

Order of ESI files

- 1: Compound 2-1-NMR
- 2: Compound 2-2-NMR
- 3: Compound 2-MS
- 4: Compound 3-MS
- 5: Compound 4-NMR
- 6: Compound 4-MS
- 7: Compound 5-HPLC
- 8: Compound 5-1-NMR
- 9: Compound 5-1-MS
- 10: Compound 5-2-MS
- 11: Compound 5-2-NMR
- 12: Compound 5-3-NMR
- 13: Compound 6-NMR
- 14: Compound 6-MS
- 15: Compound 7-NMR
- 16: Compound 7-MS
- 17: Compound 8-HPLC
- 18: Compound 8-NMR
- 19: Compound 8-MS
- 20: Compound 9-HPLC
- 21: Compound 9-NMR
- 22: Compound 9-MS

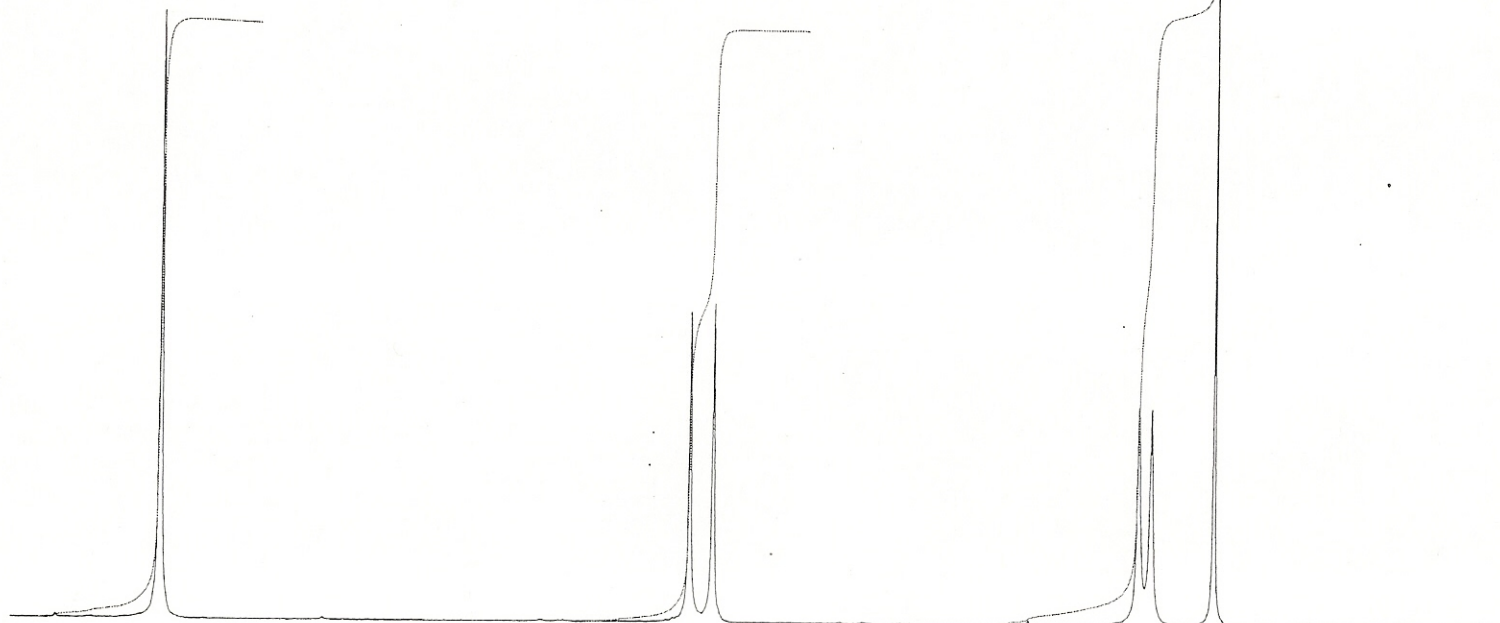
8.839
8.822
8.795
8.772
8.694
8.662

8.466

8.341

8.161
8.136
8.129
8.076
8.054
8.022
7.986
7.977
7.954
7.921
7.743
7.712
7.645
7.525
7.506
7.488
7.478
7.465
7.430
7.375
7.324
7.306
7.276
7.218
7.121
7.102
7.083
7.037
6.999
6.976
6.954

SD1-Shoarab



8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 ppm

1.60

1.59

2.64



Current Data Parameters
NAME SD1-Shourab
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date 20060227
Time 12.56
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 114
DW 60.800 usec
DE 6.00 usec
TE 290.4 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.00 usec
PL1 0.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300260 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

3.891
3.669
3.651
3.634
3.616
3.606
3.593
3.576
3.520
3.510
3.502
3.493
3.483
3.476
3.466
3.452
3.402
3.244
3.231
3.223
3.219
2.248
2.226
2.110
1.912
1.587
1.558
1.531
1.497
1.480
1.457
1.430
1.369
1.351
1.335
1.319
1.295
1.270
1.212
1.201
1.185
1.168
1.150
1.129



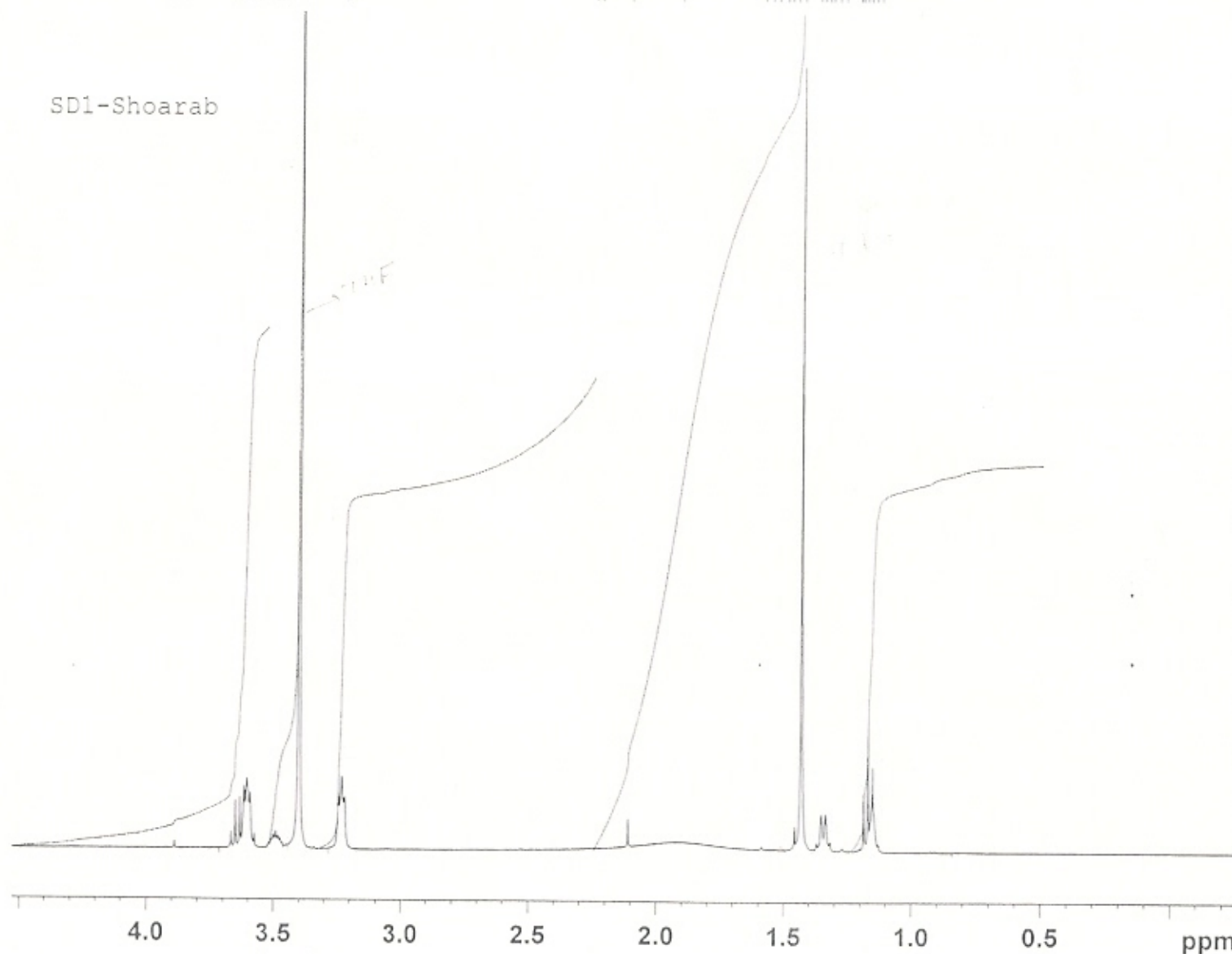
SD1-Shoarab

Current Data Parameters
NAME SD1-Shourab
EXPNO 1
PROCNO 1

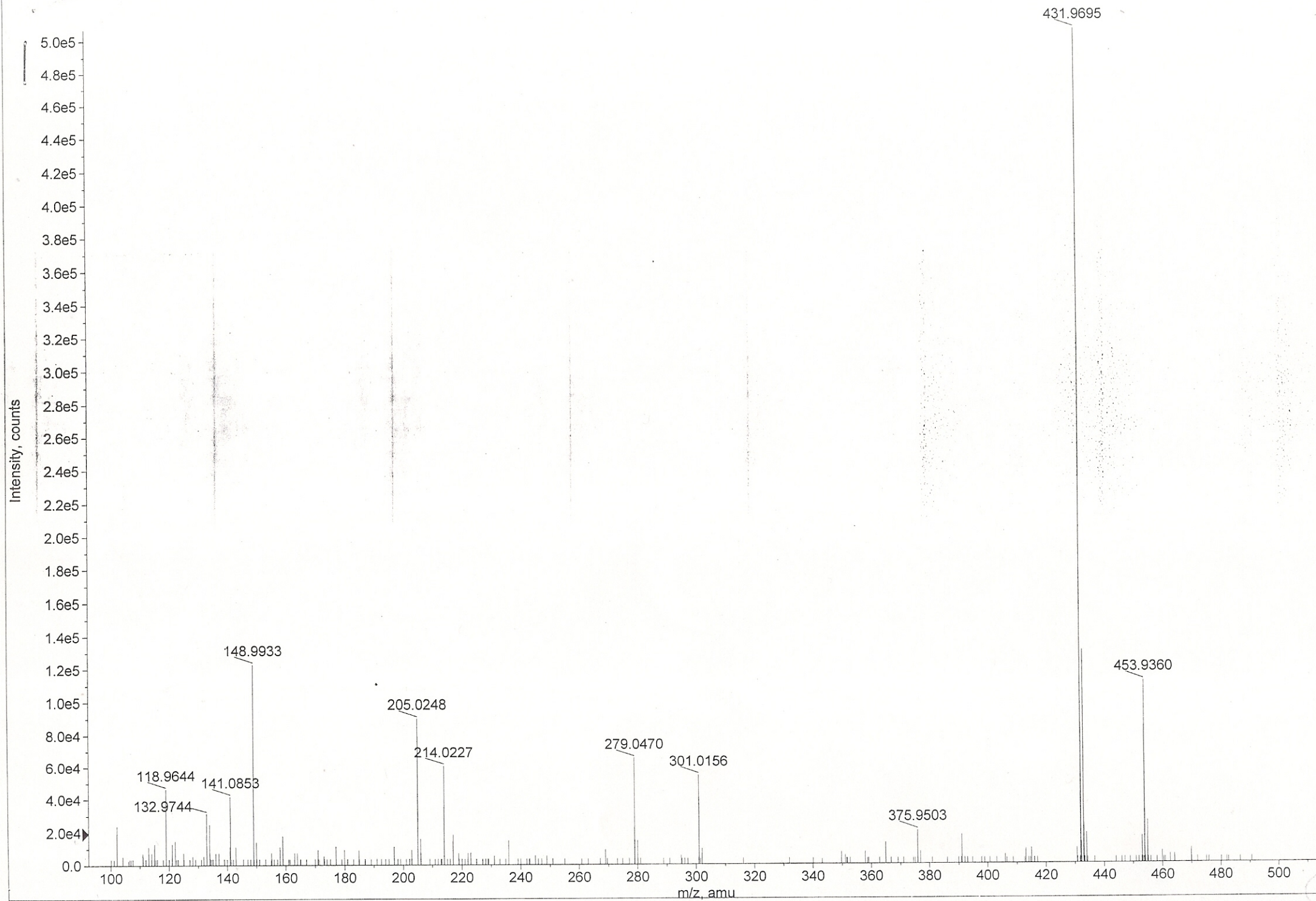
F2 - Acquisition Parameters
Date 20060227
Time 12.56
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 114
DW 60.800 usec
DE 6.00 usec
TE 290.4 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.00 usec
PL1 0.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300260 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

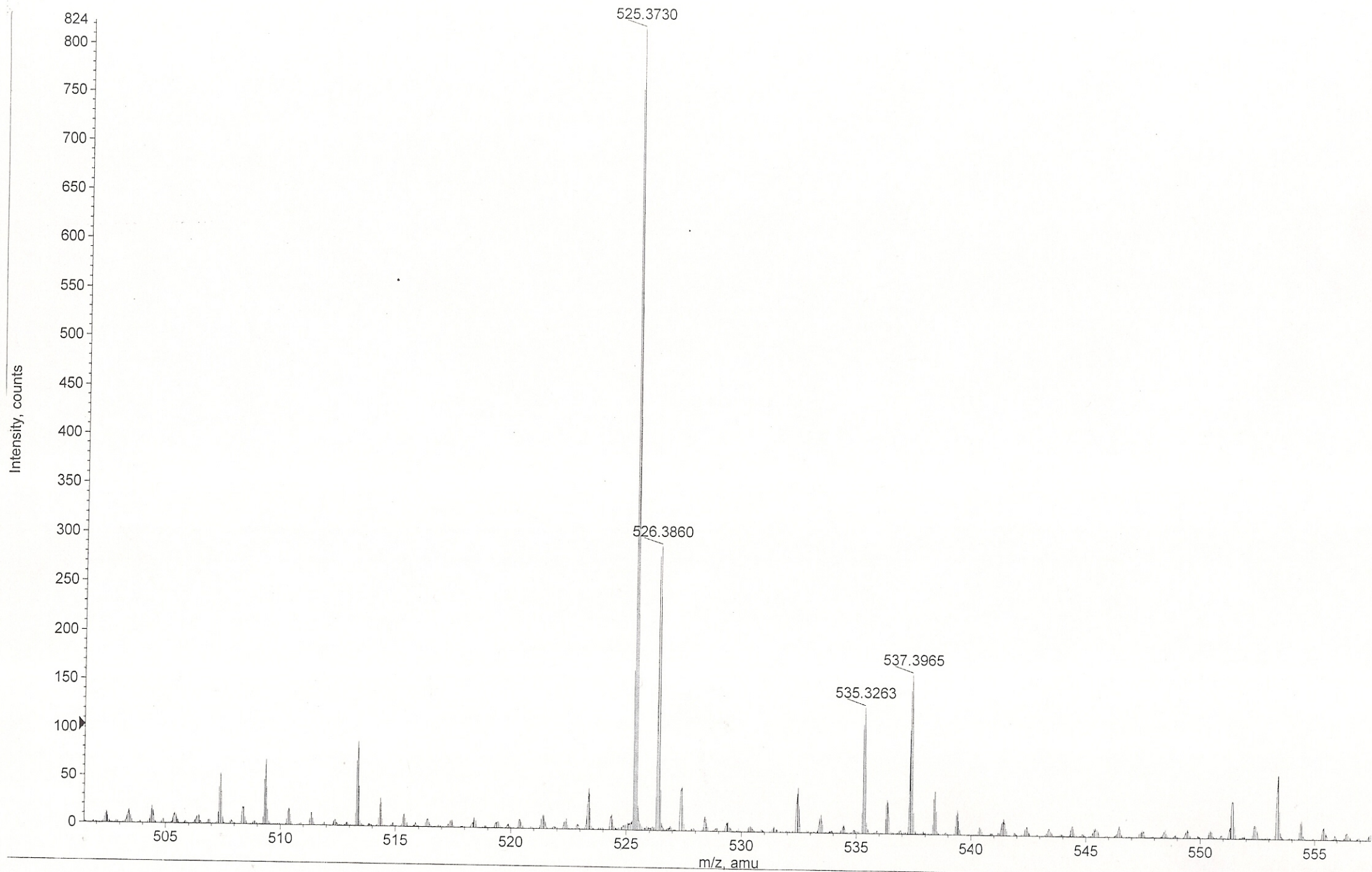


a=3.56648734867816710e-004, t0=-4.99256432894944740e+001, subtracted (8.319 to 8.920 min and 9.35 to 10.17 min)



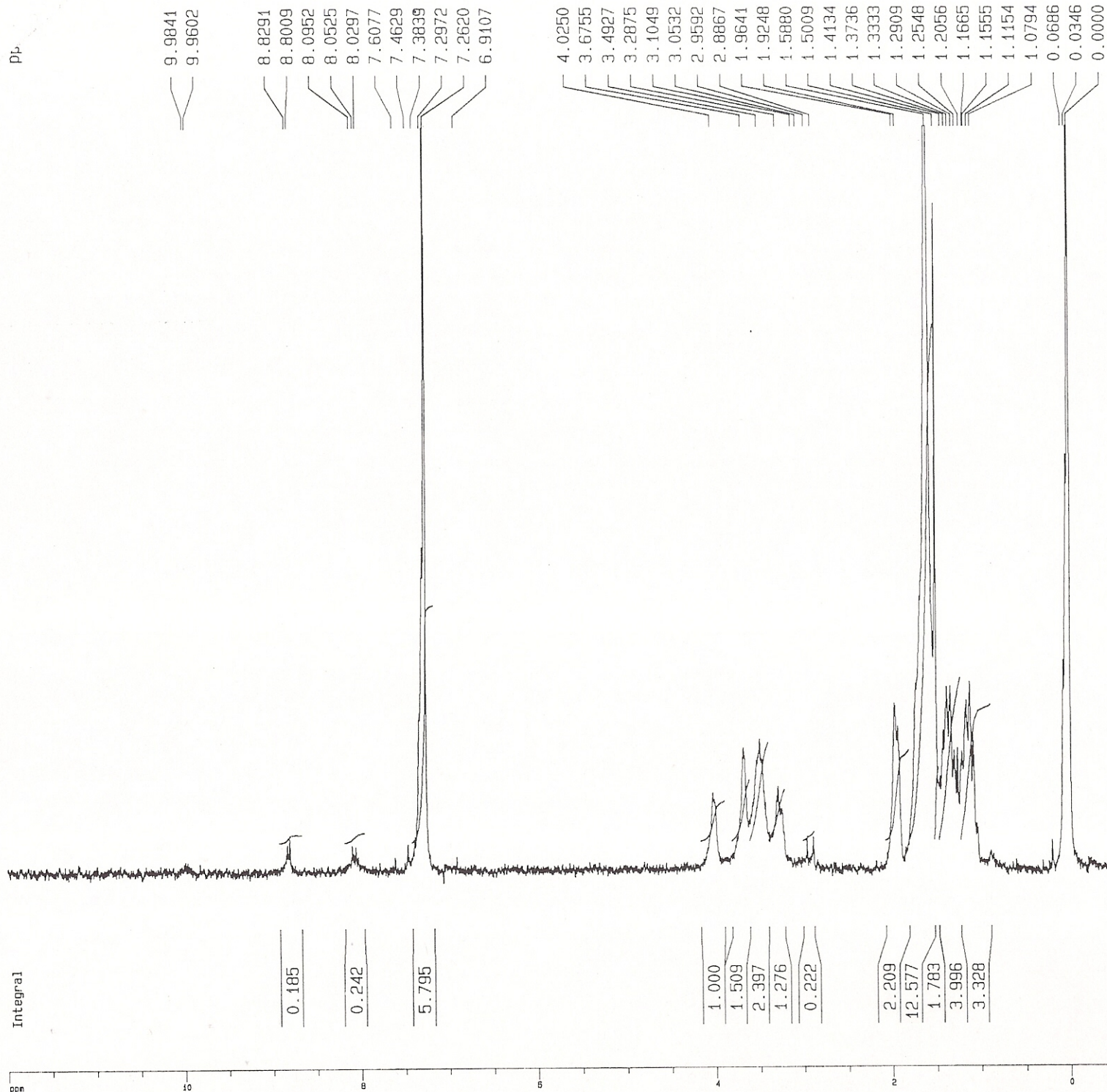
2.734 to 2.835 min from Sample 3 (sau2) of sau2.wiff
6479999999980e-004, t0=-3.48803564015000020e+001, subtracted (3.085 to 4.851 min)

Max. 1624.5 counts.



Integral

ppm



Current Data Parameters
 NAME proton
 EXPNO 593
 PROCNO 1

F2 - Acquisition Parameters

Date_ 500000
 Time 12.55
 INSTRUM dpx300
 PROBHD 5mm Dual Z5
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 8992.806 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 362
 DW 55.600 usec
 DE 4.50 usec
 TE 300.0 K
 D1 5.00000000 sec
 P1 11.35 usec
 DE 4.50 usec
 SF01 300.1342018 MHz
 NUC1 1H
 PL1 0.00 dB

F2 - Processing parameters

SI 32768
 SF 300.1300057 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters

CX 20.00 cm
 F1P 12.000 ppm
 F1 3601.56 Hz
 F2P -0.500 ppm
 F2 -150.07 Hz
 PPMCM 0.62500 ppm/cm
 HZCM 187.58125 Hz/cm

30-Oct-200609:47:16

TOF MS ES+
7.62e3

30-Oct-200609:47:16

TOF MS ES+

100

RN03 1 (0.017)

100

306.5797

%

307.6102

225.4318

247.4427

197.3489

471.8608

469.7644

528.8743

RN03 1 (0.017)

100

556.8973

544.8907

545.8826

558.9259

545.9191

568.9235

616.9791

615.0212

641.0105

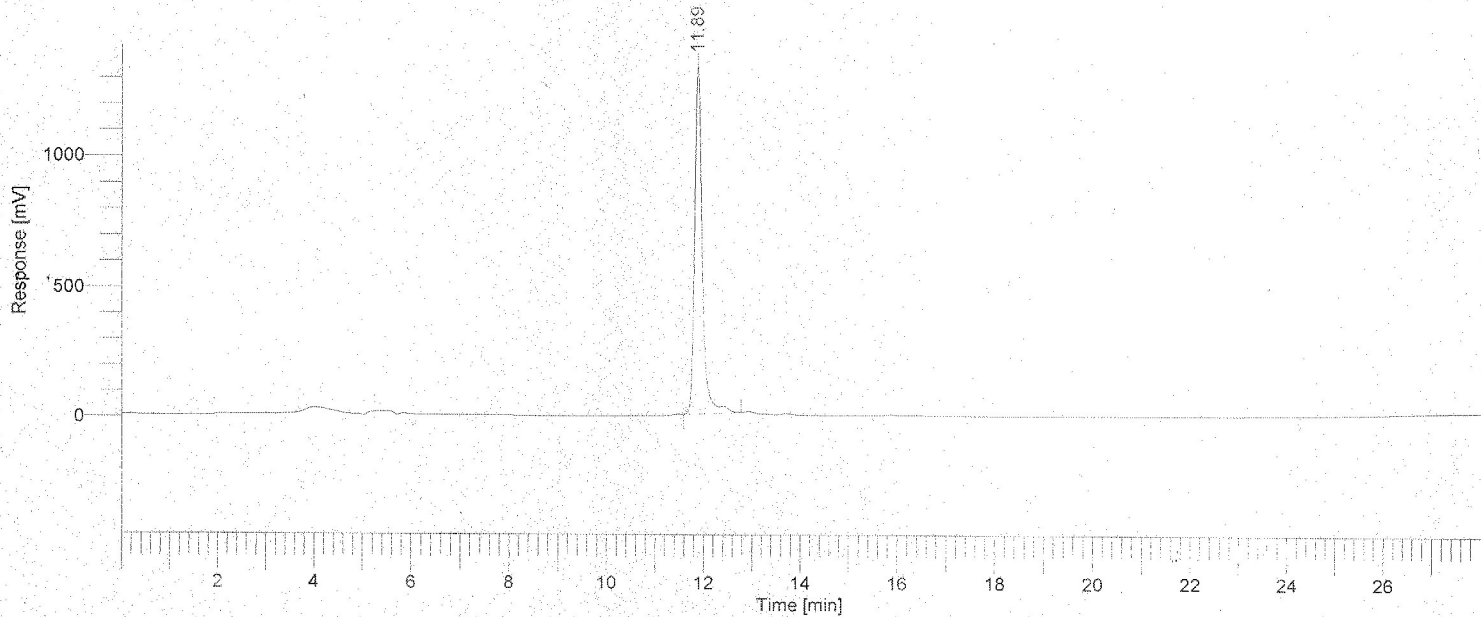
648.2394

687.1181

m/z

0

100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000



Dr M adhu Chopra CT5
PROTON128 CDC13 D:\\shubhra 1

1.960
1.952
1.930
1.921
1.729
1.719
1.708
1.656
1.590
1.410
1.400
1.371
1.338
1.308
1.300
1.258
1.168
1.147
1.138
1.115
1.109
1.089
1.082
0.904
0.885

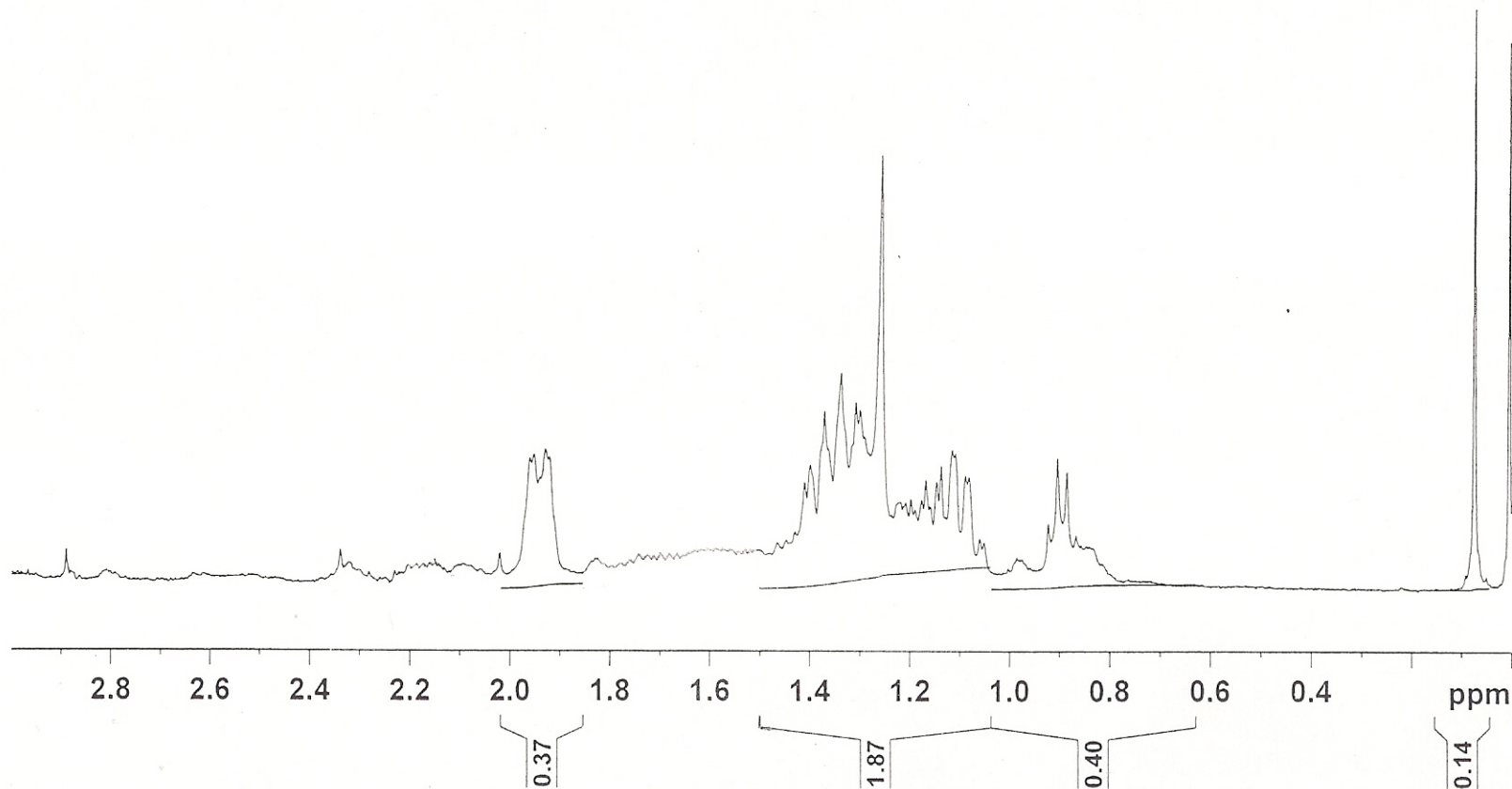
0.075

Current Data Parameters
NAME May08-2008-shubhra
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080508
Time_ 9.47
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 128
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 512
DW 60.800 usec
DE 6.00 usec
TE 293.7 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.95 usec
PL1 0.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300009 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Analysis Name: MADHUCT5000
002.D

Instrument: Agilent 6310 Ion Trap

Print Date: 4/16/2009 3:44:57 PM

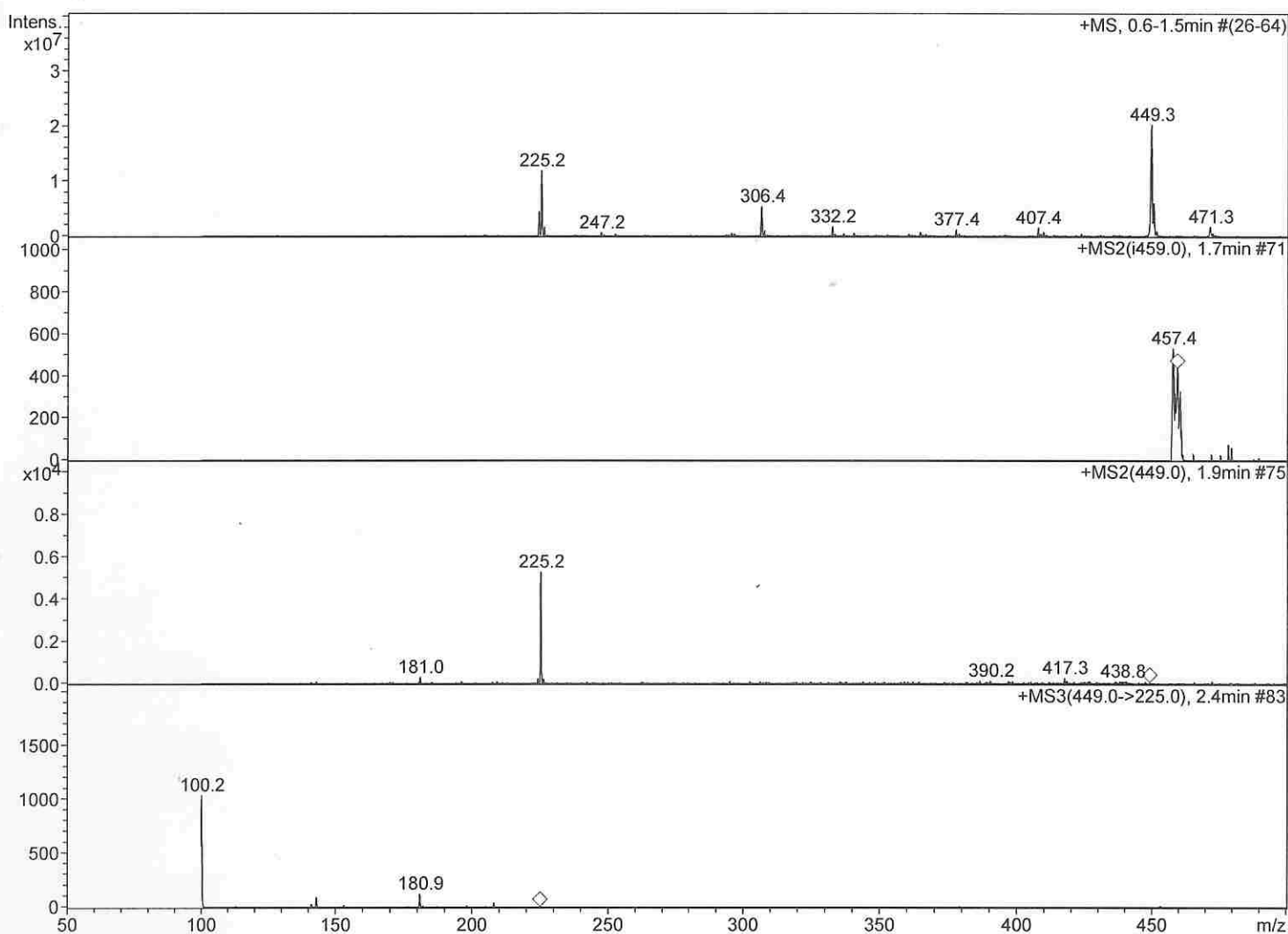
Method: DEF_LCMS.M

Operator: AK Mishra

Acq. Date: 4/16/2009 3:40:06 PM

Sample Name: CT5

Analysis Info: CT5



Display Report - Selected Window Selected Analysis

Analysis Name: MADHUCT5000
001.D

Instrument: Agilent 6310 Ion Trap

Print Date: 4/16/2009 3:45:38 PM

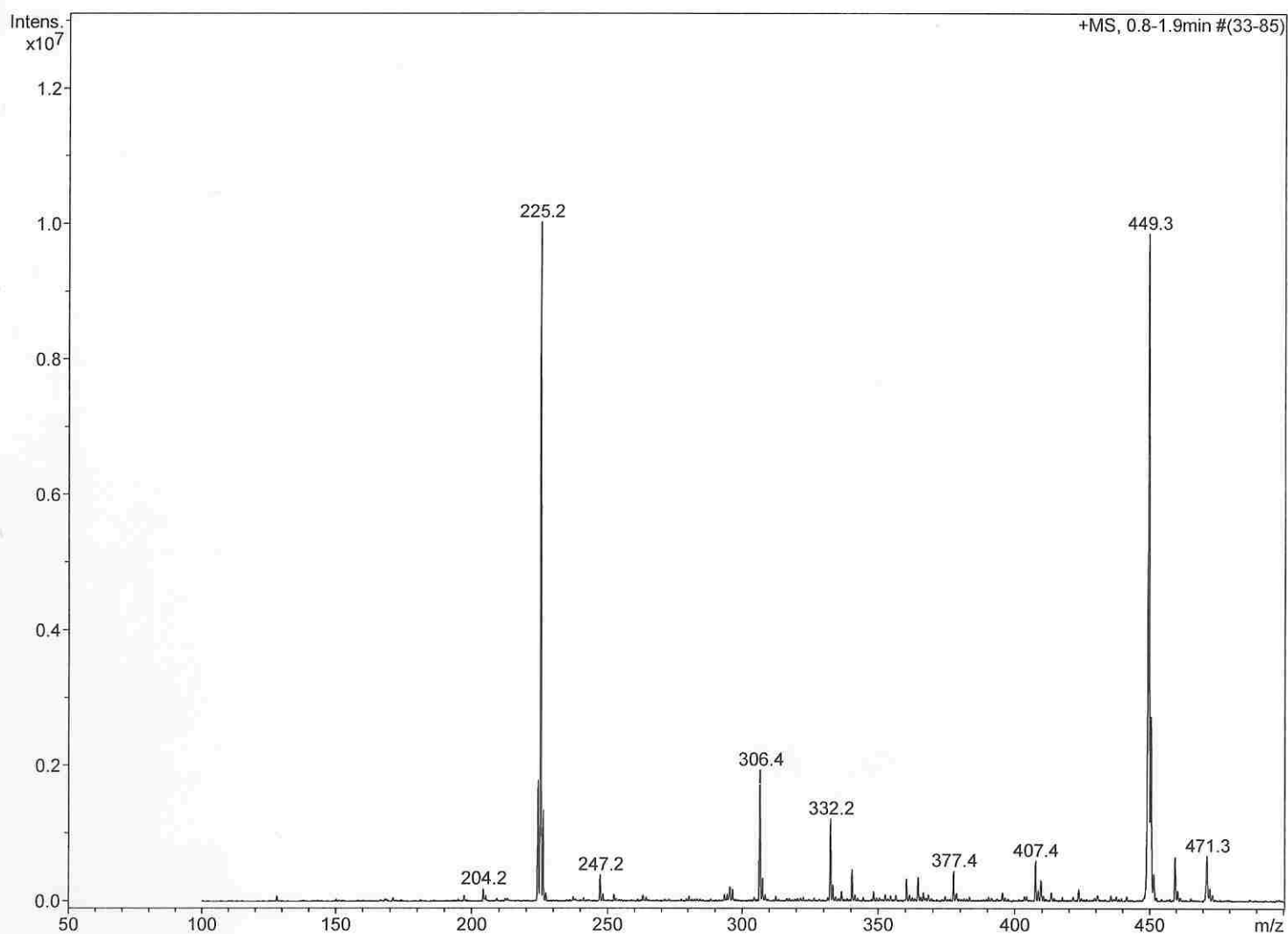
Method: DEF_LCMS.M

Operator: AK Mishra

Acq. Date: 4/16/2009 3:34:26 PM

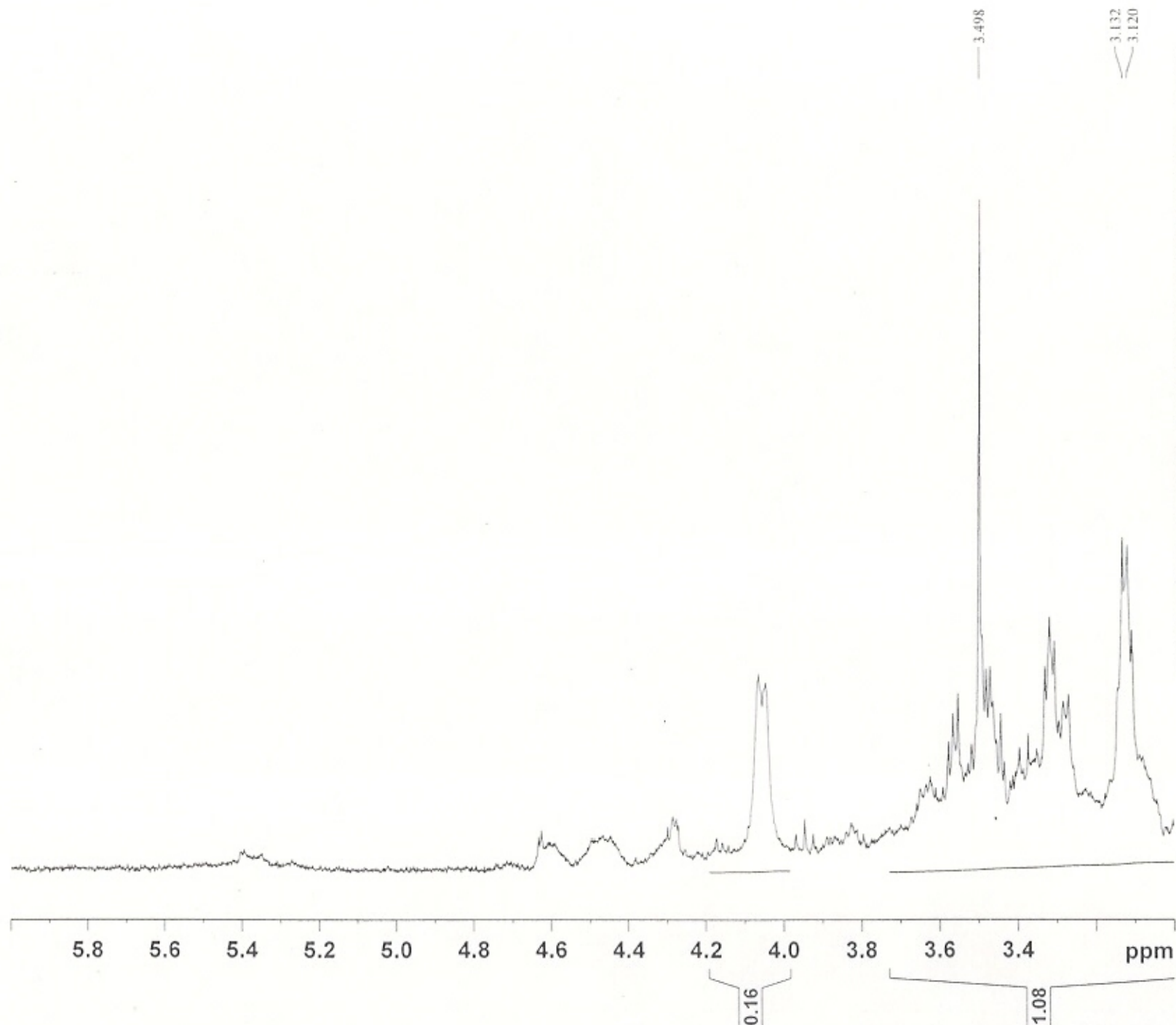
Sample Name: CT5

Analysis Info: CT5



Display Report - Selected Window Selected Analysis

Dr M adhu Chopra CT5
PROTON128 CDCl3 D:\shubhra 1



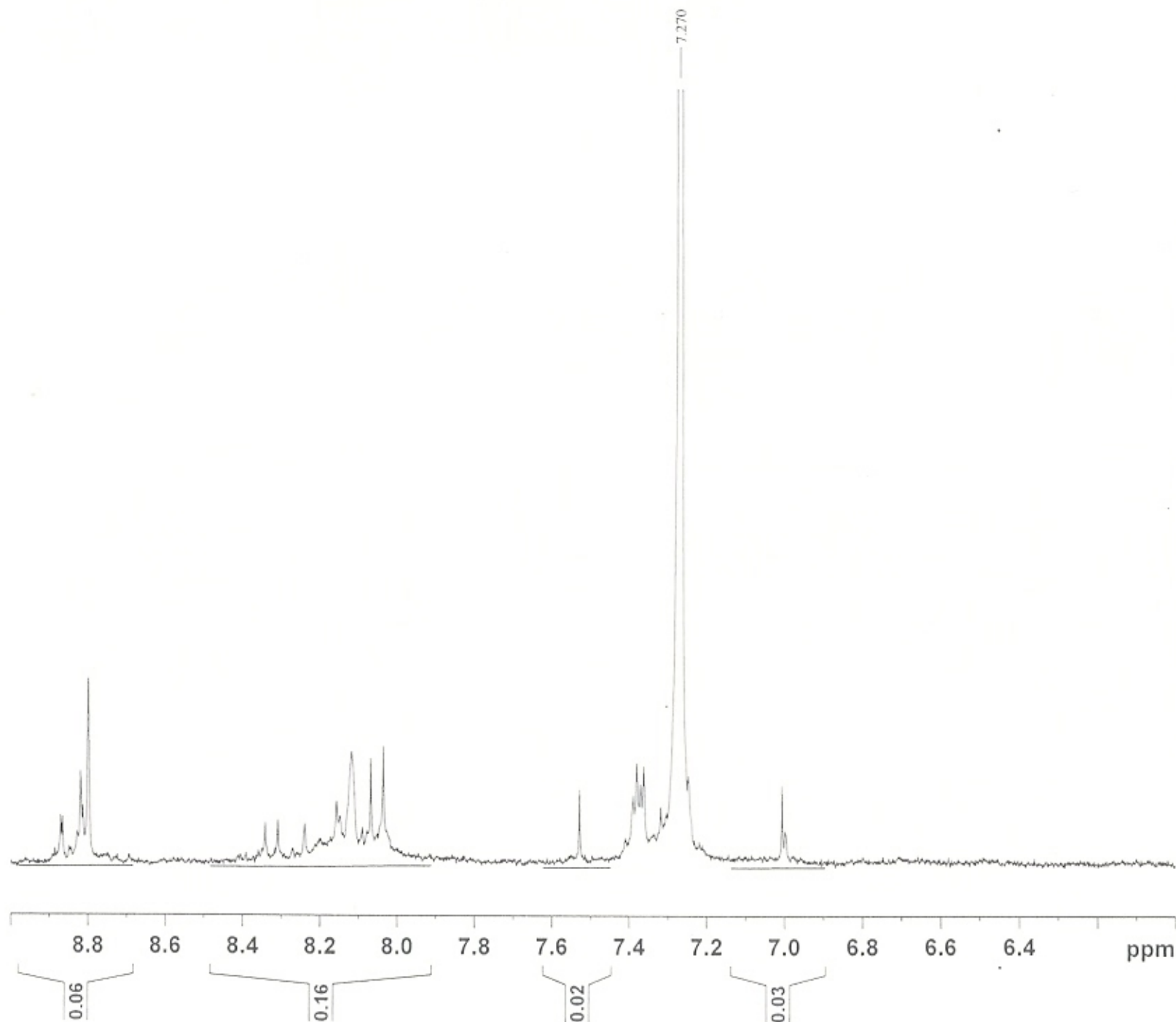
Current Data Parameters
NAME May08-2008-shubhra
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080508
Time_ 9.47
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 512
DW 60.800 usec
DE 6.00 usec
TE 293.7 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.95 usec
PL1 0.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300009 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dr M adhu Chopra CT5
PROTON128 CDC13 D:\shubhra 1



Current Data Parameters
NAME May08-2008-shubhra
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080508
Time_ 9.47
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 128
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 512
DW 60.800 usec
DE 6.00 usec
TE 293.7 K
D1 2.00000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 1H
P1 13.95 usec
PL1 0.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300009 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ppm

Integral

4.69795
3.94937
3.82097
3.65018
3.59258
3.53024
3.48081
3.41119
3.27727
3.13355
3.06403
3.04387
2.96091
1.99931
1.85960
1.71394

Current Data Parameters
NAME proton
EXPNO 359
PROCNO 1

F2 - Acquisition Parameters
Date_ 500000
Time 17.26
INSTRUM dpx300
PROBHD 5mm Dual Z5
PULPROG zg
TD 32768
SOLVENT D2O
NS 32
DS 0
SWH 8992.806 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 114
DW 55.600 usec
DE 4.50 usec
TE 300.0 K
D1 5.00000000 sec
P1 12.00 usec
DE 4.50 usec
SF01 300.1342018 MHz
NUC1 1H
PL1 0.00 dB

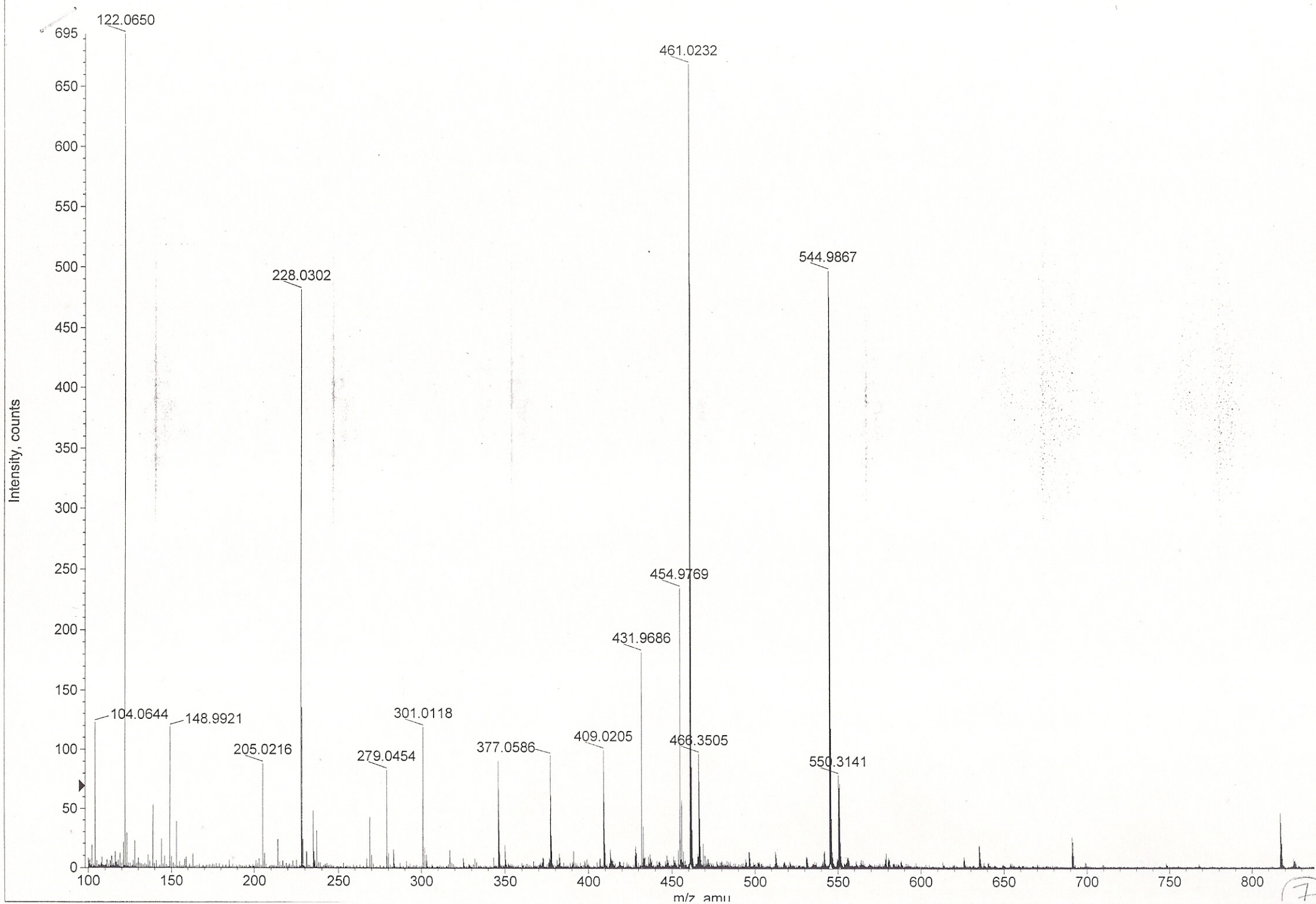
F2 - Processing parameters
SI 32768
SF 300.1299995 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
F1P 10.000 ppm
F1 3001.30 Hz
F2P -0.500 ppm
F2 -150.07 Hz
PPMCM 0.52500 ppm/cm
HZCM 157.56825 Hz/cm

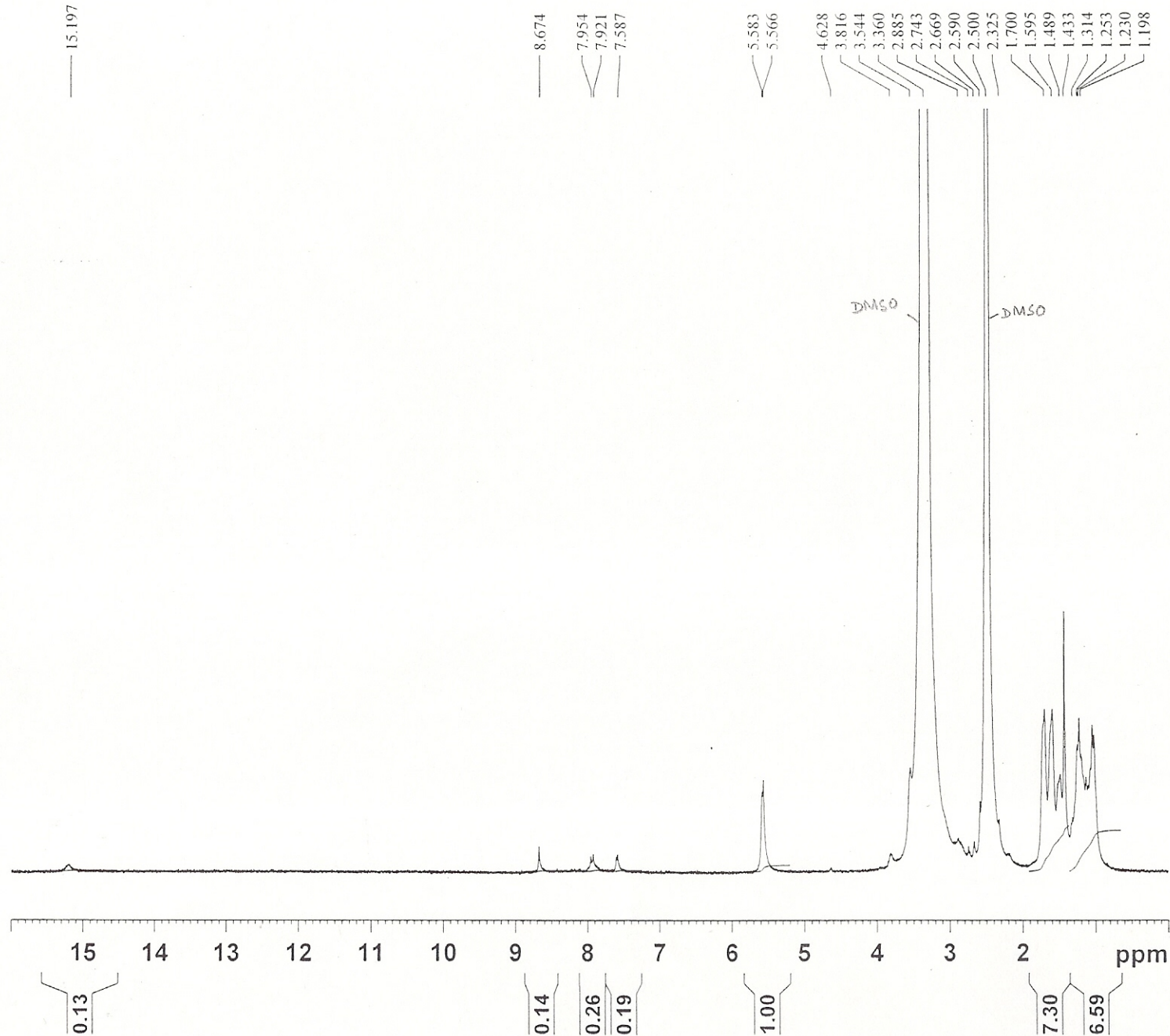
9.5549
2.1290
1.0876
3.7785
0.9614
1.0000

+TOF MS: 6.618 to 6.685 min from MT20070416143514.wiff
a=3.56648734867816710e-004, t0=-4.99256432894944740e+001, subtracted (6.502 to 6.552 min and 6.69 to 6.74 min)

Max. 694.7 counts.



DR Madhu CD6
PROTON128 DMSO D:\shubhra 3



Current Data Parameters
NAME May14-2008-shubhra
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080514
Time_ 15.14
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 128
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 362
DW 60.800 usec
DE 6.00 usec
TE 290.5 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.95 usec
PL1 0.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1299962 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

Analysis Name: MADHUCD6000
005.D

Instrument: Agilent 6310 Ion Trap

Print Date: 4/16/2009 5:02:00 PM

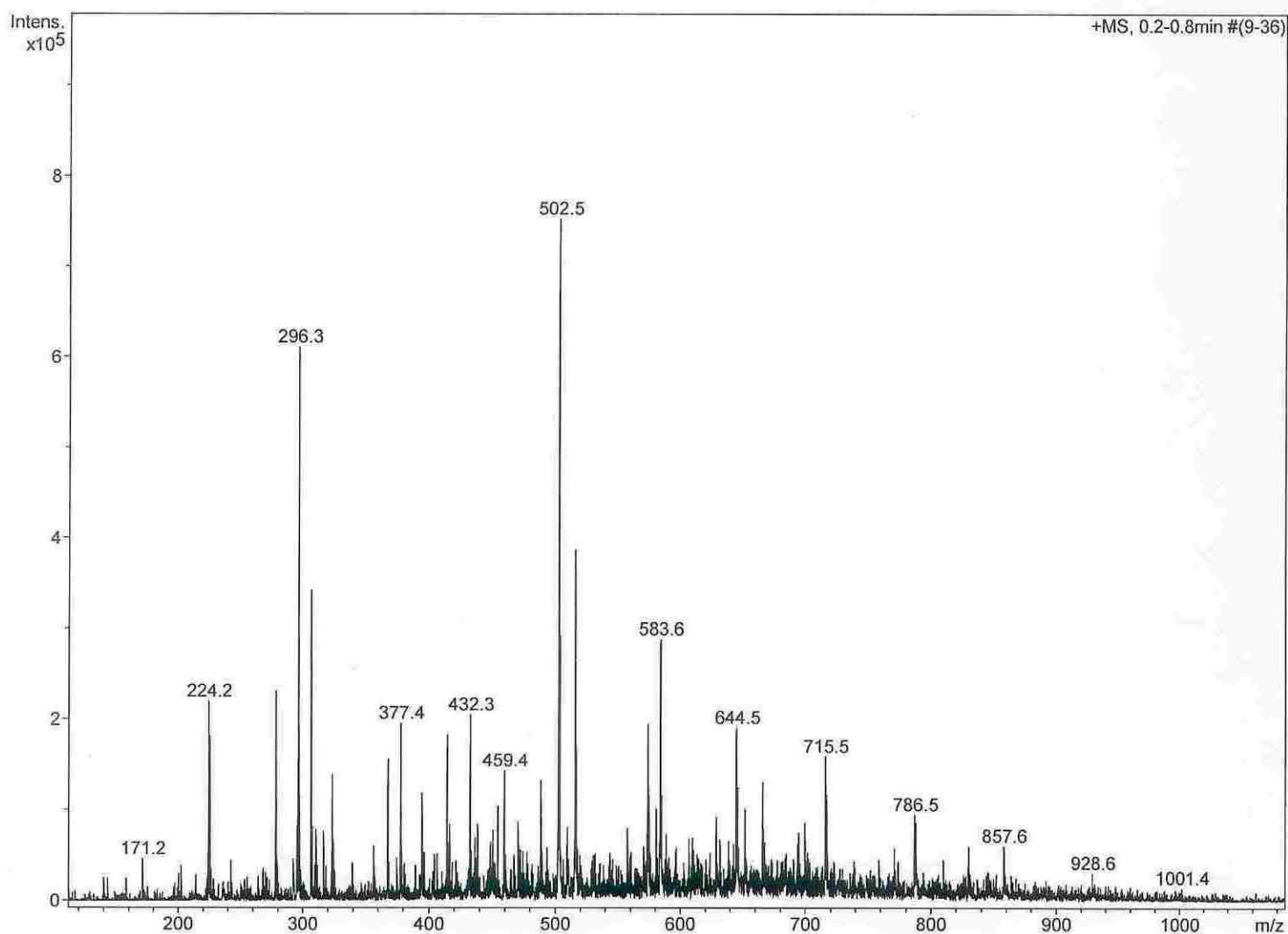
Method: DEF_LCMS.M

Operator: AK Mishra

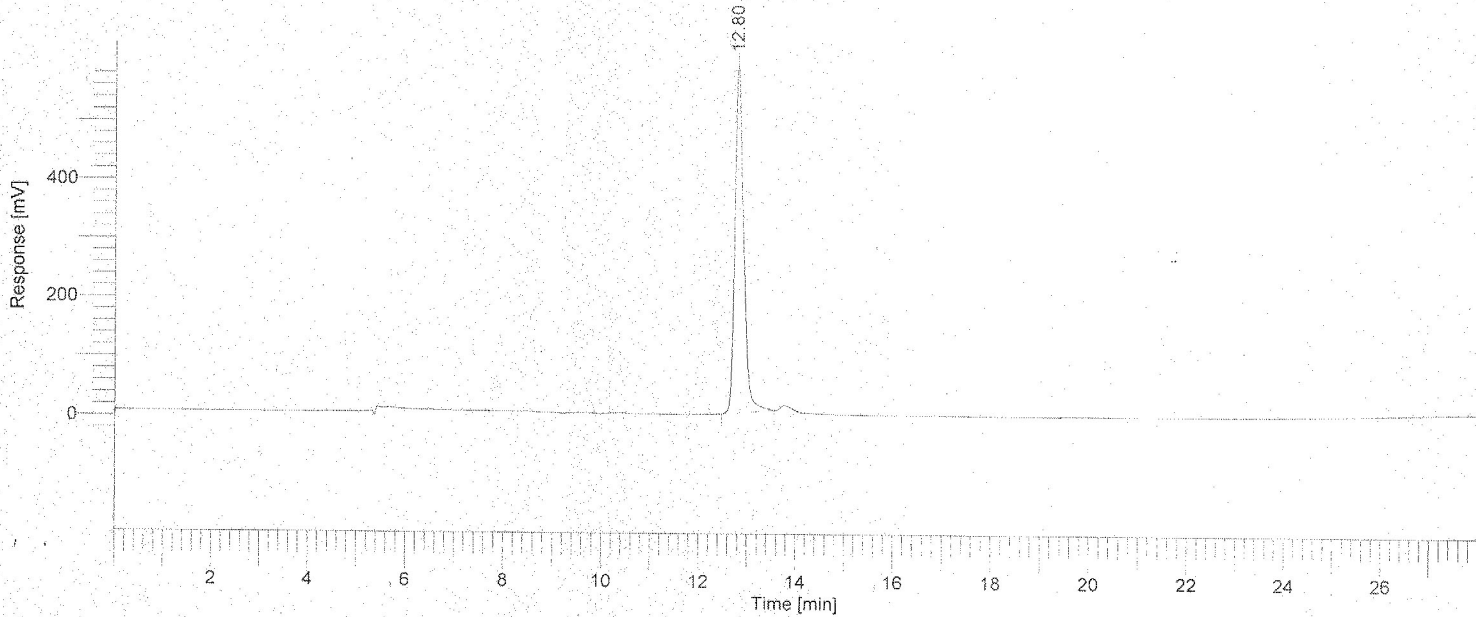
Acq. Date: 4/16/2009 4:55:30 PM

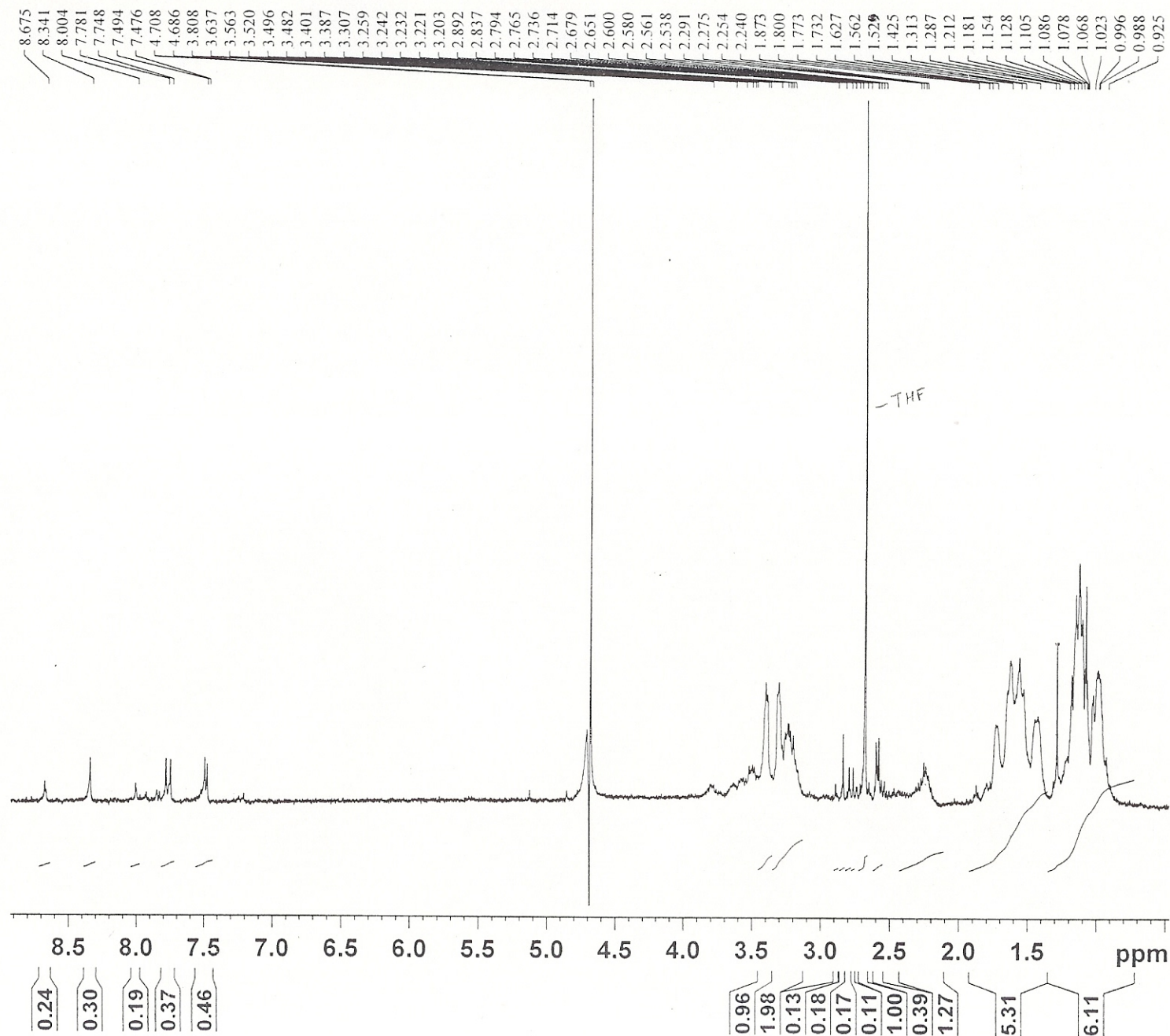
Sample Name: CD6

Analysis Info: CD6



Display Report - Selected Window Selected Analysis





Current Data Parameters
 NAME madhu chopra
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080514
 Time_ 14.39
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpr
 TD 65536
 SOLVENT D2O ✓
 NS 128
 DS 4
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 362
 DW 60.800 usec
 DE 6.00 usec
 TE 290.2 K
 D1 1.00000000 sec
 d12 0.00002000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.95 usec
 PL1 0.00 dB
 PL9 51.09 dB
 SFO1 400.1318749 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.40

Analysis Name: MADHUCD7000
001.D

Instrument: Agilent 6310 Ion Trap

Print Date: 4/16/2009 5:15:33 PM

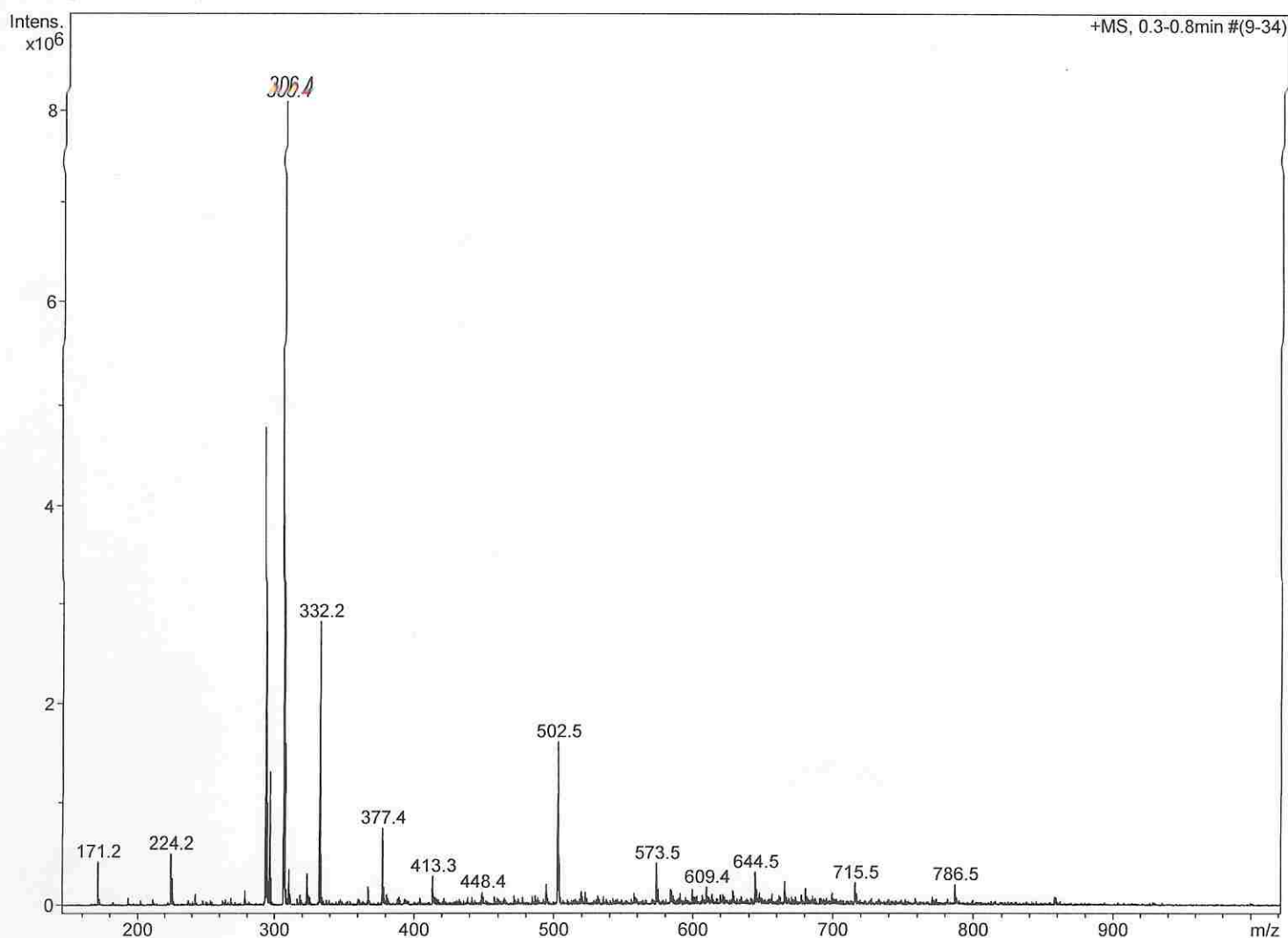
Method: DEF_LCMS.M

Operator: AK Mishra

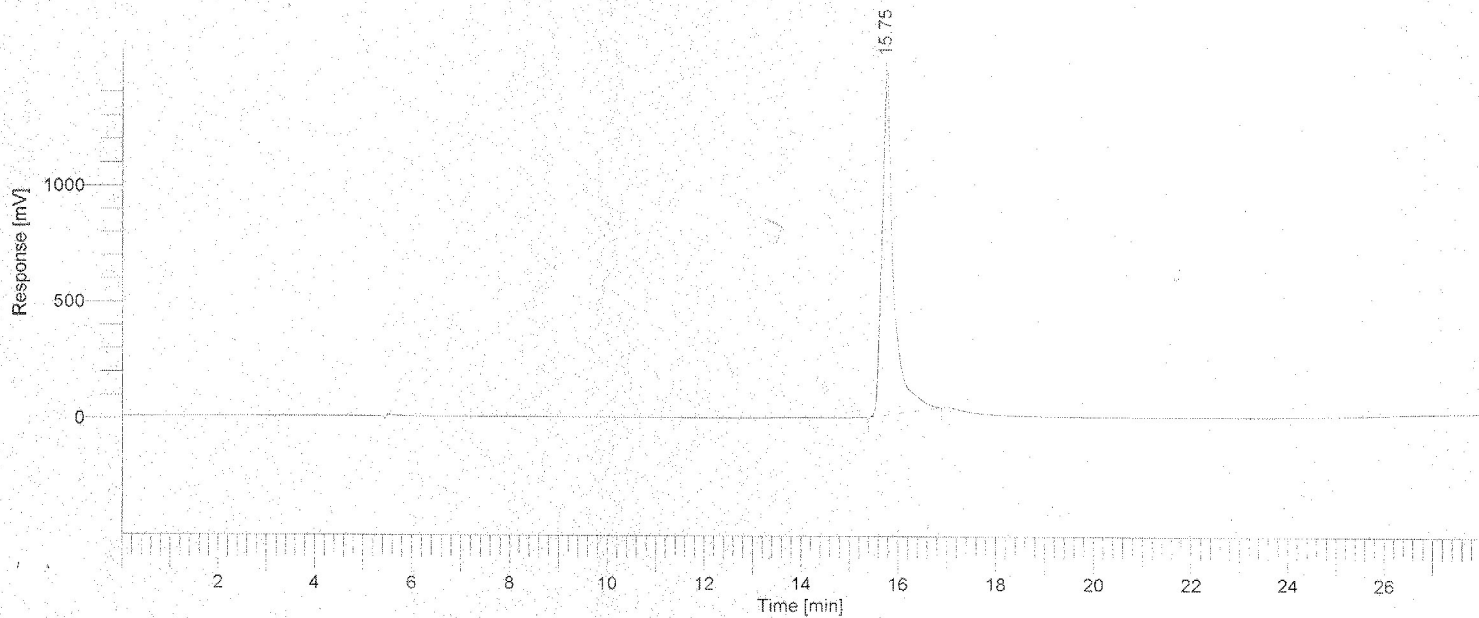
Acq. Date: 4/16/2009 5:07:14 PM

Sample Name: CD7

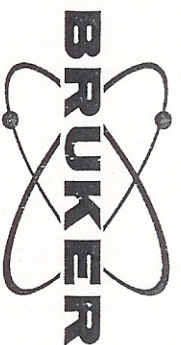
Analysis Info: CD7



Display Report - Selected Window Selected Analysis



DU M Chop SD 03 07



- 8.329
- 8.262
- 8.128
- 7.541
- 7.507
- 7.370
- 7.352
- 6.978
- 6.943
- 4.663
- 4.112
- 3.754
- 3.655
- 3.587
- 3.553
- 3.458
- 3.398
- 3.359
- 3.247
- 3.217
- 3.110
- 2.999
- 2.905
- 2.890
- 2.874
- 2.782
- 2.767
- 2.484
- 2.447
- 2.367
- 2.329

Current Data Parameters
NAME DU M Chop SD 03 07
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070328
Time_ 10.43
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT D2O
NS 24
DS 2
SWH 9615.385 Hz
FIDRES 0.146719 Hz
AQ 3.4079220 sec
RG 228
DW 52.000 usec
DE 6.00 usec
TE 290.9 K
D1 5.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.00 usec
PL1 0.00 dB
SFO1 400.1332010 MHz

F2 - Processing Parameters
SI 32768
SF 400.1300106 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm

0.28
0.23
0.27
0.30
0.50

0.56
4.95
3.54
0.66
6.73
1.68
1.84
1.95
1.00
0.99
1.29
1.34

+TOF MS: 0.750 to 0.767 min from Sample 4 (Rajni) of SD03.wiff
a=3.56877768712611110e-004, t0=-3.83104637123287830e+001, subtracted (0.150 to 0.650 min)

Max. 1627.0 counts.

