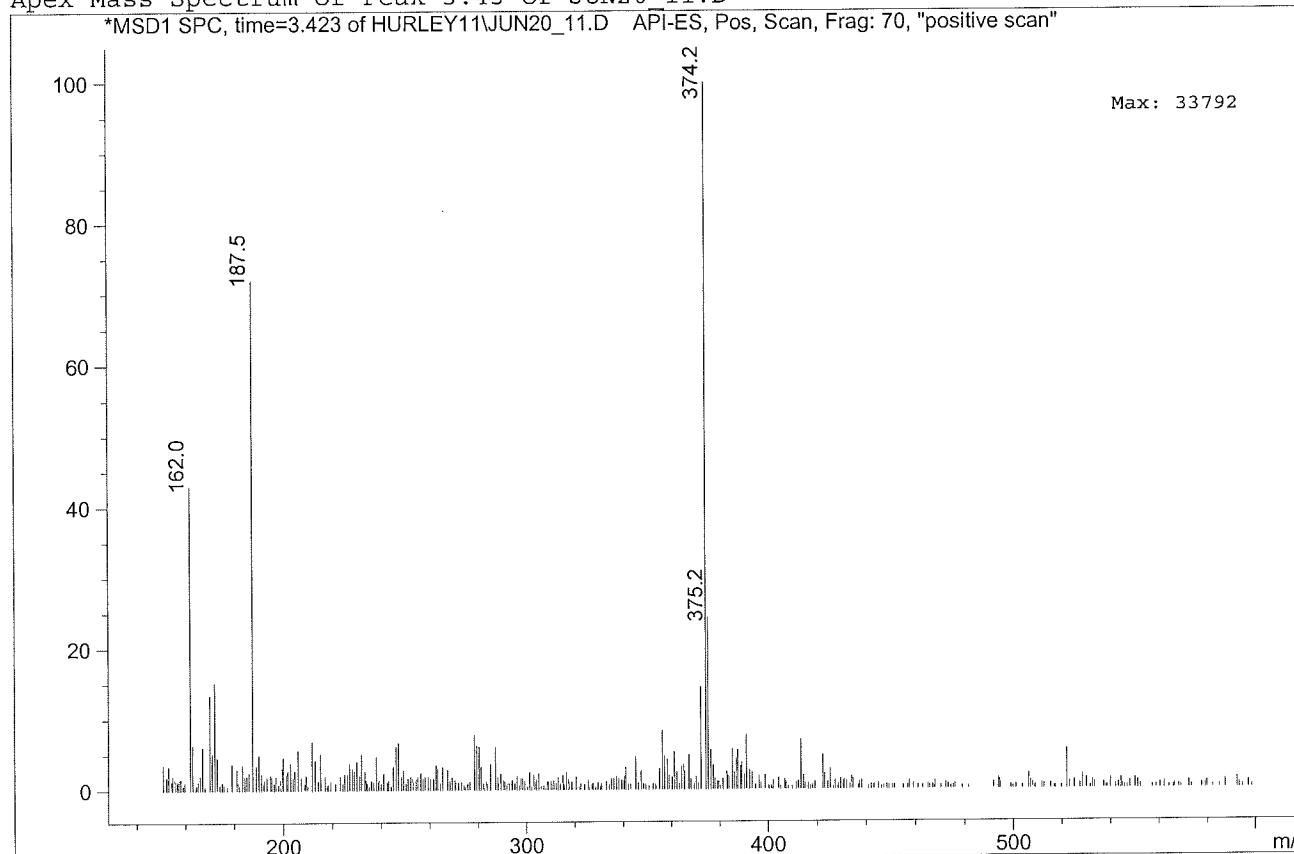
=====
*** End of Report ***

```
=====
Injection Date   : 6/20/2011 4:58:56 PM
Sample Name      : KS-GSA-01-166
Acq. Operator    : Karen
Acq. Instrument  : Instrument 1
Method           : C:\HPCHEM\1\METHODS\LC_MS_UV.M
Last changed     : 6/20/2011 5:09:49 PM by Karen
                  (modified after loading)
Zorbax SB C18,150 x 4.6, 3.5u,40/60/0.25,MeOH/water/formic, POS, 150-600; frag 70; 25C, cap volt
2500, gas temp 350; drying gas 10
=====
```

Current Chromatogram(s)

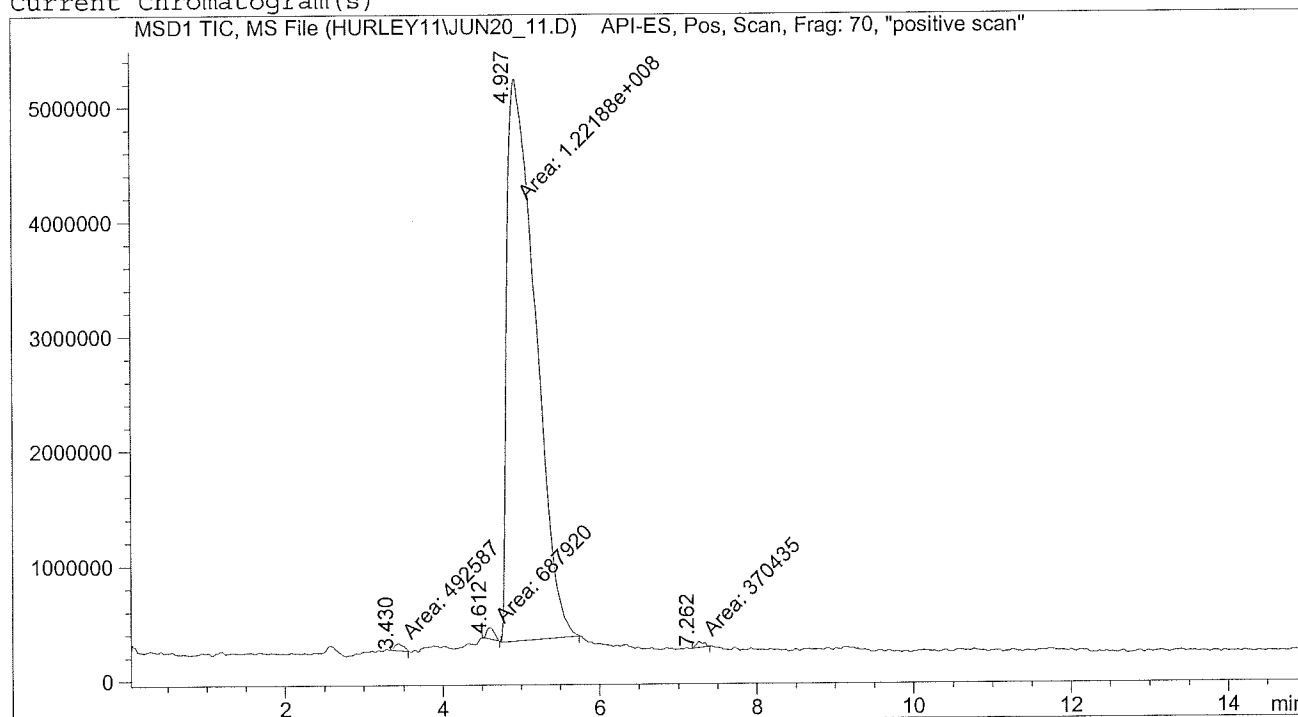


Apex Mass Spectrum of Peak 3.43 of JUN20_11.D

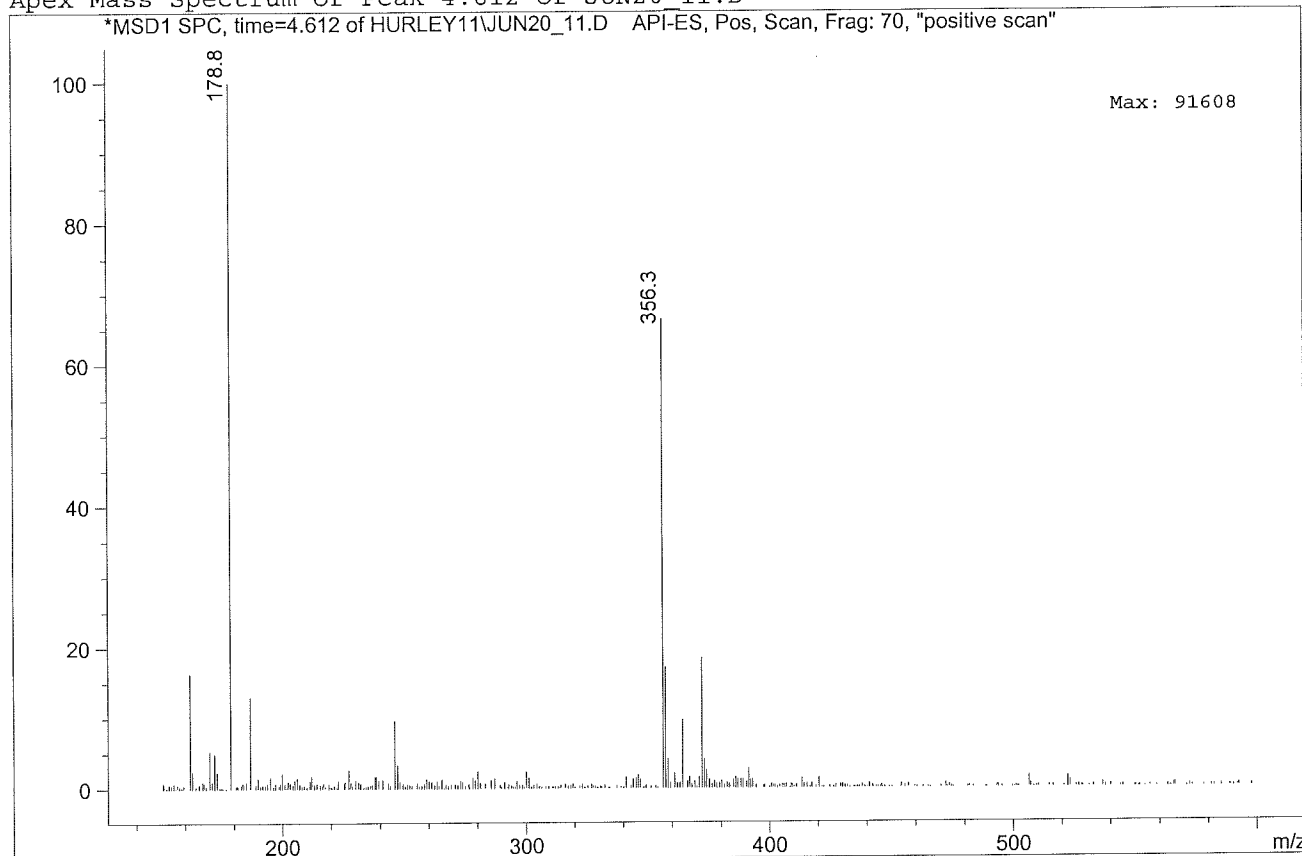


```
=====
Injection Date   : 6/20/2011 4:58:56 PM
Sample Name      : KS-GSA-01-166
Acq. Operator    : Karen
Acq. Instrument  : Instrument 1
Method           : C:\HPCHEM\1\METHODS\LC_MS_UV.M
Last changed     : 6/20/2011 5:09:49 PM by Karen
                  (modified after loading)
Zorbax SB C18,150 x 4.6, 3.5u,40/60/0.25,MeOH/water/formic, POS, 150-600; frag 70; 25C,
cap volt 2500, gas temp 350; drying gas 10
=====
```

Current Chromatogram(s)

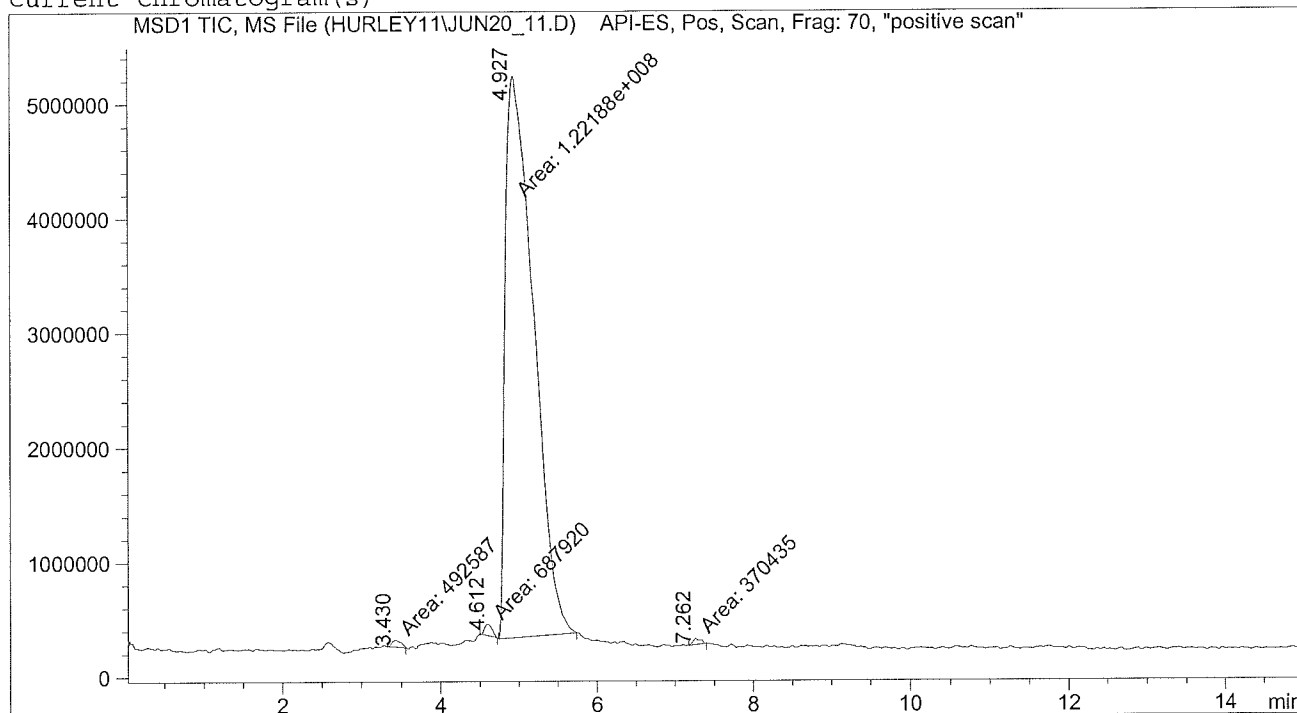


Apex Mass Spectrum of Peak 4.612 of JUN20_11.D

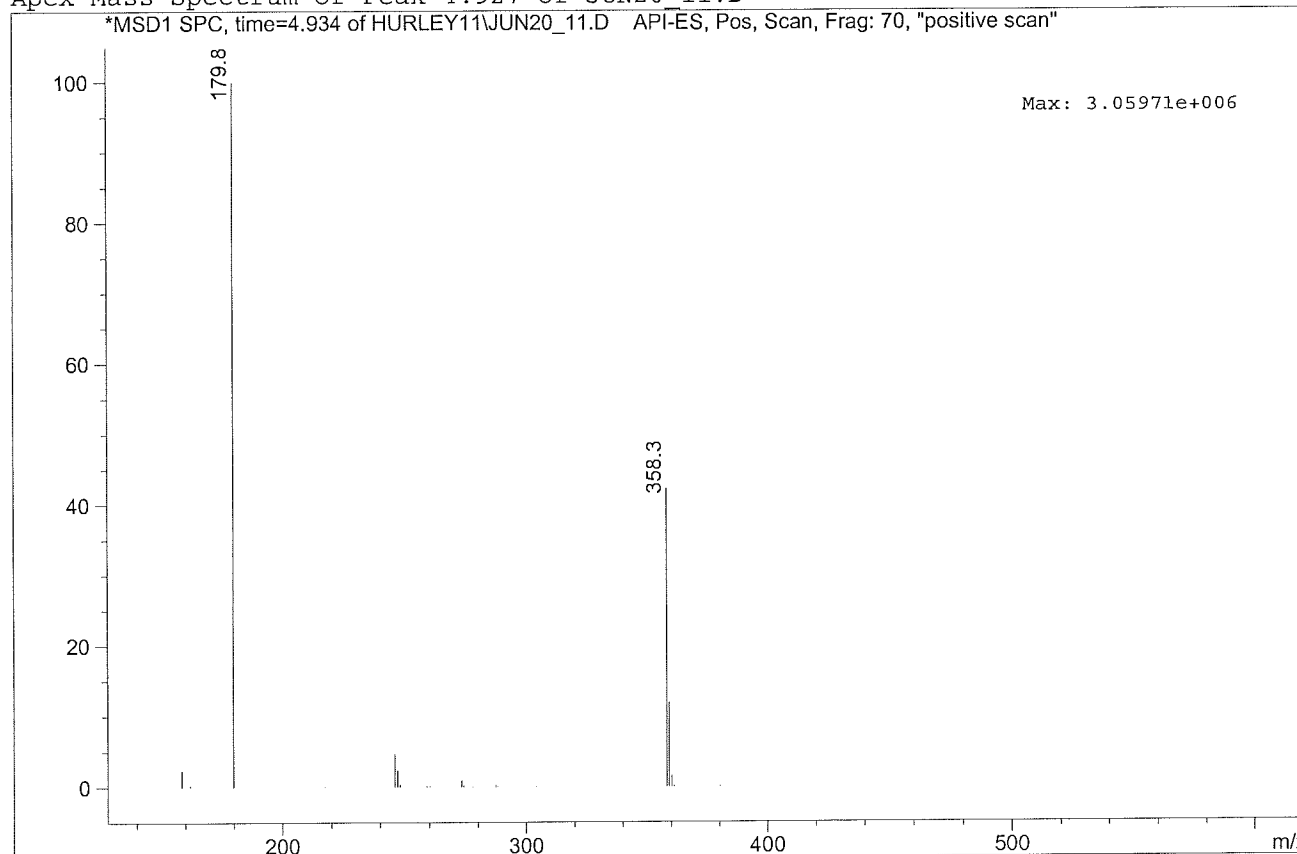


```
=====
Injection Date   : 6/20/2011 4:58:56 PM
Sample Name      : KS-GSA-01-166
Acq. Operator    : Karen
Acq. Instrument  : Instrument 1
Method           : C:\HPCHEM\1\METHODS\LC_MS_UV.M
Last changed     : 6/20/2011 5:09:49 PM by Karen
                  (modified after loading)
Zorbax SB C18,150 x 4.6, 3.5u,40/60/0.25,MeOH/water/formic, POS, 150-600; frag 70; 25C,
cap volt 2500, gas temp 350; drying gas 10
=====
```

Current Chromatogram(s)

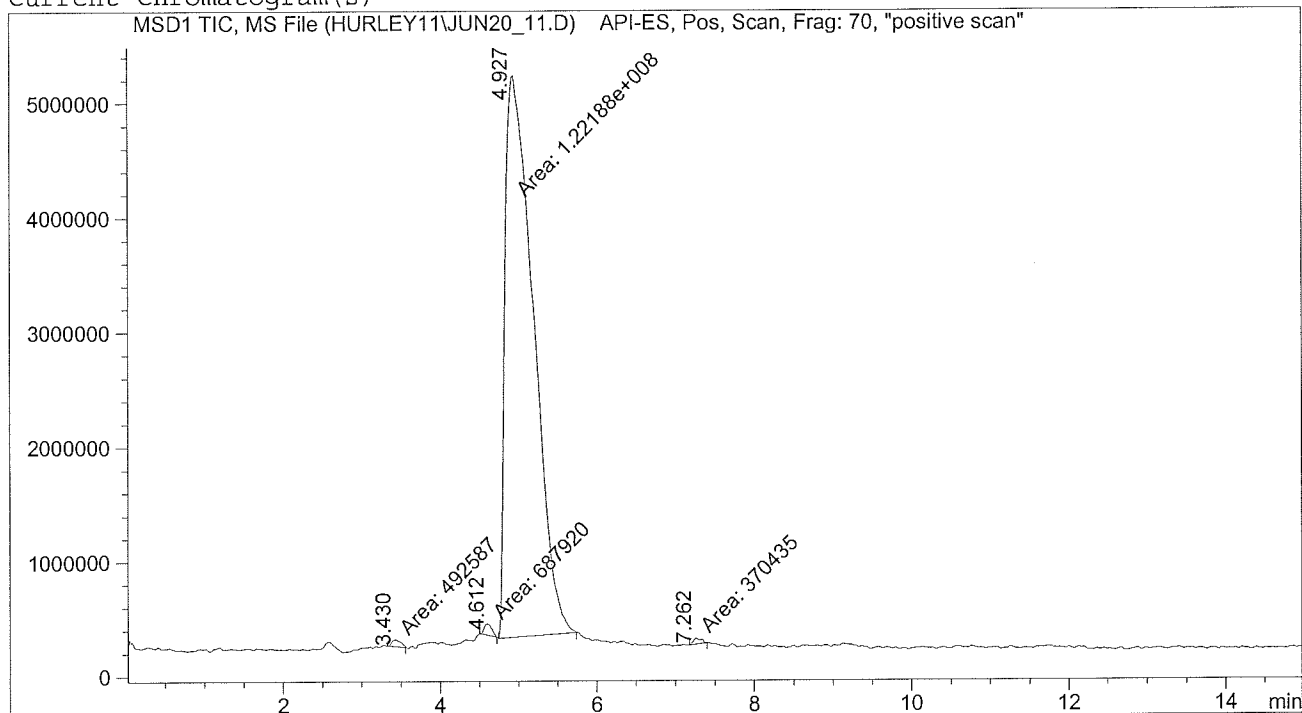


Apex Mass Spectrum of Peak 4.927 of JUN20_11.D

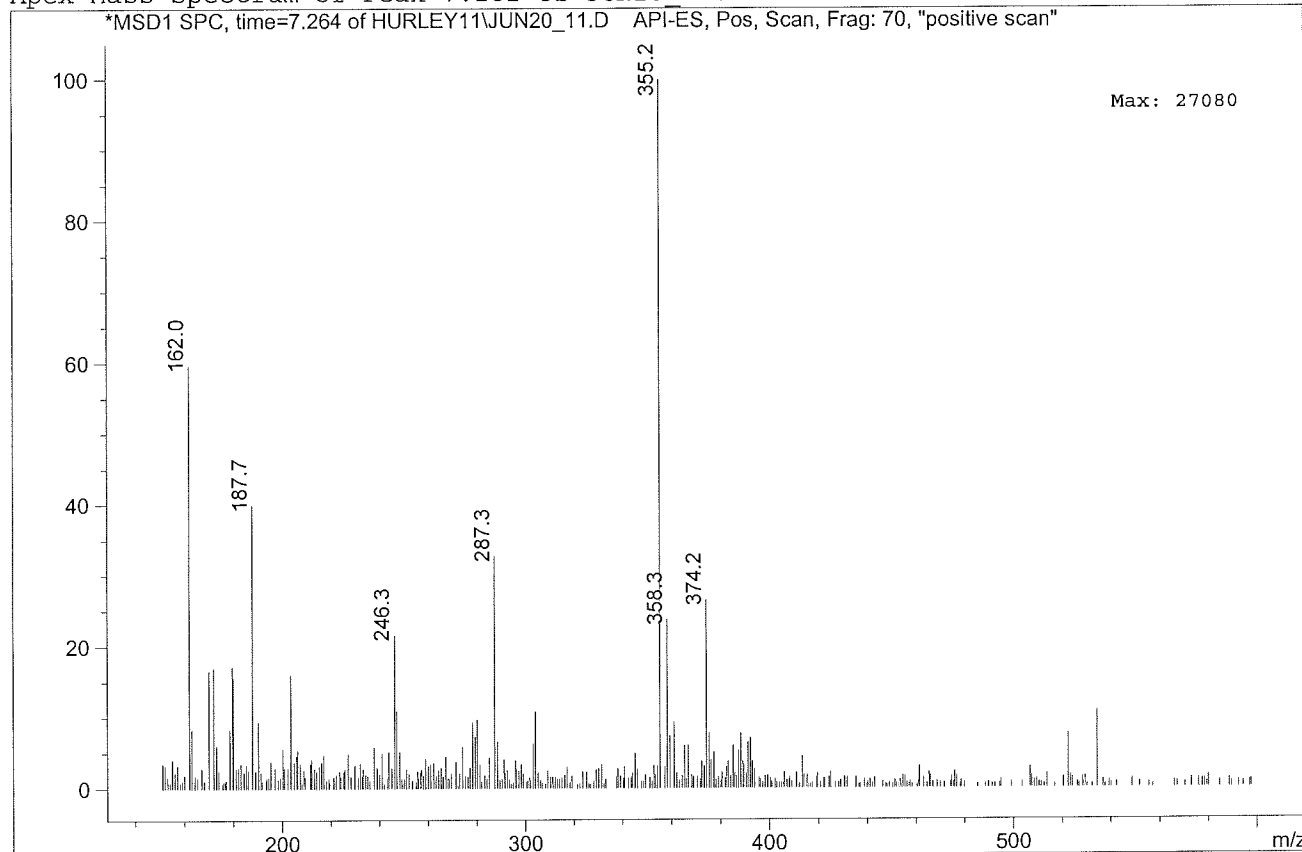


```
=====
Injection Date   : 6/20/2011 4:58:56 PM
Sample Name      : KS-GSA-01-166
Acq. Operator    : Karen
Acq. Instrument  : Instrument 1
Method           : C:\HPCHEM\1\METHODS\LC_MS_UV.M
Last changed     : 6/20/2011 5:09:49 PM by Karen
                  (modified after loading)
Zorbax SB C18,150 x 4.6, 3.5u,40/60/0.25,MeOH/water/formic, POS, 150-600; frag 70; 25C,
cap volt 2500, gas temp 350; drying gas 10
=====
```

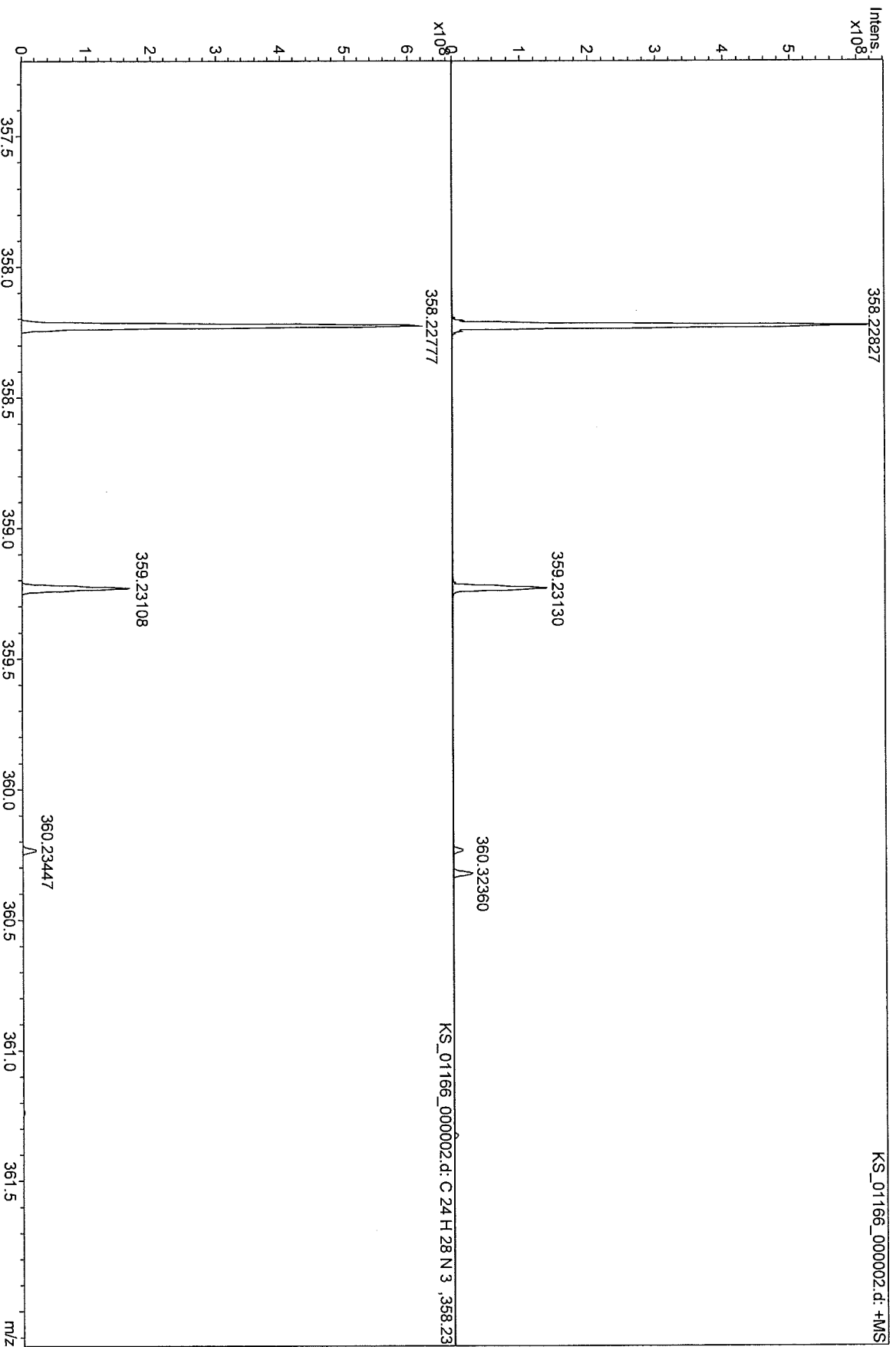
Current Chromatogram(s)



Apex Mass Spectrum of Peak 7.262 of JUN20_11.D



Generic Display Report (all)



SmartFormula Manually



Min

C20H25N2

Generate

Max

C 20-n, H 25-n, N 2-n

Help

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

Measured m/z

358.22827

Tolerance

2

ppm

Charge

1

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
358.22827	1	<chem>C24H28N3</chem>	100.00	358.22777	-0.5	-1.4	26.2	12.5	even	ok

☐ 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 KS-GSA-01-16 H1
 EXPNO 7
 PROCNO 1

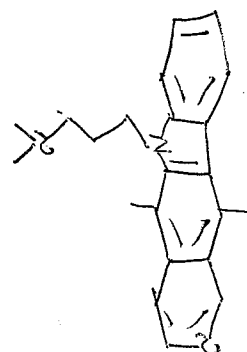
F2 - Acquisition Parameters

Date_ 20110610
 Time 15.43
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 64
 DS 2
 SMH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 406.4
 DM 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
 GB 0
 PC 1.00

9.690
 9.672
 8.459
 8.449
 8.438
 8.421
 8.389
 8.363
 8.022
 8.002
 7.673
 7.646
 7.615
 7.591
 7.565
 7.330
 7.305
 7.282



4.631
 4.606
 4.583

3.204
 2.968
 2.504
 2.279
 2.257
 2.236
 2.136
 2.120
 2.096
 1.904
 1.882
 1.860

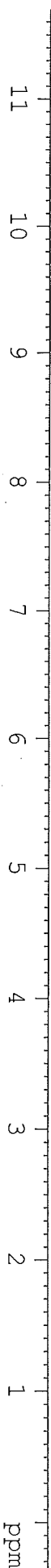
0.000
 -0.010
 -0.017

1.000
 1.037
 1.000
 1.005
 2.031
 1.014

1.970

3.128
 3.012

2.076
 5.950
 2.076



9.690
9.672

8.459
8.449
8.438
8.421
8.389
8.363

8.022
8.002

7.673
7.646
7.615
7.591
7.565

7.330
7.305
7.282

Current Data Parameters
NAME KS-GSA-01-166 H1
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters

Date_ 20110610
Time 15.43
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 2
SWH 6172.839 Hz
FIDRES 0.094130 Hz
AQ 5.3084660 sec
RG 406.4
DM 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

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

MUCL 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

1.000

1.037
1.000

1.005

2.031

1.014

10.0
9.5
9.0
8.5
8.0
7.5
7.0
ppm

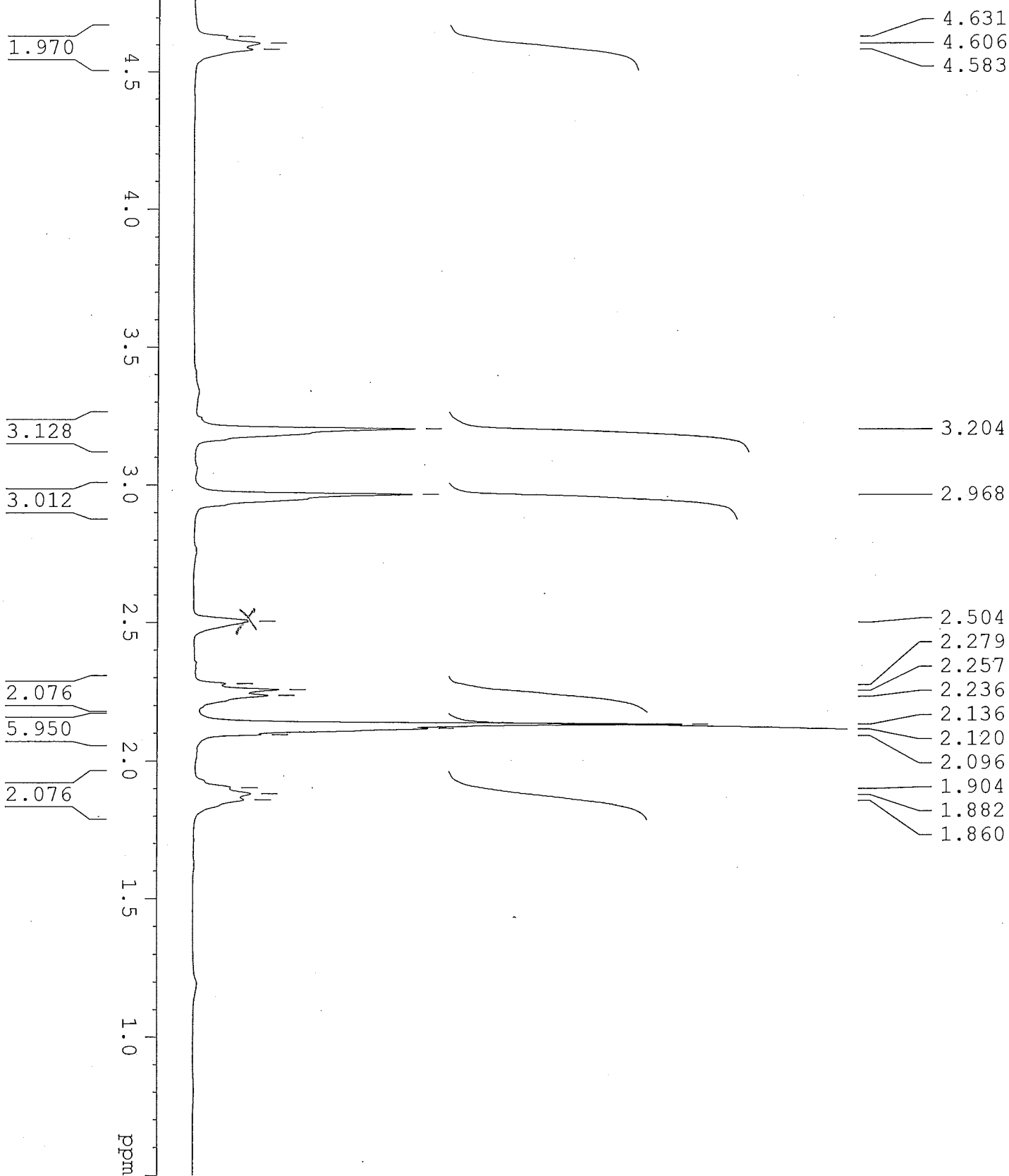
Current Data Parameters
NAME KS-GSA-01-166 H1
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters

Date_ 20110610
Time 15.43
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 406.4
DM 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
GB 0
PC 1.00



16513C

Current Data Parameters
NAME KS-GSA-01-14-13C
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110611
Time 10.57

INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30

TD 65536
SOLVENT CDCl3
NS 18000

DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz

AQ 1.8219508 sec
RG 2580.3
DW 27.800 usec

DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec

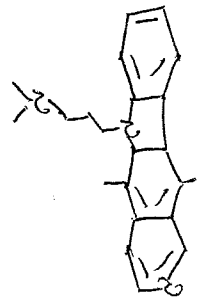
d11 0.03000000 sec
d12 0.00002000 sec

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

===== CHANNEL f2 =====
CDEPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB

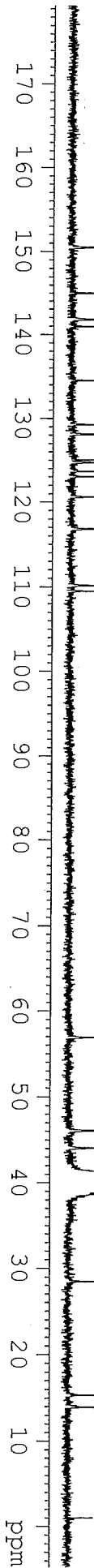
PL12 19.47 dB
PL13 19.00 dB
SFO2 300.1312005 MHz

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



- 150.422
- 144.997
- 141.782
- 140.950
- 134.516
- 129.265
- 128.092
- 125.036
- 124.706
- 123.637
- 123.000
- 120.576
- 116.785
- 110.129
- 109.462

- 56.878
- 46.058
- 44.042
- 41.216
- 40.938
- 40.660
- 40.382
- 40.104
- 39.826
- 39.548
- 39.182
- 28.442
- 15.312
- 13.929



Current Data Parameters
NAME KS-GSA-01-166.13C
EXPNO 7
PROCNO 1

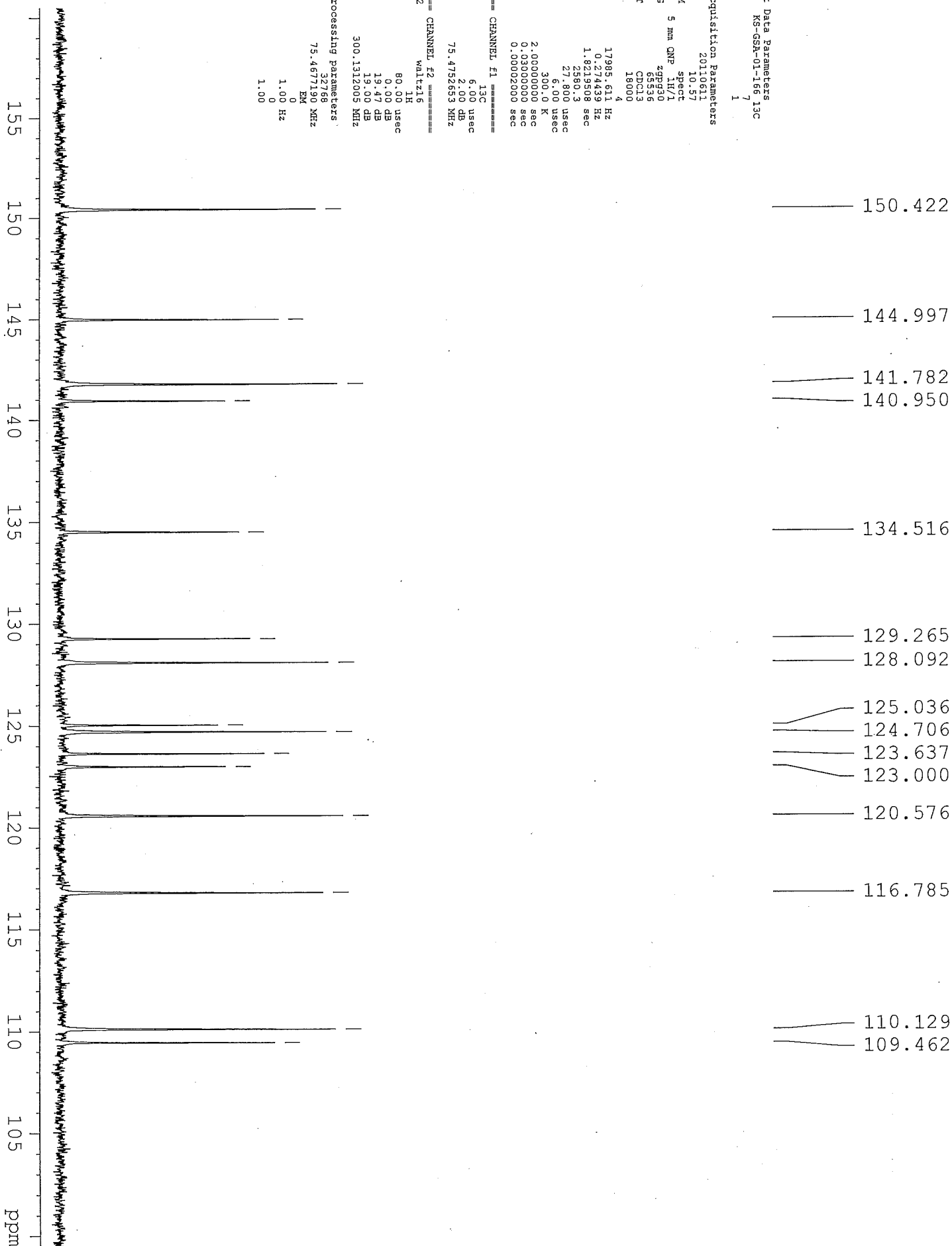
F2 - Acquisition Parameters

Date_ 20110611
Time 10:57
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 18000
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2580.3
DM 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.0002000 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 18.47 dB
PL13 18.00 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



Current Data Parameters
NAME KS-GSA-01-166 13C
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters

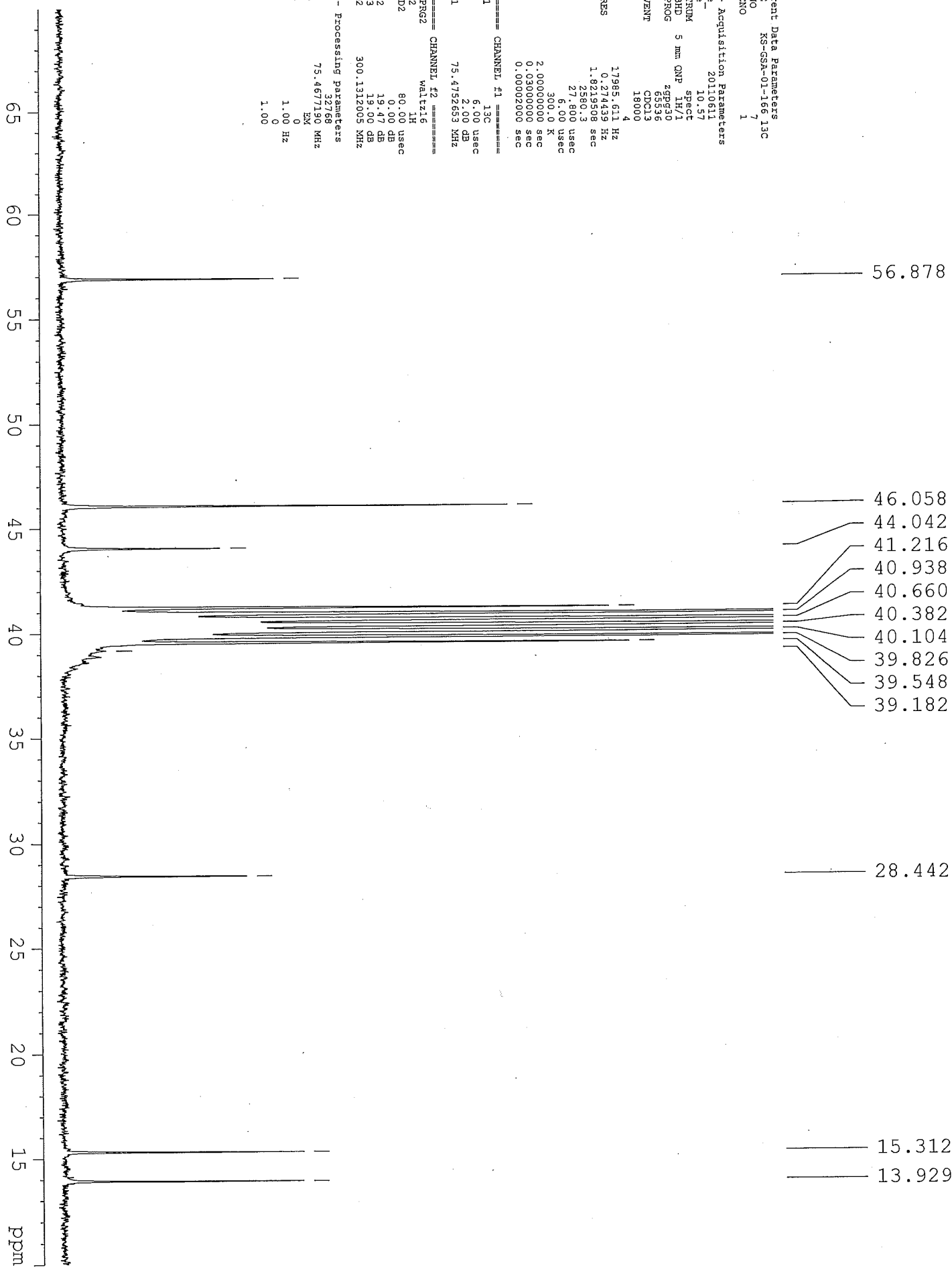
Date_ 20110611
Time 10.37
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 18000
DS 4
SWH 17965.611 Hz
FIDRES 0.274439 Hz
AQ 1.6218508 sec
RG 2560.3
DM 27.800 usec
DE 300.0 K
TE 6.00 usec
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 6.00 usec
PL1 2.50 dB
SFO1 75.4752653 MHz

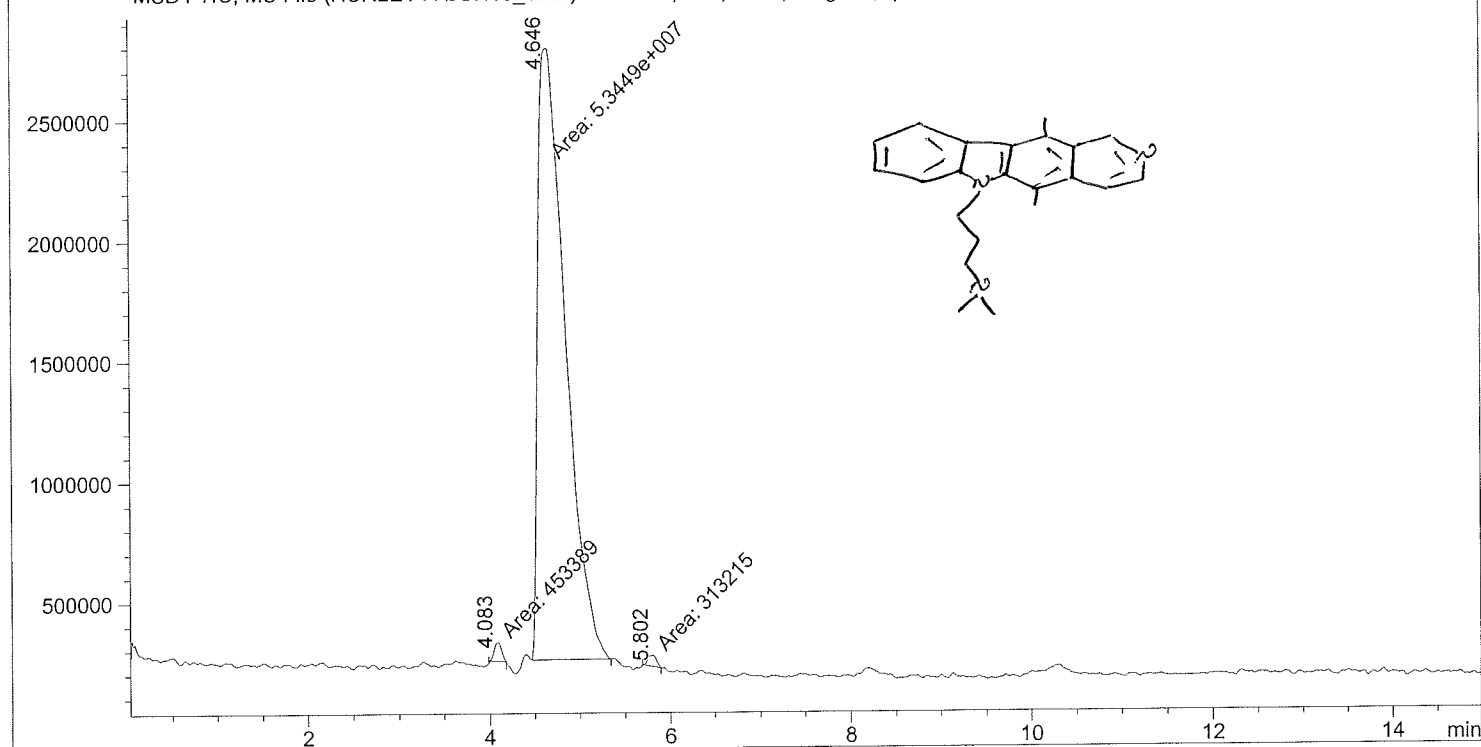
===== CHANNEL f2 =====
CPRRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 19.47 dB
PL13 19.00 dB
SFO2 300.1312005 MHz

F2 - Processing Parameters

SI 32768
SF 75.4677190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00



MSD1 TIC, MS File (HURLEY11\JUN13_16.D) API-ES, Pos, Scan, Frag: 70, "positive scan"



```
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	4.083	MM	0.0952	4.53389e5	7.93571e4	0.8363
2	4.646	MM	0.3510	5.34490e7	2.53773e6	98.5860
3	5.802	MM	0.1118	3.13215e5	4.67125e4	0.5777

Totals :	5.42156e7	2.66380e6
----------	-----------	-----------

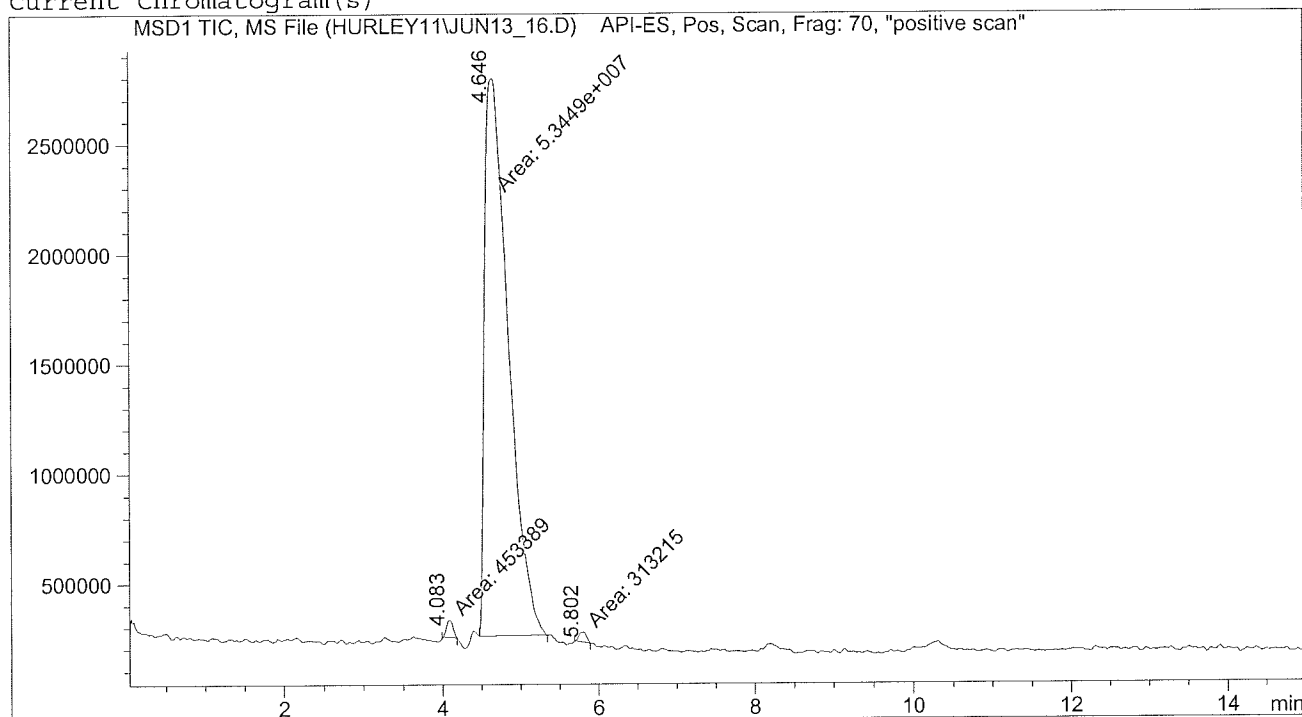
*** End of Report ***

=====

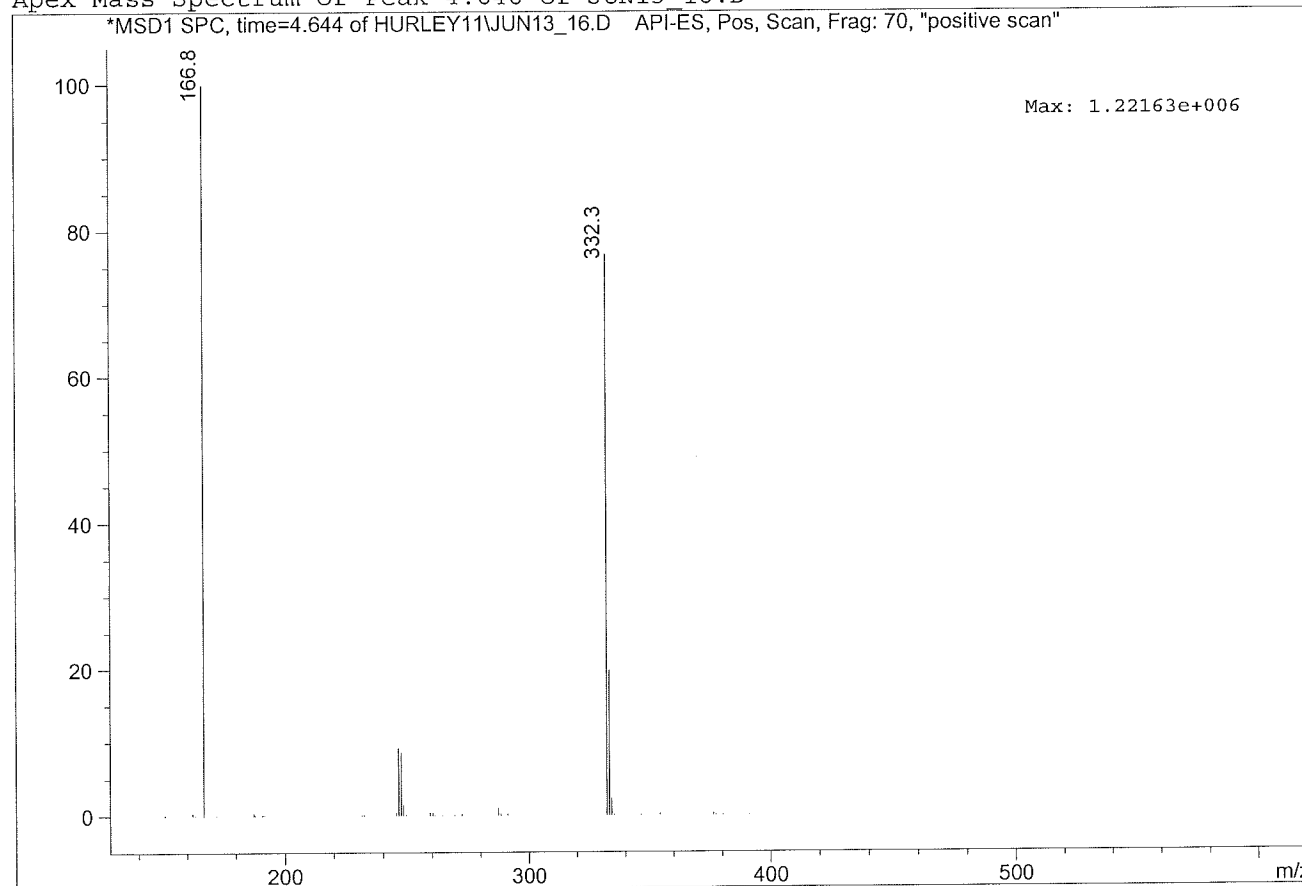
Injection Date	: 6/13/2011 6:17:29 PM	Location	: Vial 4
Sample Name	: KS-GSA-01-165	Inj	: 1
Acq. Operator	: Karen	Inj Volume	: 0.1 µl
Acq. Instrument	: Instrument 1		
Method	: C:\HPCHEM\1\METHODS\LC_MS_UV.M		
Last changed	: 6/13/2011 6:15:43 PM by Karen		

Zorbax SB C18, 150 x 4.6, 3.5µ, 40/60/0.25, MeOH/water/formic, POS, 150-600; frag 70; 25C, cap volt 2500, gas temp 350; drying gas 10

Current Chromatogram(s)

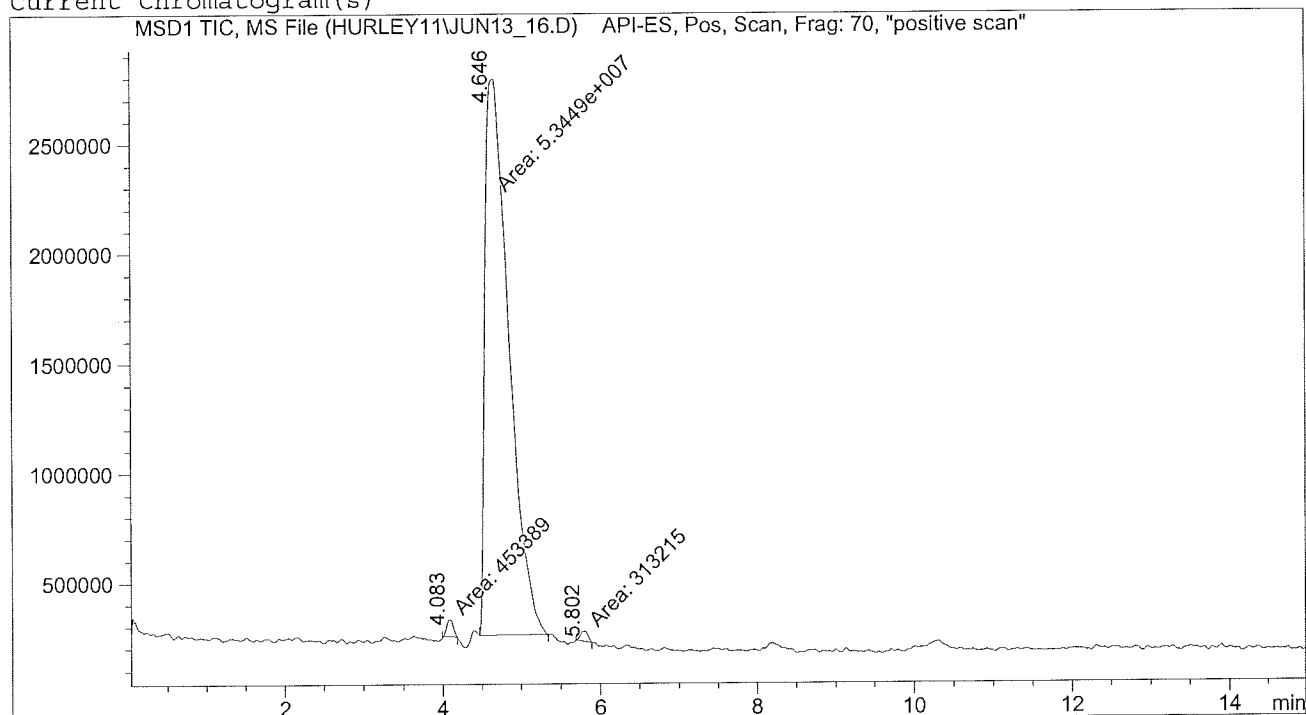


Apex Mass Spectrum of Peak 4.646 of JUN13_16.D

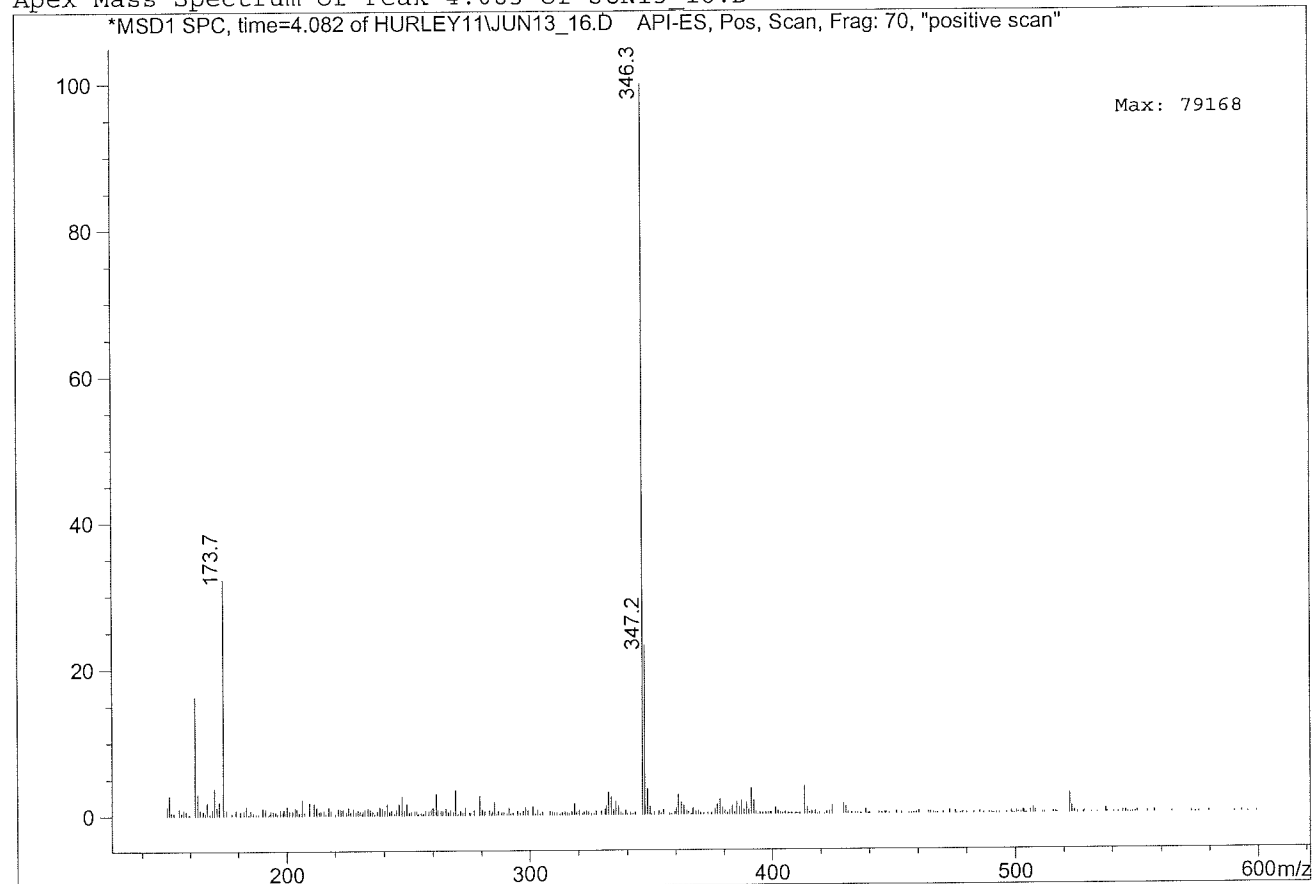


```
=====
Injection Date   : 6/13/2011 6:17:29 PM
Sample Name      : KS-GSA-01-165
Acq. Operator    : Karen
Acq. Instrument  : Instrument 1
Method           : C:\HPCHEM\1\METHODS\LC_MS_UV.M
Last changed     : 6/13/2011 6:15:43 PM by Karen
Zorbax SB C18,150 x 4.6, 3.5u,40/60/0.25,MeOH/water/formic, POS, 150-600; frag 70; 25C, cap volt
2500, gas temp 350; drying gas 10
=====
```

Current Chromatogram(s)



Apex Mass Spectrum of Peak 4.083 of JUN13_16.D

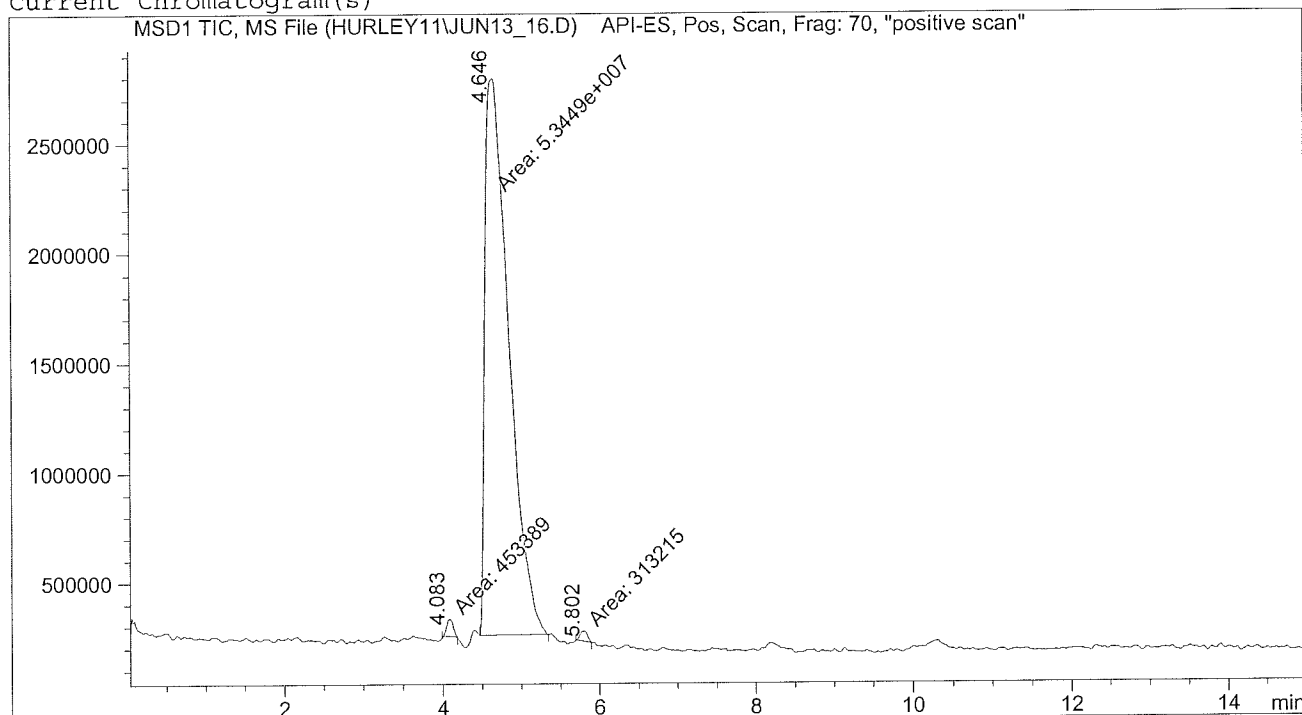


=====

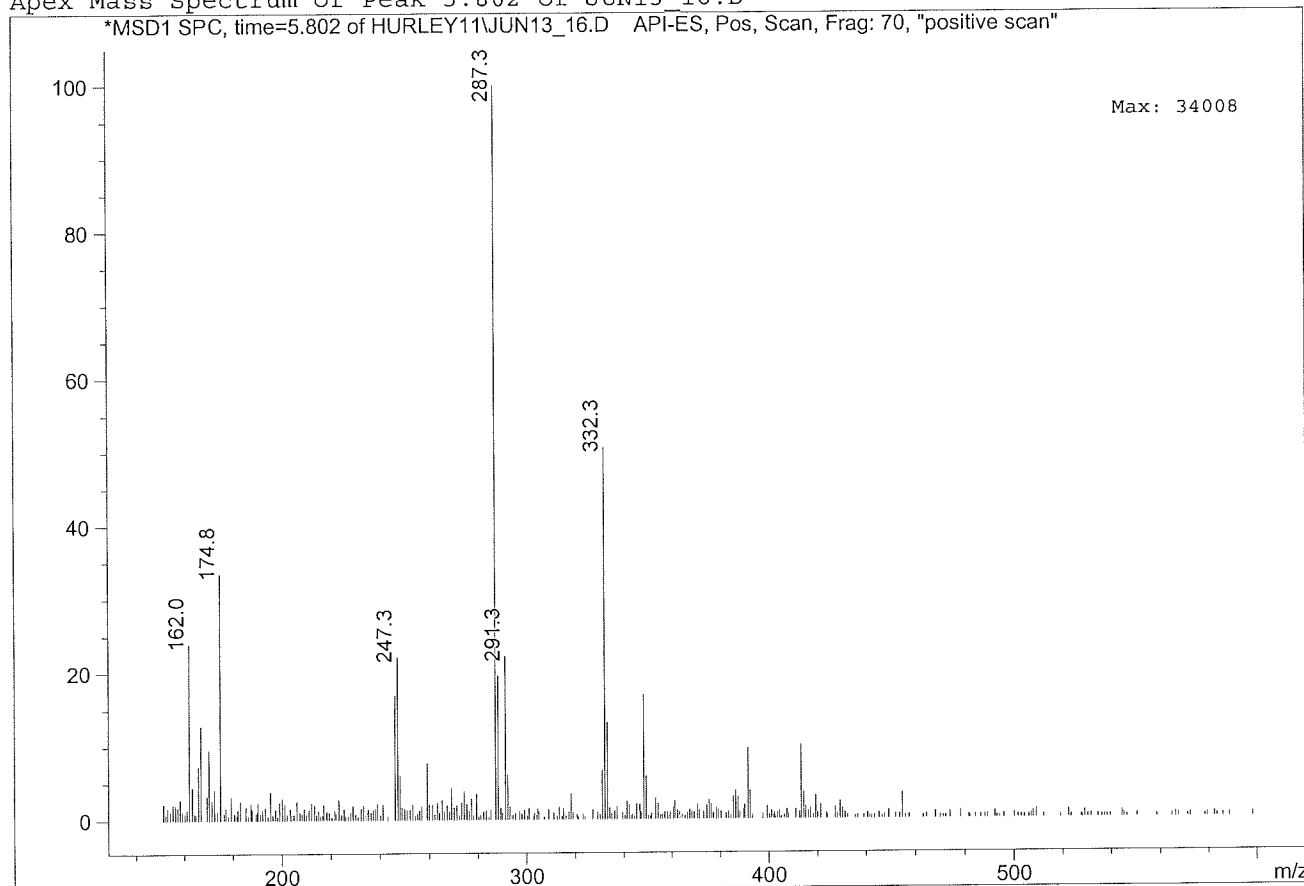
Injection Date	: 6/13/2011 6:17:29 PM	Location	: Vial 4
Sample Name	: KS-GSA-01-165	Inj	: 1
Acq. Operator	: Karen	Inj Volume	: 0.1 µl
Acq. Instrument	: Instrument 1		
Method	: C:\HPCHEM\1\METHODS\LC_MS_UV.M		
Last changed	: 6/13/2011 6:15:43 PM by Karen		

Zorbax SB C18, 150 x 4.6, 3.5µ, 40/60/0.25, MeOH/water/formic, POS, 150-600; frag 70; 25C, cap volt 2500, gas temp 350; drying gas 10

Current Chromatogram(s)



Apex Mass Spectrum of Peak 5.802 of JUN13_16.D

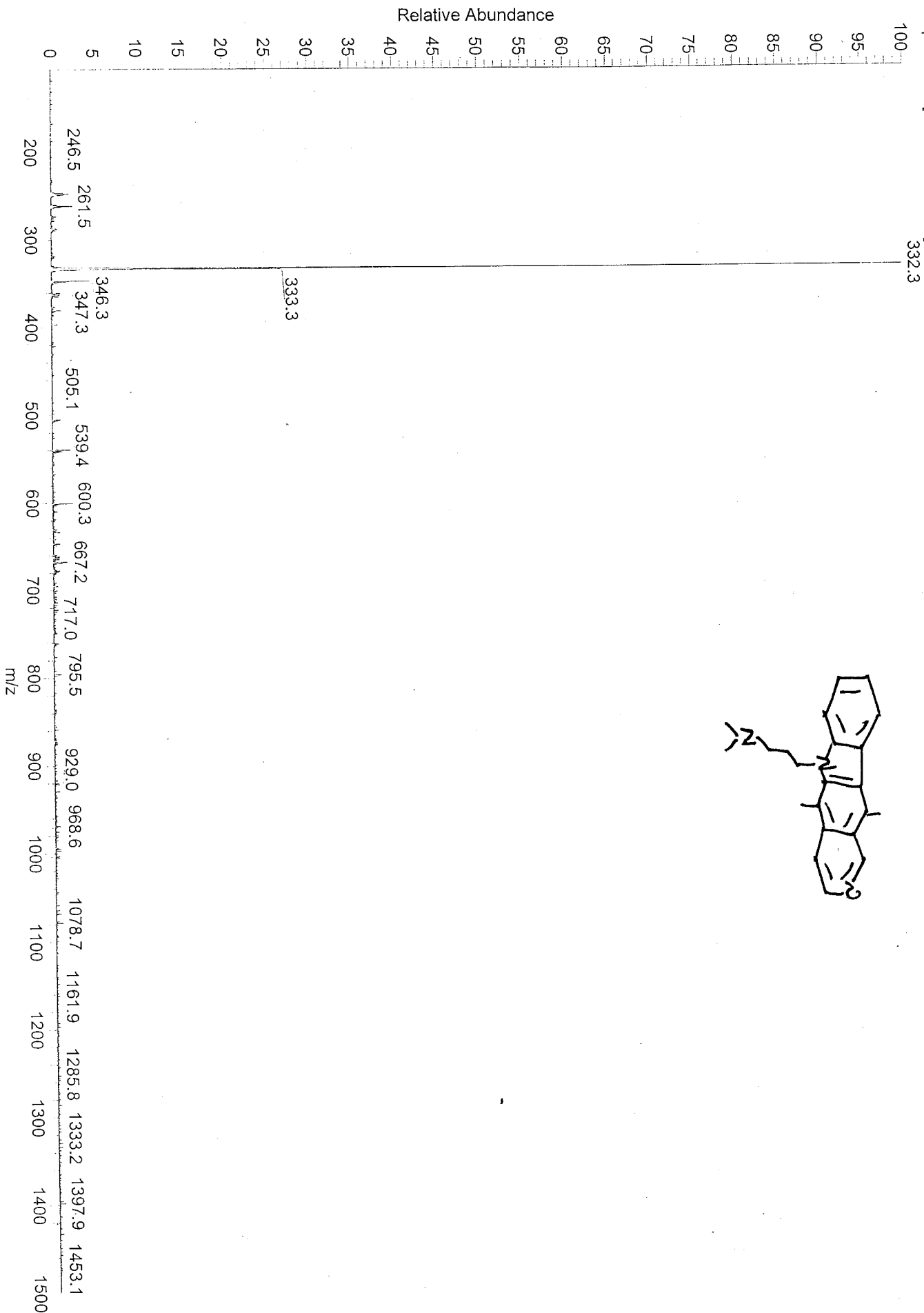


E:\MSLab\LCQ\KS_GSA_01_165
Srinivasa Kota, ACN:MeOH

06/14/2011 04:24:01 PM

KS_GSA_01_165

KS_GSA_01_165 #22-25 RT: 0.58-0.66 AV: 4 NL: 2.47E7
T: + p Full ms [105.00-1500.00]

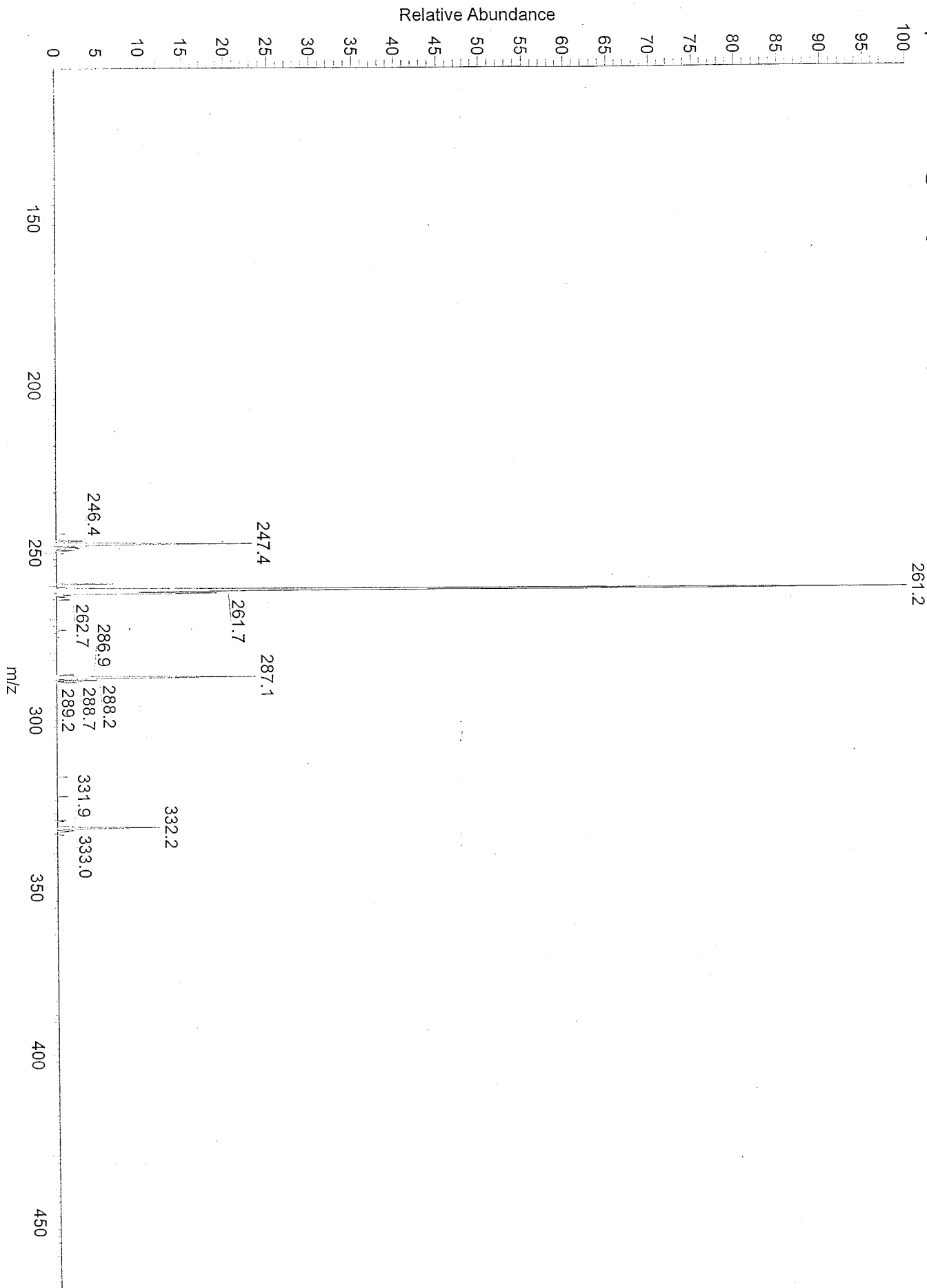


E:\MSLab\LCQ\KS_GSA_01_165
Srinivasa Kota, ACN:MeOH

06/14/2011 04:24:01 PM

KS_GSA_01_165

KS_GSA_01_165 #11-16 RT: 0.28-0.42 AV: 6 NL: 3.50E6
T: + p Full ms2 332.00@35.00 [105.00-1500.00]



SmartFormula Manually



Min

C₁₃

Generate

Max

C₁₃-n

Help

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

Measured m/z 332.21233

Tolerance 10

mDa

Charge 1

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdB	e ⁻ Conf	N-Rule
332.21233	1	C ₁₇ H ₂₆ N ₅ O ₂	4.75	332.20810	-4.2	-12.7	7.7	7.5	even	ok
	2	C ₁₆ H ₂₆ N ₇ O	0.06	332.21933	7.0	21.1	10.1	7.5	even	ok
	3	C ₂₂ H ₂₆ N ₄	100.00	332.21212	-0.2	-0.6	19.6	11.5	even	ok
	4	C ₁₃ H ₂₂ N ₁₁	0.06	332.20542	-6.9	-20.8	20.5	8.5	even	ok
	5	C ₁₆ H ₃₀ N ₆ O	0.55	332.20676	-5.6	-16.8	22.5	2.5	even	ok
	6	C ₁₅ H ₃₀ N ₃ O ₅	0.45	332.21800	5.7	17.1	24.4	2.5	even	ok

☐ 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

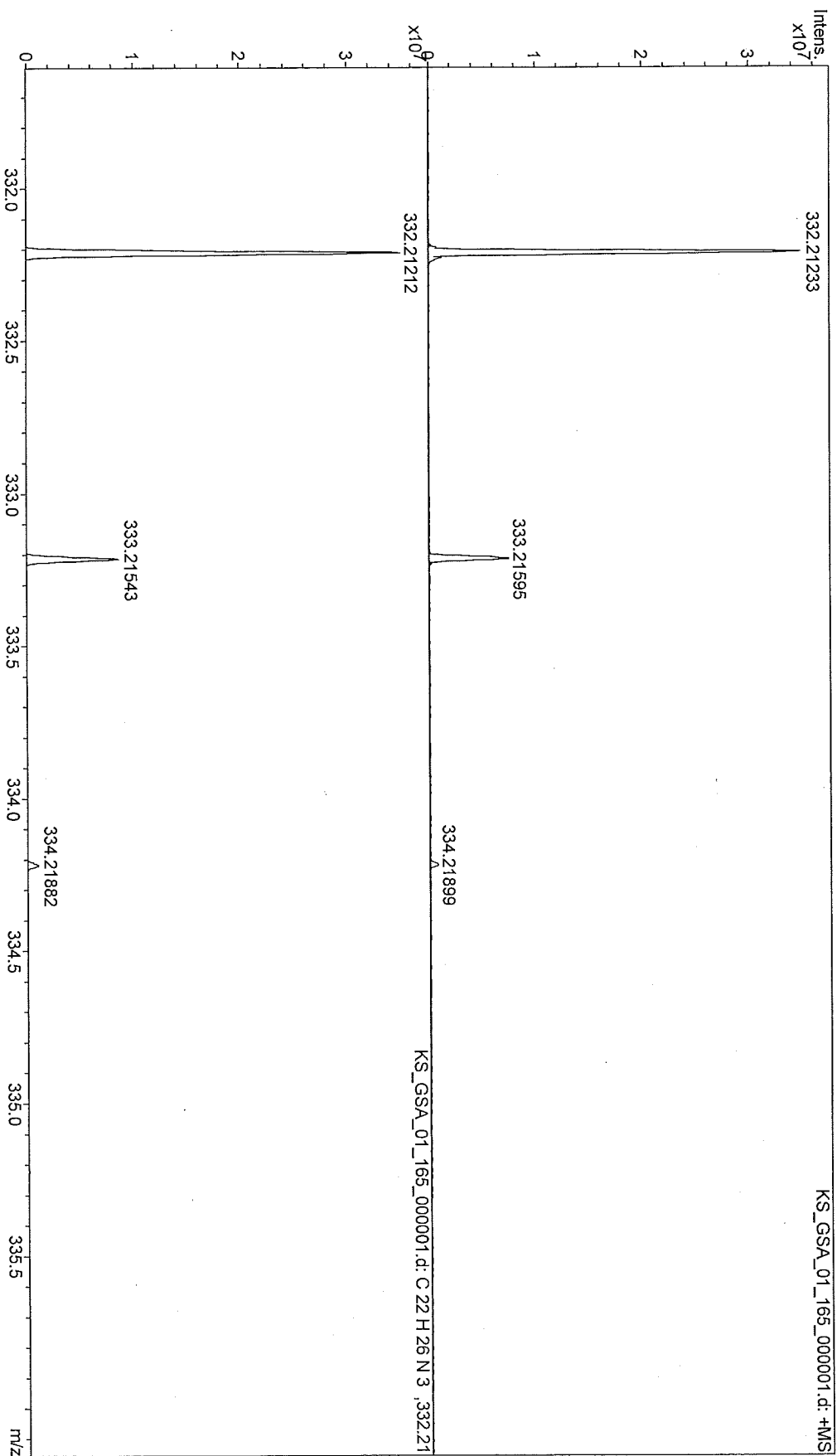
Generic Display Report

Analysis Info

Analysis Name D:\DATA\Facility_June_11\KS_GSA_01_165_000001.d
Method Scott_tune
Sample Name KS_GSA_01_165
Comment Srinivasa Kota, ACN:MeOH

Acquisition Date 6/14/2011 4:26:03 PM

Operator
Instrument apex-Ultra



Current Data Parameters
 NAME VB-GSA-0336-2
 EXPNO 341
 PROCNO 1

F2 - Acquisition Parameters:
 Date_ 20110524
 Time 15.45

INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg30
 TD 65536
 SOLVENT DMSO

NS 2
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 724.1
 DW 81.000 use
 DE 6.00 use
 TE 300.0 K
 D1 1.00000000 sec

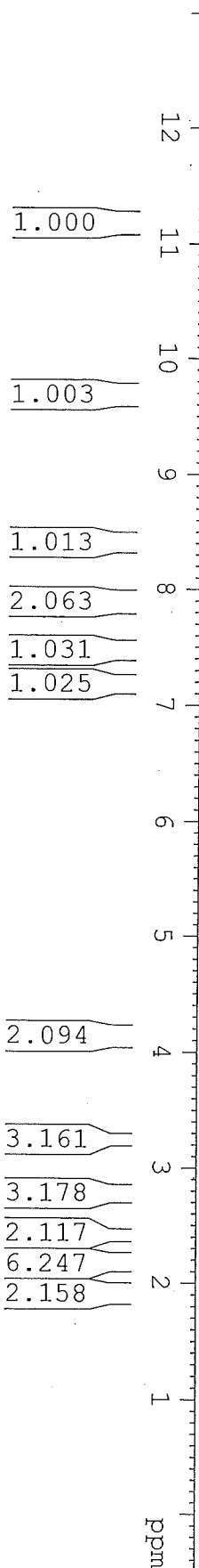
===== CHANNEL f1 =====
 NUC1 1H
 P1 8.50 use
 PL1 0.00 dB
 SFO1 300.1318534 MHz

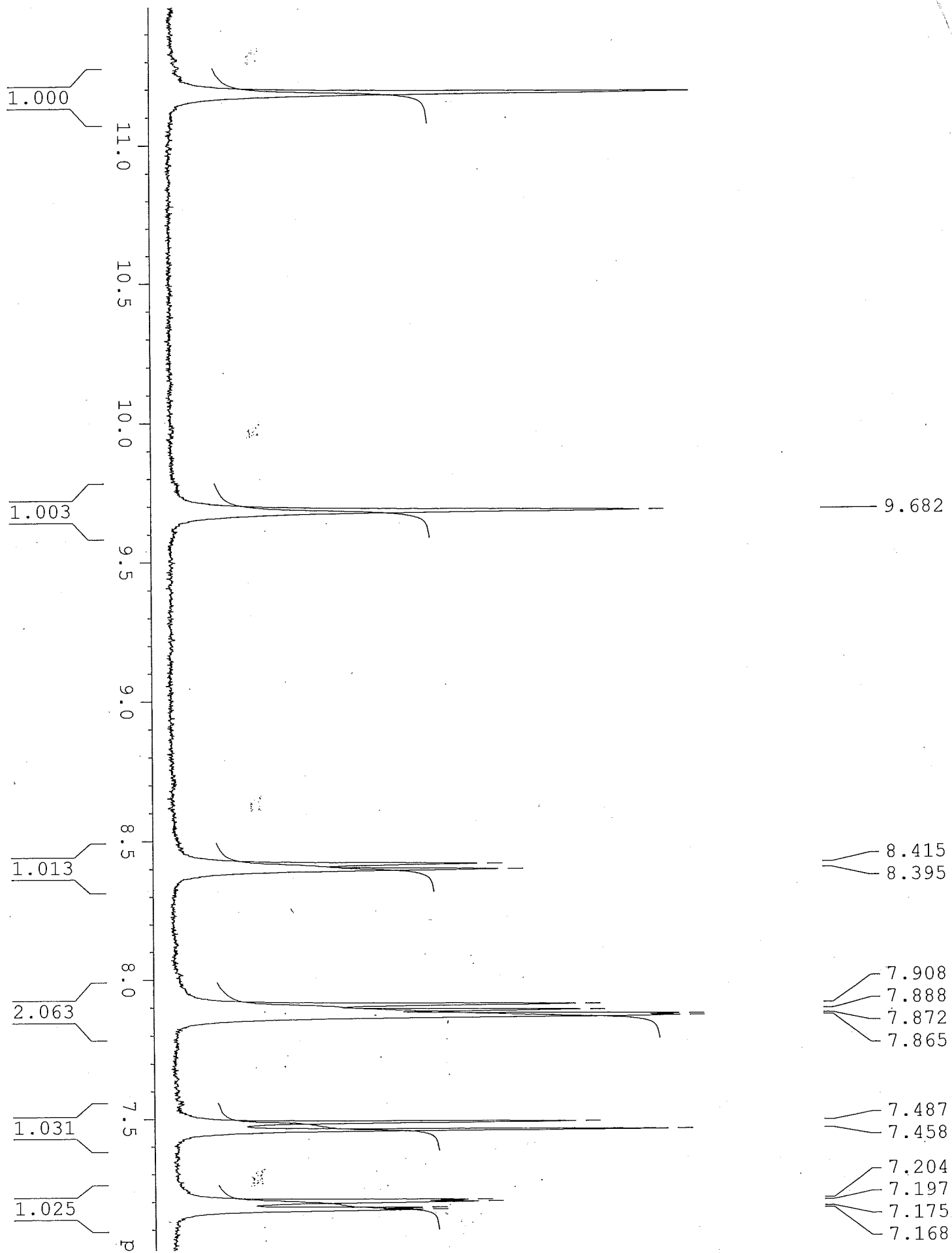
F2 - Processing Parameters
 SI 32768
 SF 300.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

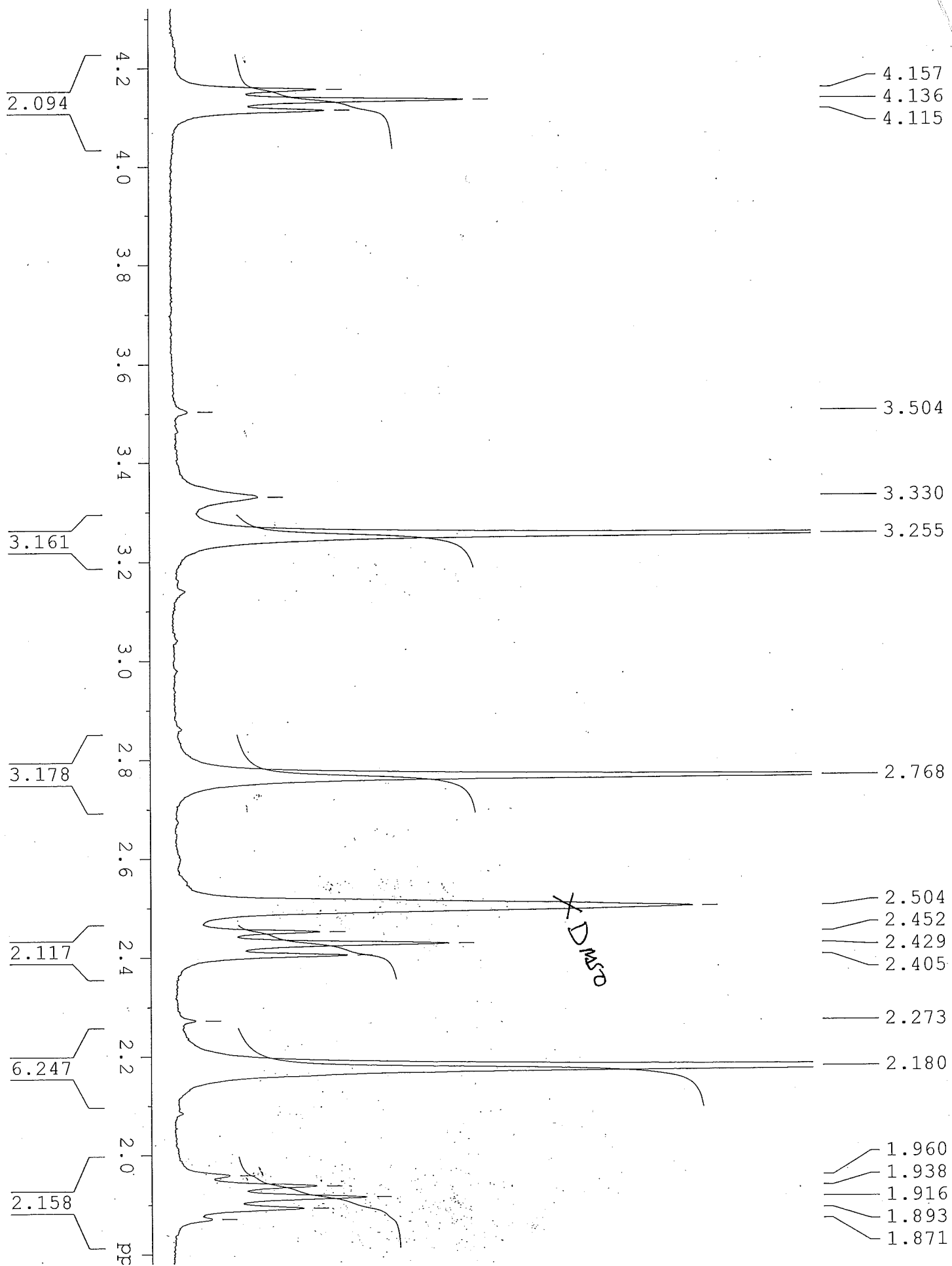
- 9.682
- 8.415
- 8.395
- 7.908
- 7.888
- 7.872
- 7.865
- 7.487
- 7.458
- 7.204
- 7.197
- 7.175
- 7.168
- 4.157
- 4.136
- 4.115
- 3.504
- 3.330
- 3.255
- 2.768
- 2.504
- 2.452
- 2.429
- 2.405
- 2.273
- 2.180
- 1.960
- 1.938
- 1.916
- 1.893
- 1.871
- 1.225
- 0.001



VB-GSA-0336







Current Data Parameters
 NAME VB-GSA-0336-2
 EXPNO 341
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110525
 Time 7.50

INSTRUM spect
 PROBD 5 mm QNP 1H/1
 PULPROG zgpg30

TD 65536
 SOLVENT DMSO-d₆
 NS 15000
 DS 4

SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec

RG 1824.6
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K

D1 2.00000000 sec
 d11 0.03000000 sec
 d12 0.0002000 sec

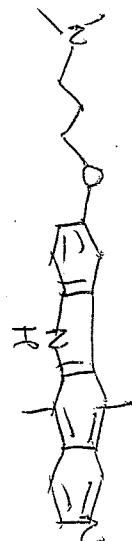
===== CHANNEL f1 =====
 NUC1 13C
 P1 6.00 usec
 PL1 2.00 dB
 SFO1 75.4752653 MHz

===== 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

153.320
 150.616
 142.079
 141.282
 138.199
 133.194
 129.065
 124.439
 124.273
 122.548
 116.642
 111.983
 109.649
 108.738

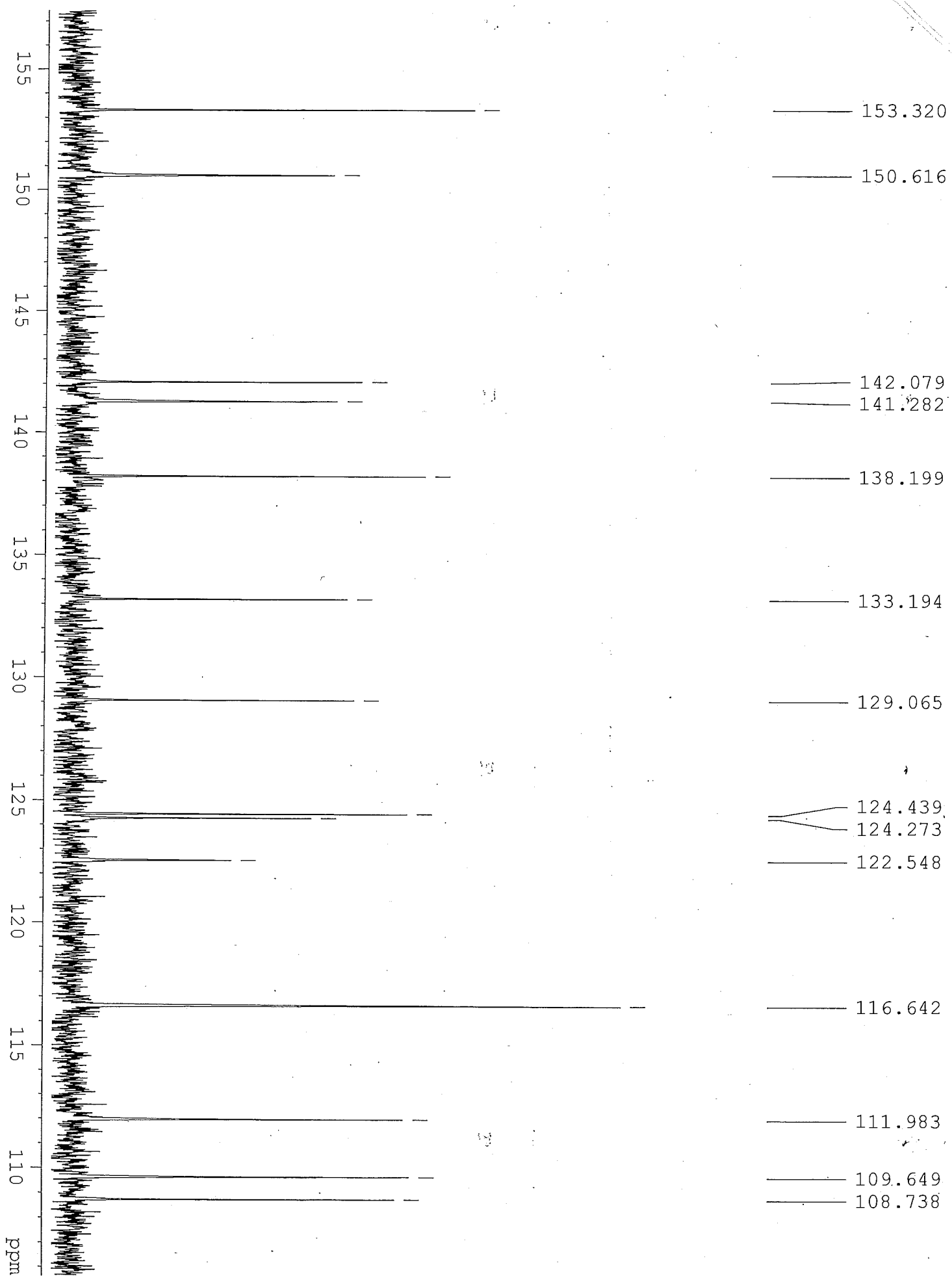
67.630
 56.740
 46.145
 41.222
 40.944
 40.666
 40.388
 40.109
 39.831
 39.552
 39.227
 38.946
 28.096
 15.152
 12.774
 0.969

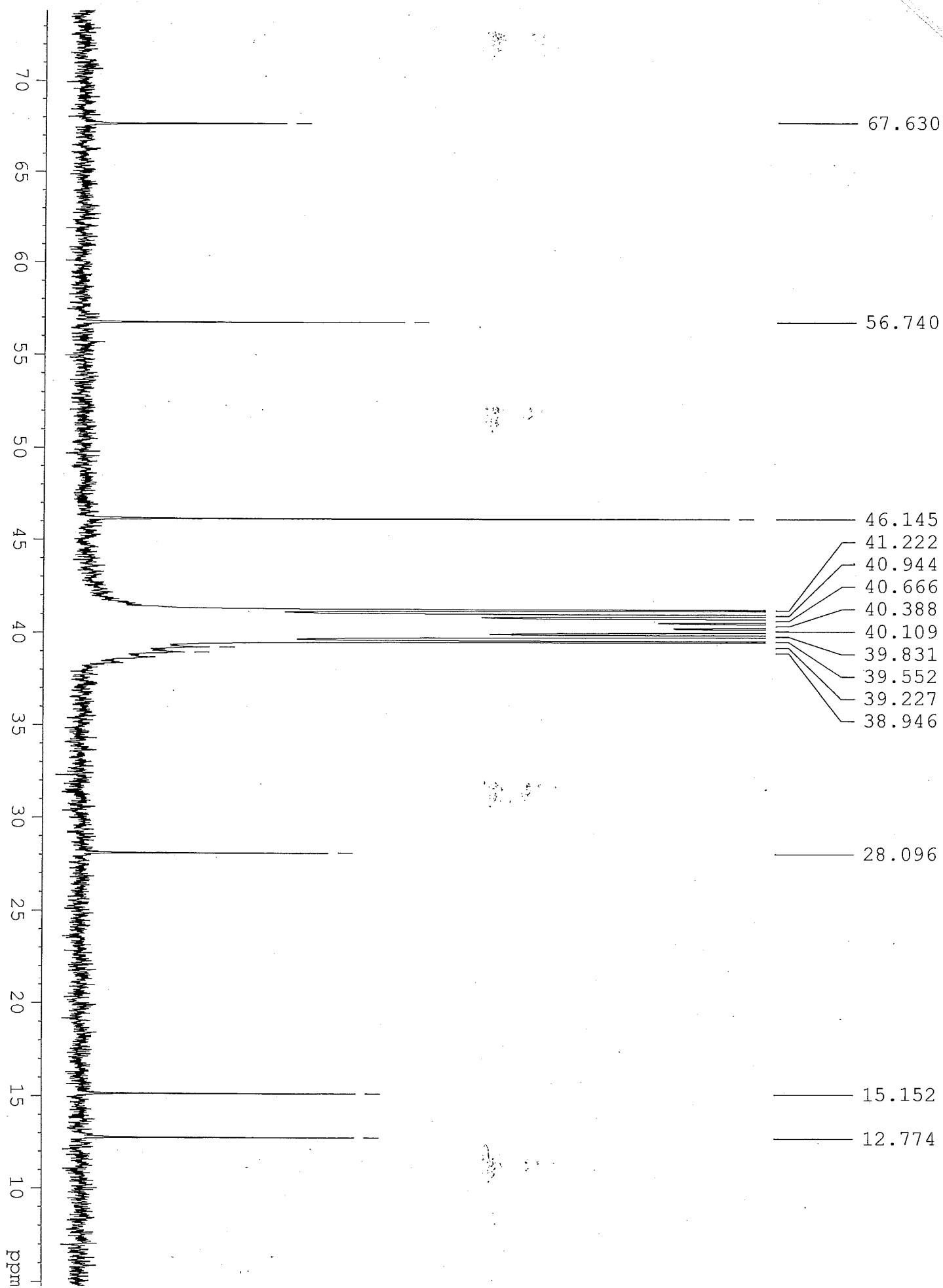


VB-GSA-0336

X DMSO

170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm





Injection Date : 5/23/2011 5:35:18 PM

Sample Name : VB-GSA-0336

Location : Vial 1

Acq. Operator : Karen

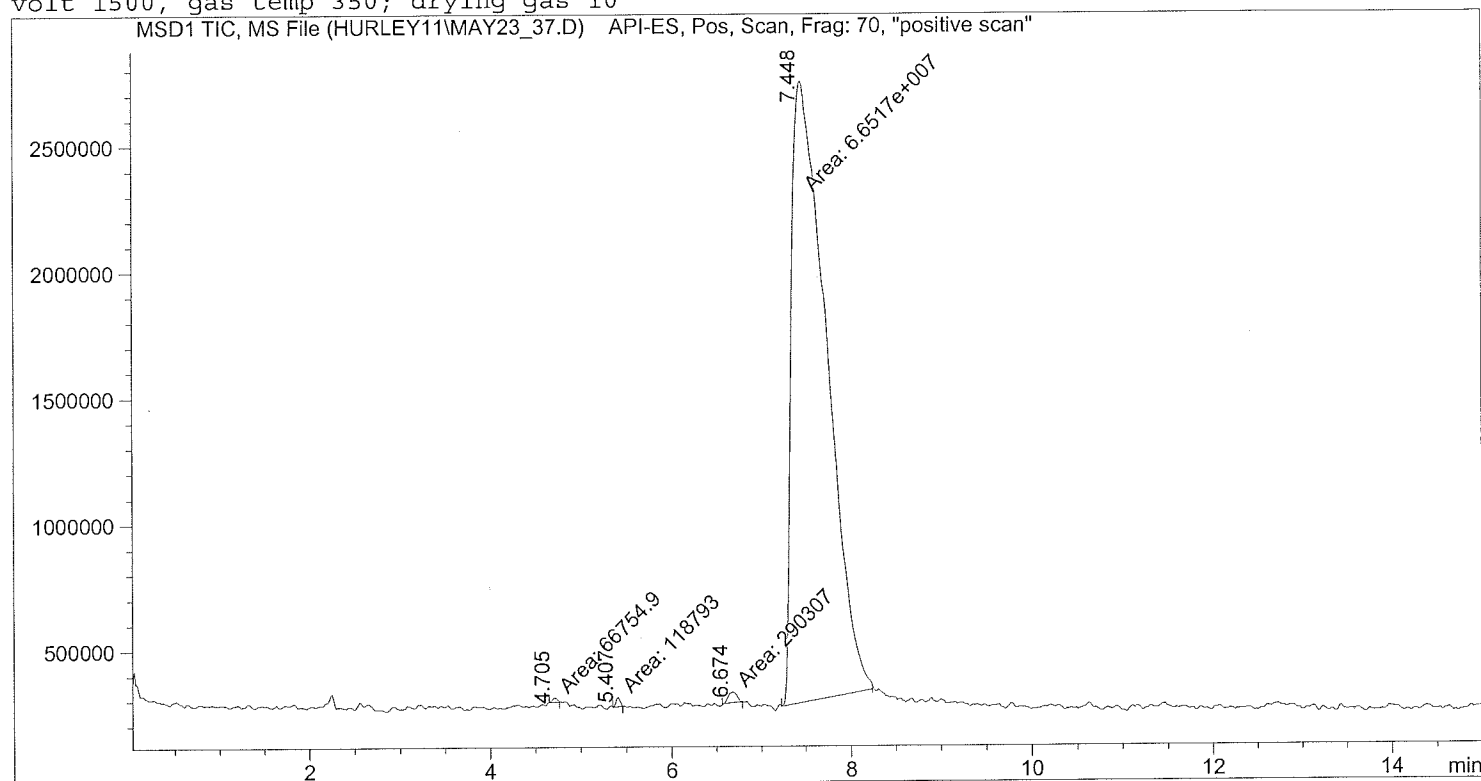
Inj : 1

Acq. Instrument : Instrument 1

Inj Volume : 0.1 µl

Method : C:\HPCHEM\1\METHODS\LC_MS_UV.M

Last changed : 5/23/2011 5:17:50 PM by Karen

Zorbax SB C18, 150 x 4.6, 3.5µ, 35/65/0.25, MeOH/water/formic, POS, 150-500; frag 70; 30C, cap
volt 1500, 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 [min]	Type	Width [min]	Area	Height	Area %
1	4.705	MM	0.0604	6.67549e4	1.84083e4	0.0996
2	5.407	MM	0.0502	1.18793e5	3.94212e4	0.1773
3	6.674	MM	0.1090	2.90307e5	4.43800e4	0.4333
4	7.448	MM	0.4492	6.65170e7	2.46805e6	99.2897

Totals : 6.69928e7 2.57026e6

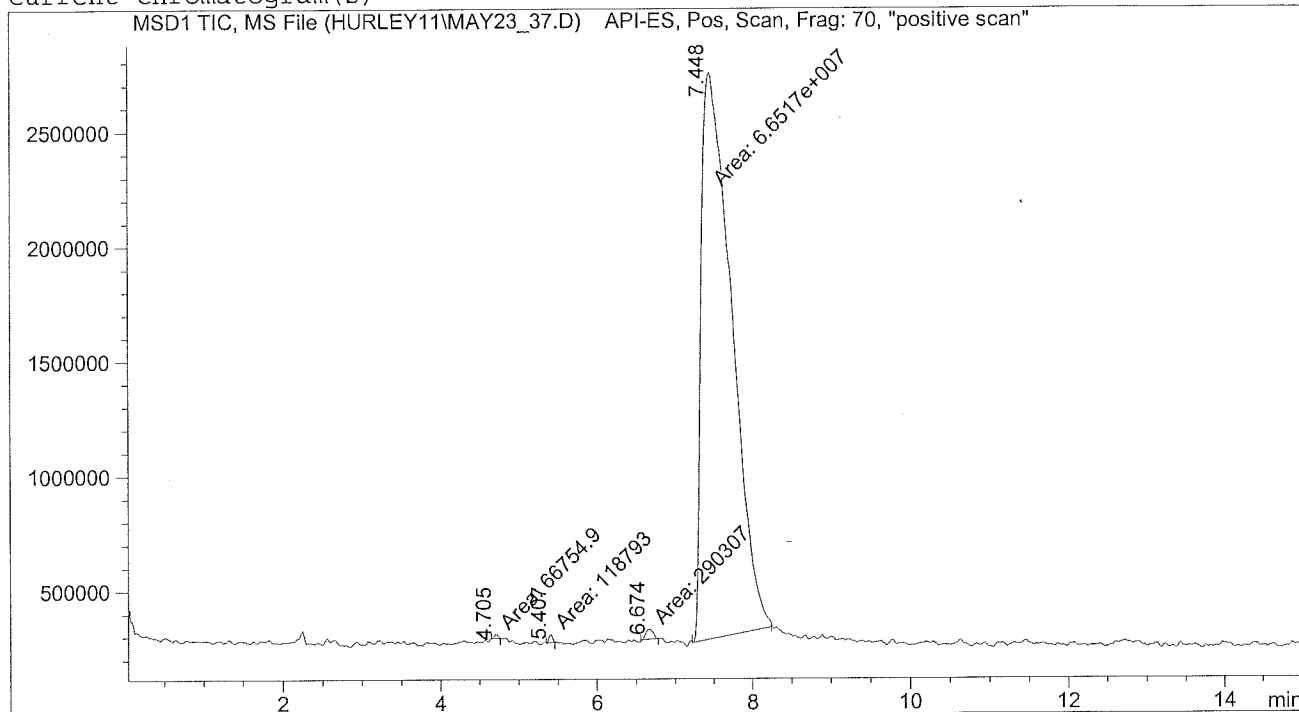
*** End of Report ***



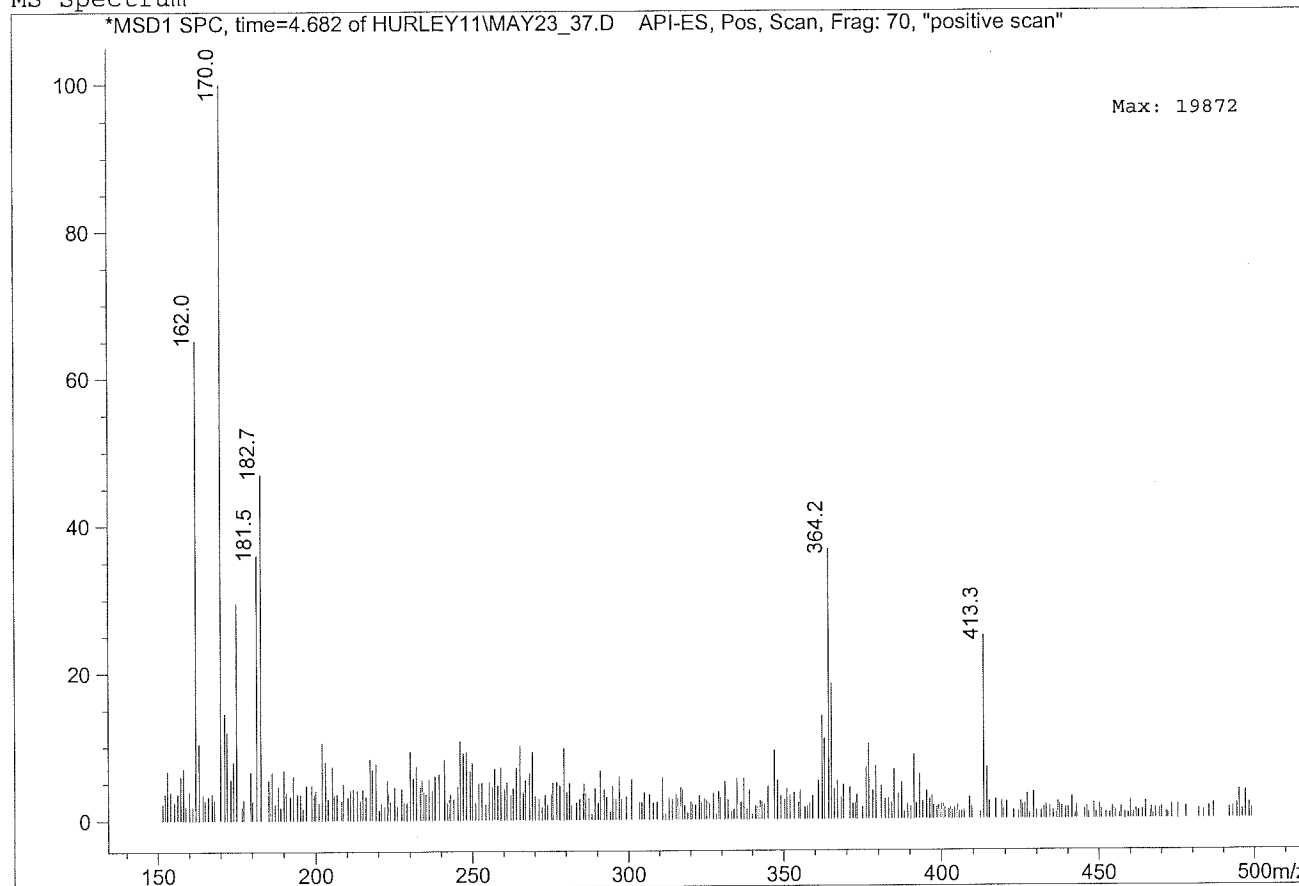
VB-GSA-0336

```
=====
Injection Date   : 5/23/2011 5:35:18 PM
Sample Name      : VB-GSA-0336
Acq. Operator    : Karen
Acq. Instrument  : Instrument 1
Method           : C:\HPCHEM\1\METHODS\LC_MS_UV.M
Last changed     : 5/23/2011 5:17:50 PM by Karen
Zorbax SB C18, 150 x 4.6, 3.5u, 35/65/0.25, MeOH/water/formic, POS, 150-500; frag 70; 30C, cap
volt 1500, gas temp 350; drying gas 10
=====
```

Current Chromatogram(s)



MS Spectrum

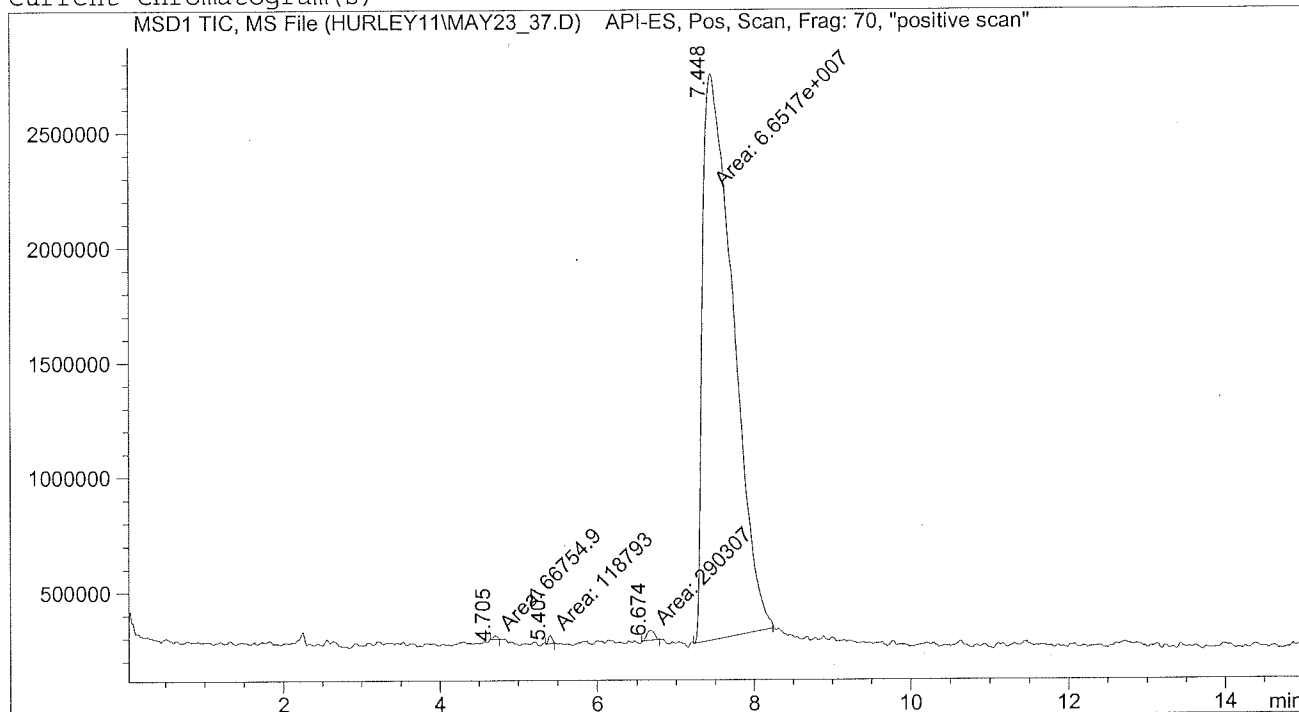


=====

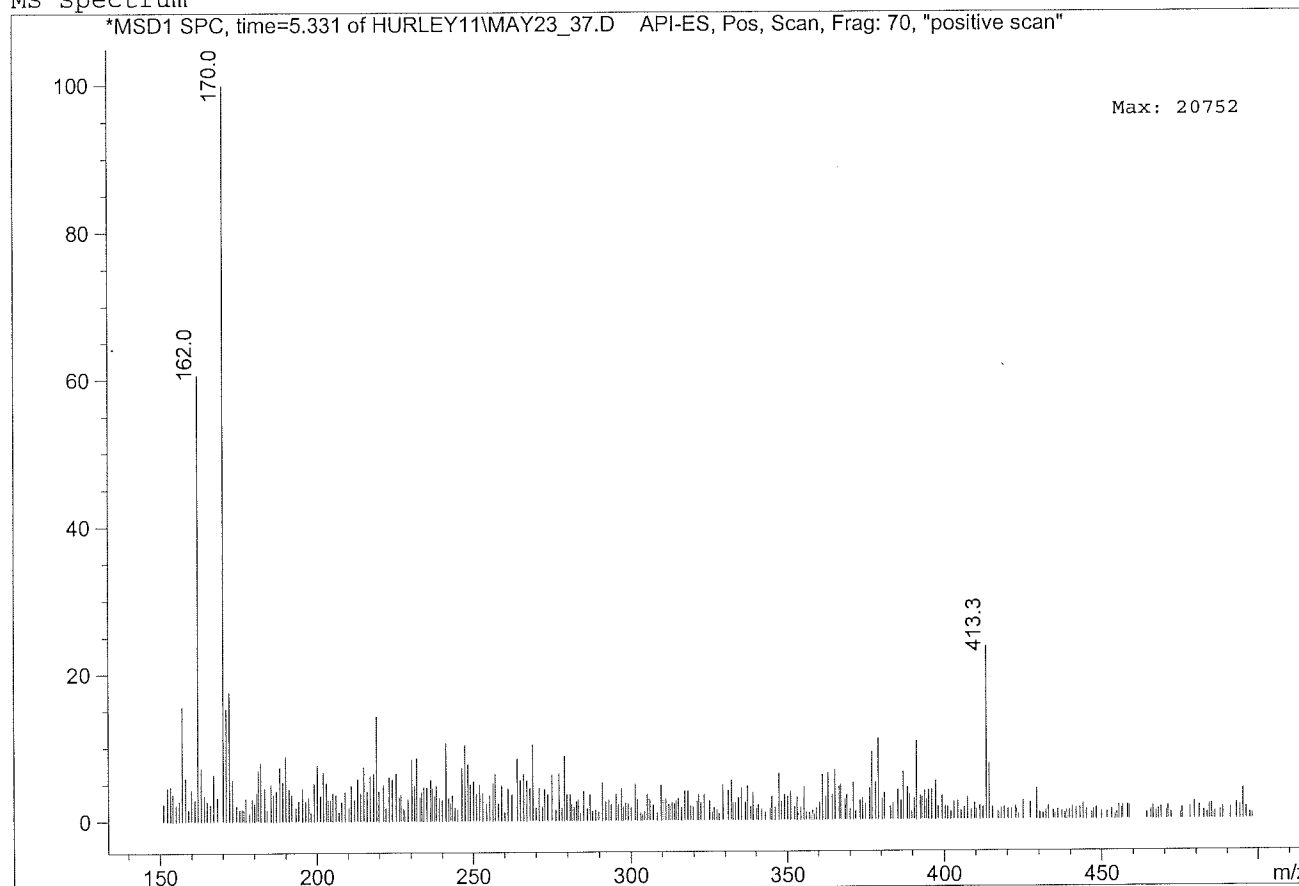
Injection Date	: 5/23/2011 5:35:18 PM	Location	: Vial 1
Sample Name	: VB-GSA-0336	Inj	: 1
Acq. Operator	: Karen	Inj Volume	: 0.1 μ l
Acq. Instrument	: Instrument 1		
Method	: C:\HPCHEM\1\METHODS\LC_MS_UV.M		
Last changed	: 5/23/2011 5:17:50 PM by Karen		

Zorbax SB C18, 150 x 4.6, 3.5 μ , 35/65/0.25, MeOH/water/formic, POS, 150-500; frag 70; 30C, cap volt 1500, gas temp 350; drying gas 10

Current Chromatogram(s)

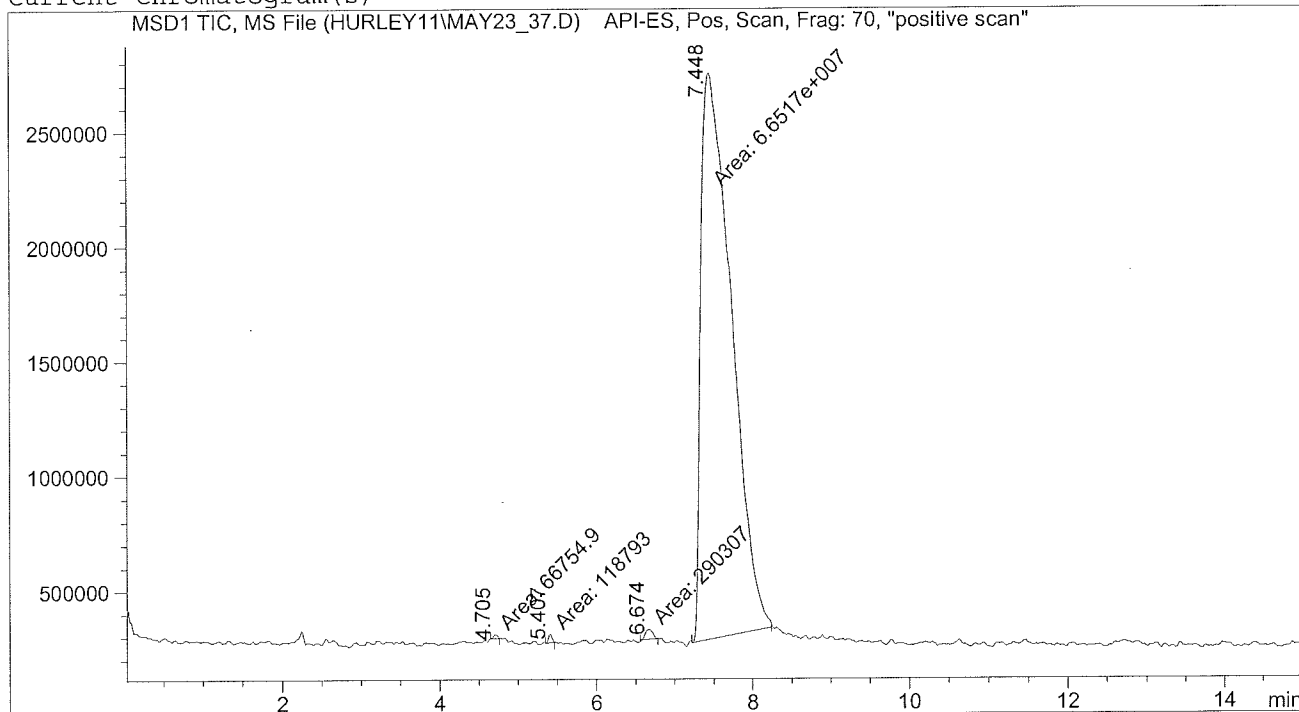


MS Spectrum

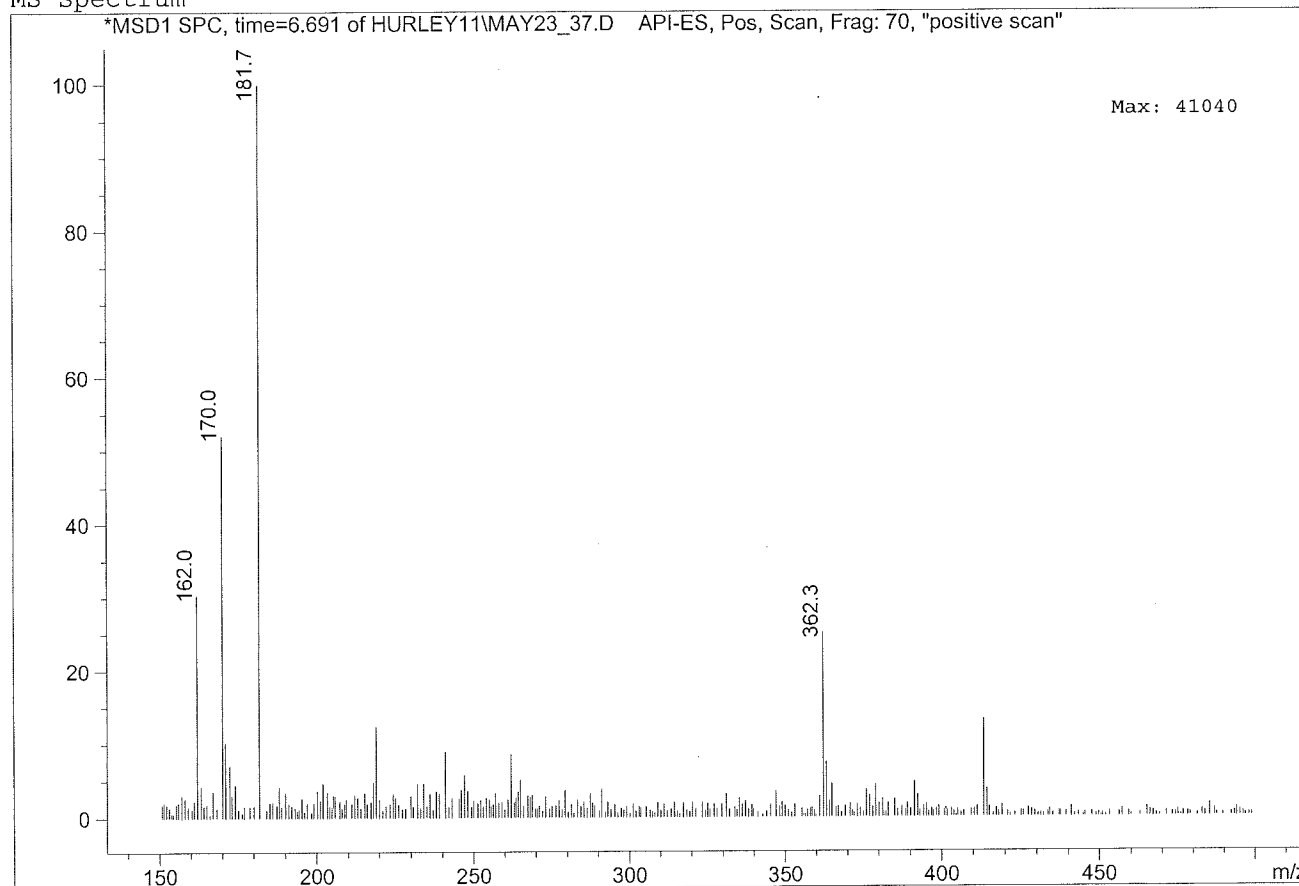



```
=====
Injection Date   : 5/23/2011 5:35:18 PM
Sample Name      : VB-GSA-0336
Acq. Operator    : Karen
Acq. Instrument  : Instrument 1
Method           : C:\HPCHEM\1\METHODS\LC_MS_UV.M
Last changed     : 5/23/2011 5:17:50 PM by Karen
Zorbax SB C18, 150 x 4.6, 3.5u, 35/65/0.25, MeOH/water/formic, POS, 150-500; frag 70; 30C,
cap volt 1500, gas temp 350; drying gas 10
=====
```

Current Chromatogram(s)

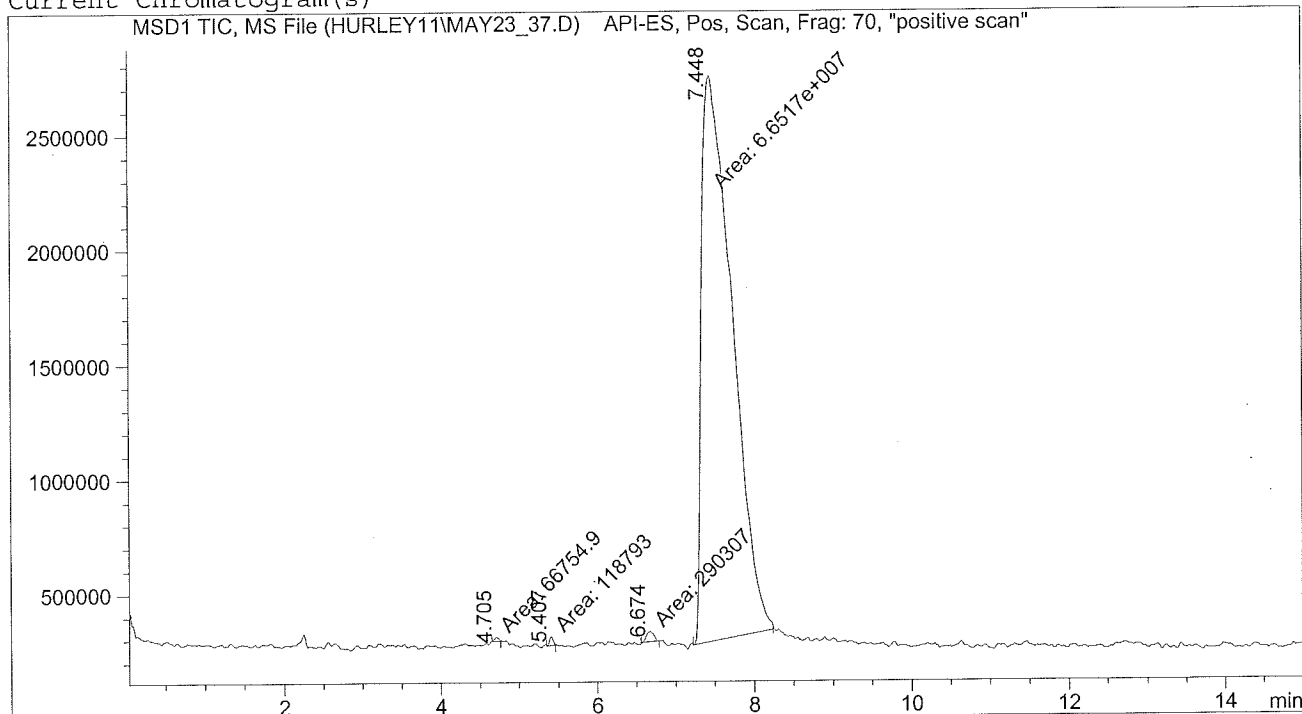


MS Spectrum

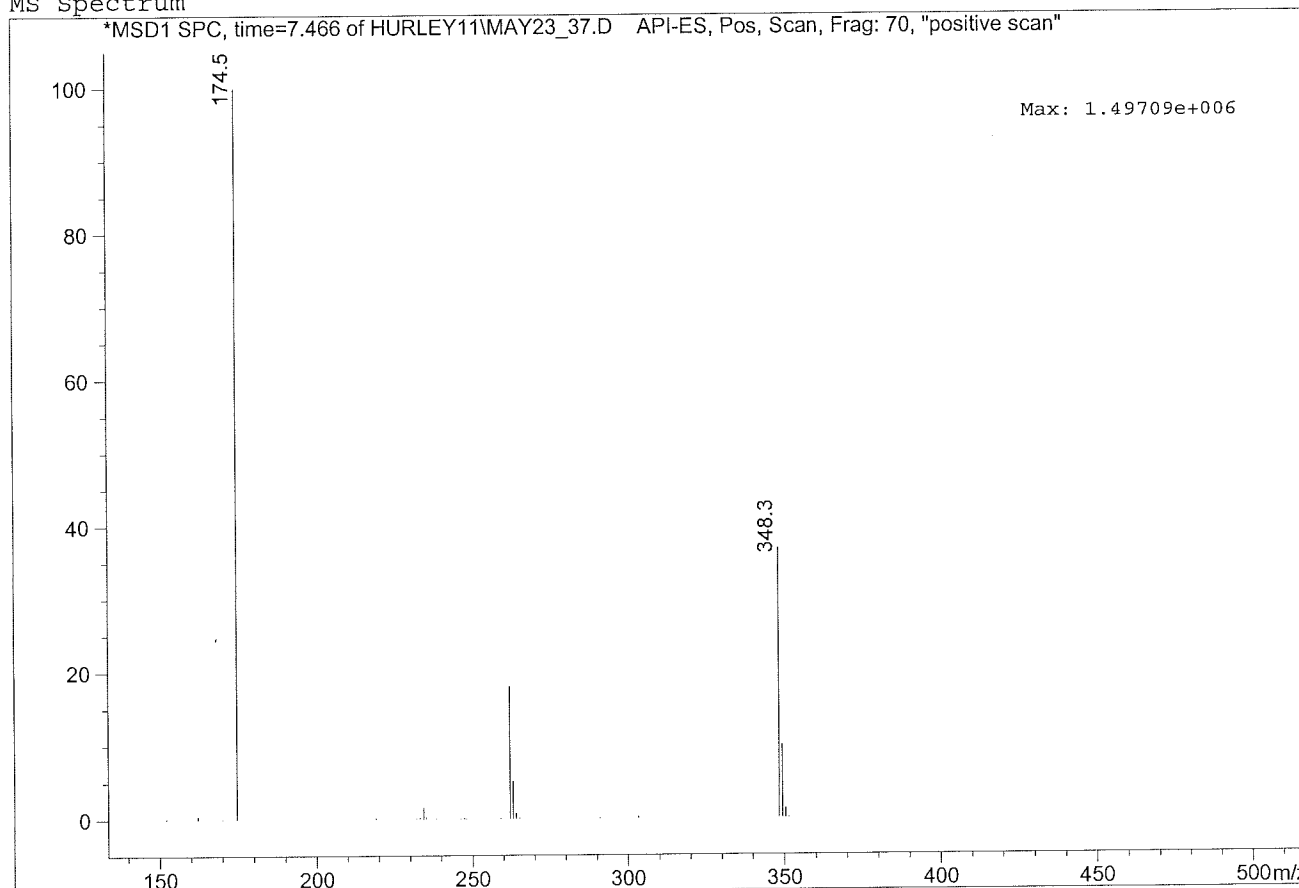


```
=====
Injection Date   : 5/23/2011 5:35:18 PM
Sample Name      : VB-GSA-0336
Acq. Operator    : Karen
Acq. Instrument  : Instrument 1
Method           : C:\HPCHEM\1\METHODS\LC_MS_UV.M
Last changed     : 5/23/2011 5:17:50 PM by Karen
Zorbax SB C18, 150 x 4.6, 3.5u,35/65/0.25,MeOH/water/formic, POS, 150-500; frag 70; 30C,
cap volt 1500, gas temp 350; drying gas 10
Location         : Vial 1
Inj              : 1
Inj Volume       : 0.1 µl
=====
```

Current Chromatogram(s)



MS Spectrum



Generic Display Report

Analysis Info

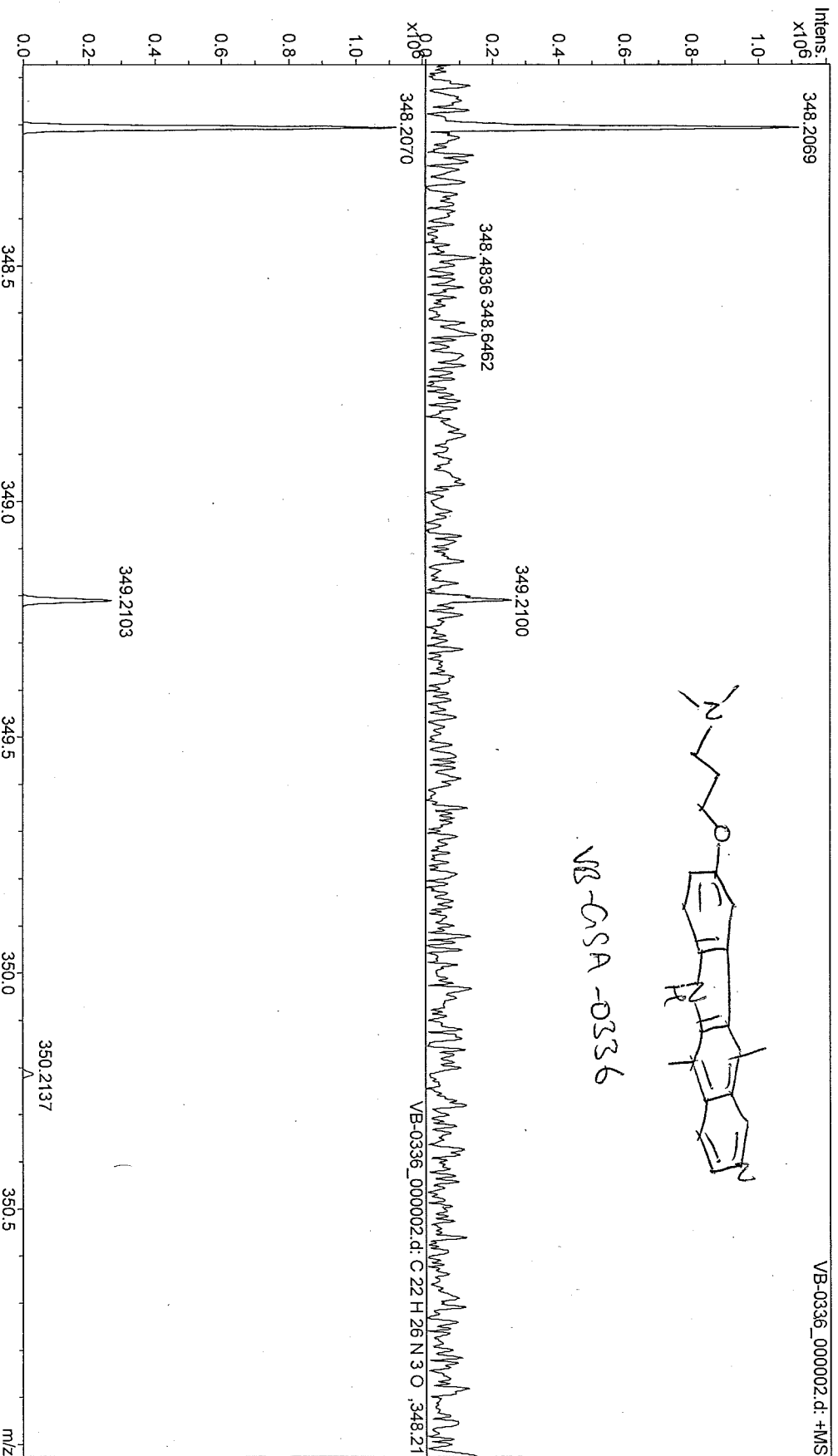
Analysis Name D:\DATA\Facility_May_11\VB-0336_000002.d
Method Scott_tune
Sample Name VB-0336
Comment Venkat B., ACN:H2O 1:1:0.1%FA

Acquisition Date

5/26/2011 9:36:01 AM

Operator
Instrument

apex-Ultra



SmartFormula Manually



Min

C₁₅

Generate

Max

C₁₅-n

Help

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

Measured m/z

348.2069

Tolerance

2

mDa



Charge

1



Meas. m/z

#

Formula

Score

m/z

err [mDa]

err [ppm]

mSigma

rdB

e-Conf

N-Rule

ok

348.2069 1 C₁₅H₂₆N₃O 100.00 348.2070 0.2 0.4 20.0 11.5 even

☐ 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