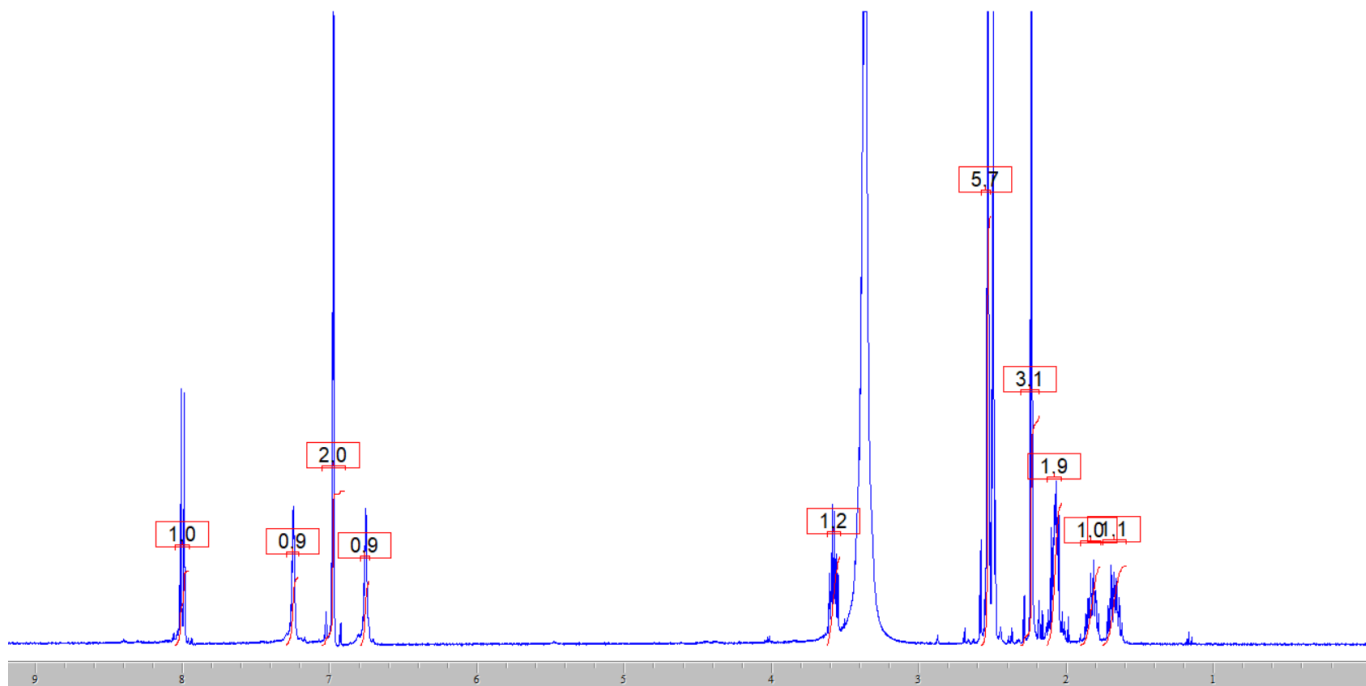
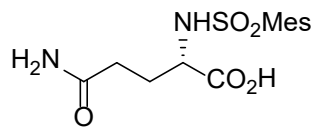


Supplementary data: spectra

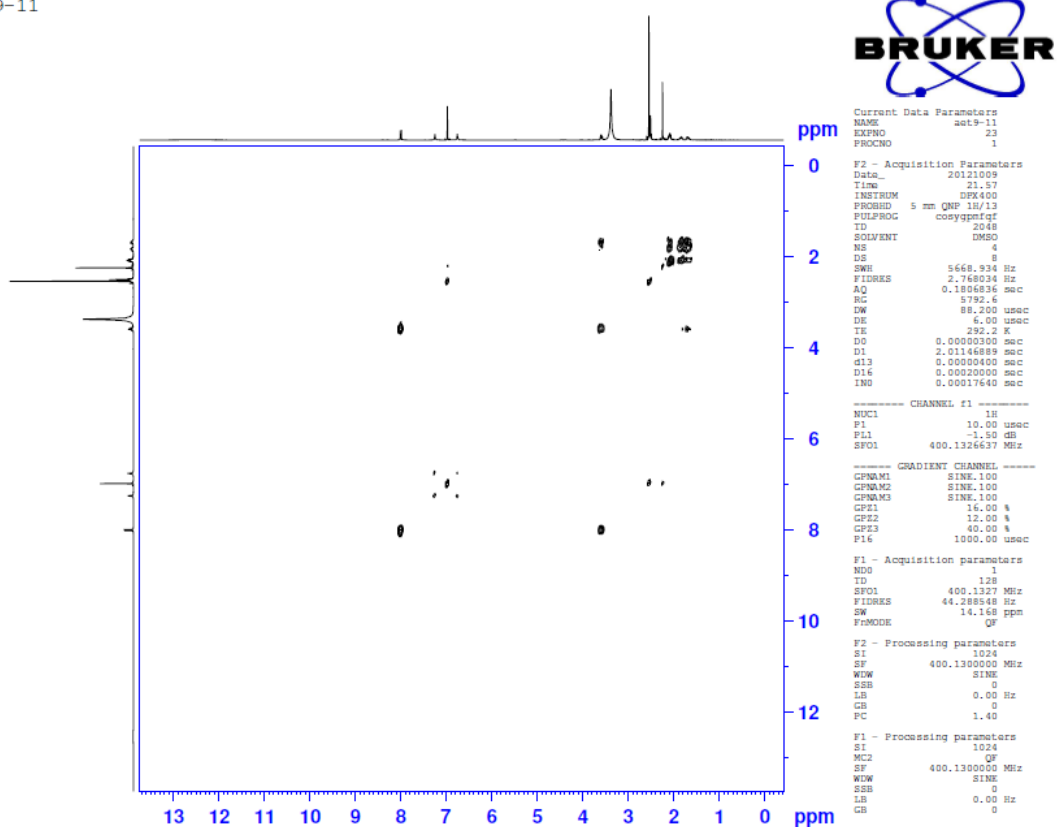
Section 1 ^1H and ^{13}C NMR spectra of novel compounds. Pages 2-106

Section 2: HRMS data of novel compounds. Pages 107 onwards

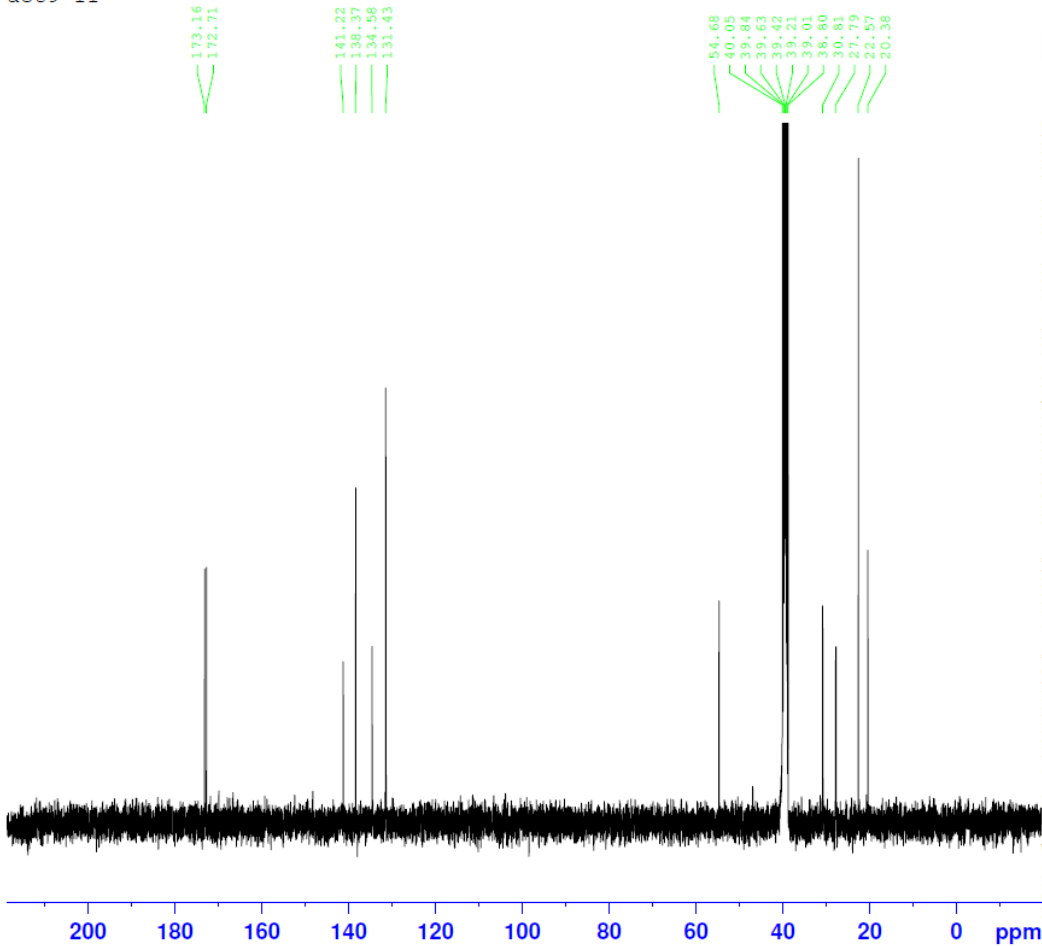
(Mesitylsulfonyl)-L-glutamine [Compound 4]



aet9-11



aet9-11



```

Current Data Parameters
NAME          aet9-11
EXPNO         21
PROCNO        1

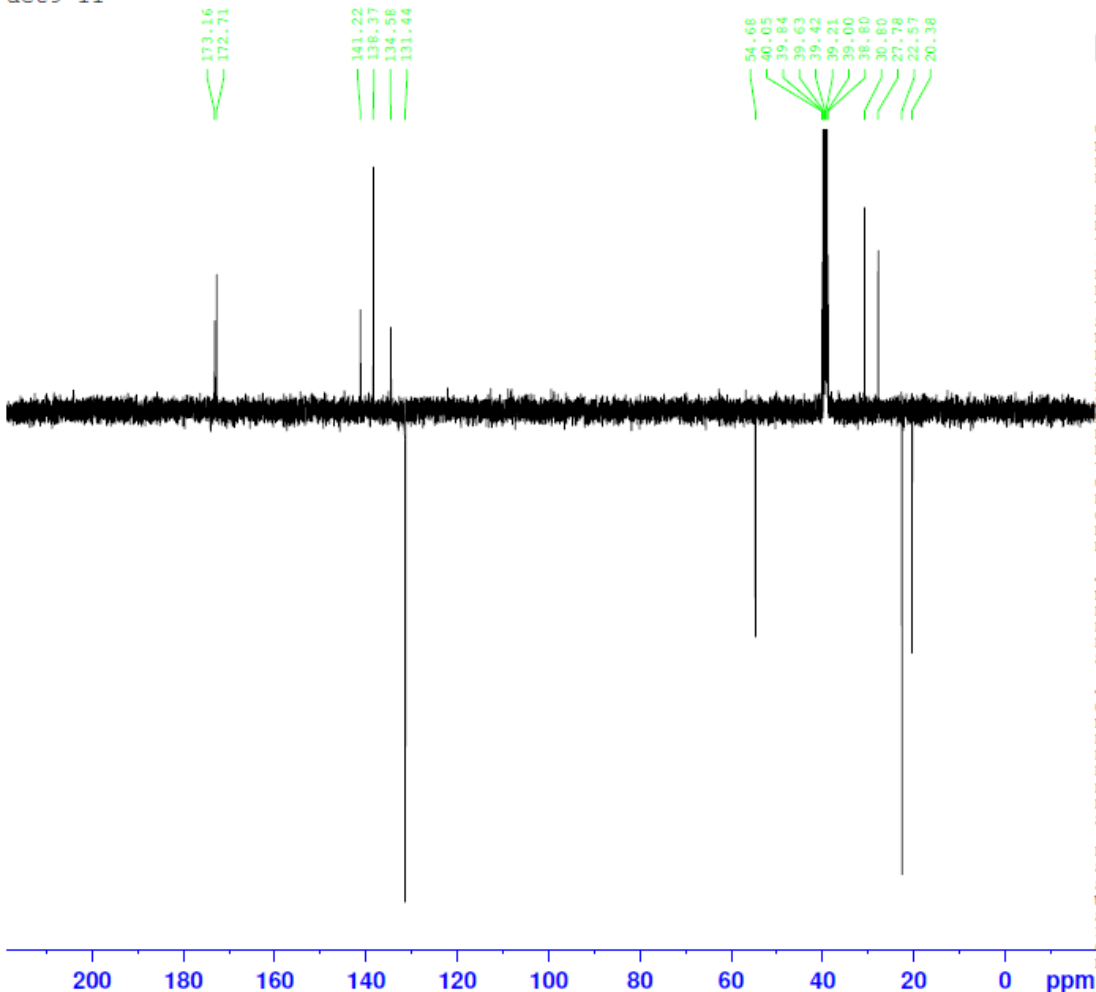
F2 - Acquisition Parameters
Date_         20121009
Time          21.26
INSTRUM       DPX400
PROBHD        5 mm QNP 1H/13
PULPROG       zgpg30
TD            65536
SOLVENT       DMSO
NS            1024
DS            4
SWH           23980.814 Hz
FIDRES        0.365918 Hz
AQ            1.3664756 sec
RG            1290.2
DW            20.850 usec
DE            6.00 usec
TE            293.2 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0           1

===== CHANNEL f1 =====
NUC1          13C
P1            8.50 usec
PL1           -2.60 dB
SFO1          100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           -1.50 dB
PL12          17.50 dB
PL13          17.50 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI            32768
SF            100.6128193 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```

aet9-11



```

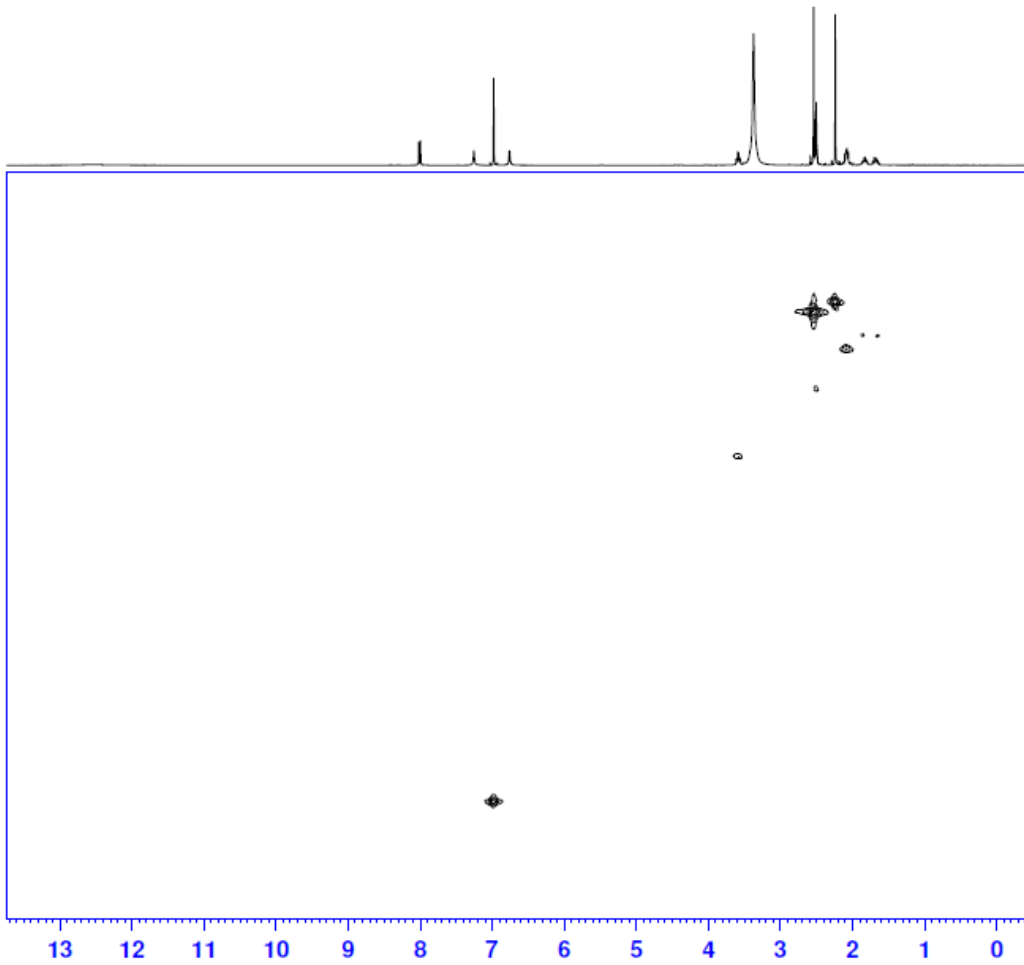
Current Data Parameters
NAME          aet9-11
EXPNO         22
PROCNO        1

F2 - Acquisition Parameters
Date_         20121009
Time          21.57
INSTRUM       DPX400
PROBHD        5 mm QNP 1H/13
PULPROG       deptg_135
TD            65536
SOLVENT       DMSO
NS            512
DS            4
SWH           23980.814 Hz
FIDRES        0.365918 Hz
AQ            1.3664756 sec
RG            11585.2
DW            20.850 usec
DE            6.00 usec
TE            292.2 K
CNSI2         145.0000000
D1            2.00000000 sec
d2            0.00344828 sec
D11           0.03000000 sec
DELTA         0.00001082 sec

===== CHANNEL f1 =====
NUC1          13C
P1            8.50 usec
P2            17.00 usec
PL1           -2.60 dB
SFO1          100.6228300 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
P3            10.00 usec
P4            20.00 usec
PCPD2         80.00 usec
PL2           -1.50 dB
PL12          17.50 dB
SFO2          400.1316000 MHz

F2 - Processing parameters
SI            32768
SF            100.6128193 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```



Current Data Parameters
 NAME aet9-11
 EXPNO 24
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121003
 Time 22.17
 INSTRUM spect
 PULPROG zgpg30
 ID 1024
 SOLVENT dmsc
 NS 4
 DS 16
 SWH 5669.934 Hz
 FIDRES 5.536068 Hz
 AQ 0.0903665 sec
 RG 24000
 DW 88.200 usec
 DE 6.00 usec
 TK 292.2 K
 CNST2 145.0000000
 d0 0.0000000 sec
 d1 1.53696404 sec
 d2 0.00344828 sec
 d12 0.00000000 sec
 d13 0.00000400 sec
 d16 0.00200000 sec
 DELTA1 0.00222428 sec
 IN0 0.00000000 sec

----- CHANNEL f1 -----
 NUC1 1H
 P1 10.00 usec
 PL1 20.00 dB
 PL12 -1.50 dB
 SFO1 400.1326637 MHz

----- CHANNEL f2 -----
 CPDPRG2 zgpg30
 NUC2 13C
 P3 8.00 usec
 PL3 74.00 dB
 PL12 -3.00 dB
 PL122 -18.00 dB
 SFO2 100.6203140 MHz

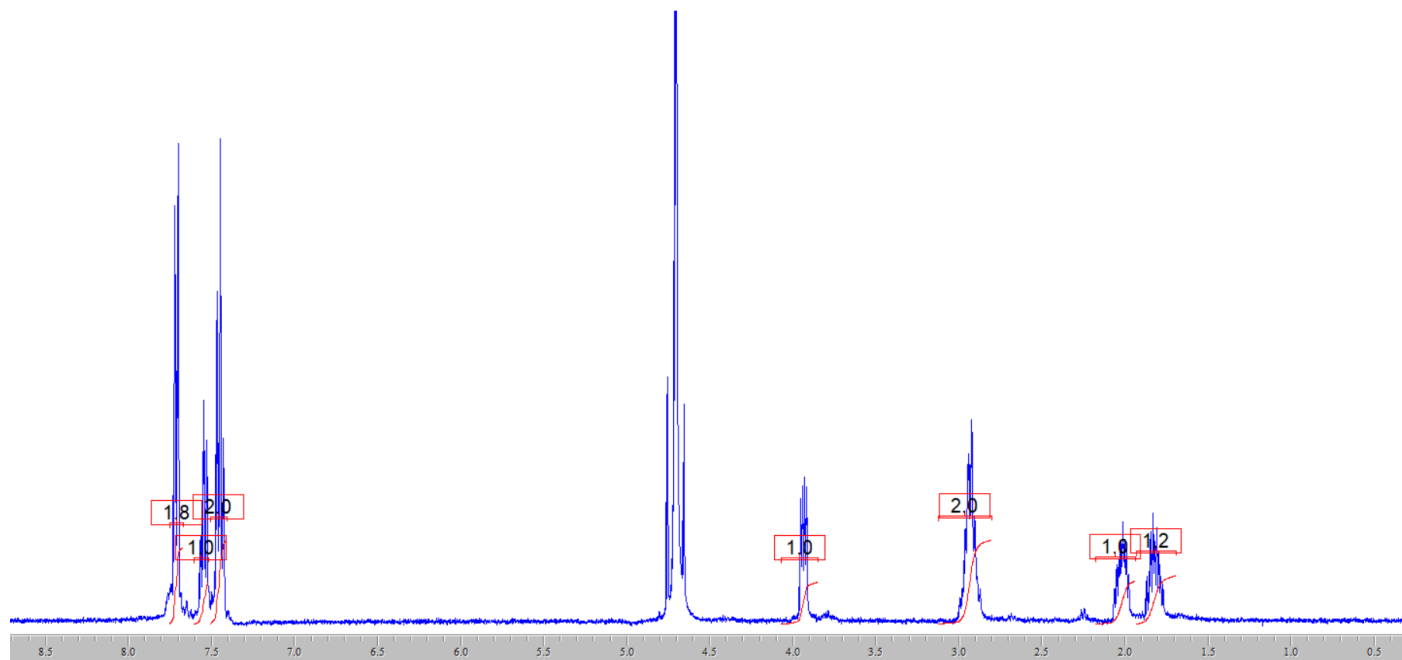
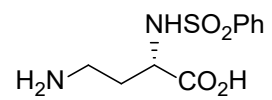
----- GRADIENT CHANNEL -----
 GPRAM1 SINE.100
 GPRAM2 SINE.100
 GPRAM3 SINE.100
 GPE1 50.00 %
 GPE2 30.00 %
 GPE3 40.10 %
 P16 1000.00 usec

F1 - Acquisition parameters
 NS0 2
 ID 128
 SFO1 100.6203 MHz
 FIDRES 130.208328 Hz
 SW 165.639 ppm
 PrMODEK QF

F2 - Processing parameters
 SI 1024
 SF 400.1300000 MHz
 MSW QSINE
 SSR 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 SF 100.6127690 MHz
 MSW QSINE
 SSR 2
 LB 0.00 Hz
 GB 0

(S)-4-Amino-2-(phenylsulfonamido)butanoic acid 5



aet9-9 1 drop TFA
aet9-9 (1 drop TFA)

173.19

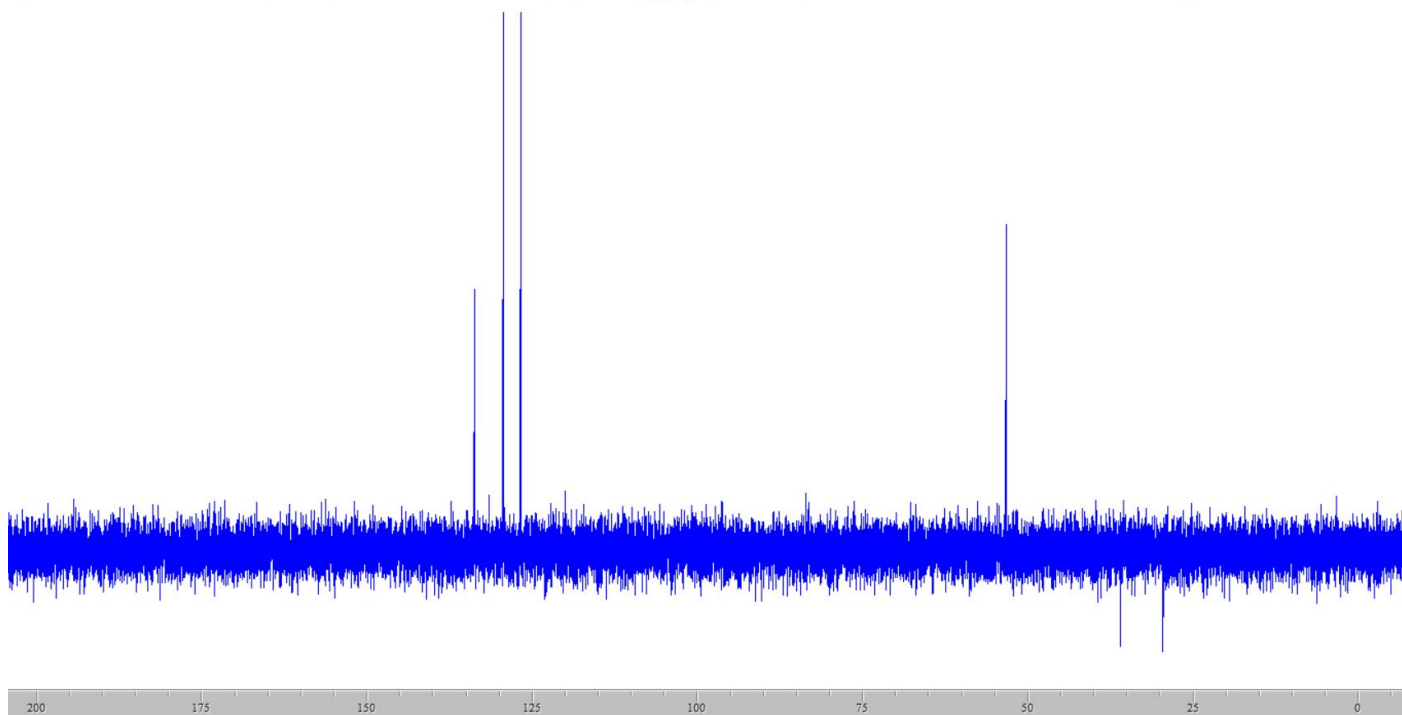
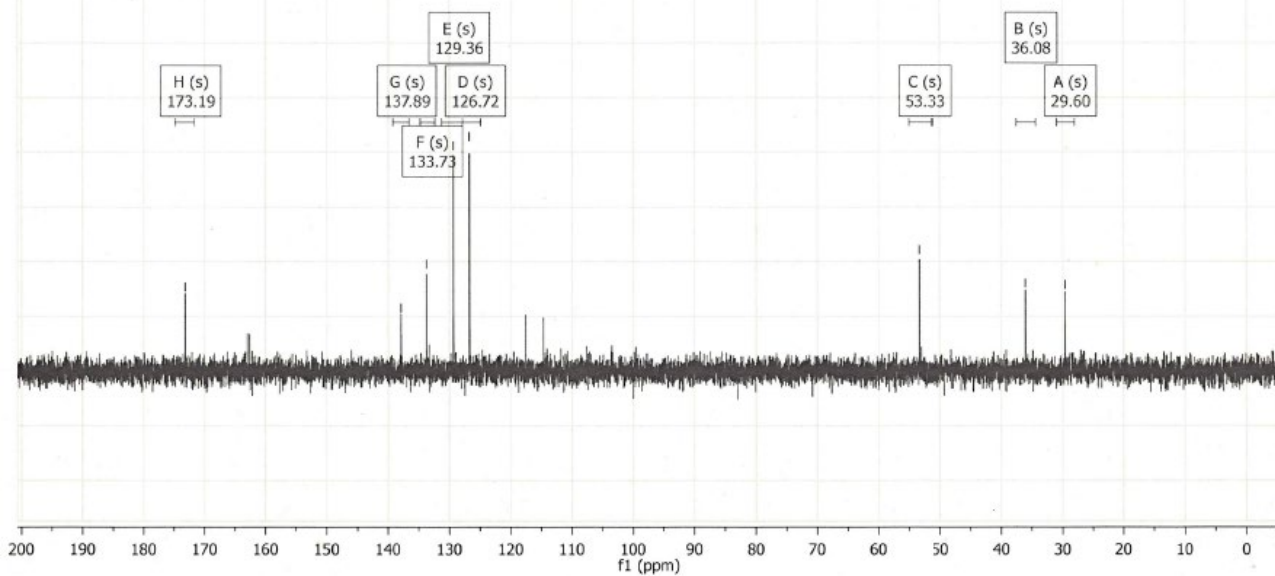
137.89
133.73
129.36
126.72

53.33

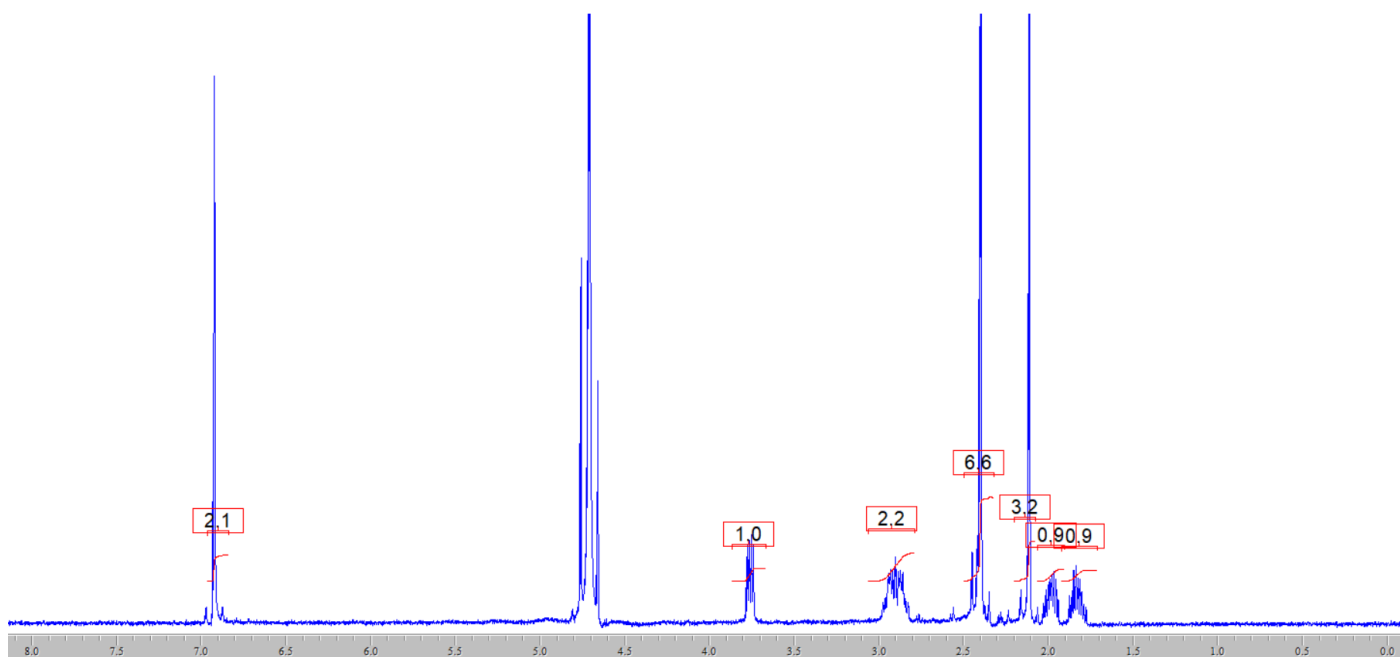
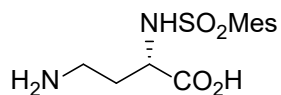
36.08

29.60

^{13}C NMR (101 MHz, D_2O) δ 173.19 (C), 137.89 (C), 133.73 (CH), 129.36 (CH), 126.72 (CH), 53.33 (CH),
36.08 (CH_2), 29.60 (CH_2);



(S)-4-Amino-2-(2,4,6-trimethylphenylsulfonamido)butanoic acid [Compound 6]:



aet9-13



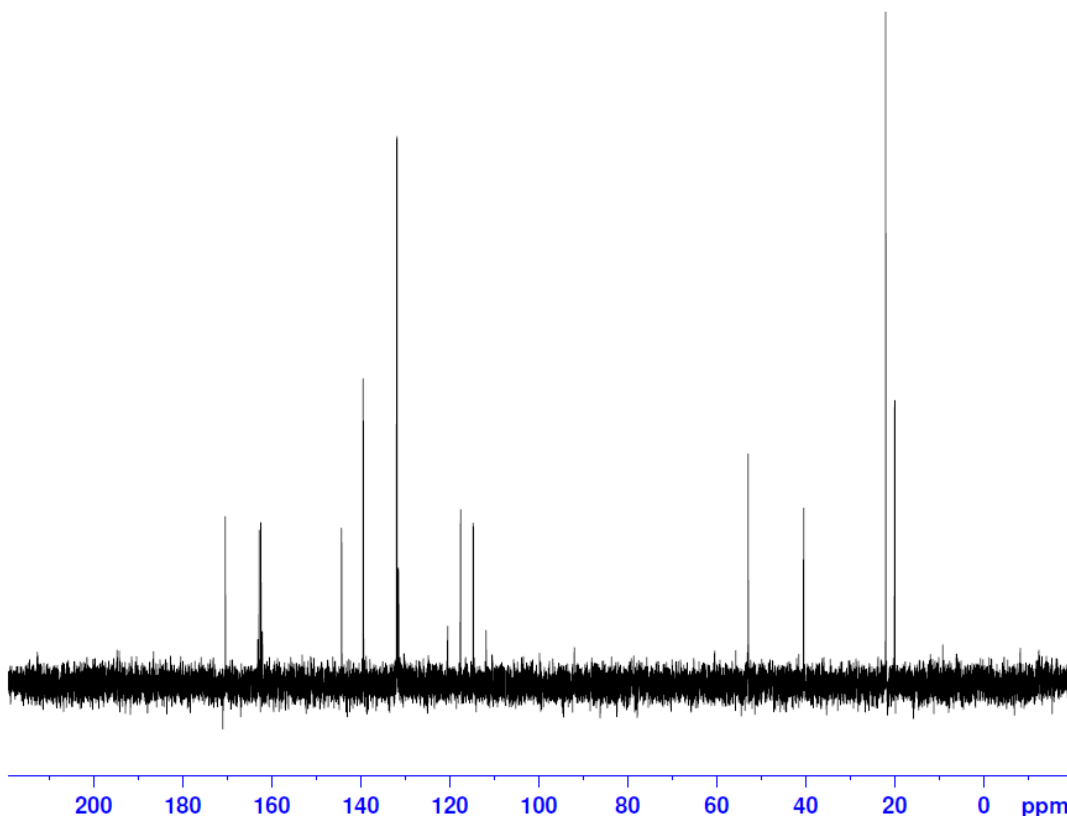
Current Data Parameters
 NAME aet9-13
 EXPNO 10
 PROCNO 1

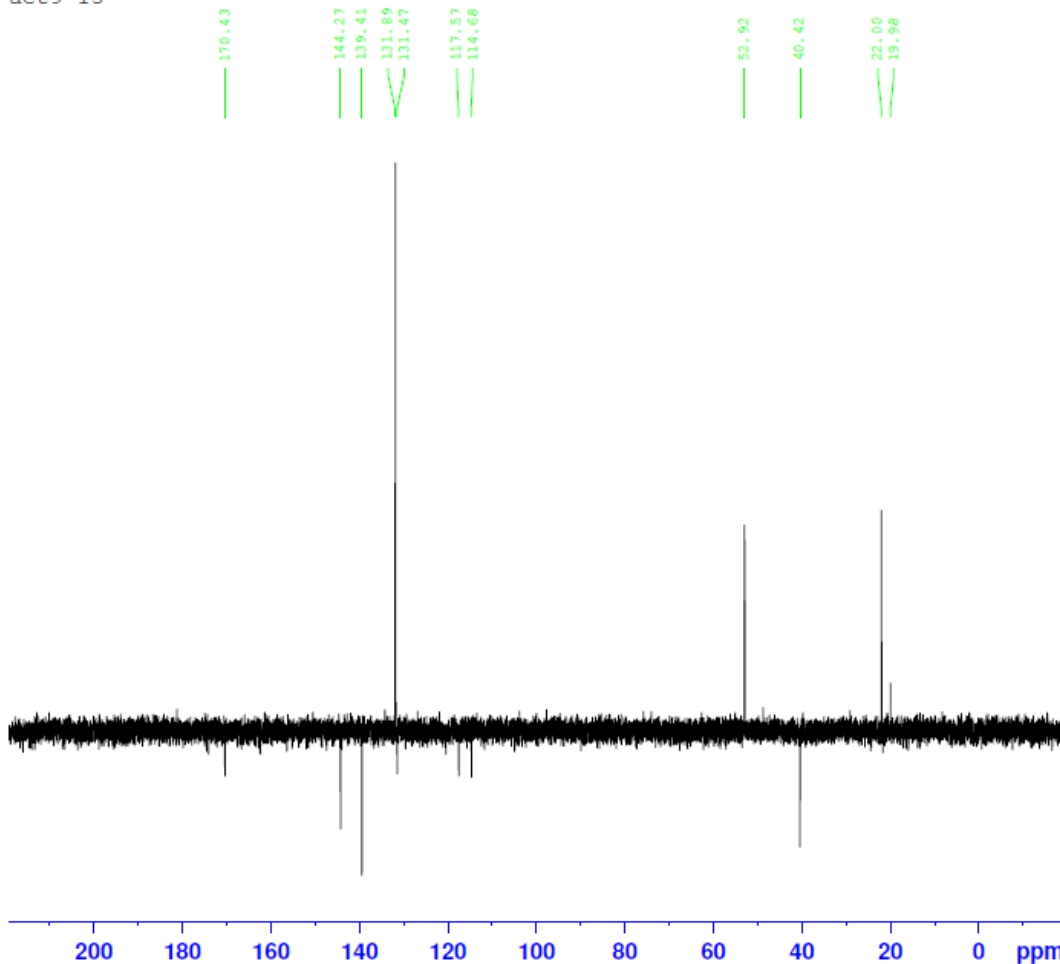
F2 - Acquisition Parameters
 Date_ 20130102
 Time 13.04
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT D2O
 NS 1024
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 2580.3
 DW 20.850 usec
 DE 6.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 PL1 -2.60 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 PL13 17.50 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40





Current Data Parameters
 NAME act9-13
 EXPNO 11
 PROCNO 1

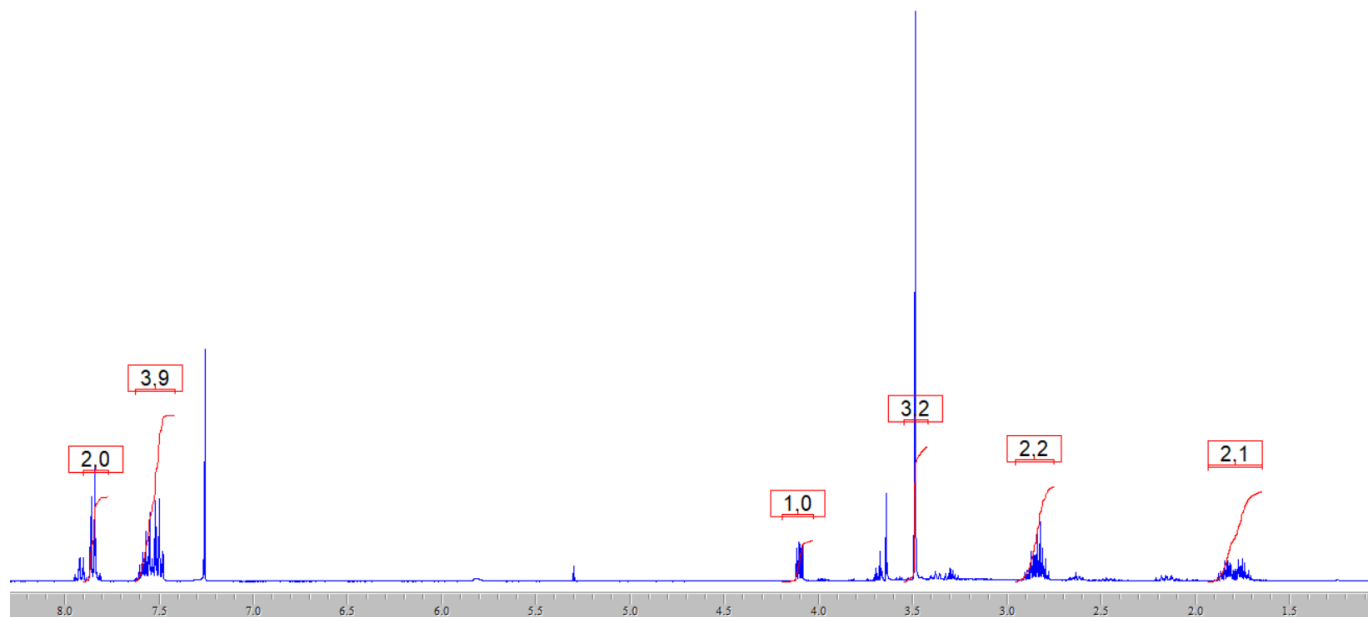
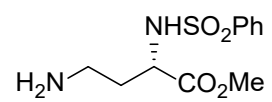
F2 - Acquisition Parameters
 Date_ 20130102
 Time_ 13.34
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG deptg_135
 ID 65536
 SOLVENT D2O
 NS 512
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 16384
 DW 20.850 usec
 DE 6.00 usec
 TE 298.2 K
 CNST2 145.0000000
 D1 2.00000000 sec
 d2 0.00344828 sec
 D11 0.03000000 sec
 DELTA 0.00001082 sec

----- CHANNEL f1 -----
 NUC1 13C
 P1 8.50 usec
 P2 17.00 usec
 PL1 -2.60 dB
 SFO1 100.6228300 MHz

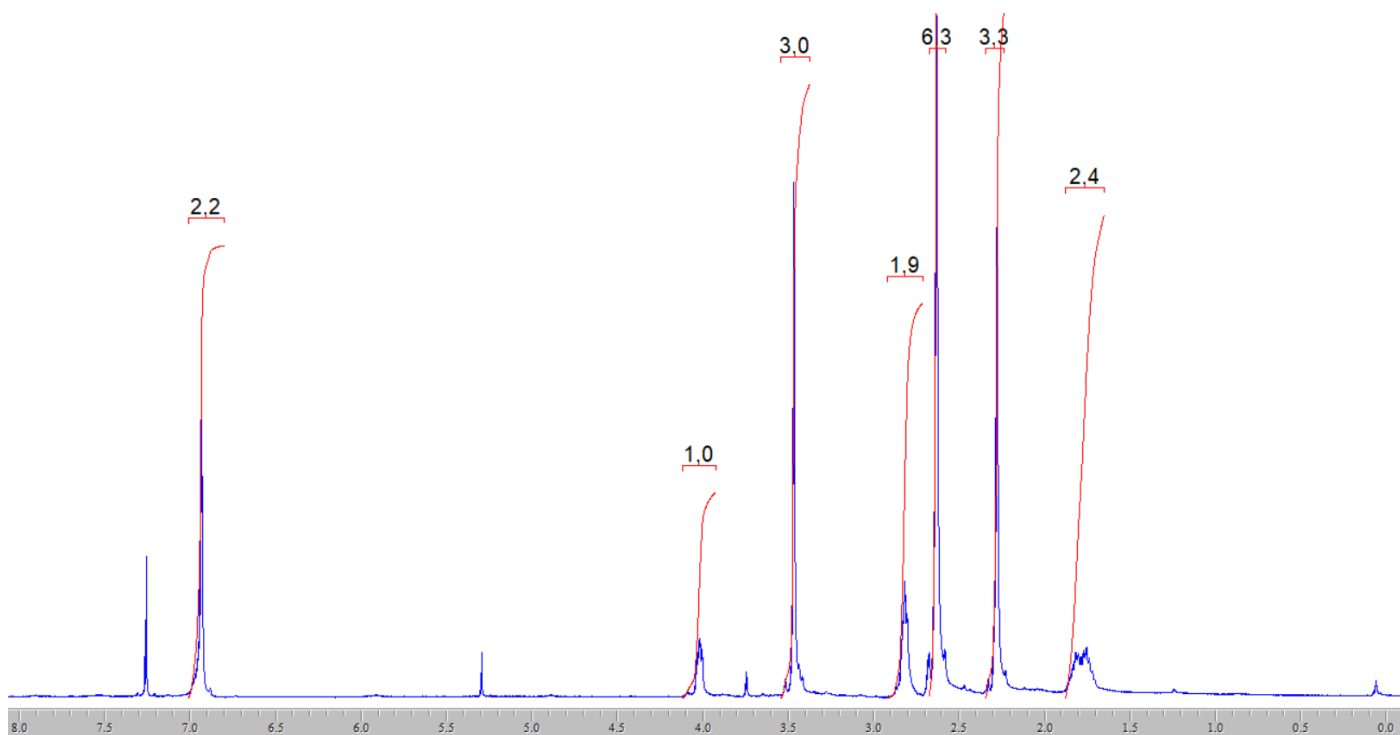
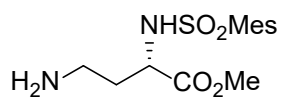
----- CHANNEL f2 -----
 CPDPRG2 waltz16
 NUC2 1H
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 SFO2 400.1316000 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

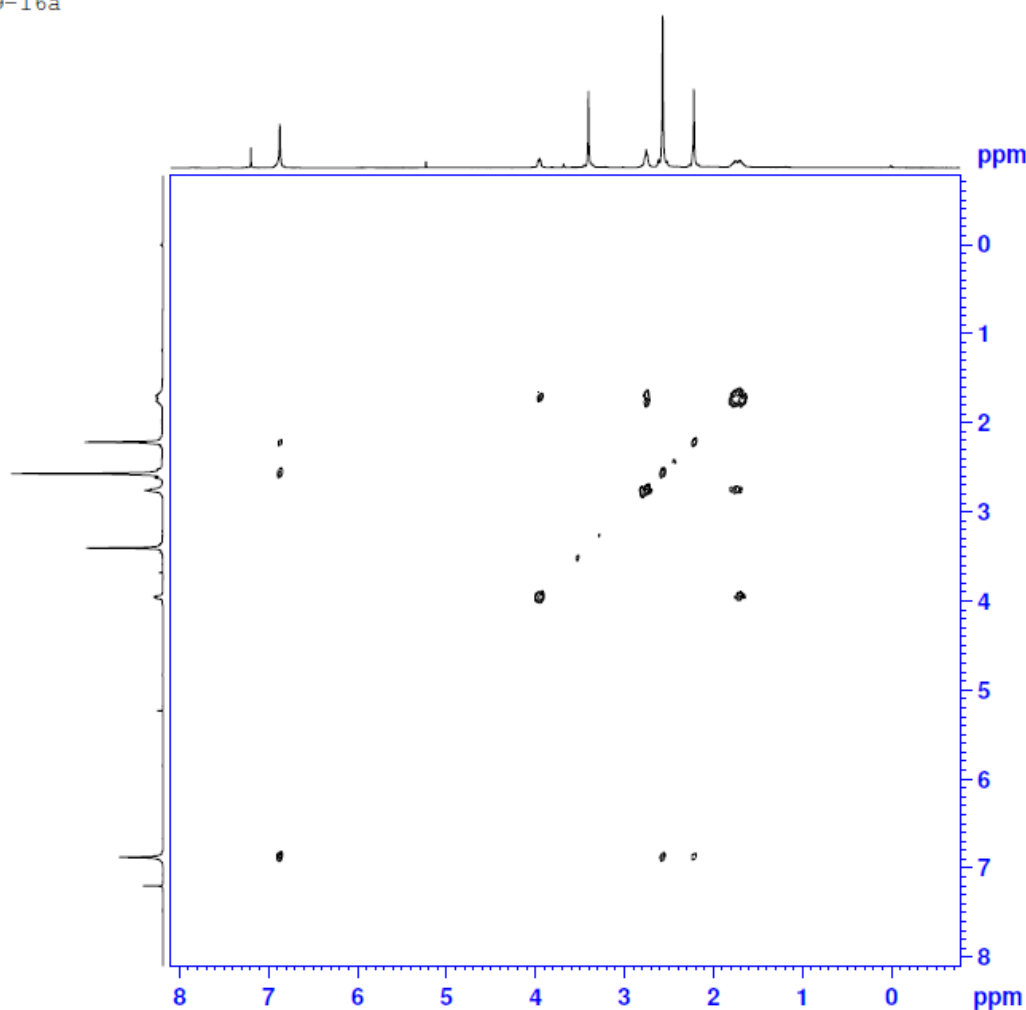
Methyl (*S*)-4-amino-2-(phenylsulfonamido)butanoate [Compound 7]



Methyl (S)-4-amino-2-(2,4,6-trimethylphenylsulfonamido)butanoate [Compound 8]



aet9-16a



Current Data Parameters
 NAME aet9-16a
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121018
 Time 19.04
 INSTRUM DFX400
 PROBRD 5 mm QNP 1H/13
 PULPROG cosygpmfzf
 ID 2048
 SOLVENT CDCl3
 NS 4
 DS 8
 SWH 3551.136 Hz
 FIDRES 1.733953 Hz
 AQ 0.2884084 sec
 RG 4597.6
 DW 140.800 usec
 DE 6.00 usec
 TE 293.2 K
 D0 0.00000300 sec
 D1 1.90292501 sec
 d13 0.00000400 sec
 D16 0.00020000 sec
 IN0 0.00028160 sec

----- CHANNEL f1 -----
 NUC1 1H
 P1 10.00 usec
 PL1 -1.50 dB
 SFO1 400.1314986 MHz

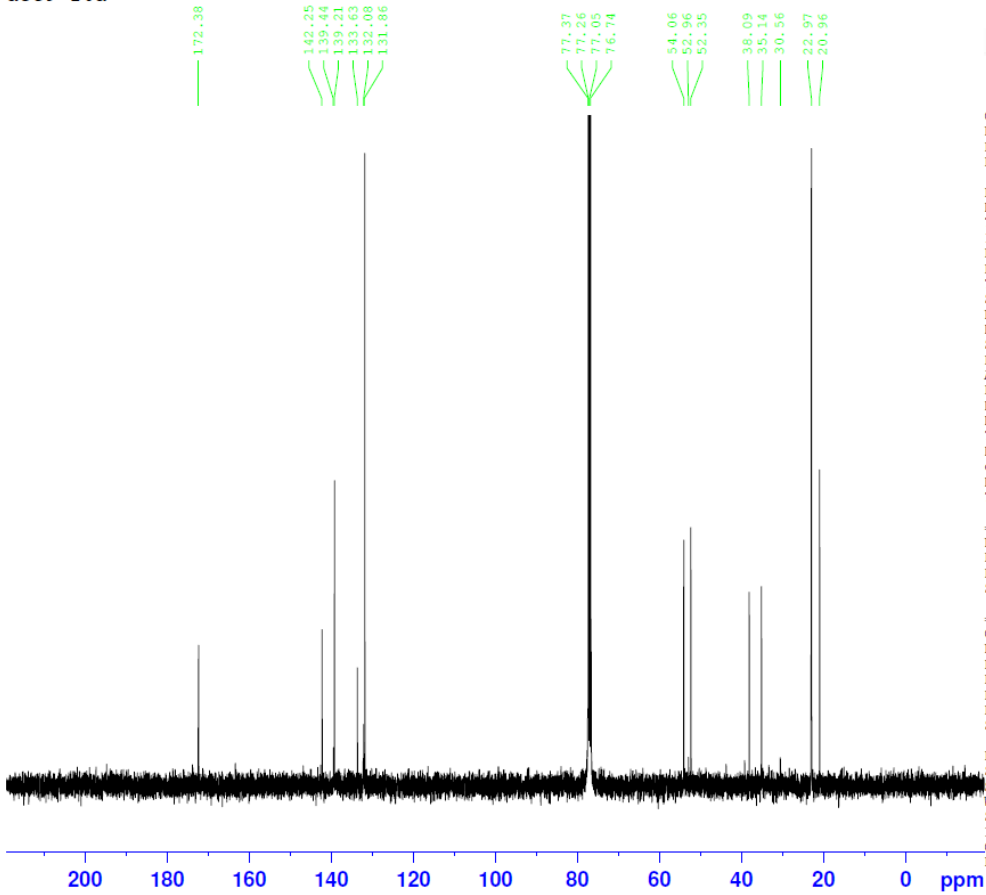
----- GRADIENT CHANNEL -----
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPNAM3 SINE.100
 CPZ1 16.00 %
 CPZ2 12.00 %
 CPZ3 40.00 %
 P16 1000.00 usec

F1 - Acquisition parameters
 ND0 1
 ID 128
 SFO1 400.1315 MHz
 FIDRES 27.743254 Hz
 SW 8.875 ppm
 FMODE QF

F2 - Processing parameters
 SI 1024
 SF 400.1300349 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 400.1300349 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

aet9-16a



Current Data Parameters
 NAME aet9-16a
 EXPNO 11
 PROCNO 1

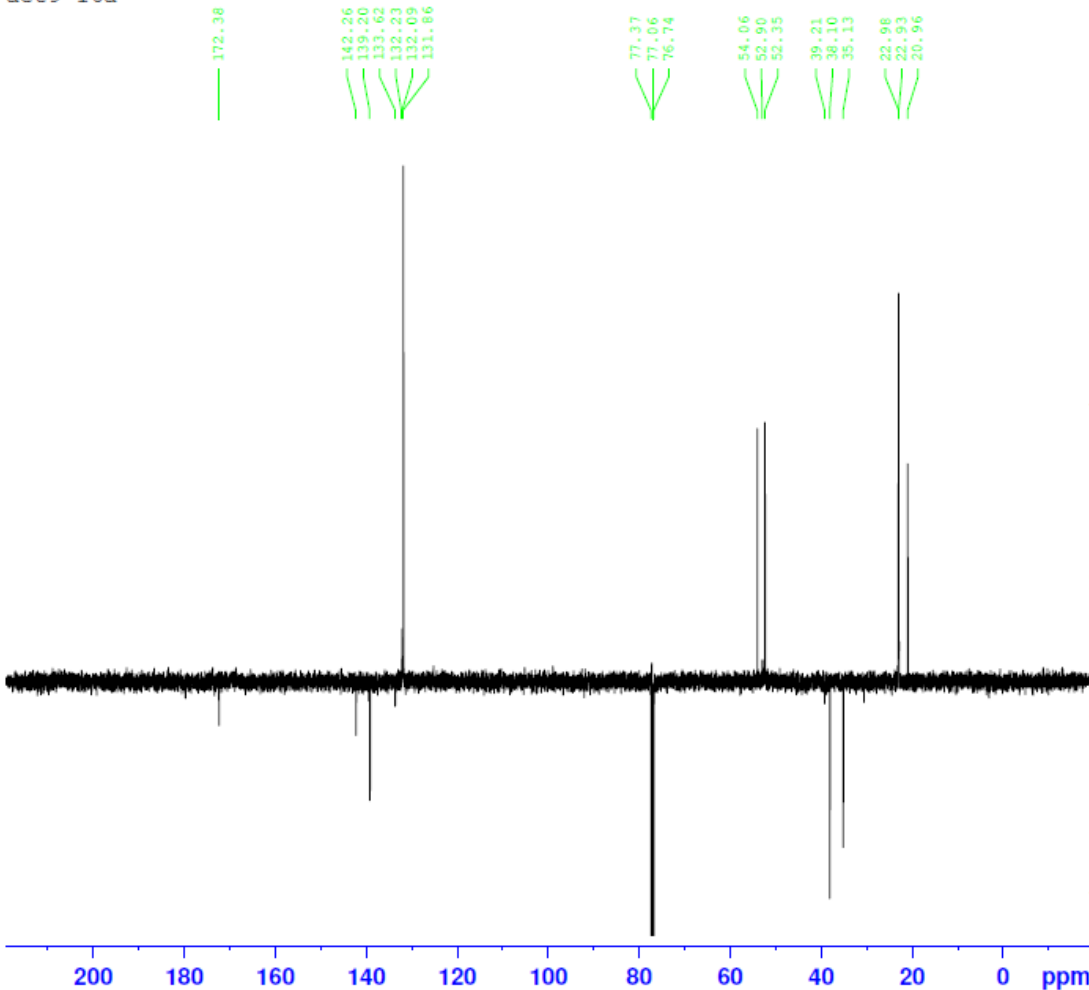
F2 - Acquisition Parameters
 Date_ 20121018
 Time 19.03
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 812.7
 DW 20.850 usec
 DE 6.00 usec
 TE 293.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 PL1 -2.60 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 PL13 17.50 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

aet9-16a



Current Data Parameters
 NAME aet9-16a
 EXPNO 13
 PROCNO 1

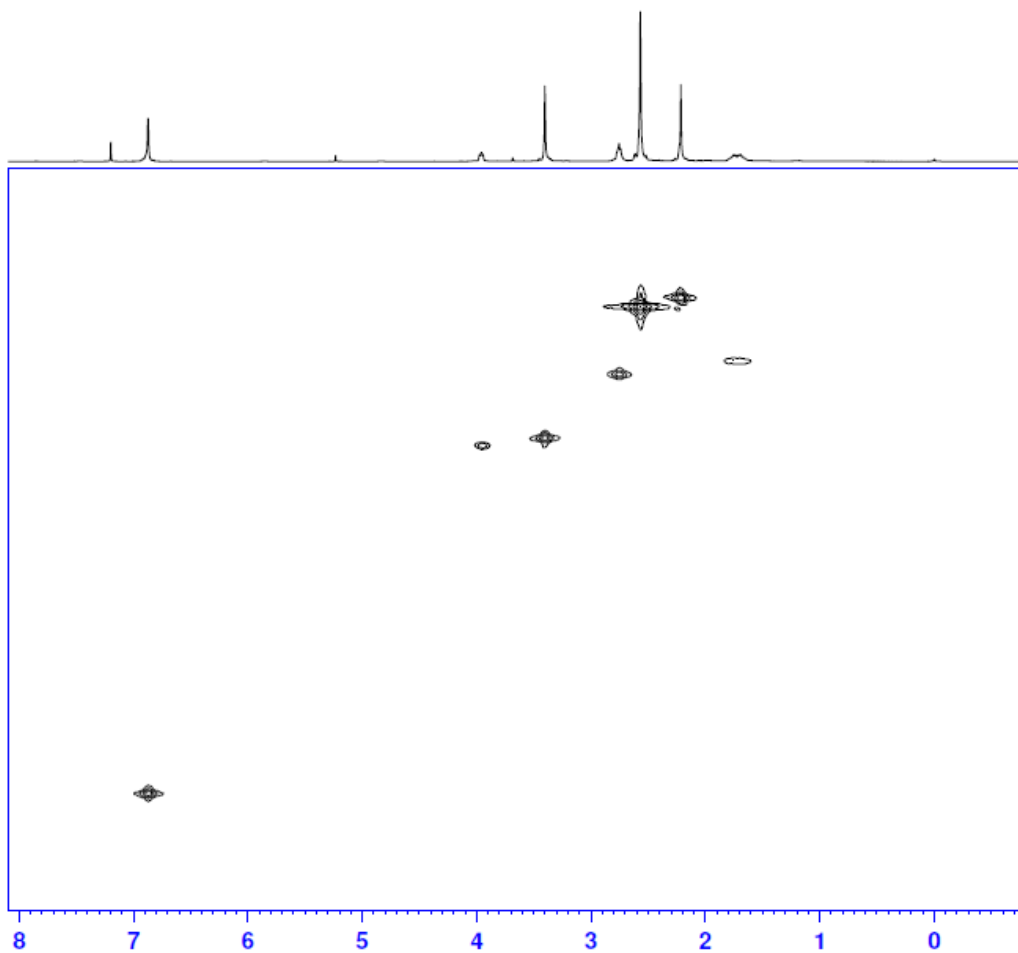
F2 - Acquisition Parameters
 Date_ 20121018
 Time 19.53
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG deptq_135
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 11585.2
 DW 20.850 usec
 DE 6.00 usec
 TE 292.2 K
 CNST2 145.0000000
 D1 2.00000000 sec
 d2 0.00344828 sec
 D11 0.03000000 sec
 DELTA 0.00001082 sec

----- CHANNEL f1 -----
 NUC1 13C
 P1 8.50 usec
 P2 17.00 usec
 PL1 -2.60 dB
 SFO1 100.6228300 MHz

----- CHANNEL f2 -----
 CPDPRG2 waltz16
 NUC2 1H
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 SFO2 400.1316000 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

aet9-16a



Current Data Parameters
NAME aet9-16a
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121016
Time 19.54
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 1024
SOLVENT ccd13
NS 4
DS 16
SWH 355.176 Hz
FIDRES 3.467907 Hz
AQ 0.1442292 sec
RG 395
DM 140.800 usec
DE 6.00 usec
TE 300.2
CMT2 145.0000000
d0 0.0000000 sec
d1 1.4819199 sec
d2 0.00344828 sec
d3 0.00000000 sec
d4 0.00000400 sec
d5 0.00020000 sec
DELTA1 0.0022424 sec
IND 0.00003000 sec

----- CHANNEL F1 -----
NUC1 1H
P1 10.00 usec
PC 20.00 usec
PL1 -1.50 dB
SFO1 400.1314984 MHz

----- CHANNEL F2 -----
CPDPRG2 zgpg30
NUC2 13C
P3 8.00 usec
PCPD2 74.00 usec
PL2 -2.00 dB
PL12 18.00 dB
SFO2 100.6203140 MHz

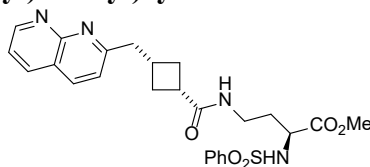
----- GRADIENT CHANNEL -----
GPRAM1 SINE.100
GPRAM2 SINE.100
GPRAM3 SINE.100
GPE1 50.00 %
GPE2 30.00 %
GPE3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
RG 2
TD 128
SFO1 100.6203 MHz
FIDRES 130.208328 Hz
SW 165.639 ppm
F2MODE QF

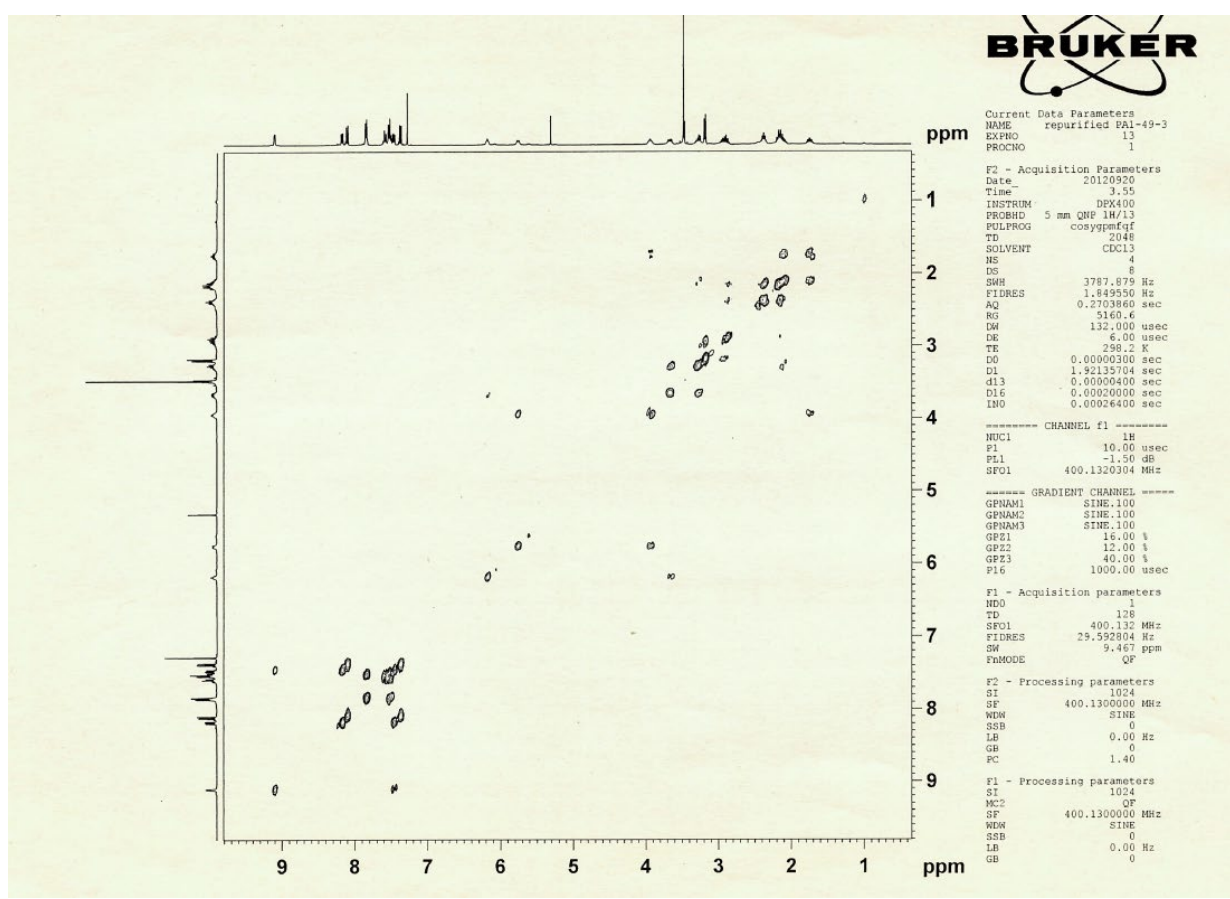
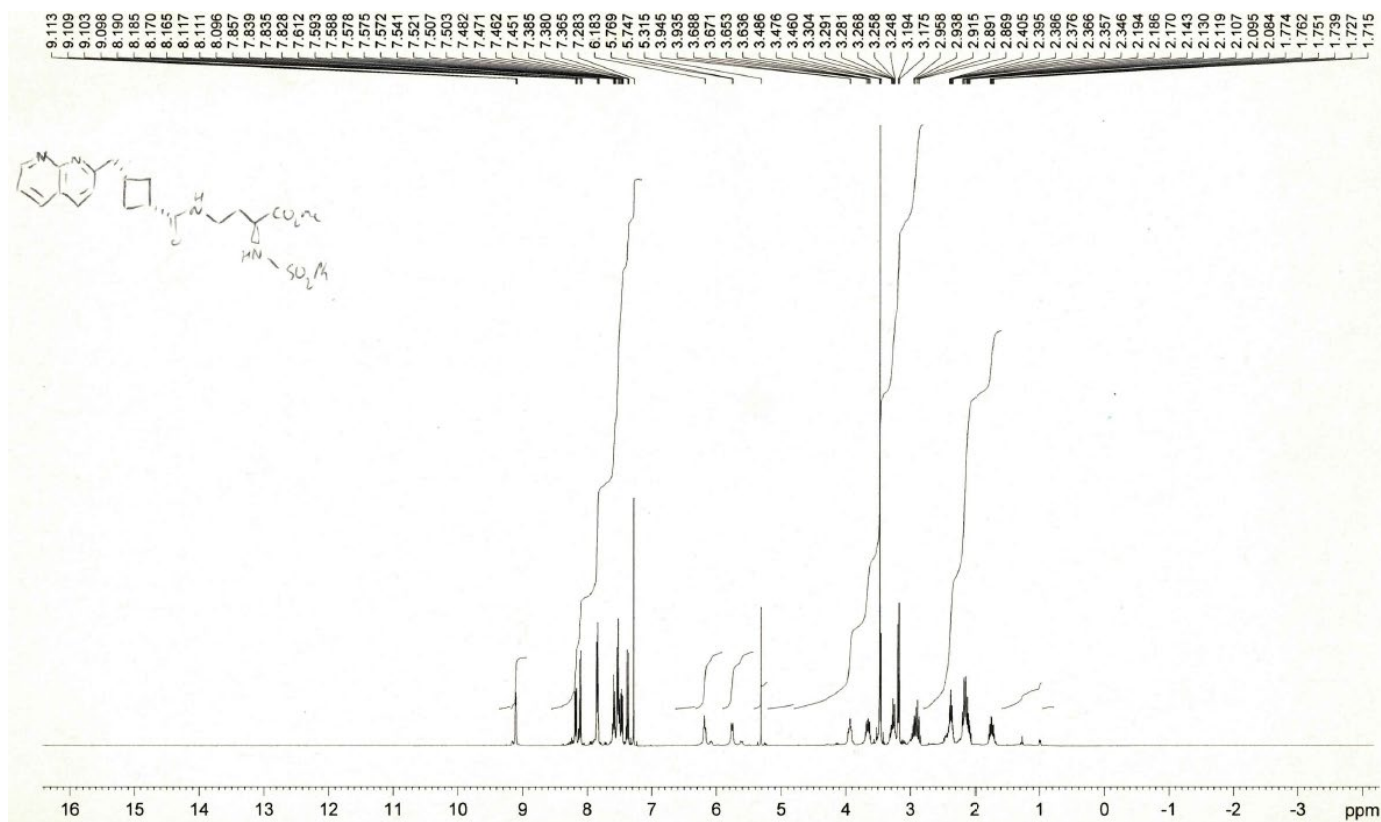
F2 - Processing parameters
SI 1024
SF 400.130349 MHz
WDW QF
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

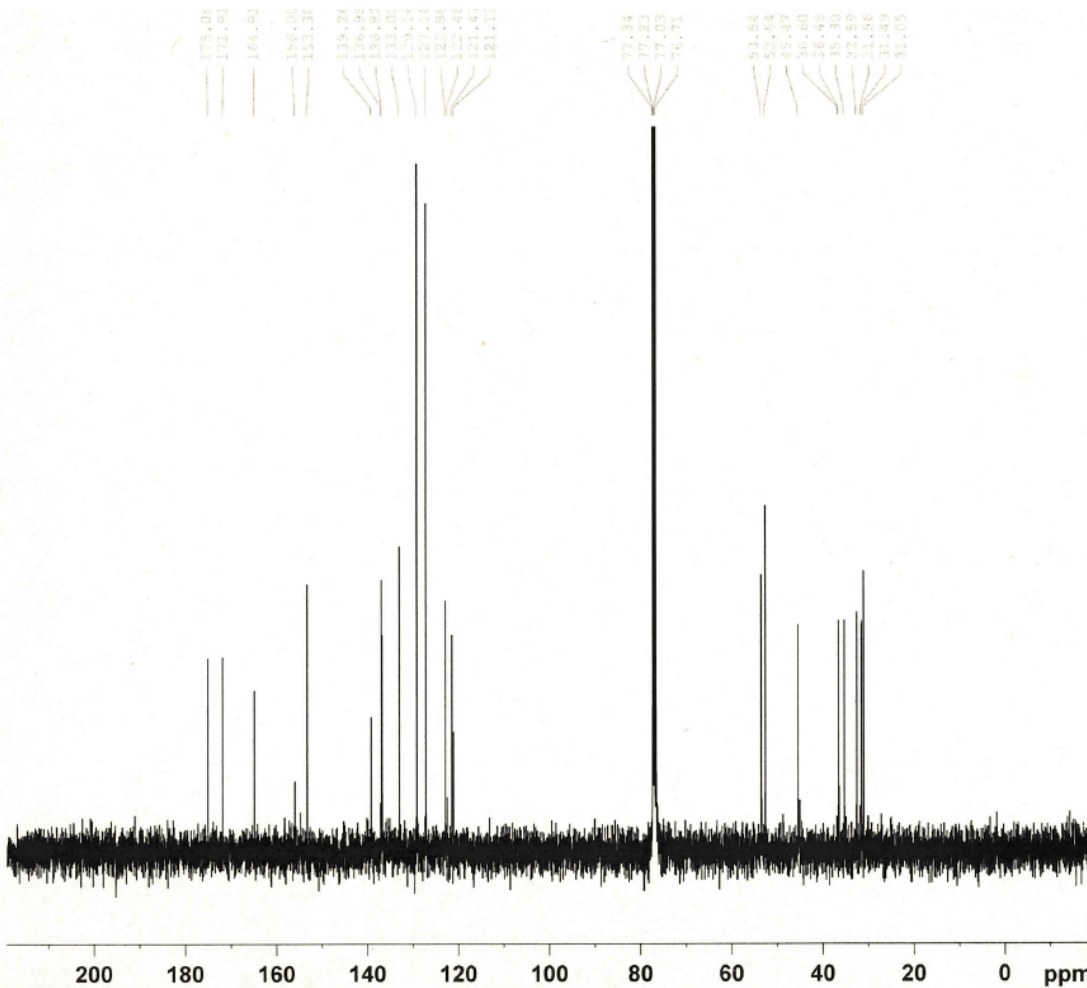
F1 - Processing parameters
SI 1024
MC2 QF
SF 100.6127630 MHz
WDW QF
SSB 0
LB 0.00 Hz
GB 0

Methyl (S)-4-((1*S**,3*R**)-3-((1,8-naphthyridin-2-yl)methyl)cyclobutane-1-carboxamido)-2-



(phenylsulfonamido)butanoate [Compound 17]





Current Data Parameters
 NAME repurified PA1-49-3
 EXPNO 11
 PROCNO 1

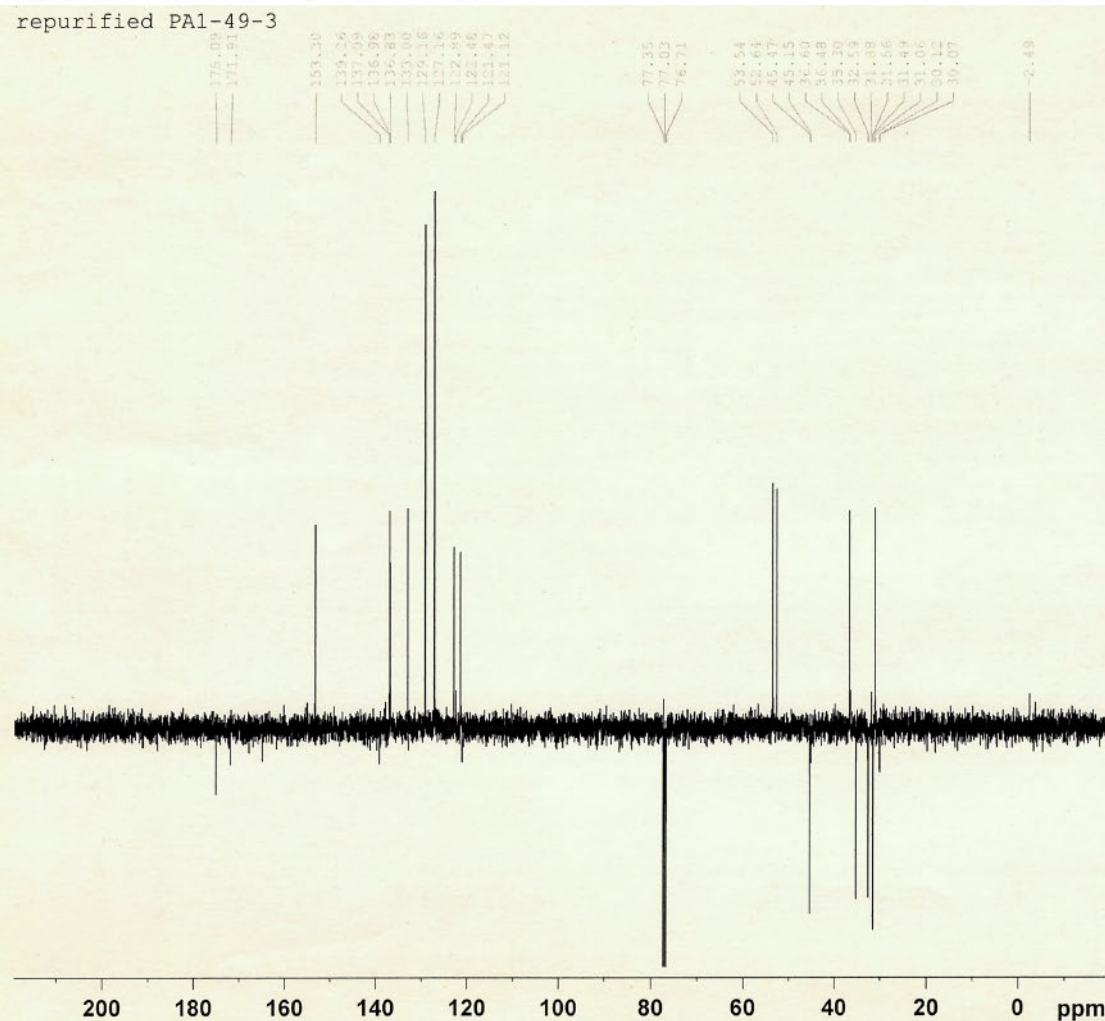
F2 - Acquisition Parameters
 Date 20120920
 Time 3.24
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 1024
 DW 20.850 usec
 DE 6.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 PL1 -2.60 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 PL13 17.50 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

repurified PA1-49-3



Current Data Parameters
 NAME repurified PA1-49-3
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date 20120920
 Time 3.54
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG deptq 135
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 11585.2
 DW 20.850 usec
 DE 6.00 usec
 TE 298.2 K
 CNST2 145.0000000
 D1 2.00000000 sec
 d2 0.00344828 sec
 D11 0.03000000 sec
 DELTA 0.00001082 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 P2 17.00 usec
 PL1 -2.60 dB
 SFO1 100.6228300 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 SFO2 400.1316000 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
NAME repurified P1-49-3
EXPRO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120920
Time_ 4.15

INSTRUM DEX400
PROBHD 5 mm QNP 1H/13
PULPROG hmqcpgpgf
TD 1024
SOLVENT CDCl3
NS 4
DS 16
SWH 3787.879 Hz
FIDRES 3.699100 Hz
AQ 0.1352180 sec
RG 26008
RW 132.000 usec
DE 6.00 usec
TE 298.2 K
CHST2 145.000000
d0 0.0000300 sec
d1 1.49180806 sec
d2 0.00344828 sec
d12 0.00002000 sec
d13 0.00000400 sec
d16 0.00020000 sec
DELTA1 0.00222428 sec
IN0 0.00003000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PC 20.00 usec
PL1 -1.50 dB
SFO1 400.1320304 MHz

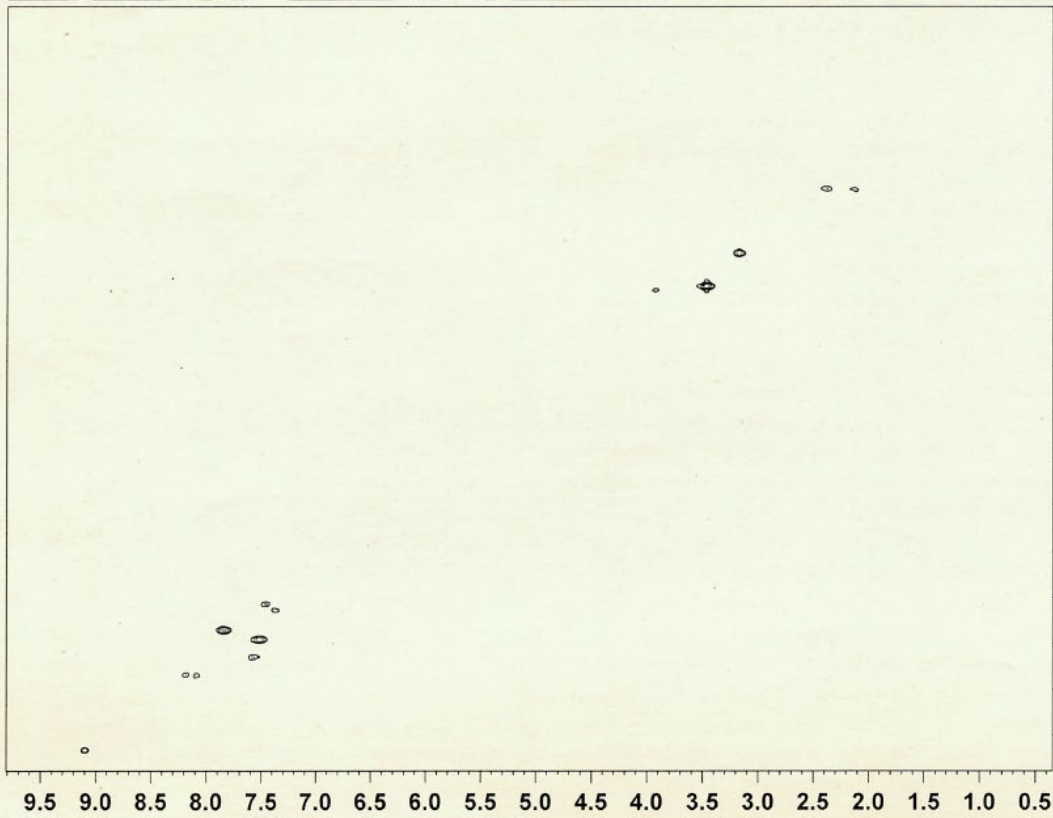
===== CHANNEL f2 =====
CPDPRG2 gmp
NUC2 13C
P3 8.00 usec
PCPD2 74.00 usec
PL2 -3.00 dB
PL12 18.00 dB
SFO2 100.6203140 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

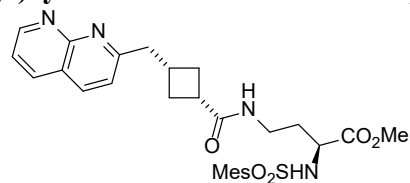
F1 - Acquisition parameters
ND0 2
TD 128
SFO1 100.6203140 MHz
FIDRES 130.208328 Hz
SW 165.639 ppm
FMODE QF

F2 - Processing parameters
SI 1024
SF 400.1300000 MHz
WEN QSIGN
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

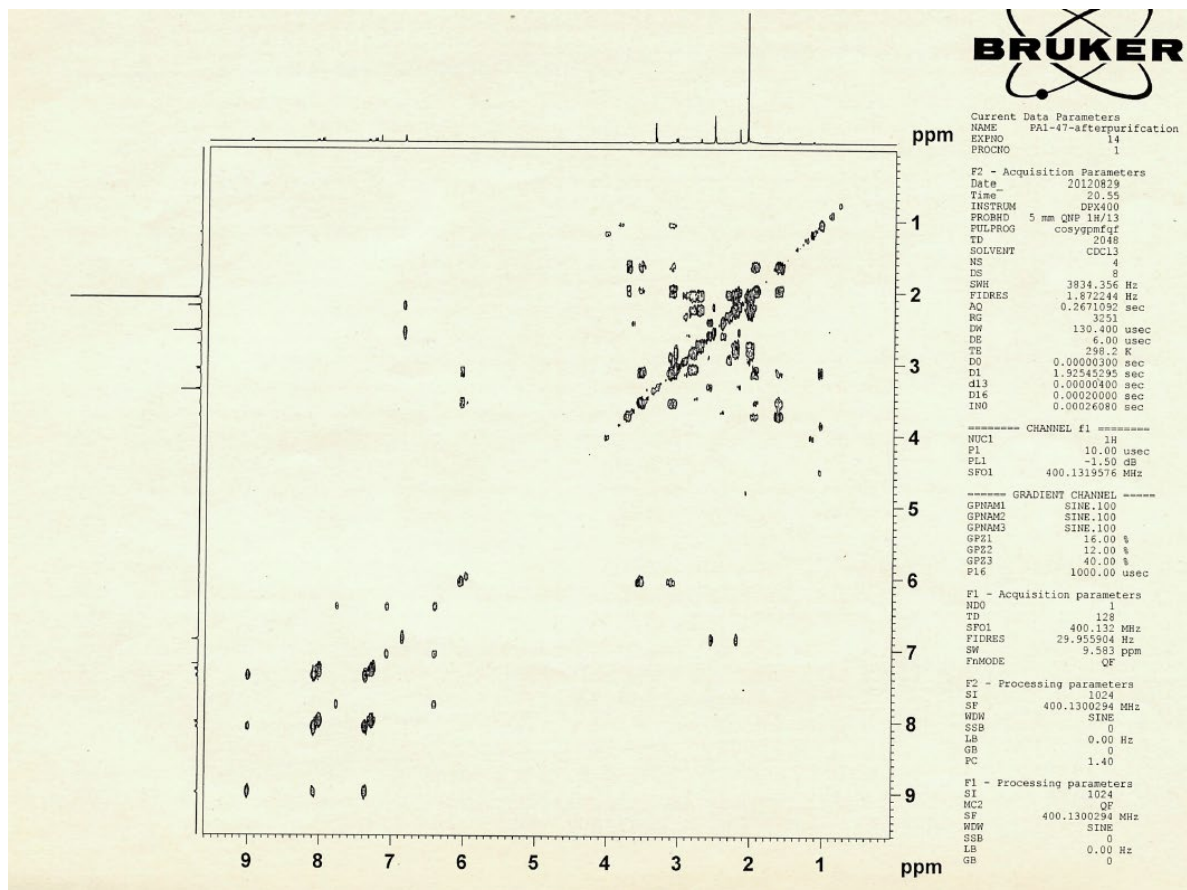
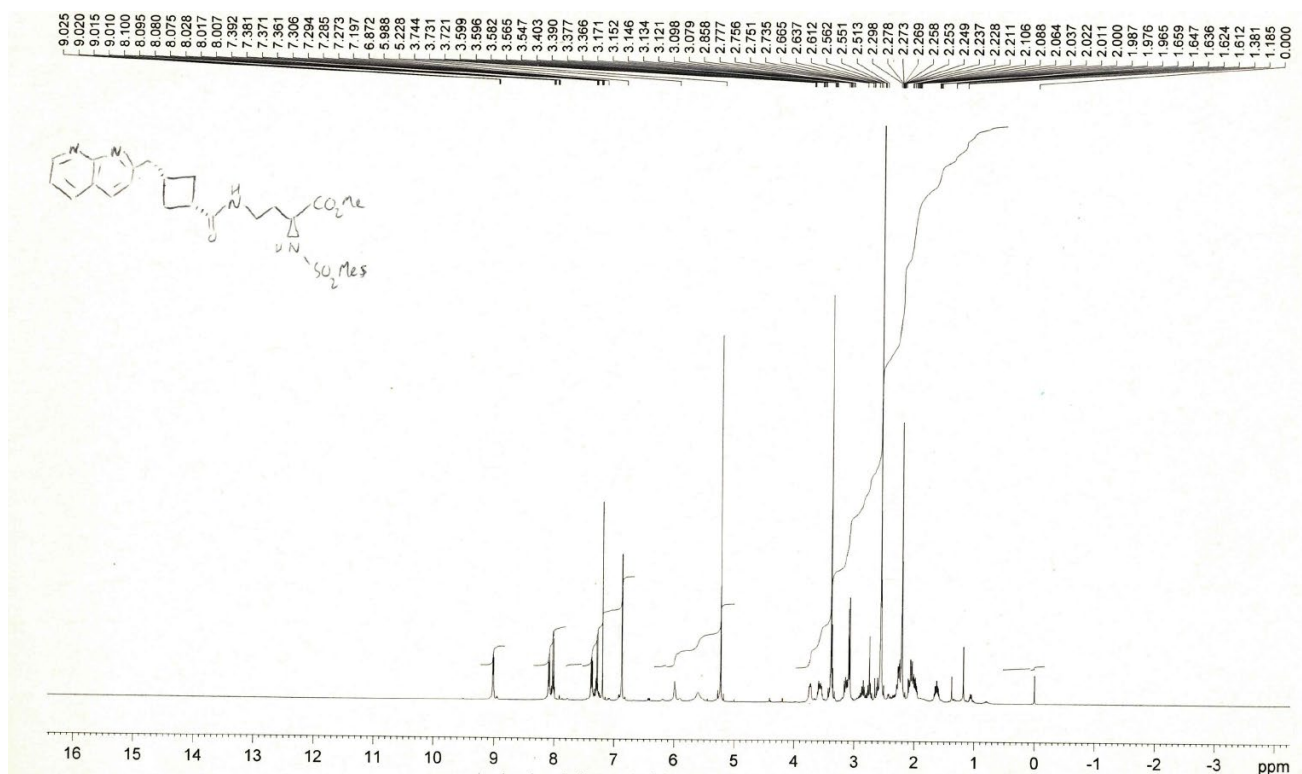
F1 - Processing parameters
SI 1024
MC2 QF
SF 100.6127690 MHz
WEN QSIGN
SSB 2
LB 0.00 Hz
GB 0



Methyl (S)-4-((1*s**,3*R**)-3-((1,8-naphthyridin-2-yl)methyl)cyclobutane-1-carboxamido)-2-(2,4,6-



trimethylphenylsulfonamido)butanoate [Compound 18]





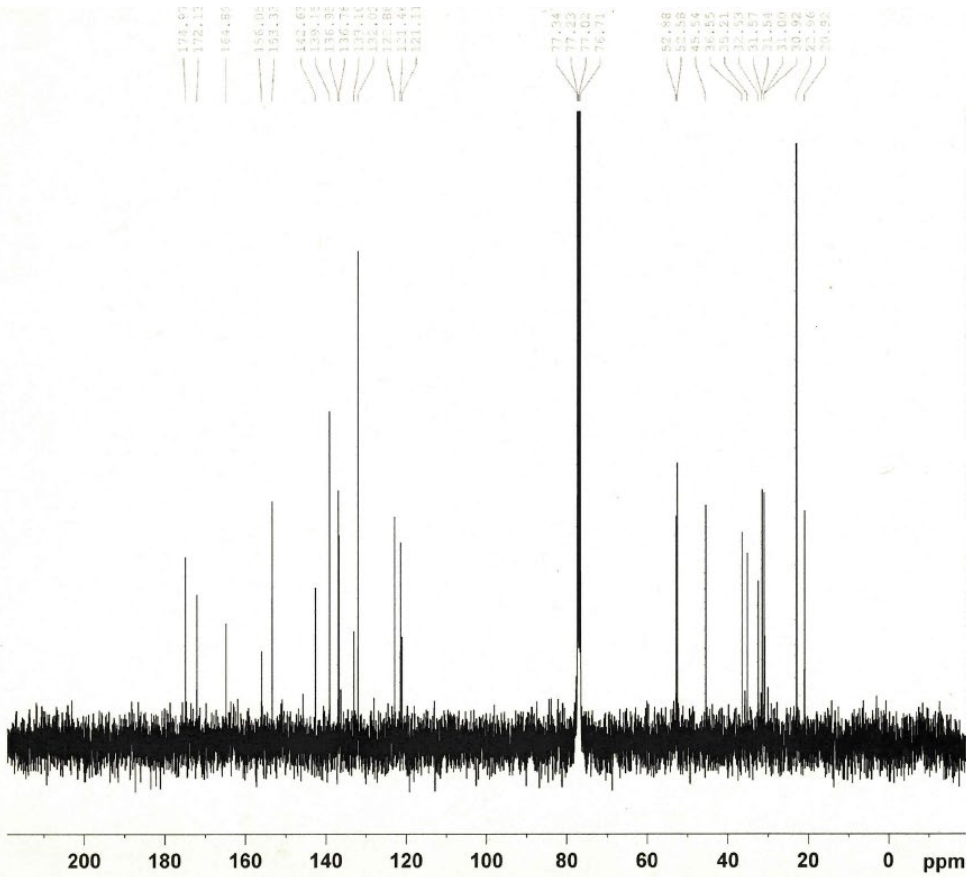
Current Data Parameters
 NAME PA1-47-afterpurification
 EXPNO 20
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120829
 Time 22.16
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 1149.4
 DW 20.850 usec
 DE 6.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13c
 P1 8.50 usec
 PL1 -2.60 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 PL13 17.50 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



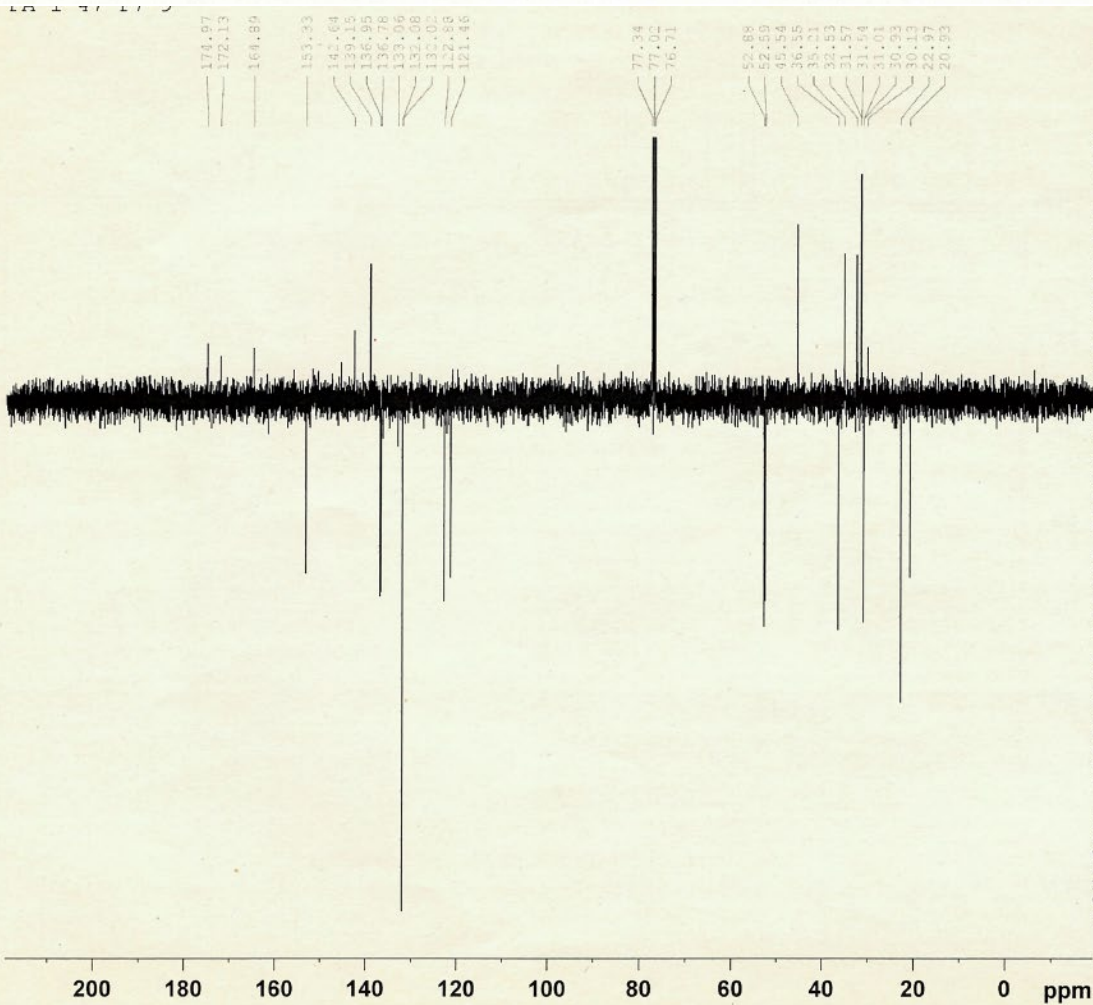
Current Data Parameters
 NAME PA1-47-afterpurificati
 EXPNO 22
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120829
 Time 22.48
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG deptq 135
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 11585.2
 DW 20.850 usec
 DE 6.00 usec
 TE 298.2 K
 CNST2 145.0000000
 D1 2.00000000 sec
 d2 0.00344828 sec
 d11 0.03000000 sec
 DELTA 0.00001082 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 P2 17.00 usec
 PL1 -2.60 dB
 SFO1 100.6228300 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 SFO2 400.1316000 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
 NAME PA1-47-afterpurification
 EXPRO 1
 PROCNO 1

ppm

0

20

40

60

80

100

120

140

ppm

```

F2 - Acquisition Parameters
Date_      20120829
Time       20.40
INSTRUM    DFX400
PROBHD     5 mm QNP 1H/13
PULPROG    zgpg30
TD         1024
SOLVENT    CDCl3
NS         4
DS         16
SMH        3834.356 Hz
FIDRES     3.744488 Hz
AQ         0.1335786 sec
RG         7298.2
DM         130.400 usec
DE         6.00 usec
TE         298.2 K
CHST1     145.0000000
d0         0.0000100 sec
d1         1.49385595 sec
d2         0.00344828 sec
d12        0.0000300 sec
d13        0.00006400 sec
d15        0.00020000 sec
DELTA1     0.0022428 sec
IN0        0.00003000 sec

----- CHANNEL f1 -----
NUC1       1H
P1         10.00 usec
P2         20.00 usec
FL1        -1.50 dB
SFO1       400.1319576 MHz

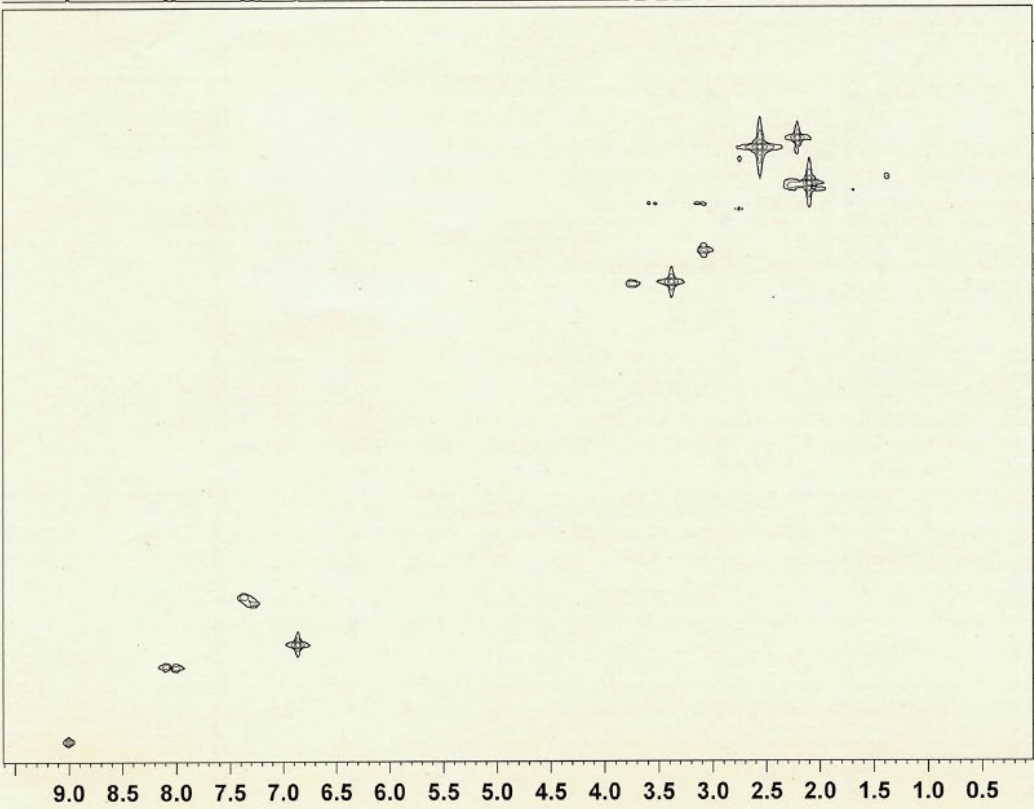
----- CHANNEL f2 -----
CPDPRG2    garp
NUC2       13C
P3         8.00 usec
PCPD2      74.00 usec
FL2        -1.00 dB
FL12       18.00 dB
SFO2       100.6203140 MHz

----- GRADIENT CHANNEL -----
GPMAM1     SINE.100
GPMAM2     SINE.100
GPMAM3     SINE.100
GPZ1       50.00 %
GPZ2       30.00 %
GPZ3       40.10 %
P16        1000.00 usec

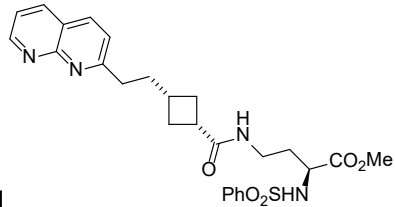
F1 - Acquisition parameters
ND0        2
TD         128
SFO1       100.6203 MHz
FIDRES     130.208320 Hz
SW         165.628 ppm
ENMODE     QF

F2 - Processing parameters
SI         1024
SF         400.1300294 MHz
WDW        QSINE
SSB        2
LB         0.60 Hz
GB         0
PC         1.40

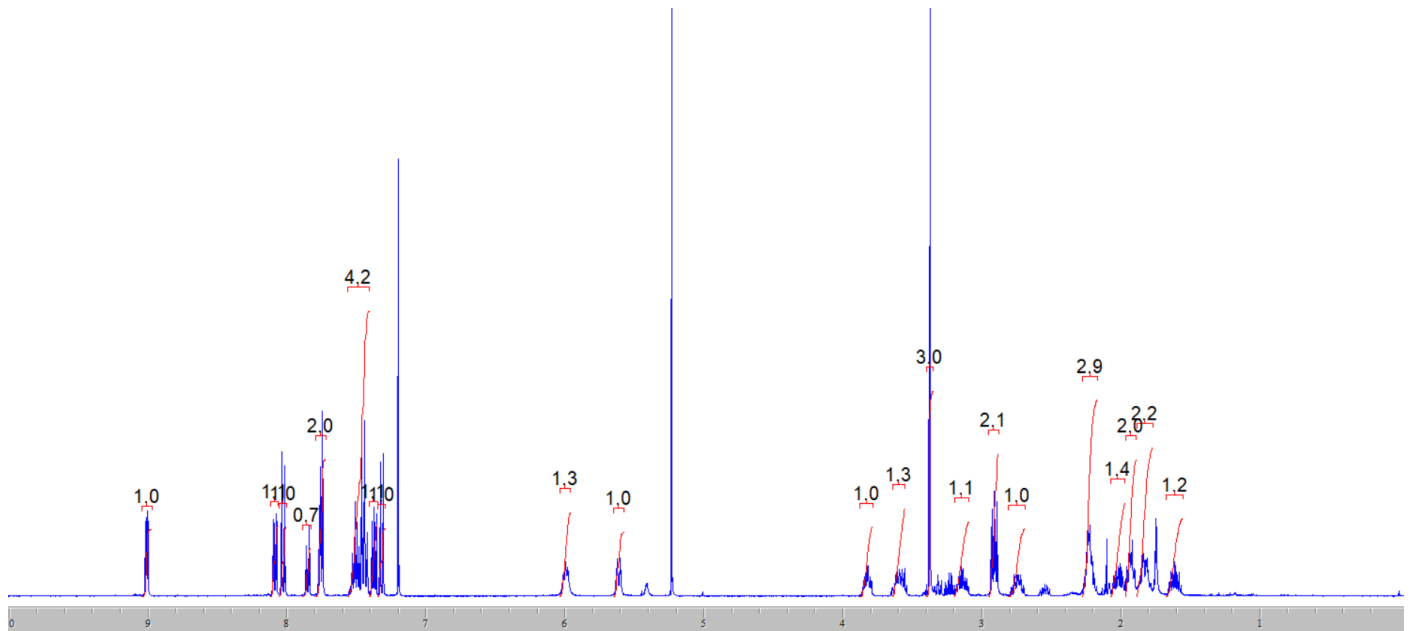
F1 - Processing parameters
SI         1024
MC2        QF
SF         100.6127680 MHz
WDW        QSINE
SSB        2
LB         0.60 Hz
GB         0
  
```



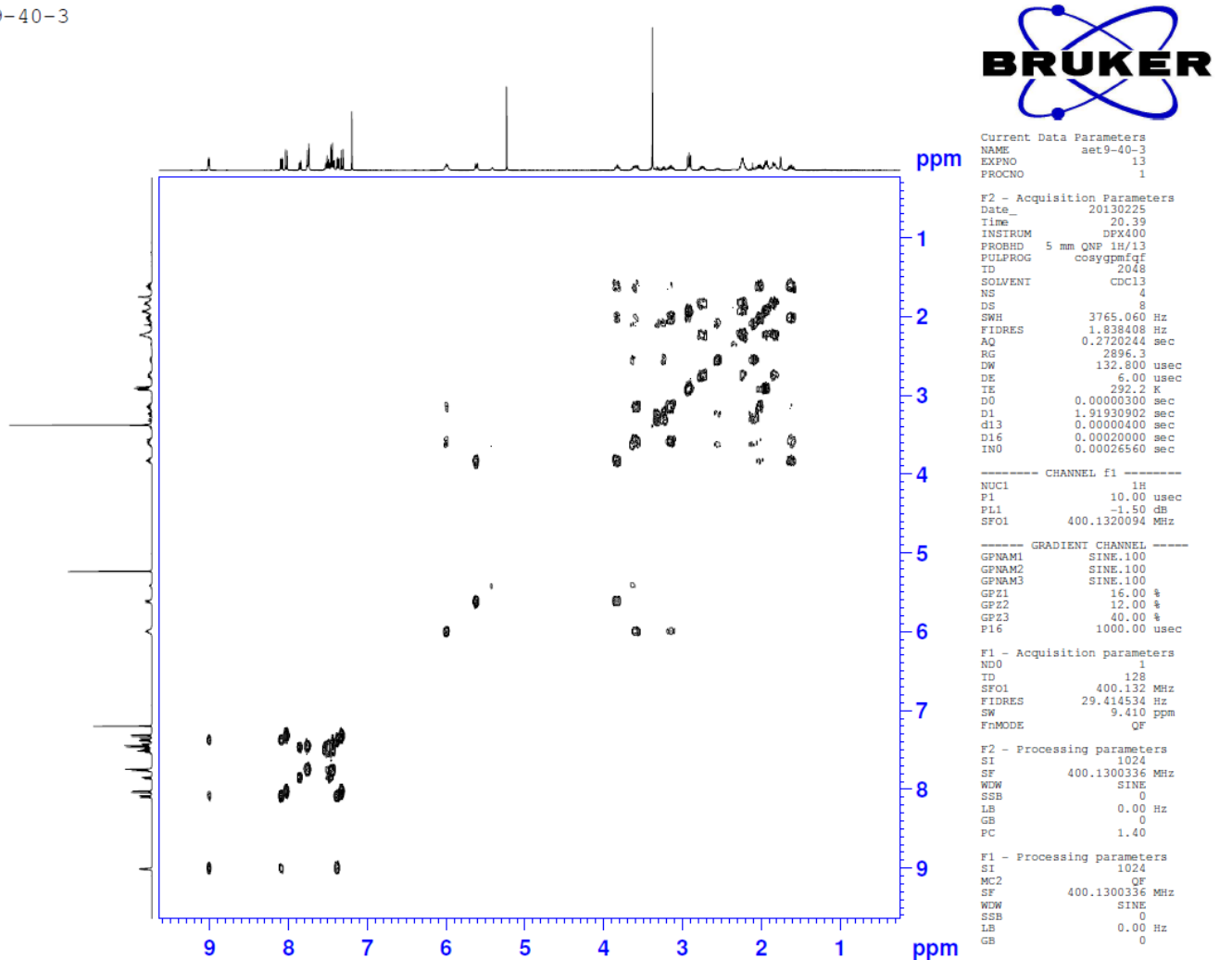
Methyl (*S*)-4-((1*r**,3*R**)-3-(2-(1,8-naphthyridin-2-yl)ethyl)cyclobutane-1-carboxamido)-2-



(phenylsulfonamido)butanoate [Compound 19]



aet9-40-3



Current Data Parameters
NAME aet9-40-3
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130225
Time 20.39
INSTRUM DPX400
PROBHD 5 mm QNP 1H/13
PULPROG cosygmrfqf
TD 2048
SOLVENT CDCl3
NS 4
DS 8
SWH 3765.060 Hz
FIDRES 1.838408 Hz
AQ 0.2720244 sec
RG 2896.3
DW 132.800 usec
DE 6.00 usec
TE 292.2 K
DO 0.00000300 sec
D1 1.91930902 sec
d13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00026560 sec

----- CHANNEL f1 -----
NUC1 1H
P1 10.00 usec
PL1 -1.50 dB
SFO1 400.1320094 MHz

----- GRADIENT CHANNEL -----
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 16.00 %
GPZ2 12.00 %
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
ND0 1
TD 128
SFO1 400.132 MHz
FIDRES 29.414534 Hz
SW 9.410 ppm
FMODE QF

F2 - Processing parameters
SI 1024
SF 400.1300336 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.1300336 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

aet9-40-3



```

Current Data Parameters
NAME      aet9-40-3
EXPNO    11
PROCNO   1

F2 - Acquisition Parameters
Date_    20130225
Time     20.08
INSTRUM  DPX400
PROBHD   5 mm QNP 1H/13
PULPROG  zgpg30
TD       65536
SOLVENT  CDC13
NS       1024
DS       4
SWH      23980.814 Hz
FIDRES   0.365918 Hz
AQ       1.3664756 sec
RG       724.1
DW       20.850 usec
DE       6.00 usec
TE       293.2 K
D1       2.00000000 sec
d11      0.03000000 sec
DELTA    1.89999999 sec
TD0      1

```

```

===== CHANNEL f1 =====
NUC1     13C
P1       8.50 usec
PL1     -2.60 dB
SFO1    100.6228298 MHz

```

```

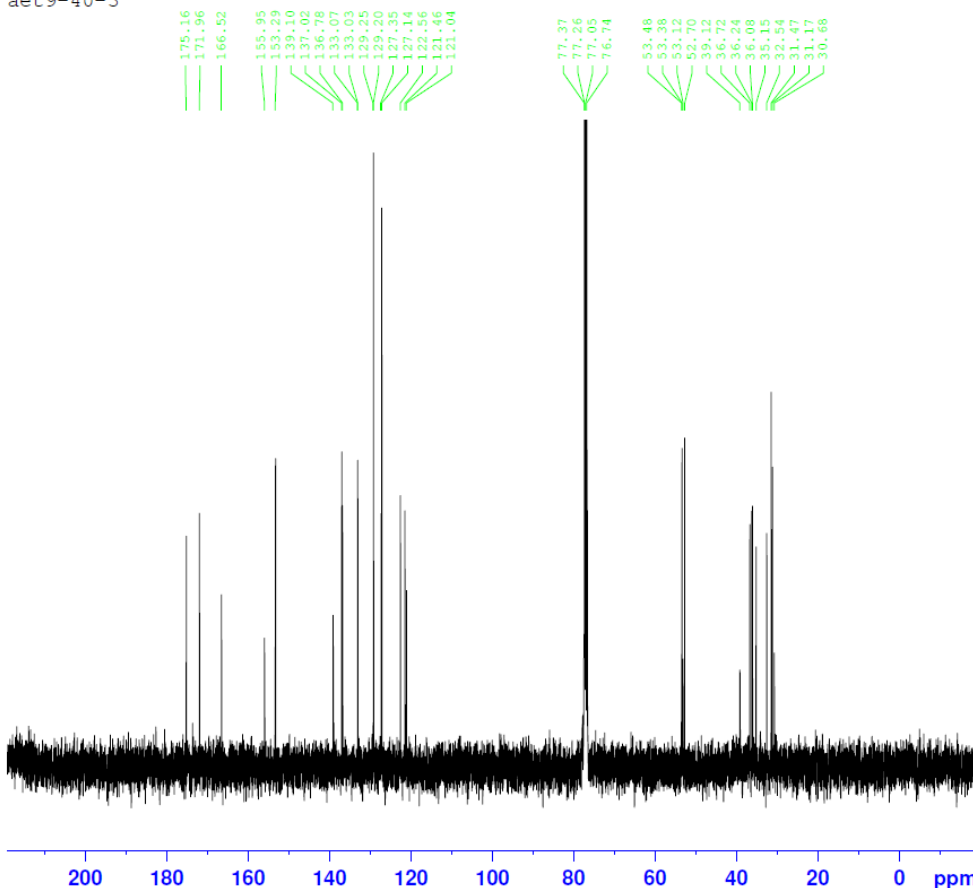
===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2     1H
PCPD2    80.00 usec
PL2     -1.50 dB
PL12    17.50 dB
PL13    17.50 dB
SFO2    400.1316005 MHz

```

```

F2 - Processing parameters
SI       32768
SF       100.6127690 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40

```



```

Current Data Parameters
NAME      aet9-40-3
EXPNO    12
PROCNO   1

```

```

F2 - Acquisition Parameters
Date_    20130225
Time     20.38
INSTRUM  DPX400
PROBHD   5 mm QNP 1H/13
PULPROG  deptq_135
TD       65536
SOLVENT  CDC13
NS       512
DS       4
SWH      23980.814 Hz
FIDRES   0.365918 Hz
AQ       1.3664756 sec
RG       18390.4
DW       20.850 usec
DE       6.00 usec
TE       293.2 K
CNST2    145.0000000
D1       2.00000000 sec
d2       0.00344828 sec
D11      0.03000000 sec
DELTA    0.00001082 sec

```

```

===== CHANNEL f1 =====
NUC1     13C
P1       8.50 usec
P2       17.00 usec
PL1     -2.60 dB
SFO1    100.6228300 MHz

```

```

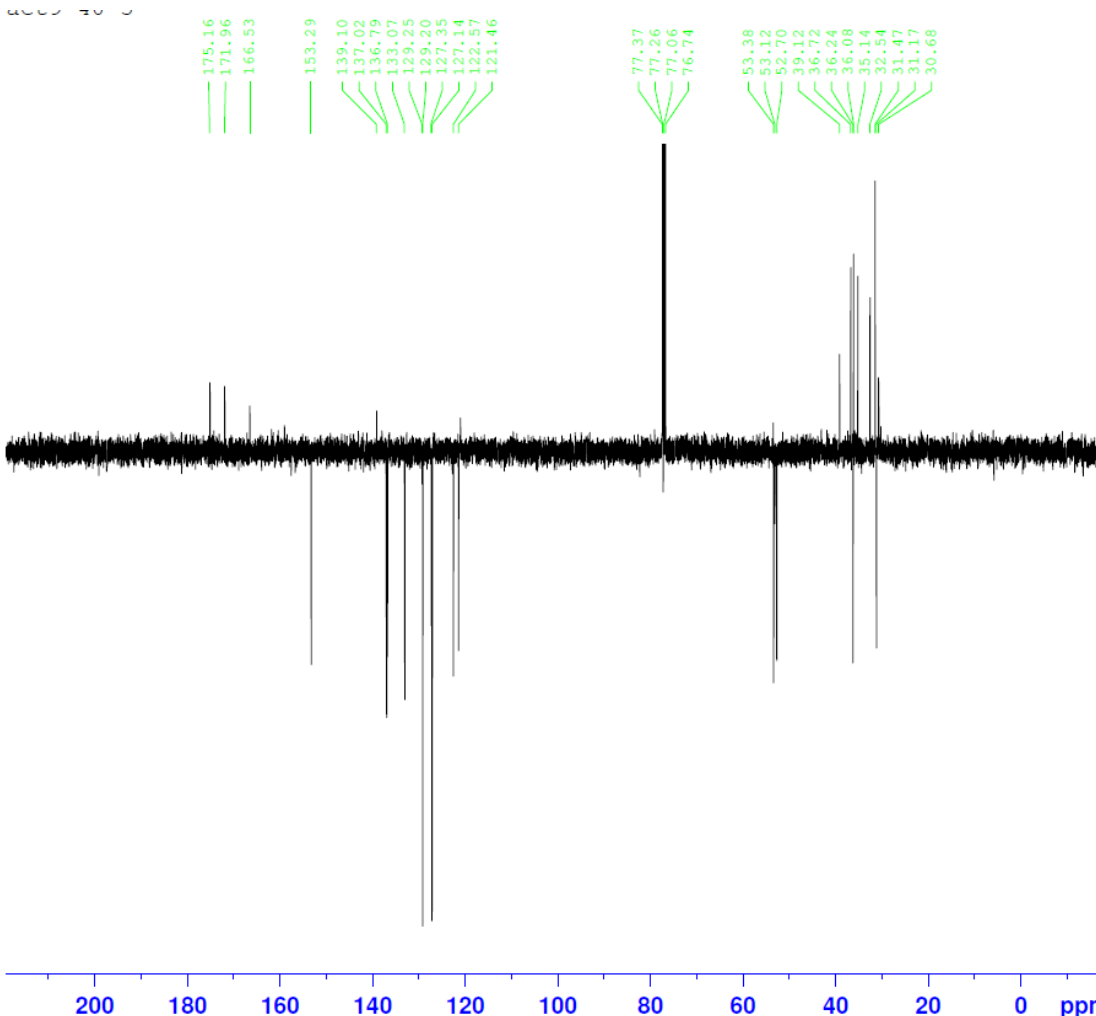
===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2     1H
P3       10.00 usec
P4       20.00 usec
PCPD2    80.00 usec
PL2     -1.50 dB
PL12    17.50 dB
SFO2    400.1316000 MHz

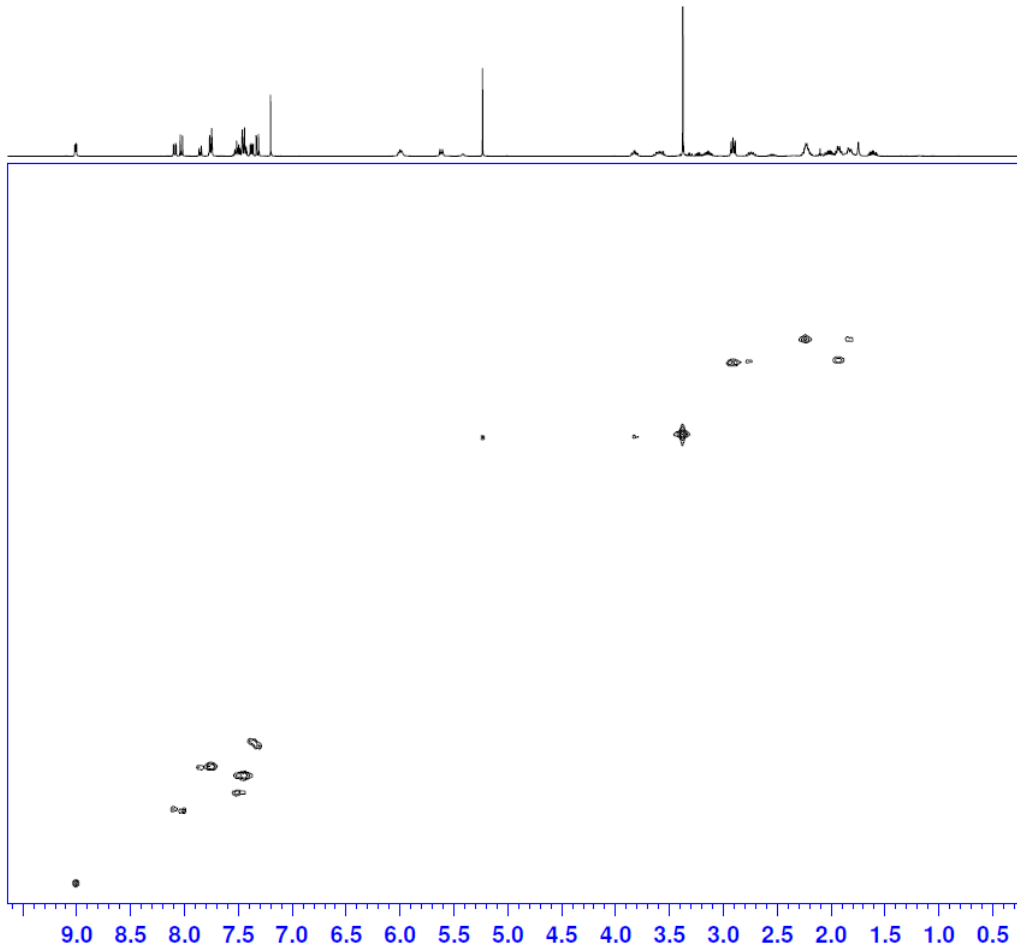
```

```

F2 - Processing parameters
SI       32768
SF       100.6127690 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40

```





```

Current Data Parameters
NAME      aet9-40-3
EXPNO     14
PROCNO    1

F2 - Acquisition Parameters
Date_     20130225
Time      20.59
INSTRUM   DPK400
PROBHD    5 mm QNP 1H/13
PULPROG   zgpg30
TD         1024
SOLVENT   CDCl3
NS         4
DS         16
SWH        3765.060 Hz
FIDRES     3.676817 Hz
AQ         0.1360372 sec
RG         5782.6
DW         132.800 usec
DE         6.00 usec
TE         292.2 K
CNST2     145.0000000
d0         0.0000000 sec
d1         1.49078405 sec
d2         0.00344828 sec
d12        0.00002000 sec
d13        0.00000400 sec
d16        0.00020000 sec
DELTA1    0.00222428 sec
INO        0.00000000 sec

===== CHANNEL f1 =====
NUC1       1H
P1         10.00 usec
P2         20.00 usec
PL1        -1.50 dB
SFO1       400.1320094 MHz

===== CHANNEL F2 =====
CPDPRG2   gspg
NUC2       13C
P3         8.00 usec
PCPD2     74.00 usec
PL2        -3.00 dB
PL12       18.00 dB
SFO2       100.6203140 MHz

===== GRADIENT CHANNEL =====
GFNAM1     SINE.100
GFNAM2     SINE.100
GFNAM3     SINE.100
GPZ1       50.00 %
GPZ2       30.00 %
GPZ3       40.10 %
P16        1000.00 usec

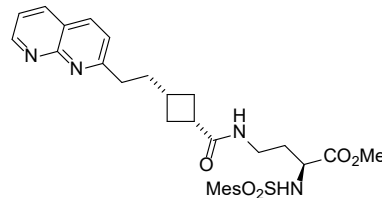
F1 - Acquisition parameters
ND0        2
TD         128
SFO1       100.6203 MHz
FIDRES     130.208328 Hz
SW         145.439 ppm
Fsmode     QF

F2 - Processing parameters
SI         1024
SF         400.1300336 MHz
WFW        QSINE
SBB        2
LB         0.00 Hz
GB         0
PC         1.40

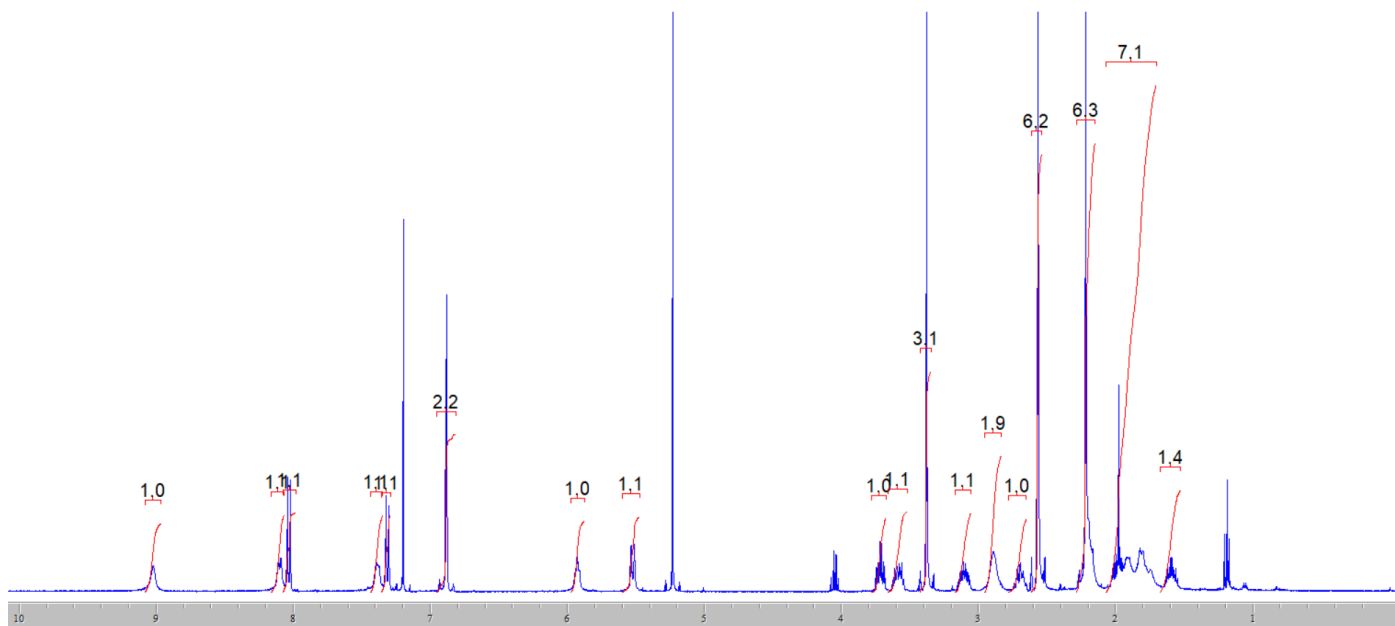
F1 - Processing parameters
SI         1024
MC2        QF
SF         100.6127690 MHz
WFW        QSINE
SBB        2
LB         0.00 Hz
GB         0

```

Methyl (S)-4-((1*r**,3*R**)-3-(2-(1,8-naphthyridin-2-yl)ethyl)cyclobutane-1-carboxamido)-2-(2,4,6-



trimethylphenylsulfonamido)butanoate [Compound 20]



Current Data Parameters
 NAME aet9-19-1
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121031
 Time 19.04
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG cosygmfzf
 TD 2048
 SOLVENT CDCl3
 NS 4
 DS 8
 SWH 3810.976 Hz
 FIDRES 1.860828 Hz
 AQ 0.2687476 sec
 RG 5792.6
 DW 131.200 usec
 DE 6.00 usec
 TE 292.2 K
 D0 0.00000300 sec
 D1 1.92340505 sec
 d13 0.00000400 sec
 D16 0.00020000 sec
 IN0 0.00026240 sec

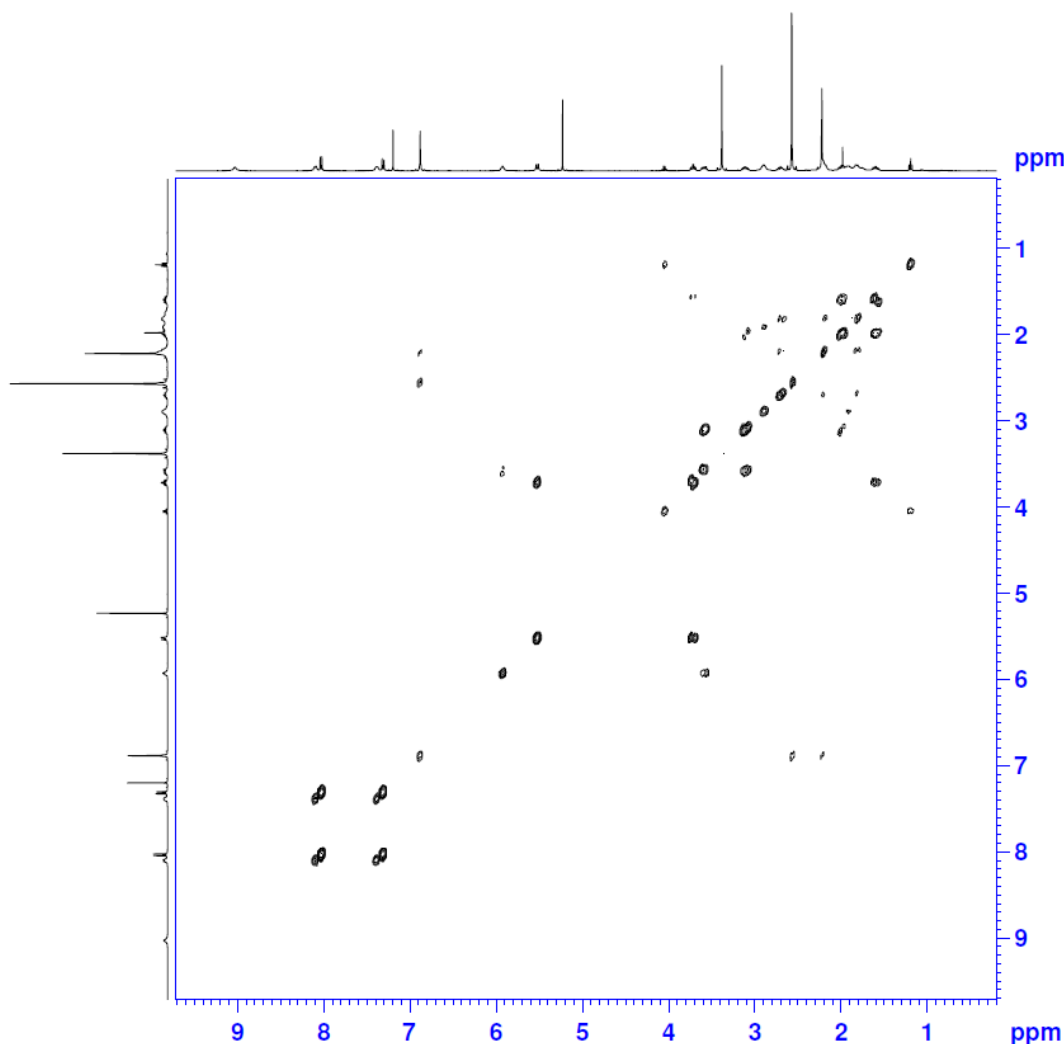
CHANNEL f1
 NUC1 1H
 P1 10.00 usec
 PL1 -1.50 dB
 SFO1 400.1320160 MHz

GRADIENT CHANNEL
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPNAM3 SINE.100
 GPZ1 16.00 %
 GPZ2 12.00 %
 GPZ3 40.00 %
 P16 1000.00 usec

F1 - Acquisition parameters
 ND0 1
 TD 128
 SFO1 400.132 MHz
 FIDRES 29.773247 Hz
 SW 9.524 ppm
 FxMODE QF

F2 - Processing parameters
 SI 1024
 SF 400.1300337 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 400.1300337 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0



aet9-19-1



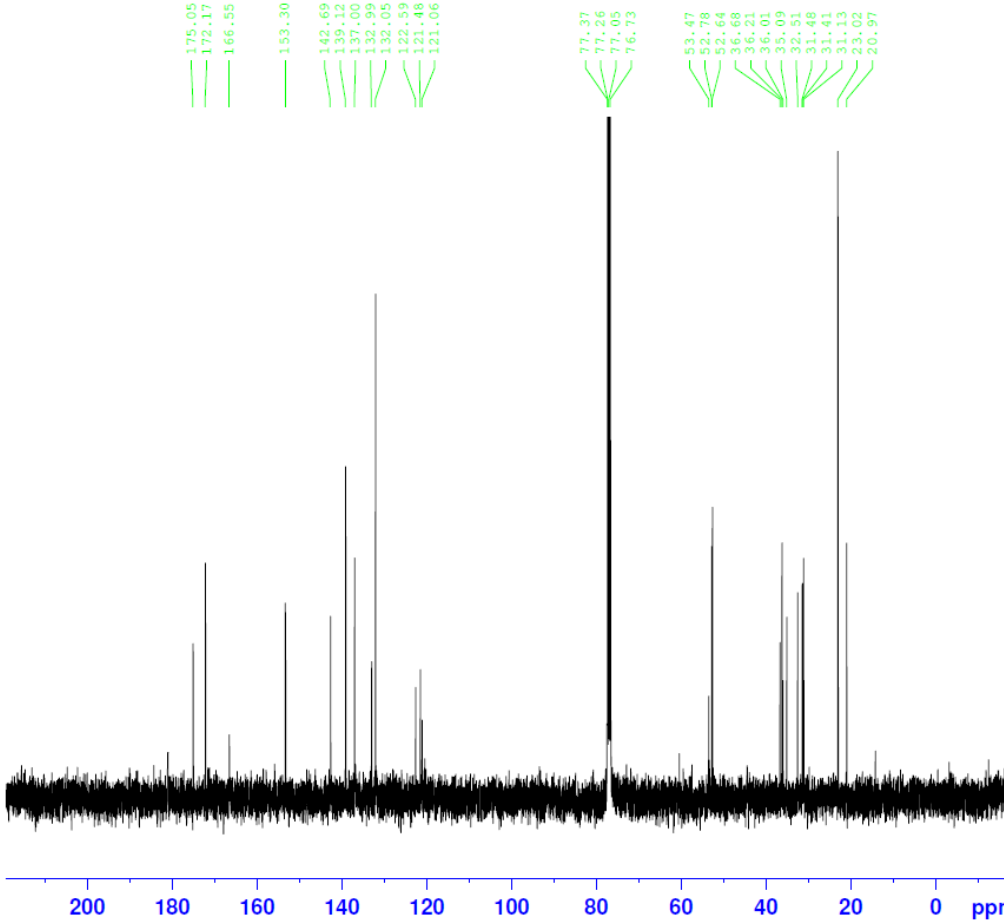
Current Data Parameters
NAME aet9-19-1
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121031
Time 19.03
INSTRUM DPX400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 812.7
DW 20.850 usec
DE 6.00 usec
TE 292.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 -2.60 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.50 dB
PL12 17.50 dB
PL13 17.50 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



aet9-19-1



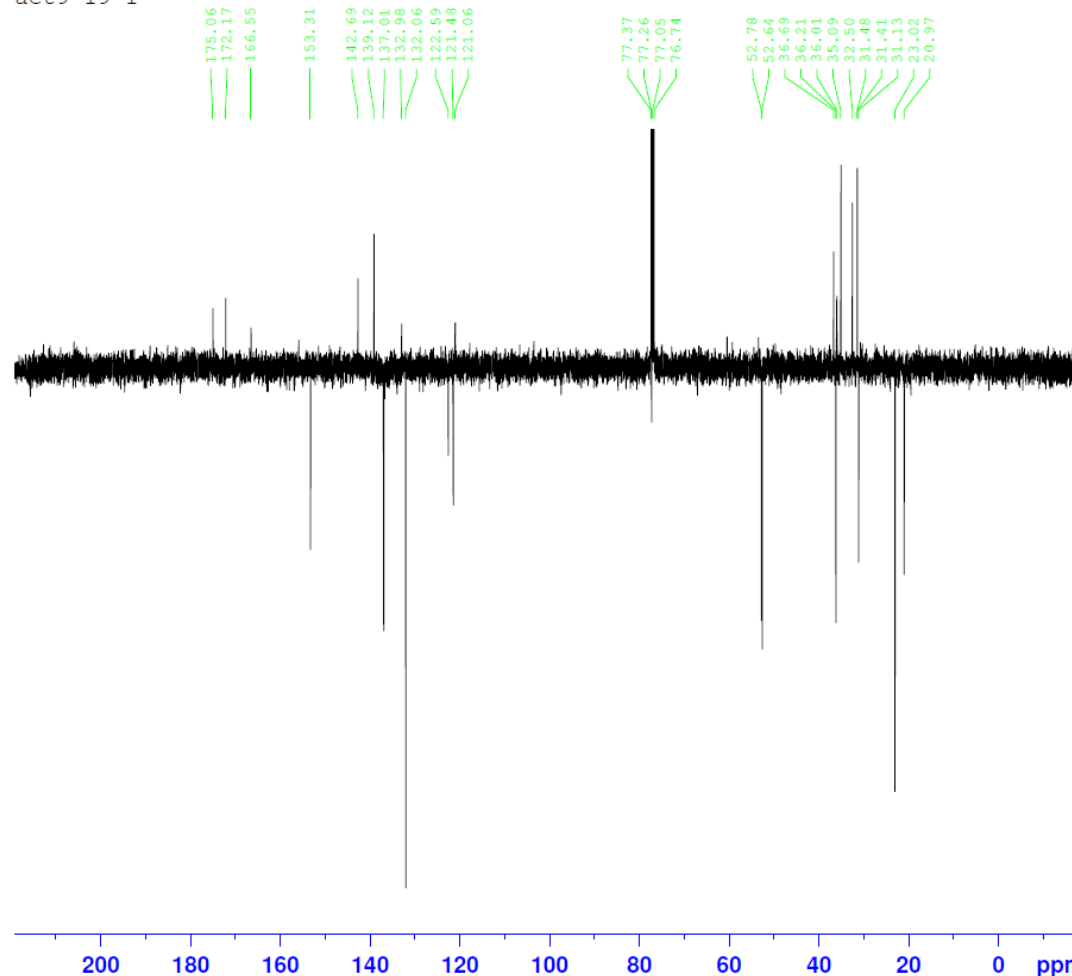
Current Data Parameters
NAME aet9-19-1
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121031
Time 19.53
INSTRUM DPX400
PROBHD 5 mm QNP 1H/13
PULPROG deptq_135
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 11585.2
DW 20.850 usec
DE 6.00 usec
TE 292.2 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
D11 0.03000000 sec
DELTA 0.00001082 sec

===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
P2 17.00 usec
PL1 -2.60 dB
SFO1 100.6228300 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 10.00 usec
P4 20.00 usec
PCPD2 80.00 usec
PL2 -1.50 dB
PL12 17.50 dB
SFO2 400.1316000 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





Current Data Parameters
NAME sec9-19-1
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121031
Time 19.54

INSTRUM DPK400
PROBHD 5 mm QNP 1H/13
PULPROG hmqcmezf
TD 1024
SOLVENT CDCl3

NS 4
DS 16
SWH 3810.976 Hz
FIDRES 3.721656 Hz

AQ 0.1343988 sec
RG 10321.3
DW 131.200 usec
DE 6.00 usec

TE 292.2 K
CNS12 145.000000 sec
d0 0.0000300 sec

D1 1.49283195 sec
d2 0.0034828 sec
d12 0.0000200 sec

d13 0.0000400 sec
D16 0.0002000 sec
DELTA1 0.0022428 sec
INO 0.0000300 sec

==== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PC 20.00 usec

==== CHANNEL f2 =====
CPDPRG2 gcp
NUC2 13C
P3 8.00 usec

PCPD2 74.00 usec
PL2 -3.00 dB
PL12 18.00 dB
SFO2 100.6203140 MHz

==== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100

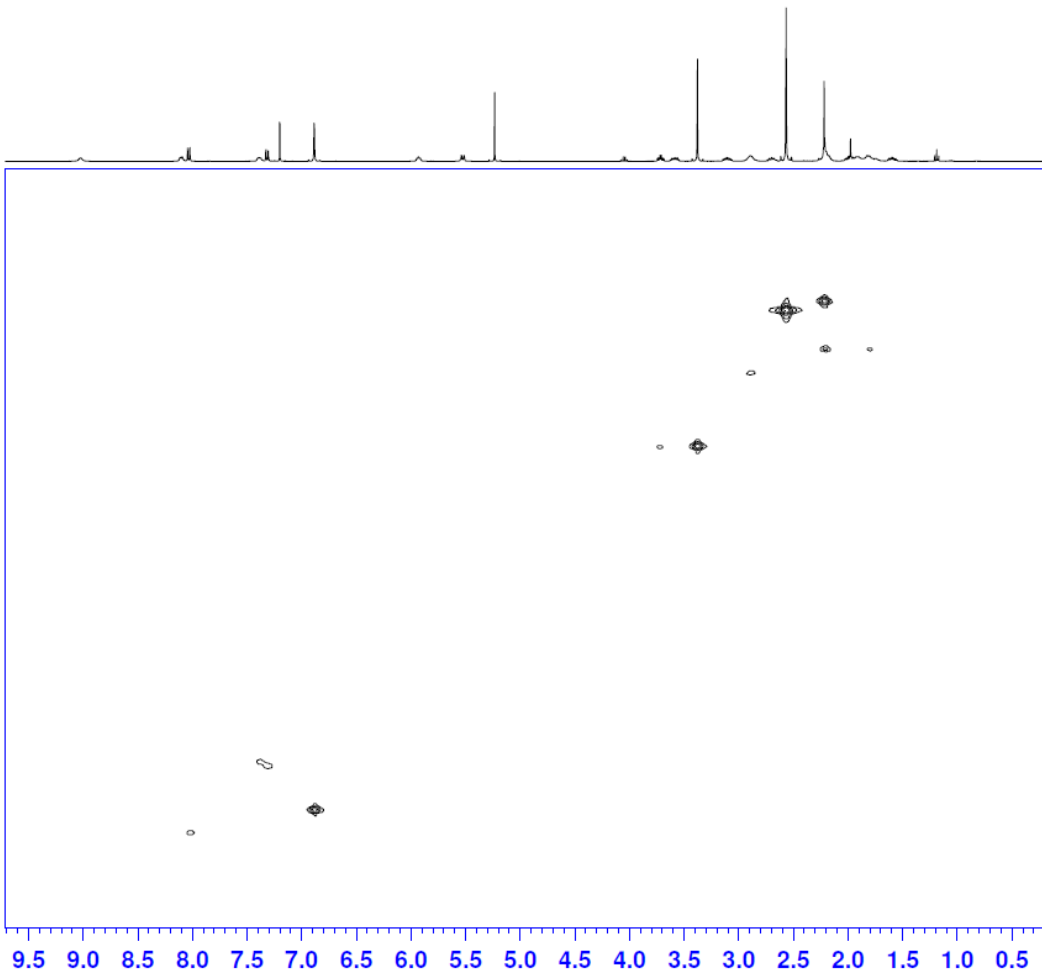
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
ND0 2
TD 128
SFO1 100.6203 MHz
FIDRES 130.208328 Hz

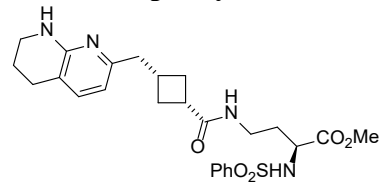
SW 165.639 ppm
FrMODE QF
F2 - Processing parameters
SI 1024
SF 400.1300337 MHz

WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

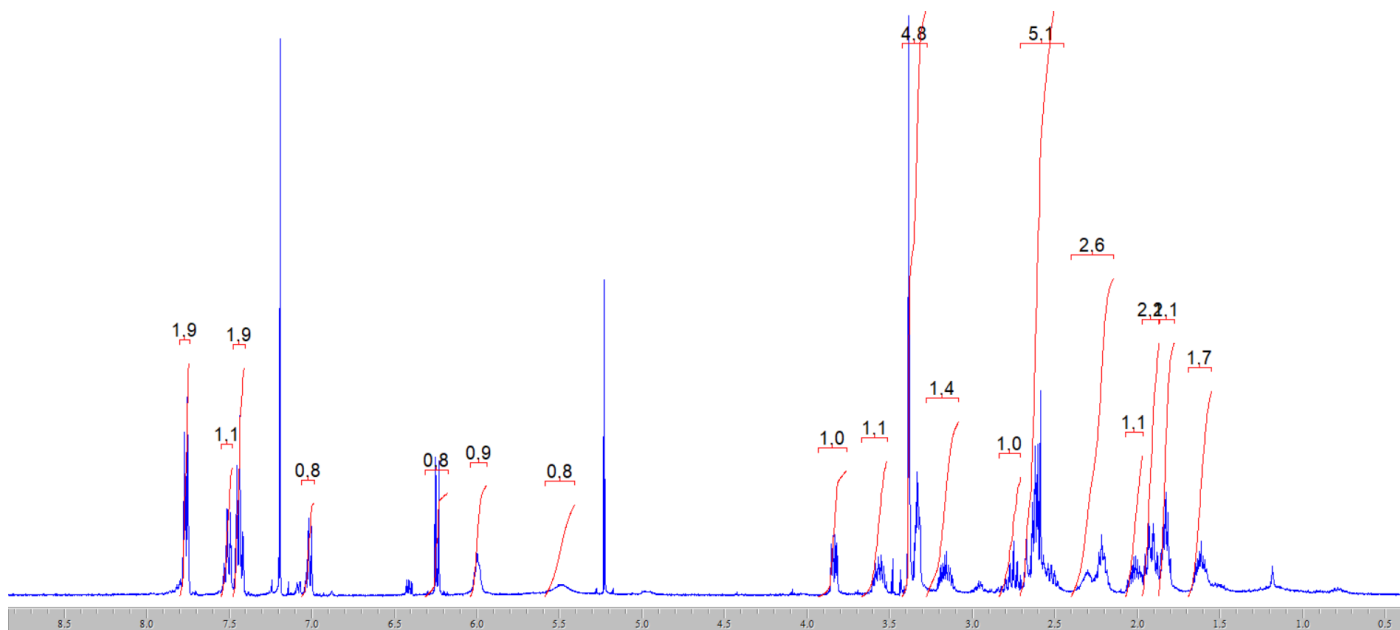
F1 - Processing parameters
SI 1024
MC2 QF
SF 100.6127690 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0



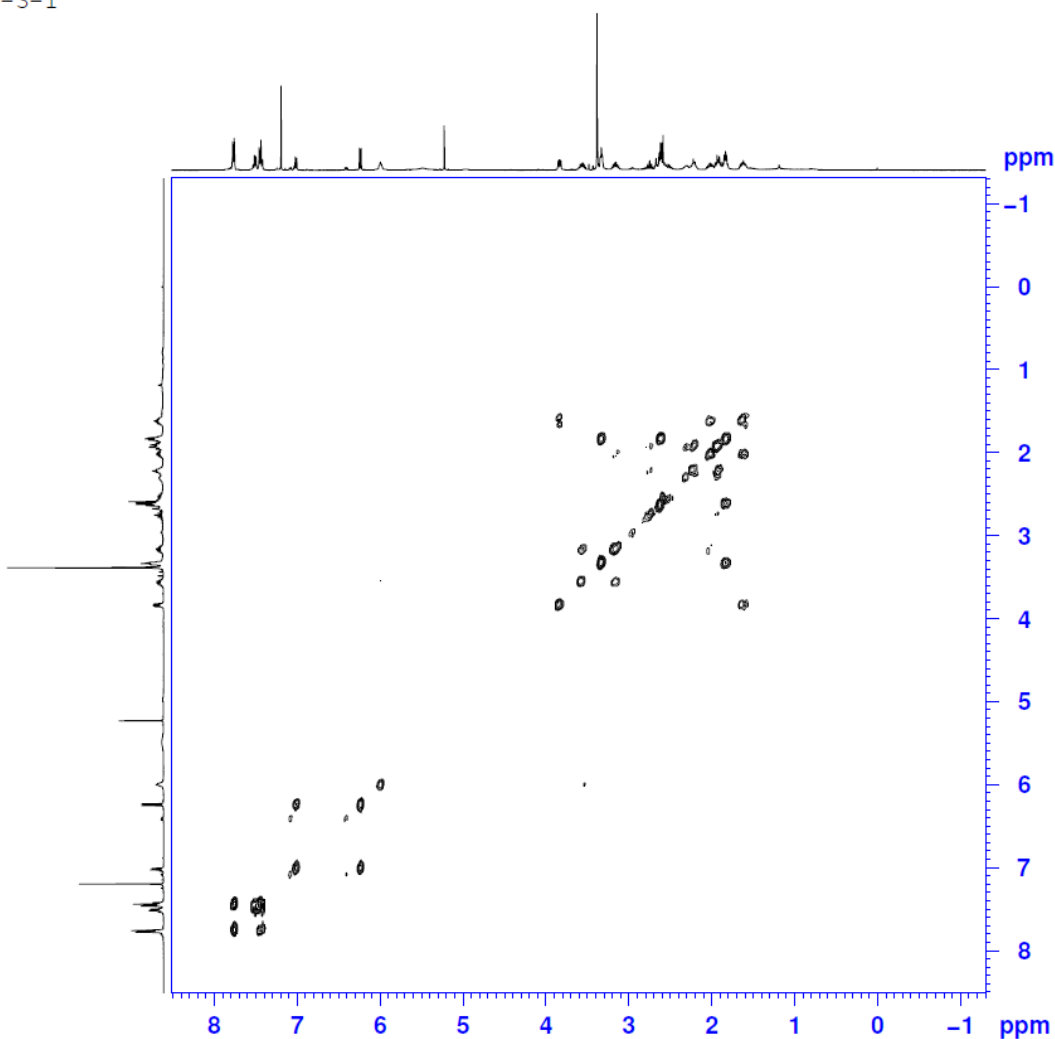
Methyl (S)-2-(phenylsulfonamido)-4-((1*S**,3*R**)-3-((5,6,7,8-tetrahydro-1,8-naphthyridin-2-



yl)methyl)cyclobutane-1-carboxamido)butanoate [Compound 21]



act9-3-1



Current Data Parameters
NAME act9-3-1
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120925
Time 22.30
INSTRUM dpx400
PROBHD 5 mm QNP 1H/13
PULPROG cosygpmfqr
ID 2048
SOLVENT CDCl3
NS 4
DS 8
SWH 3930.818 Hz
FIDRES 1.919345 Hz
AQ 0.2605556 sec
RG 7298.2
DW 127.200 usec
DE 6.00 usec
TE 298.2 K
D0 0.00000300 sec
D1 1.93159699 sec
d13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00025440 sec

----- CHANNEL f1 -----
NUC1 1H
P1 10.00 usec
PL1 -1.50 dB
SFO1 400.1314768 MHz

----- GRADIENT CHANNEL -----
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 16.00 %
GPZ2 12.00 %
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
ND0 1
ID 128
SFO1 400.1315 MHz
FIDRES 30.709513 Hz
SW 9.824 ppm
FMODE QF

F2 - Processing parameters
SI 1024
SF 400.1300356 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.1300356 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

aet9-3-1



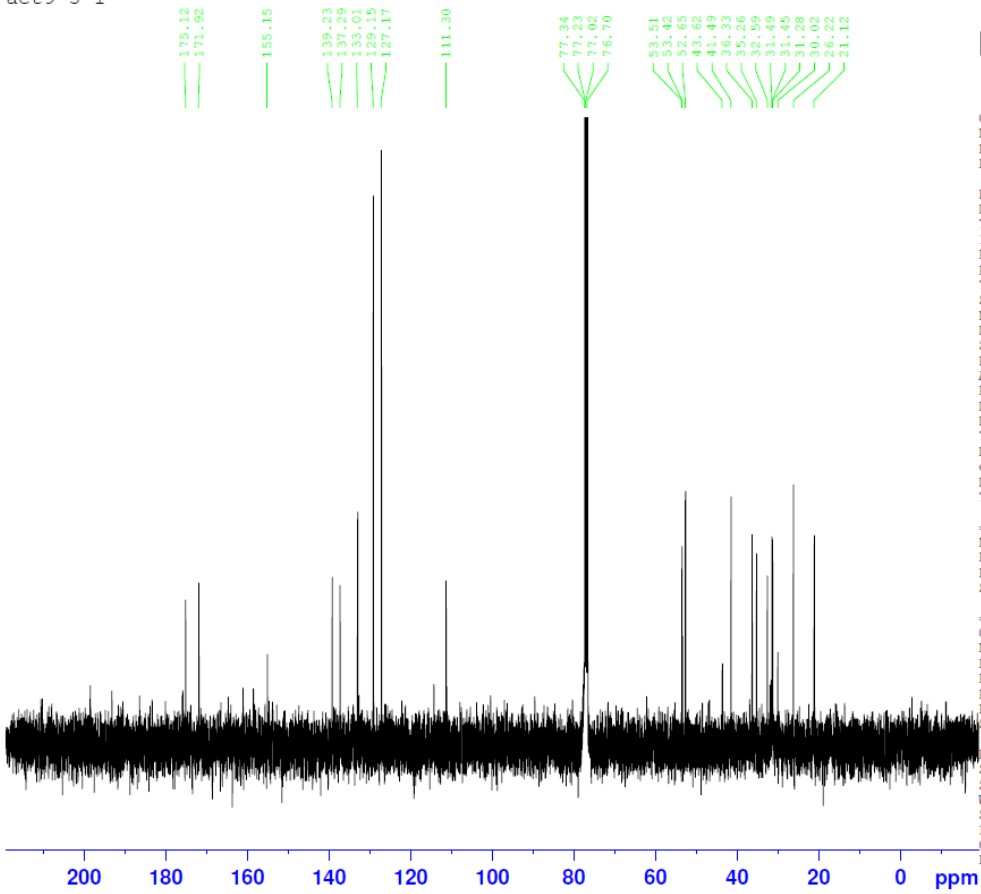
Current Data Parameters
NAME aet9-3-1
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120925
Time 21.59
INSTRUM DPX400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 912.3
DW 20.850 usec
DE 6.00 usec
TE 298.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 -2.60 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.50 dB
PL12 17.50 dB
PL13 17.50 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



aet9-3-1



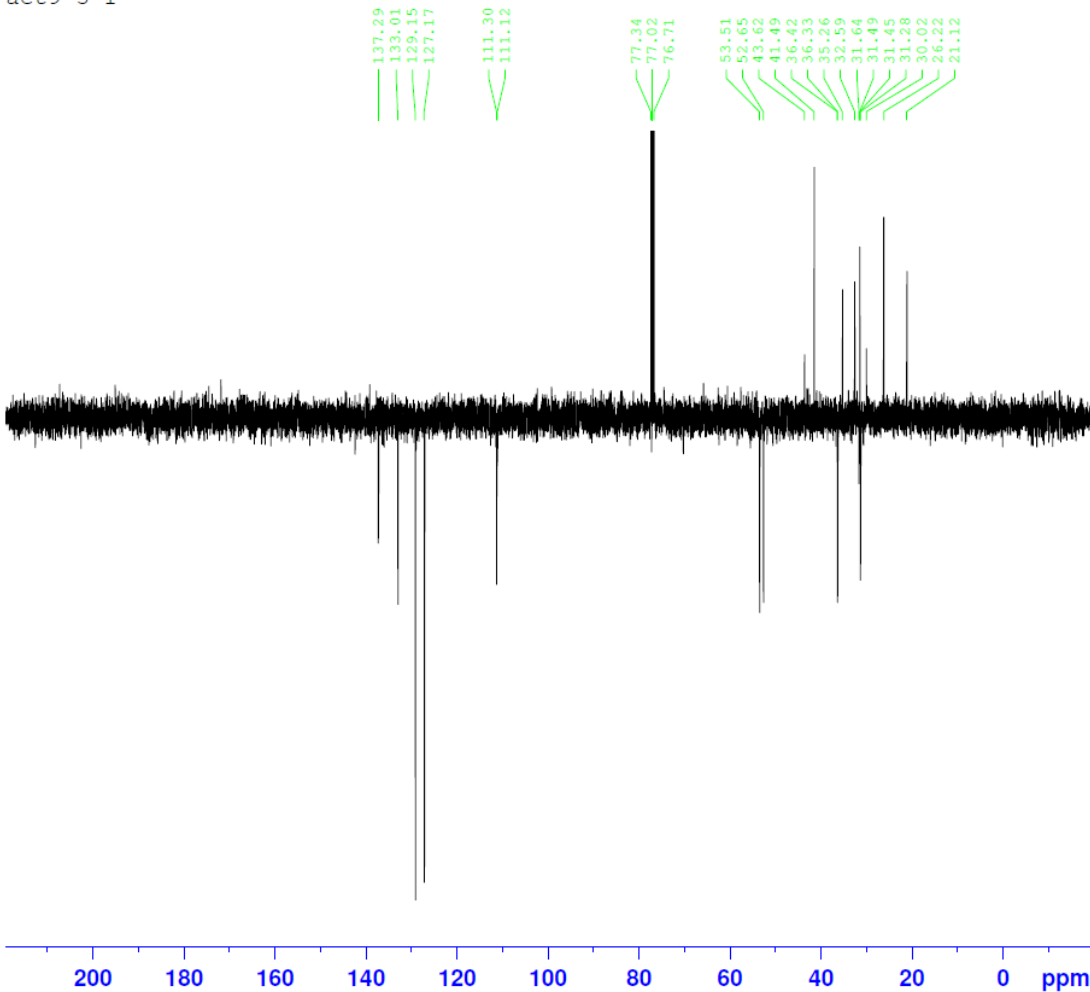
Current Data Parameters
NAME aet9-3-1
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120925
Time 22.29
INSTRUM DPX400
PROBHD 5 mm QNP 1H/13
PULPROG deptq_135
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 16384
DW 20.850 usec
DE 6.00 usec
TE 298.2 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
D11 0.03000000 sec
DELTA 0.00001082 sec

===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
P2 17.00 usec
PL1 -2.60 dB
SFO1 100.6228300 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 10.00 usec
P4 20.00 usec
PCPD2 80.00 usec
PL2 -1.50 dB
PL12 17.50 dB
SFO2 400.1316000 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





Current Data Parameters
NAME act9-3-1
EXPNO 14
PROCNO 1

P2 - Acquisition Parameters
Date_ 20120925
Time 22.50
INSTRUM QNP140
PROBHD 5 mm QNP 1H/13
PULPROG hmqcpgpgf
TD 1024
SOLVENT CDCl3
NS 4
DS 16
SWH 3930.818 Hz
FIDRES 3.838689 Hz
AQ 0.1303028 sec
RG 7288.2
DW 127.200 usec
DE 6.00 usec
TE 298.2 K
CNST2 145.000000
d0 0.0000300 sec
d1 1.4969798 sec
d2 0.00344828 sec
d12 0.00002000 sec
d13 0.00000400 sec
d16 0.00020000 sec
DELTA1 0.00222428 sec
IND 0.00003000 sec

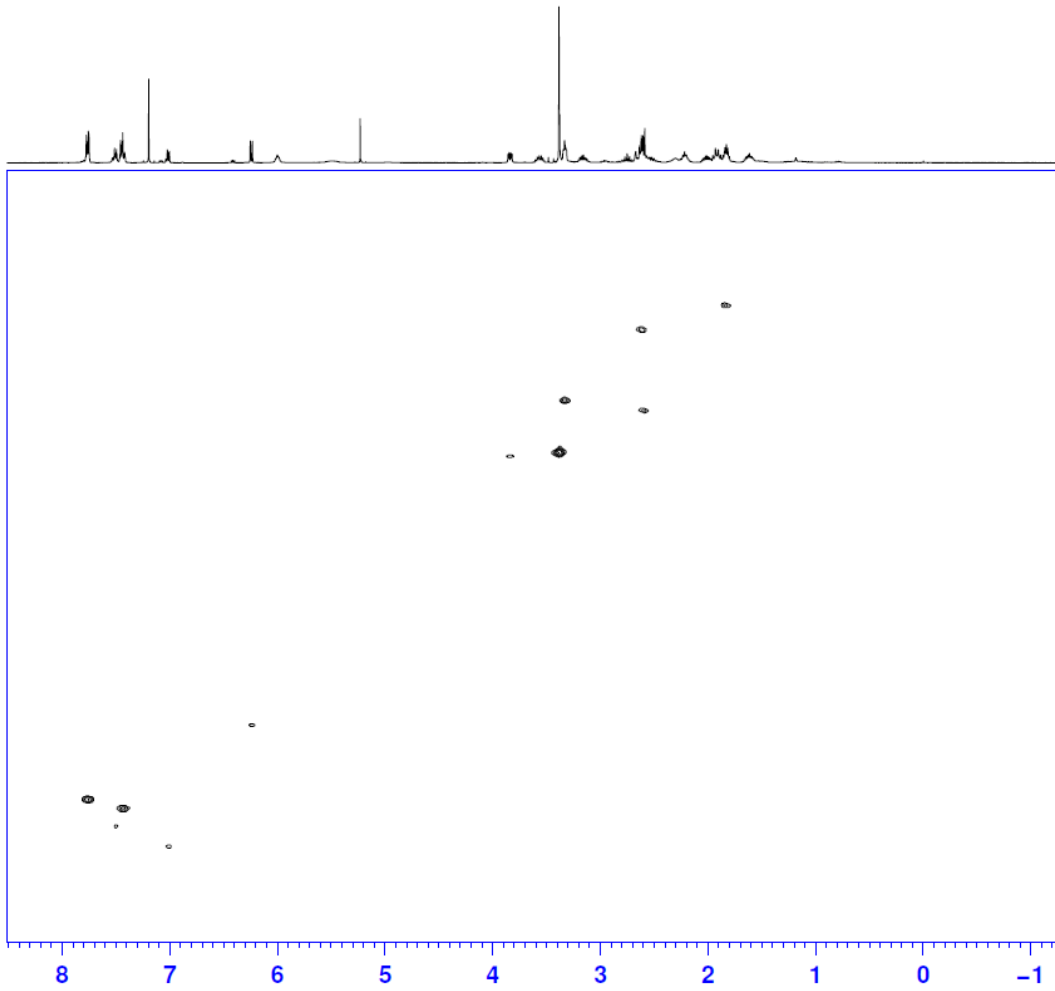
==== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
p2 20.00 usec
PL1 -1.50 dB
SFO1 400.1314728 MHz
==== CHANNEL f2 =====
CPDPRG2 garp
NUC2 13C
P3 8.00 usec
PCPD2 74.00 usec
PL2 -3.00 dB
PL12 18.00 dB
SFO2 100.6203140 MHz

==== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

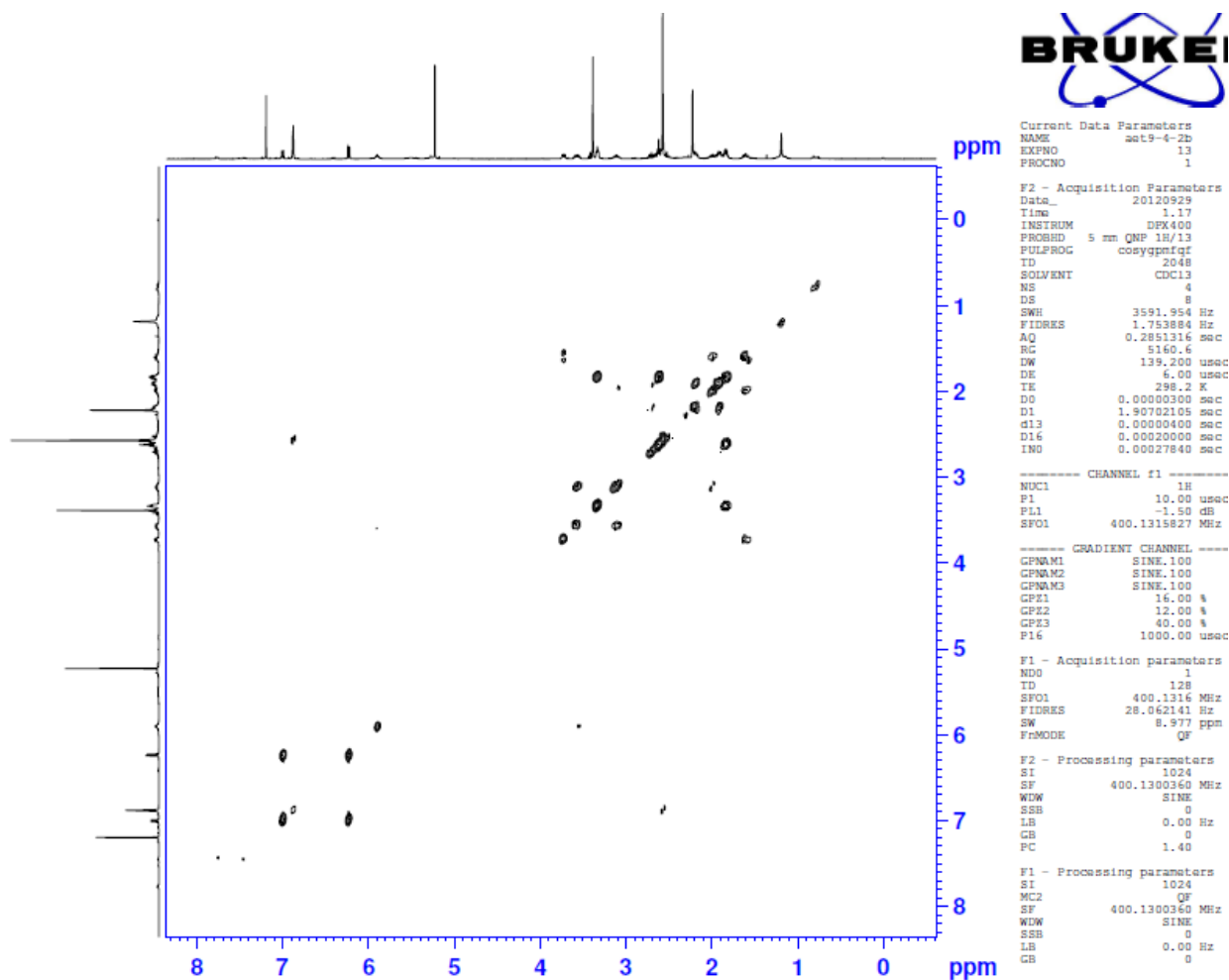
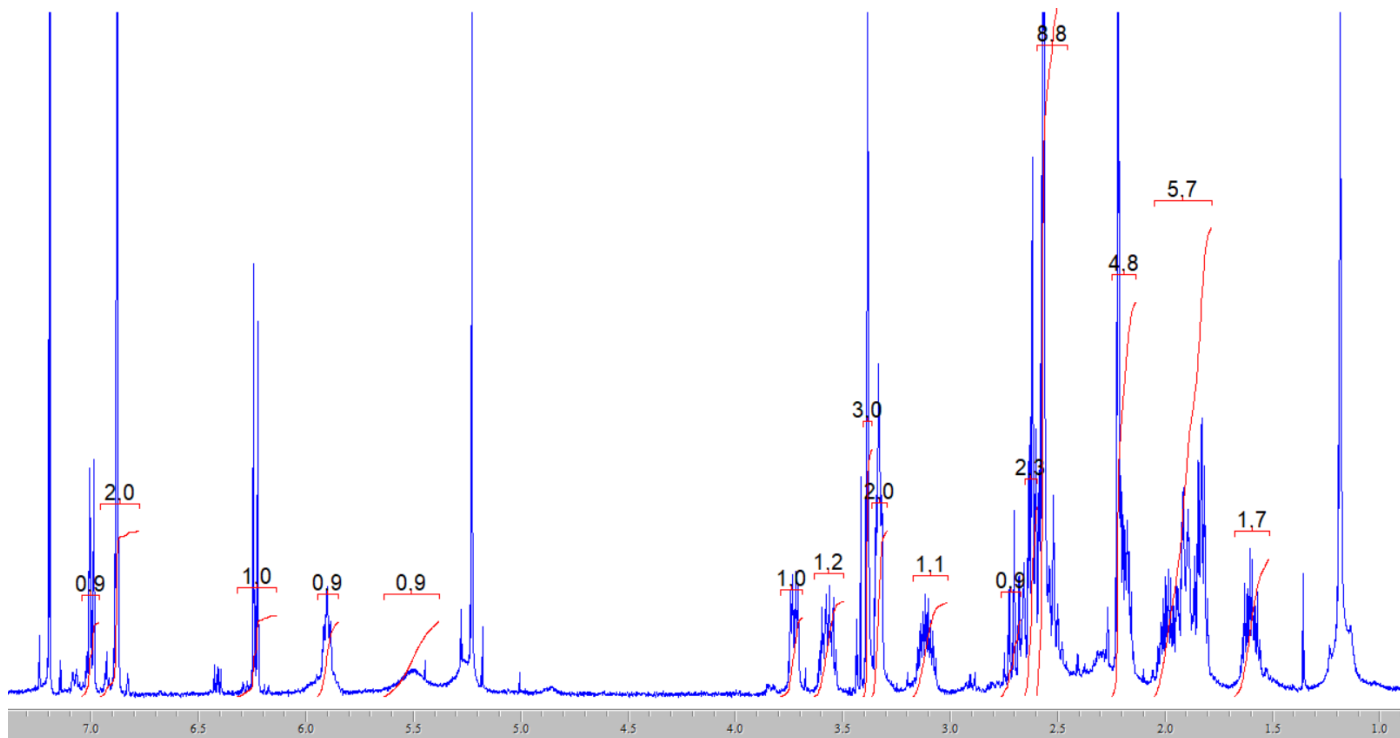
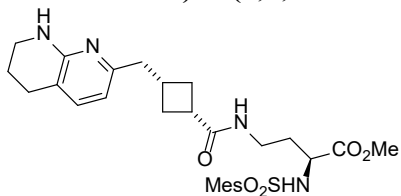
F1 - Acquisition parameters
ND0 2
TD 128
SFO1 100.6203 MHz
FIDRES 130.208328 Hz
SW 155.639 ppm
FMODE QF

P2 - Processing parameters
SI 1024
SF 400.1300356 MHz
WFW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 100.6127690 MHz
WFW QSINE
SSB 2
LB 0.00 Hz
GB 0



Methyl (*S*)-4-((1*S,3*R**)-3-((5,6,7,8-tetrahydro-1,8-naphthyridin-2-yl) methyl)cyclobutane-1-carboxamido)-2-(2,4,6-trimethylphenylsulfonamido)butanoate [Compound 22]**



Current Data Parameters
NAME act9-4-2b
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Data_ 20120929
Time 1.17
INSTRUM DPK400
PROBHD 5 mm QNP 1H/13
PULPROG cosygprfgr
TD 2048
SOLVENT CDCl3
NS 4
DS 8
SWH 3591.954 Hz
FIDRES 1.753884 Hz
AQ 0.2851316 sec
RG 5140.6
DW 139.200 usec
DE 6.00 usec
TE 298.2 K
D0 0.00000300 sec
D1 1.90702105 sec
d13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00027840 sec

----- CHANNEL f1 -----
NUC1 1H
P1 10.00 usec
PL1 -1.50 dB
SFO1 400.1315827 MHz

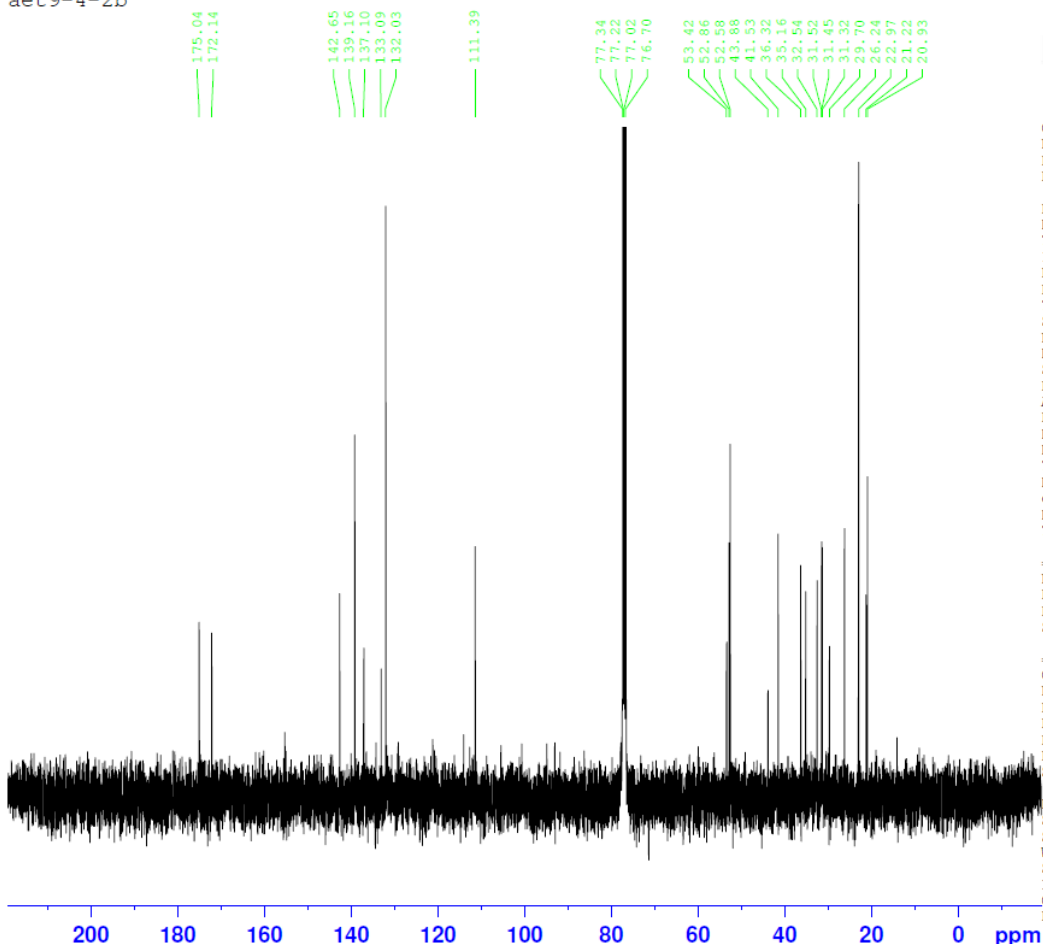
----- GRADIENT CHANNEL -----
GPMAM1 SINE.100
GPMAM2 SINE.100
GPMAM3 SINE.100
GPE1 16.00 %
GPE2 12.00 %
GPE3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
ND0 1
TD 128
SFO1 400.1316 MHz
FIDRES 28.062141 Hz
SW 8.977 ppm
FMODE QF

F2 - Processing parameters
SI 1024
SF 400.1300360 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.1300360 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

aet9-4-2b



Current Data Parameters
 NAME aet9-4-2b
 EXPNO 11
 PROCNO 1

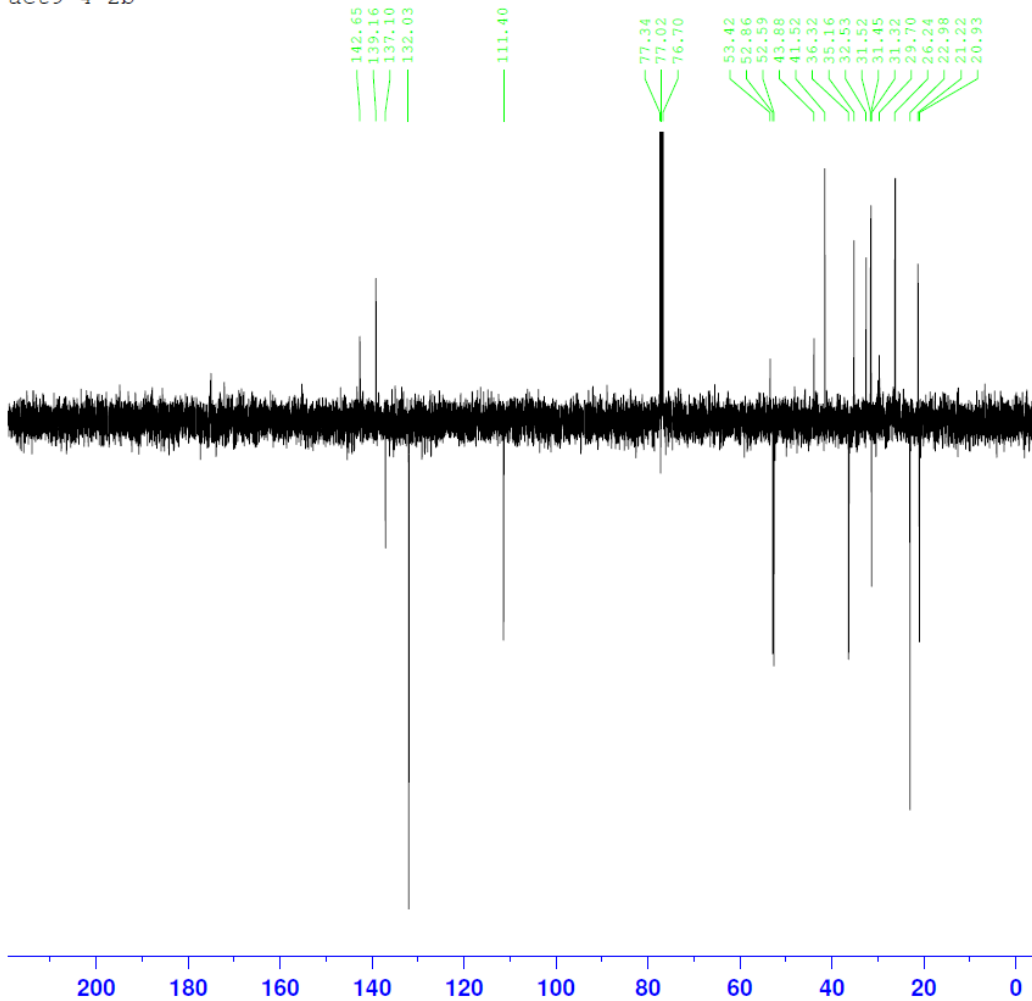
F2 - Acquisition Parameters
 Date_ 20120929
 Time 0.46
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 1149.4
 DW 20.850 usec
 DE 6.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 PL1 -2.60 dB
 SFO1 100.6228298 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 PL13 17.50 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

aet9-4-2b



Current Data Parameters
 NAME aet9-4-2b
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120929
 Time 1.16
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG deptg_135
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 18390.4
 DW 20.850 usec
 DE 6.00 usec
 TE 298.2 K
 CNST2 145.0000000
 D1 2.00000000 sec
 d2 0.00344828 sec
 D11 0.03000000 sec
 DELTA 0.00001082 sec

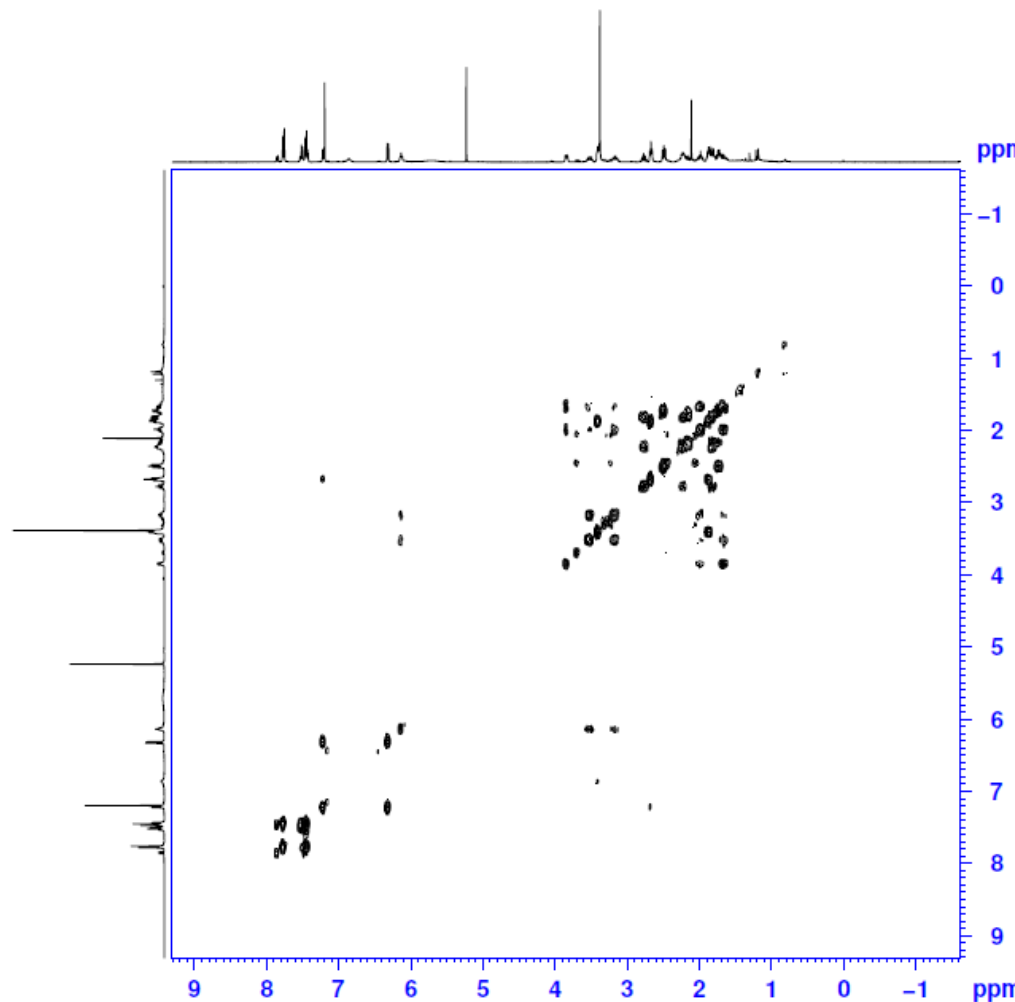
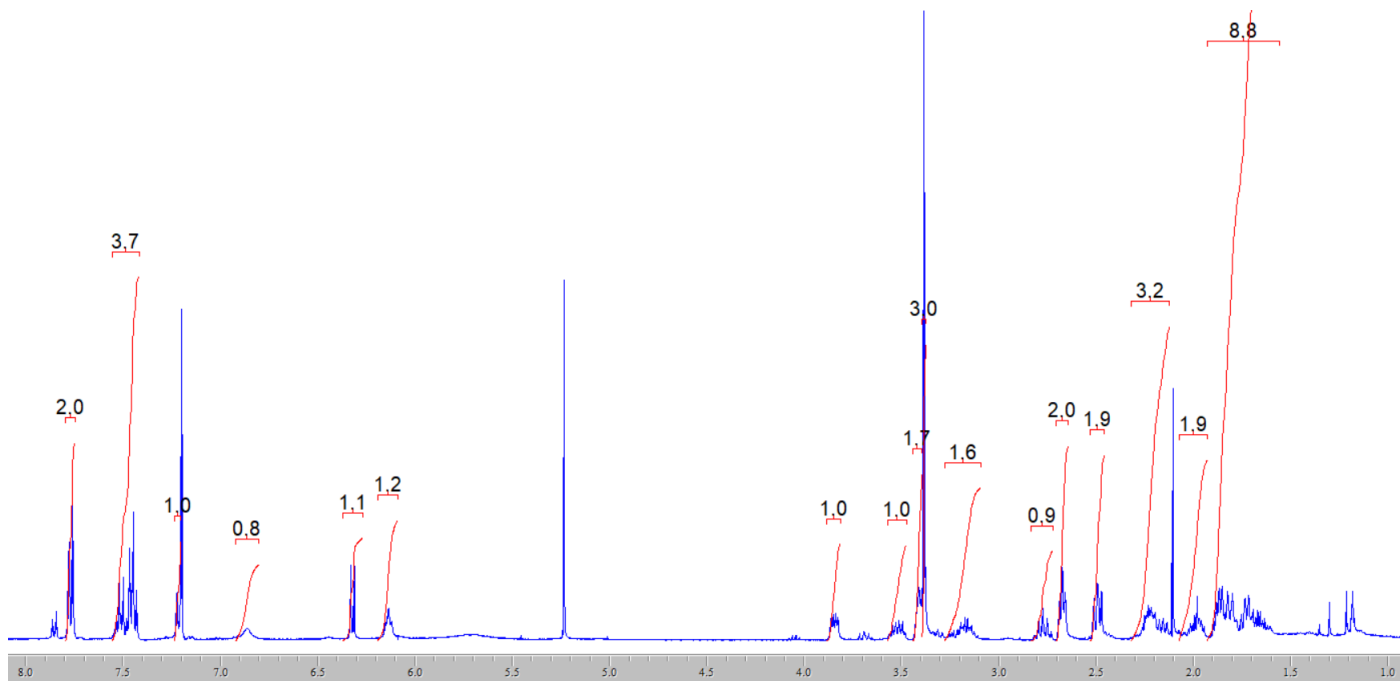
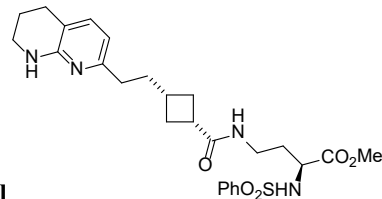
==== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 P2 17.00 usec
 PL1 -2.60 dB
 SFO1 100.6228300 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 SFO2 400.1316000 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Methyl (S)-2-(phenylsulfonamido)-4-((1*r**,3*R**)-3-(2-(5,6,7,8-tetrahydro-1,8-naphthyridin-2-

yl)ethyl)cyclobutane-1-carboxamido)butanoate [Compound 23]



Current Data Parameters
 NAME set9-41
 EXPNO 13
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130228
 Time 19.48
 INSTRUM DFX400
 PROBED 5 mm QNP 1H/13
 PULPROG cosygprf2f
 ID 2048
 SOLVENT CDCl3
 NS 4
 DS 8
 SWH 4370.629 Hz
 FIDRES 2.134096 Hz
 AQ 0.2343412 sec
 RG 3251
 LW 114.400 usec
 DE 6.00 usec
 TE 292.2 K
 DO 0.00000300 sec
 D1 1.95822096 sec
 d13 0.00000400 sec
 D16 0.00020000 sec
 INO 0.00022880 sec

----- CHANNEL f1 -----
 NUC1 1H
 P1 10.00 usec
 PL1 -1.50 dB
 SFO1 400.1315728 MHz

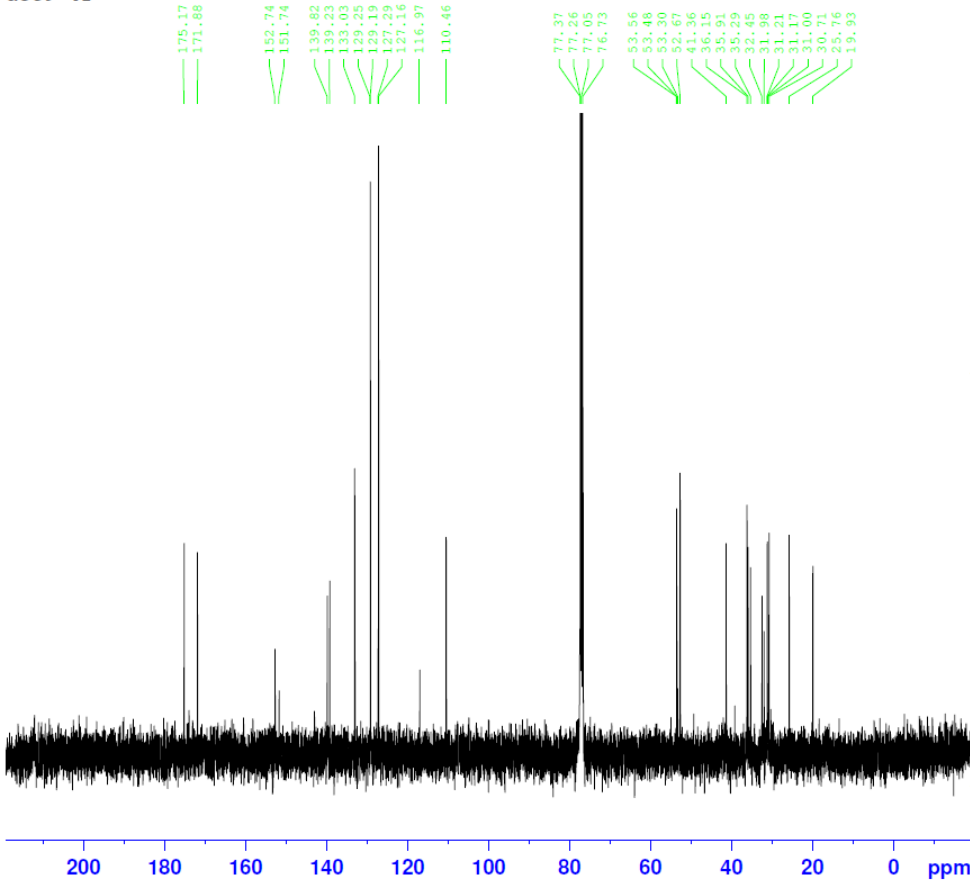
----- GRADIENT CHANNEL -----
 GPNAM1 SINK.100
 GPNAM2 SINK.100
 GPNAM3 SINK.100
 GPE1 16.00 %
 GPE2 12.00 %
 GPE3 40.00 %
 P16 1000.00 usec

F1 - Acquisition parameters
 NDO 1
 ID 128
 SFO1 400.1316 MHz
 FIDRES 34.145542 Hz
 SW 10.923 ppm
 FMODE QF

F2 - Processing parameters
 SI 1024
 SF 400.1300339 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 400.1300339 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

aet9-41



Current Data Parameters
 NAME aet9-41
 EXPNO 11
 PROCNO 1

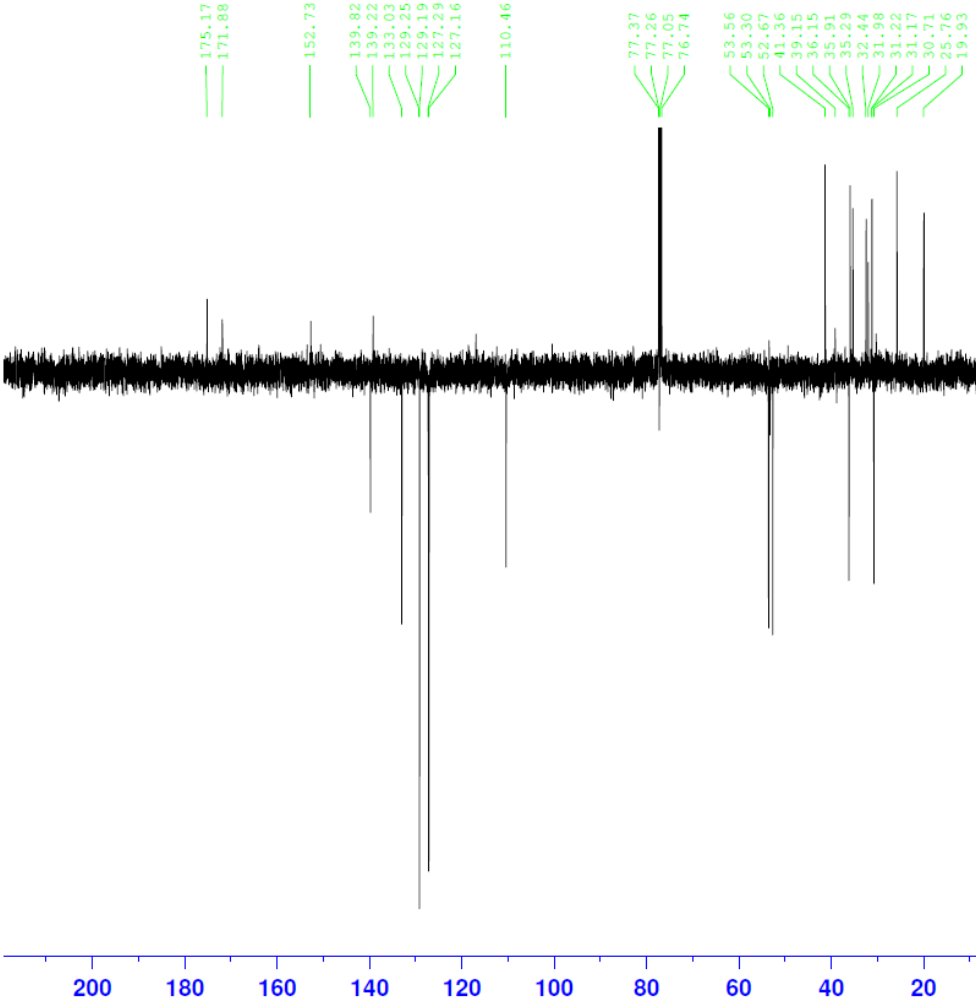
F2 - Acquisition Parameters
 Date_ 20130228
 Time 19.17
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 1024
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 1290.2
 DW 20.850 usec
 DE 6.00 usec
 TE 293.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.899999999 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 PL1 -2.60 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 PL13 17.50 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

aet9-41



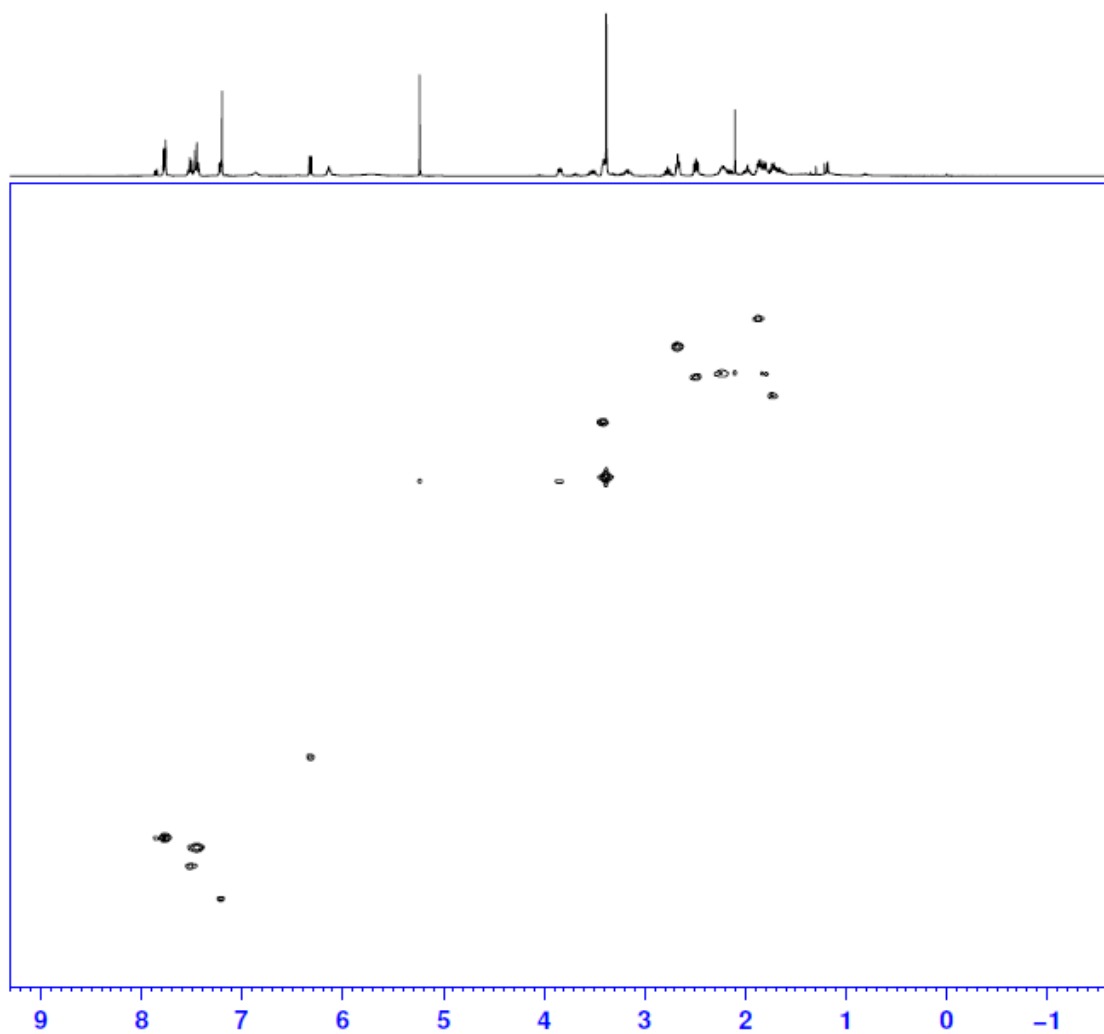
Current Data Parameters
 NAME aet9-41
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130228
 Time 19.47
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG deptq_135
 TD 65536
 SOLVENT CDC13
 NS 512
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 18390.4
 DW 20.850 usec
 DE 6.00 usec
 TE 292.2 K
 CNST2 145.0000000
 D1 2.00000000 sec
 d2 0.00344828 sec
 D11 0.03000000 sec
 DELTA 0.00001082 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 P2 17.00 usec
 PL1 -2.60 dB
 SFO1 100.6228300 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 SFO2 400.1316000 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
 NAME: test3-41
 EXPNO: 14
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20130228
 Time: 20.08
 INSTRUM: spect400
 PULPROG: zgpg30
 F2 - Acquisition Parameters
 S mm QNP 1H/13
 PULPROG: hmqcpgpgf
 TD: 1024
 SOLVENT: cdcl3
 NS: 4
 DS: 16
 SWH: 4370.639 Hz
 FIDRES: 4.258193 Hz
 AQ: 0.1171956 sec
 RG: 26008
 SW: 114.400 usec
 DE: 6.00 usec
 TE: 292.2 K
 CHGT2: 145.000000
 d0: 0.00000300 sec
 d1: 1.51023996 sec
 d2: 0.00344828 sec
 d12: 0.00002000 sec
 d13: 0.00000400 sec
 D16: 0.00020000 sec
 DELTA1: 0.0022428 sec
 IN0: 0.00003000 sec

----- CHANNEL f1 -----
 NUC1: 1H
 P1: 10.00 usec
 P2: 20.00 usec
 PL1: -1.50 dB
 SFO1: 400.1315728 MHz

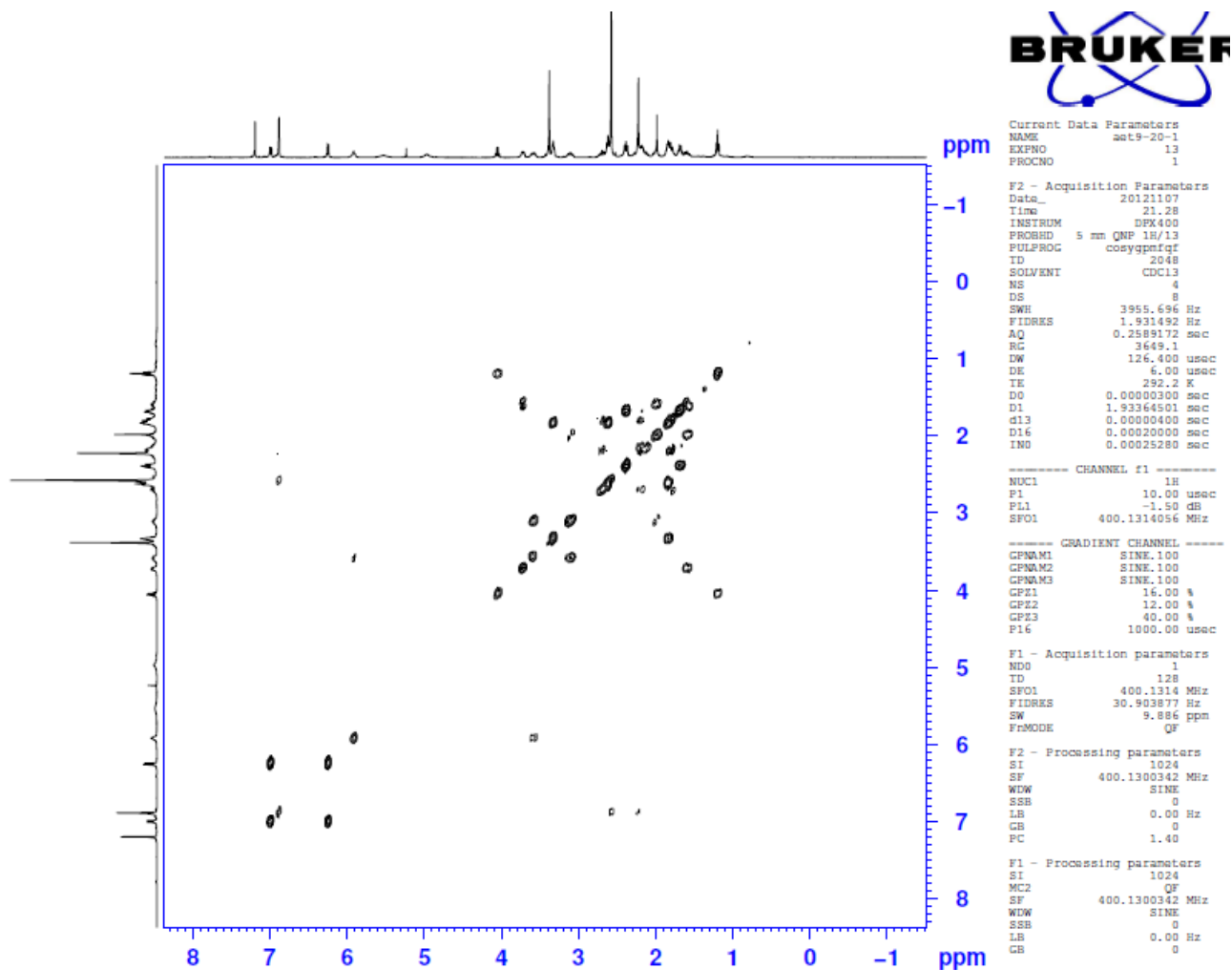
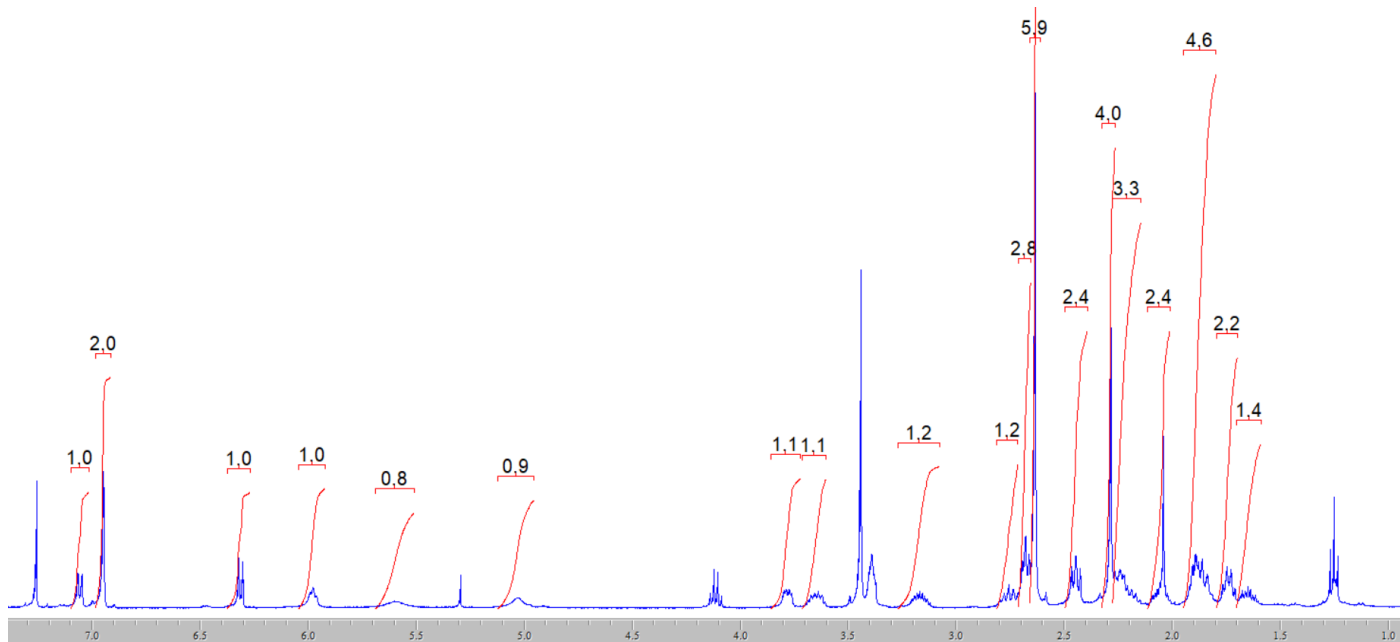
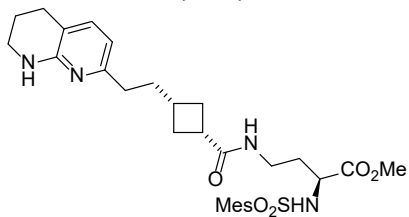
----- CHANNEL f2 -----
 CPDPRG2: gqzgpg
 NUC2: 13C
 P3: 8.00 usec
 PCDP2: 74.00 usec
 PL2: -3.00 dB
 PL12: 18.00 dB
 SFO2: 100.6203140 MHz

----- GRADIENT CHANNEL -----
 GPMAM1: SINE.100
 GPMAM2: SINE.100
 GPMAM3: SINE.100
 GPR1: 50.00 %
 GPR2: 30.00 %
 GPR3: 40.10 %
 P1G: 1000.00 usec

F1 - Acquisition parameters
 NO0: 2
 TD: 128
 SFO1: 100.6203 MHz
 FIDRES: 130.208328 Hz
 SW: 165.639 ppm
 F2 - Processing parameters
 SI: 1024
 SF: 400.1300339 MHz
 MDM: QSINE
 SSB: 2 Hz
 LB: 0 Hz
 GB: 0
 FC: 1.40

F1 - Processing parameters
 SI: 1024
 MC2: QF
 SF: 100.6127690 MHz
 MDM: QSINE
 SSB: 2 Hz
 LB: 0.00 Hz
 GB: 0

Methyl (S)-4-((1*r,3*R**)-3-(2-(5,6,7,8-tetrahydro-1,8-naphthyridin-2-yl)ethyl)cyclobutane-1-carboxamido)-2-(2,4,6-trimethylphenylsulfonamido)butanoate [Compound 24]**



BRUKER

Current Data Parameters
NAME set9-20-1
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121107
Time 21.28
INSTRUM DPX400
PROBHD 5 mm QNP 1H/13
PULPROG cosygpcfgf
ID 2048
SOLVENT CDCl3
NS 4
DS 8
SWH 3955.696 Hz
FIDRES 1.931492 Hz
AQ 0.2589172 sec
RG 3649.1
DW 126.400 usec
DE 6.00 usec
TE 292.2 K
D0 0.0000300 sec
d13 1.9364501 sec
d16 0.0000400 sec
IN0 0.00025280 sec

----- CHANNEL f1 -----
NUC1 13
P1 10.00 usec
PL1 -1.50 dB
SFO1 400.1314056 MHz

----- GRADIENT CHANNEL -----
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 16.00 %
GPZ2 12.00 %
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
ND0 1
ID 128
SFO1 400.1314 MHz
FIDRES 30.903877 Hz
SW 9.886 ppm
FMODE QF

F2 - Processing parameters
SI 1024
SF 400.1300342 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.1300342 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

aet9-20-1



```

Current Data Parameters
NAME          aet9-20-1
EXPNO         11
PROCNO        1

F2 - Acquisition Parameters
Date_         20121107
Time_         20.57
INSTRUM       DPX400
PROBHD        5 mm QNP 1H/13
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            1024
DS            4
SWH           23980.814 Hz
FIDRES        0.365918 Hz
AQ            1.3664756 sec
RG            512
DW            20.850 usec
DE            6.00 usec
TE            292.2 K
D1            2.0000000 sec
d11           0.0300000 sec
DELTA         1.89999998 sec
TDO           1

```

```

===== CHANNEL f1 =====
NUC1          13C
P1            8.50 usec
PL1           -2.60 dB
SFO1         100.6228298 MHz

```

```

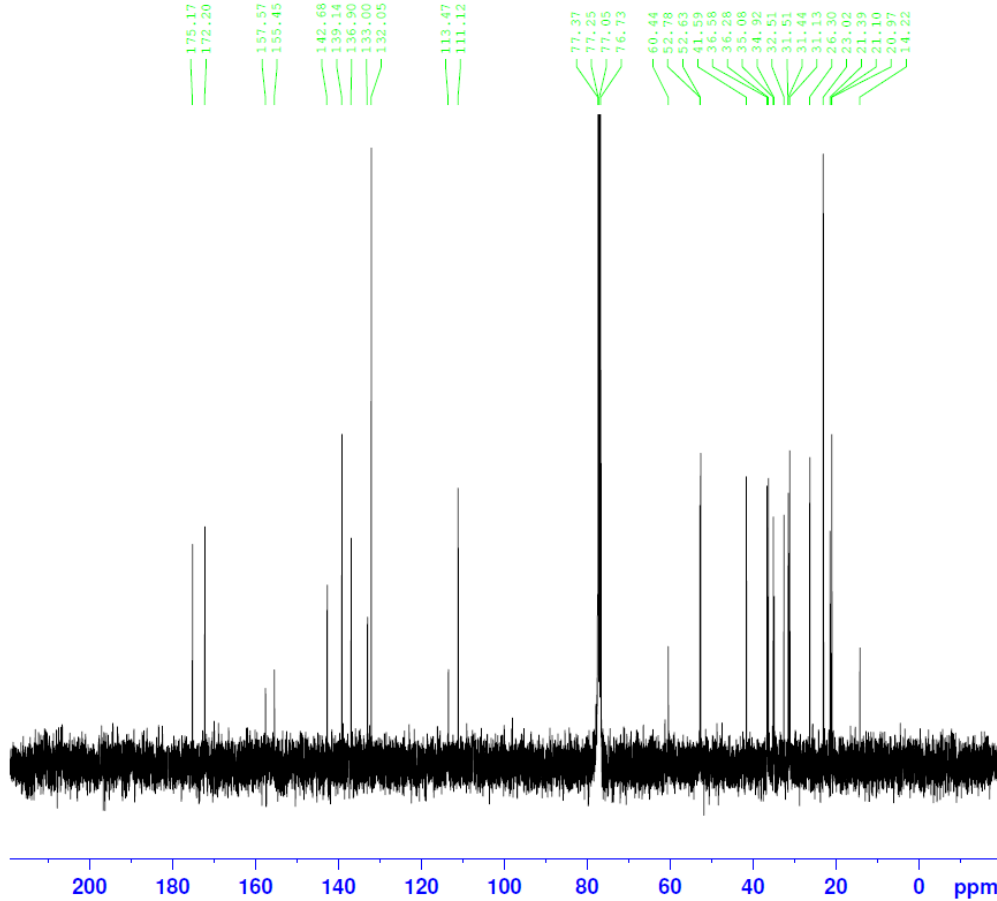
===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2          1H
PCPD2        80.00 usec
PL2           -1.50 dB
PL12         17.50 dB
PL13         17.50 dB
SFO2         400.1316005 MHz

```

```

F2 - Processing parameters
SI            32768
SF            100.6127690 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

```



```

Current Data Parameters
NAME          aet9-20-1
EXPNO         12
PROCNO        1

F2 - Acquisition Parameters
Date_         20121107
Time_         21.27
INSTRUM       DPX400
PROBHD        5 mm QNP 1H/13
PULPROG       deptq_135
TD            65536
SOLVENT       CDCl3
NS            512
DS            4
SWH           23980.814 Hz
FIDRES        0.365918 Hz
AQ            1.3664756 sec
RG            20642.5
DW            20.850 usec
DE            6.00 usec
TE            292.2 K
CNST2        145.0000000
D1            2.0000000 sec
d2            0.00344828 sec
D11           0.0300000 sec
DELTA         0.00001082 sec

```

```

===== CHANNEL f1 =====
NUC1          13C
P1            8.50 usec
P2            17.00 usec
PL1           -2.60 dB
SFO1         100.6228300 MHz

```

```

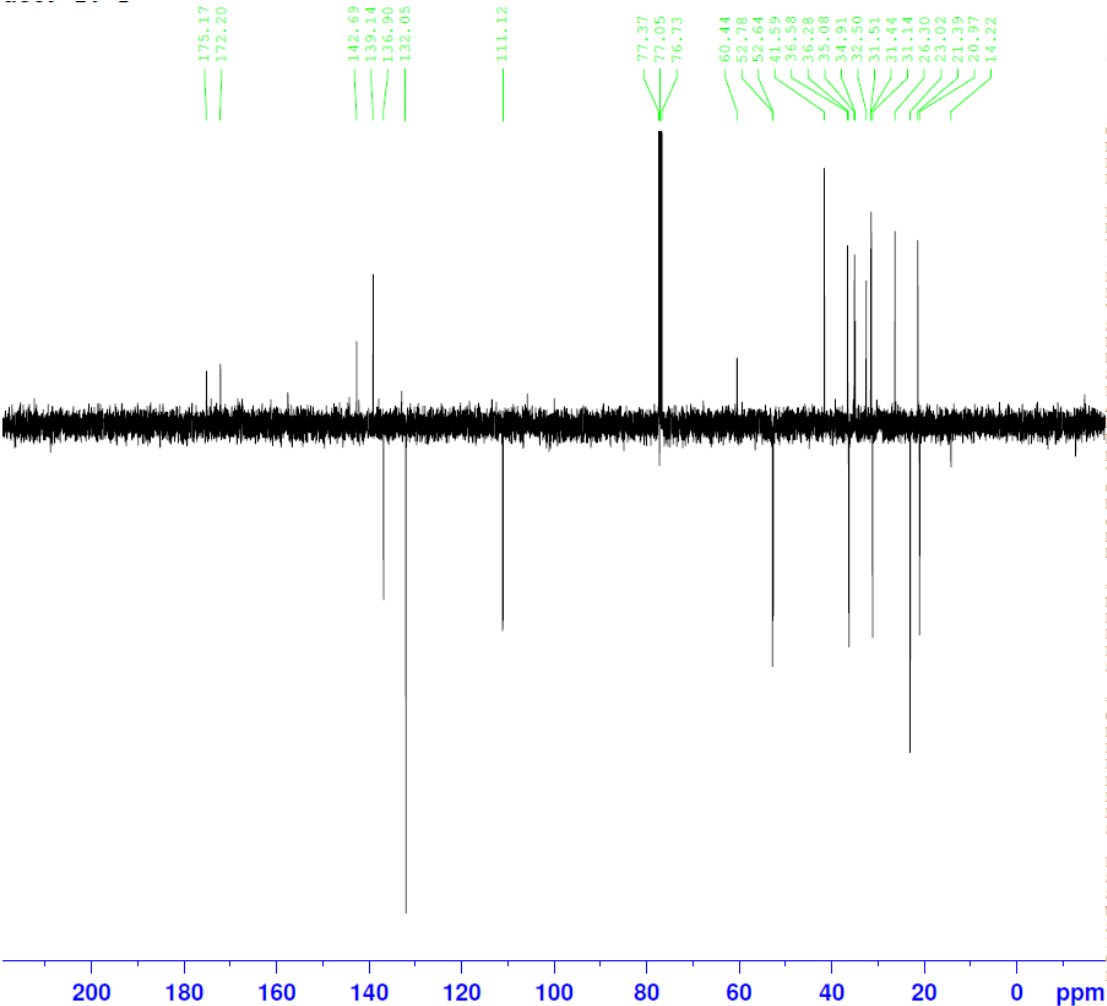
===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2          1H
P3            10.00 usec
P4            20.00 usec
PCPD2        80.00 usec
PL2           -1.50 dB
PL12         17.50 dB
SFO2         400.1316000 MHz

```

```

F2 - Processing parameters
SI            32768
SF            100.6127690 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

```



Current Data Parameters
 NAME: act9-20-1
 EXPNO: 15
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20121107
 Time: 21:50
 INSTRUM: spect
 PROBRD: 5 mm QNP 1H/13
 PULPROG: zgpg30
 TD: 1024
 SOLVENT: CDCl3
 NS: 4
 DS: 16
 SWH: 3955.694 Hz
 FIDRES: 3.862985 Hz
 AQ: 0.1294834 sec
 RG: 650
 DW: 126.400 usec
 DE: 6.00 usec
 TE: 292.2 K
 CNST2: 145.0000000
 d0: 0.0000300 sec
 d1: 1.49795198 sec
 d2: 0.00344828 sec
 d12: 0.00002000 sec
 d13: 0.00004000 sec
 d16: 0.00200000 sec
 DELTA1: 0.0022428 sec
 IN0: 0.00003000 sec

----- CHANNEL F1 -----
 NUC1: 1H
 P1: 10.00 usec
 PL: 20.00 usec
 PL1: -1.50 dB
 SFO1: 400.1314054 MHz

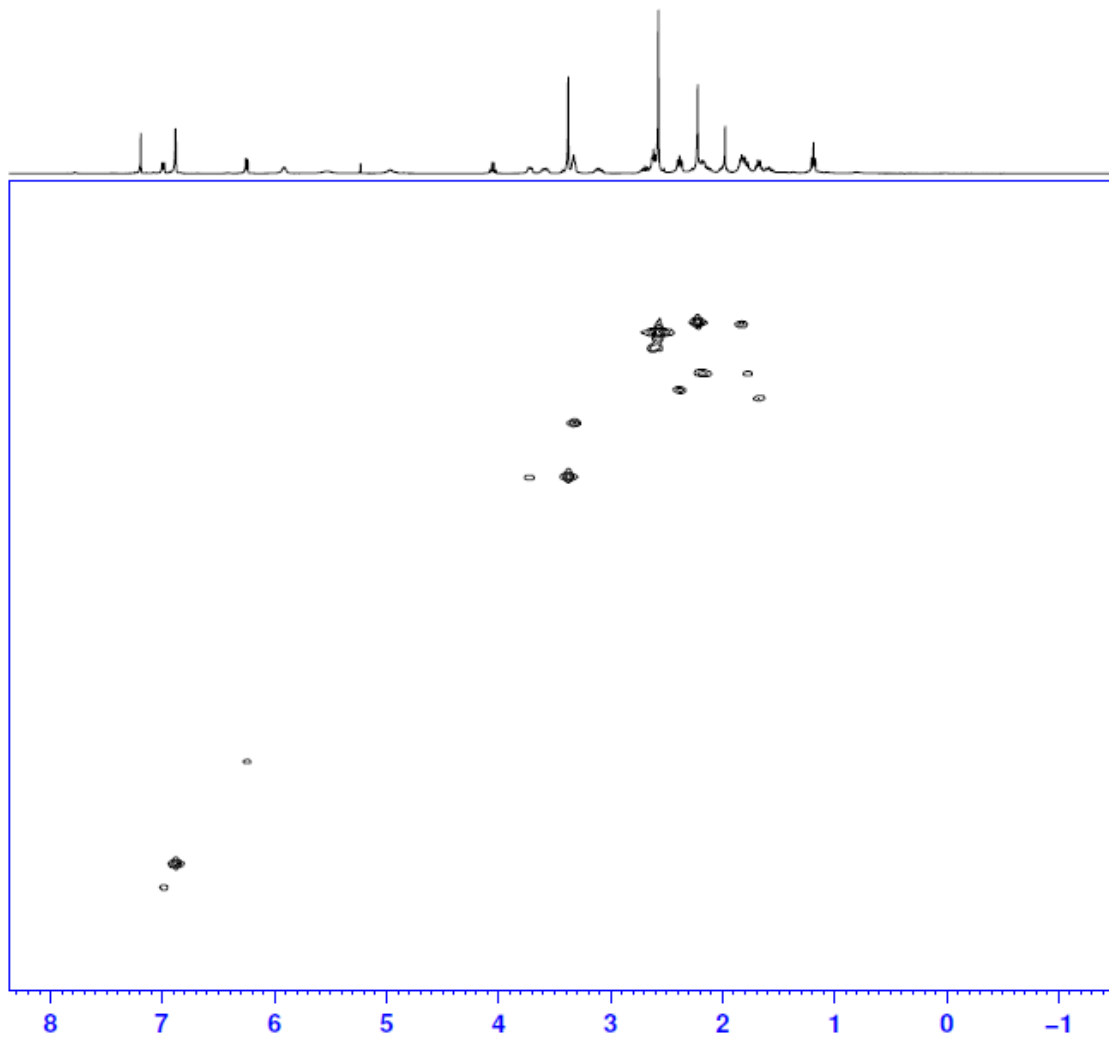
----- CHANNEL F2 -----
 CPDPRG2: gcp
 NUC2: 13C
 P3: 8.00 usec
 PCPD2: 74.00 usec
 PL2: -3.00 dB
 PL12: 18.00 dB
 SFO2: 100.6203140 MHz

----- GRADIENT CHANNEL -----
 GPMAX1: SINE.100
 GPMAX2: SINE.100
 GPMAX3: SINE.100
 GPR1: 50.00 %
 GPR2: 30.00 %
 GPR3: 40.10 %
 PLG: 1000.00 usec

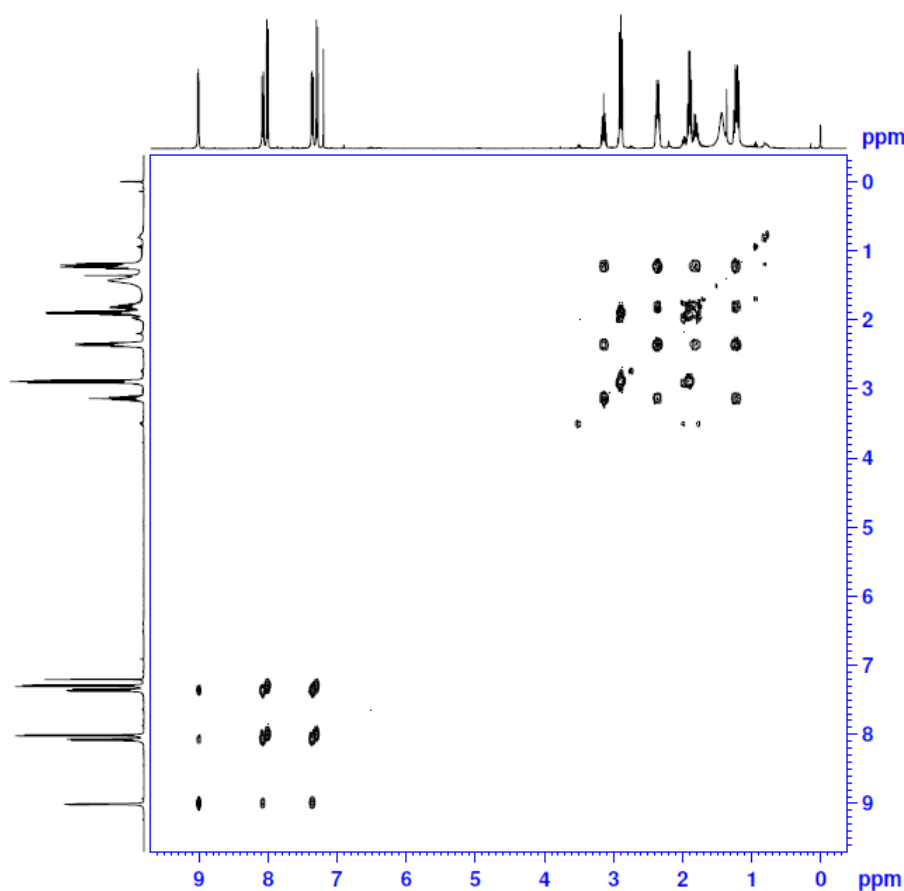
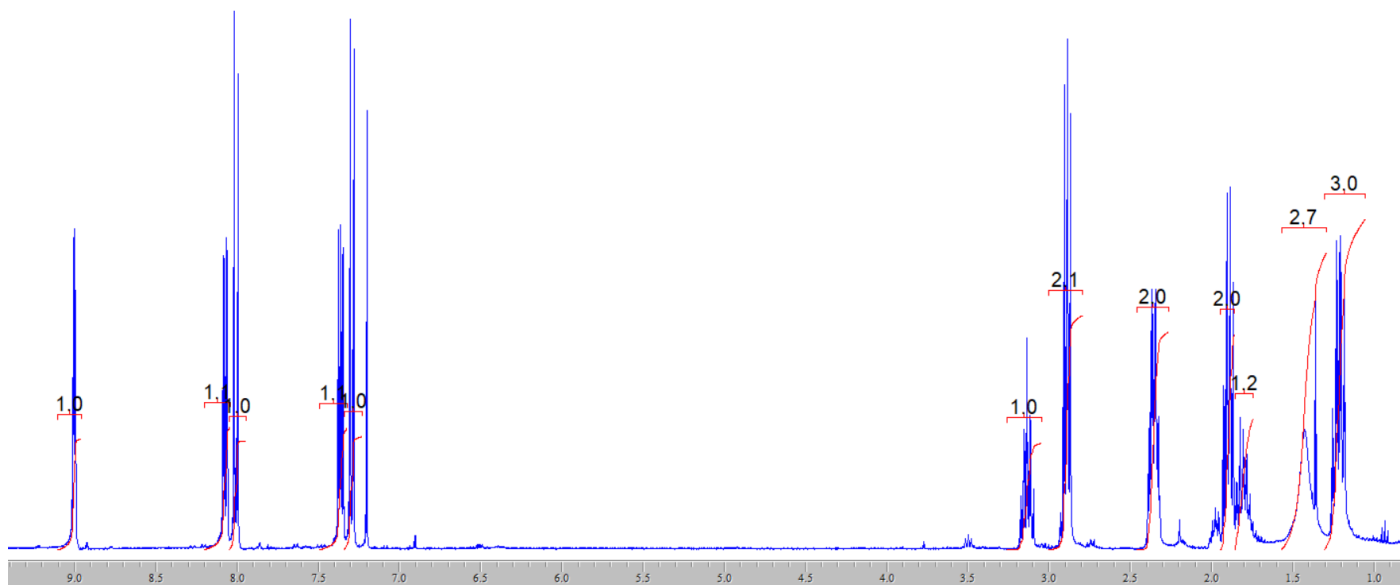
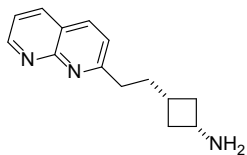
F1 - Acquisition parameters
 MD0: 2
 TD: 128
 SFO1: 100.6203 MHz
 FIDRES: 130.208328 Hz
 SW: 165.639 ppm
 FWHM: 0

F2 - Processing parameters
 SI: 1024
 SF: 400.1300342 MHz
 WDM: QCSINE
 SSB: 2
 LB: 0.00 Hz
 GB: 0
 PC: 1.40

F1 - Processing parameters
 SI: 1024
 MC2: 0
 SF: 100.6127690 MHz
 WDM: QCSINE
 SSB: 2
 LB: 0.00 Hz
 GB: 0



(1*r, 3*s**)-3-(2-(1,8-Naphthyridin-2-yl)ethyl)cyclobutan-1-amine [Compound 25]:**



Current Data Parameters
NAME set7-16
EXFNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111027
Time 0.09
INSTRUM DFX400
PROBHD 5 mm QNP 1H/13
PULPROG cosygpgmf
TD 2048
SOLVENT CDCl3
NS 4
DS 8
SWH 4032.258 Hz
FIDRES 1.968876 Hz
AQ 0.2340020 sec
RG 3251
DW 124.000 usec
DE 6.00 usec
TE 298.2 K
DD 0.00000300 sec
D1 1.93774104 sec
d13 0.00000400 sec
D16 0.00020000 sec
IND 0.00024800 sec

----- CHANNEL f1 -----
NUC1 1H
P1 10.00 usec
PL1 -1.50 dB
SFO1 400.1318955 MHz

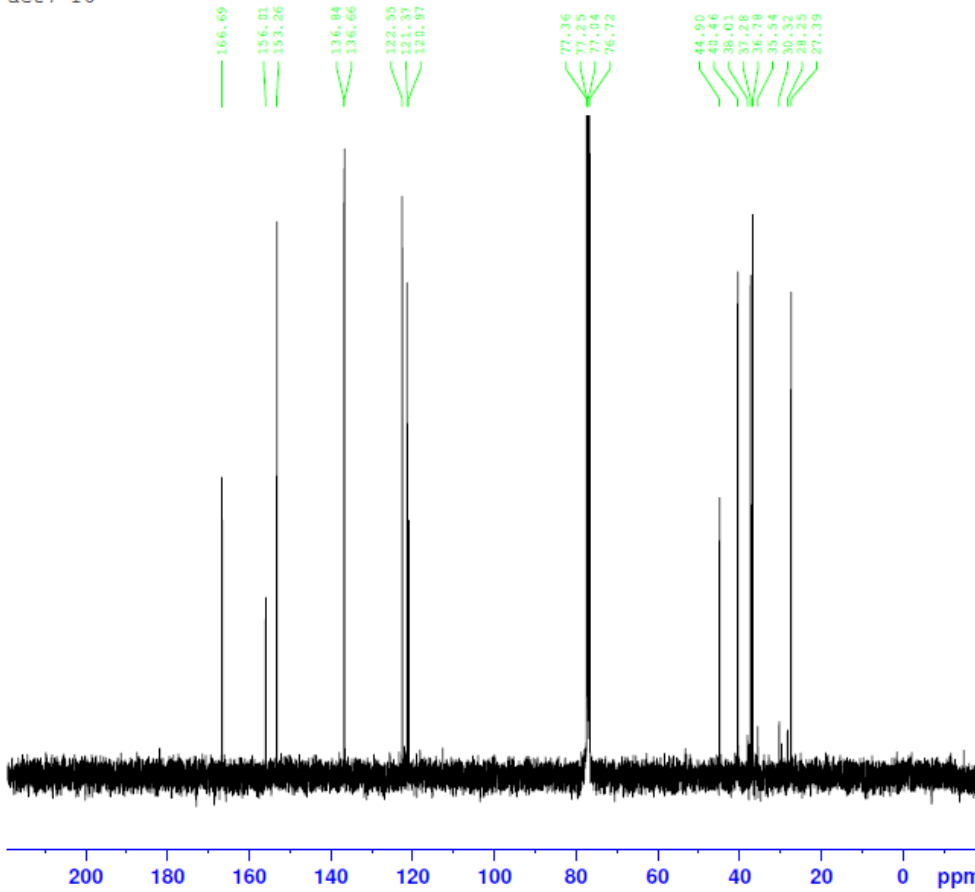
----- GRADIENT CHANNEL -----
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
CPZ1 16.00 %
CPZ2 12.00 %
CPE3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
ND0 1
TD 128
SFO1 400.1319 MHz
FIDRES 31.500016 Hz
SW 10.077 ppm
FrMODE QF

F2 - Processing parameters
SI 1024
SF 400.1300320 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.1300320 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

aet7-16



Current Data Parameters
NAME aet7-16
EXPNO 11
PROCNO 1

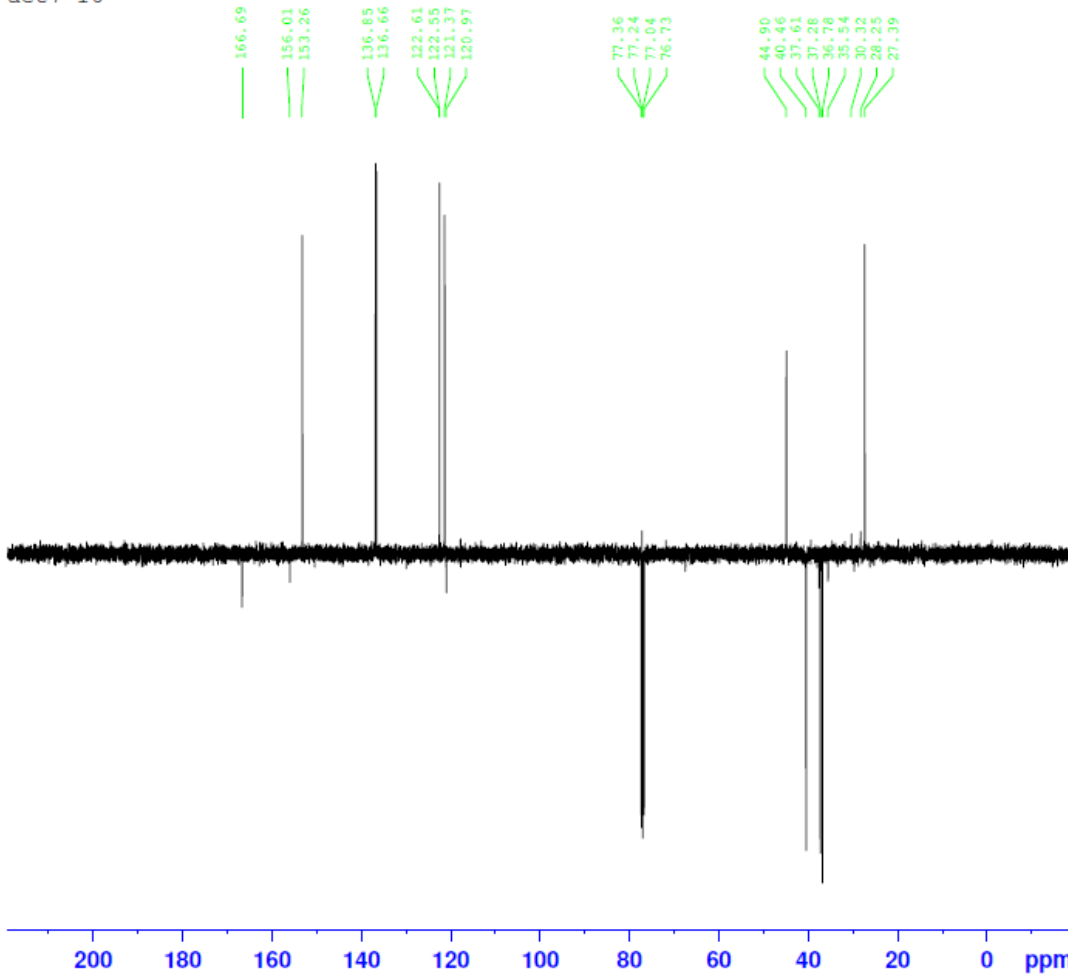
F2 - Acquisition Parameters
Date_ 20111026
Time 23.38
INSTRUM DPX400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 1824.6
DW 20.850 usec
DE 6.00 usec
TE 298.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

----- CHANNEL f1 -----
NUC1 13C
P1 8.00 usec
PL1 -2.60 dB
SFO1 100.6228298 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.50 dB
PL12 17.50 dB
PL13 17.50 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

aet7-16



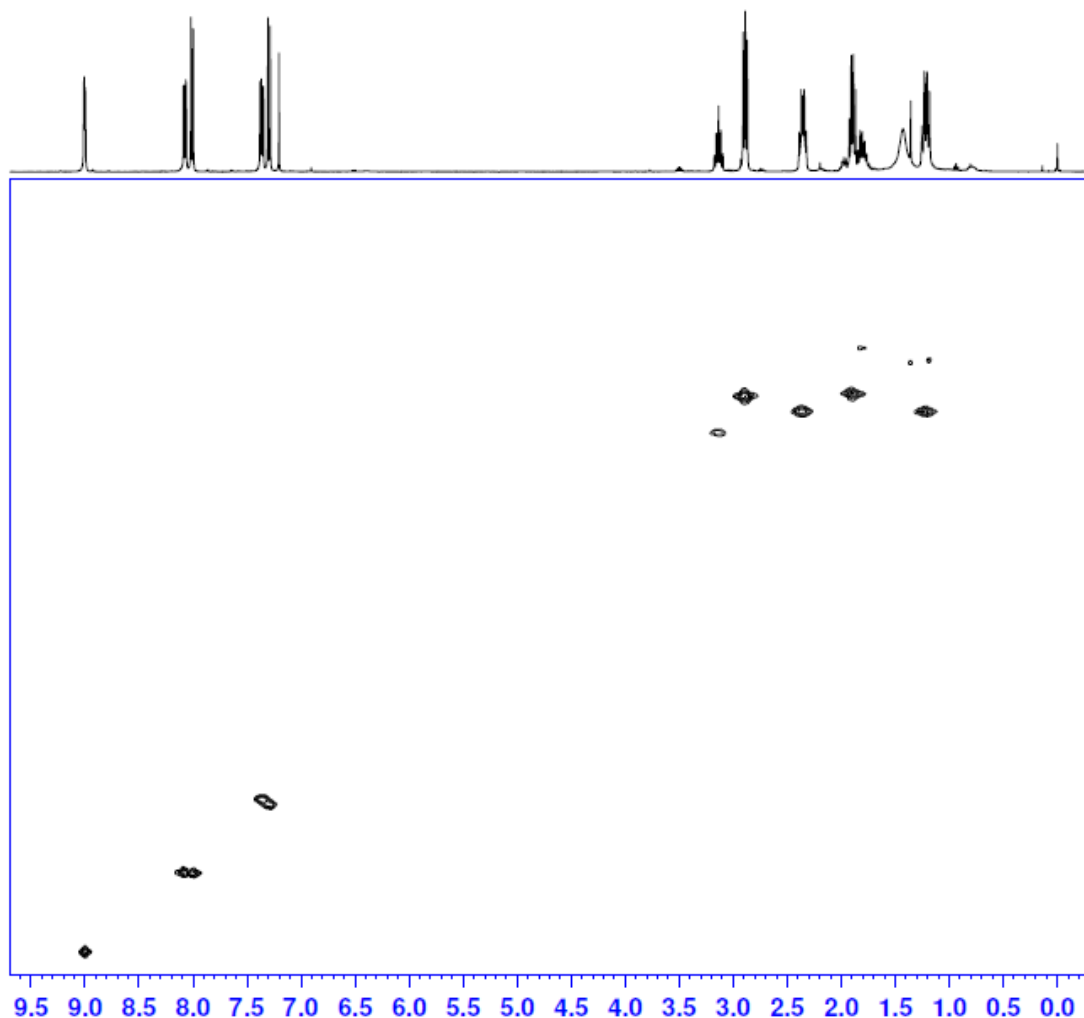
Current Data Parameters
NAME aet7-16
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111027
Time 0.08
INSTRUM DPX400
PROBHD 5 mm QNP 1H/13
PULPROG deptq_135
TD 65536
SOLVENT CDC13
NS 512
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 16384
DW 20.850 usec
DE 6.00 usec
TE 298.2 K
CNST2 145.00000000
D1 2.00000000 sec
d2 0.00344828 sec
D11 0.03000000 sec
DELTA 0.00001019 sec

----- CHANNEL f1 -----
NUC1 13C
P1 8.00 usec
P2 16.00 usec
PL1 -2.60 dB
SFO1 100.6228300 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
P3 10.00 usec
P4 20.00 usec
PCPD2 80.00 usec
PL2 -1.50 dB
PL12 17.50 dB
SFO2 400.1316000 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
 NAME act7-16
 EXPNO 14
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20111027
 Time 0.29
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG hmcqcpzg
 TD 1024
 SOLVENT cdcl3
 NS 4
 DS 16
 SWH 4032.258 Hz
 FIDRES 3.937752 Hz
 AQ 0.1270260 sec
 RG 26008
 DW 124.000 usec
 DE 6.00 usec
 TE 298.2 K
 CNST2 145.0000000
 d0 0.00000300 sec
 d1 1.50000000 sec
 d2 0.00344828 sec
 d12 0.00002000 sec
 d13 0.00000400 sec
 d16 0.00020000 sec
 DELTA1 0.00222428 sec
 IN0 0.00003000 sec

CHANNEL F1
 NUC1 1H
 P1 10.00 usec
 P2 20.00 usec
 PL1 -1.50 dB
 SFO1 400.1318955 MHz

CHANNEL E2
 CPDPRG2 gaitp
 NUC2 13C
 P3 8.00 usec
 PCPD2 74.00 usec
 PL2 -3.00 dB
 PL12 18.00 dB
 SFO2 100.6203140 MHz

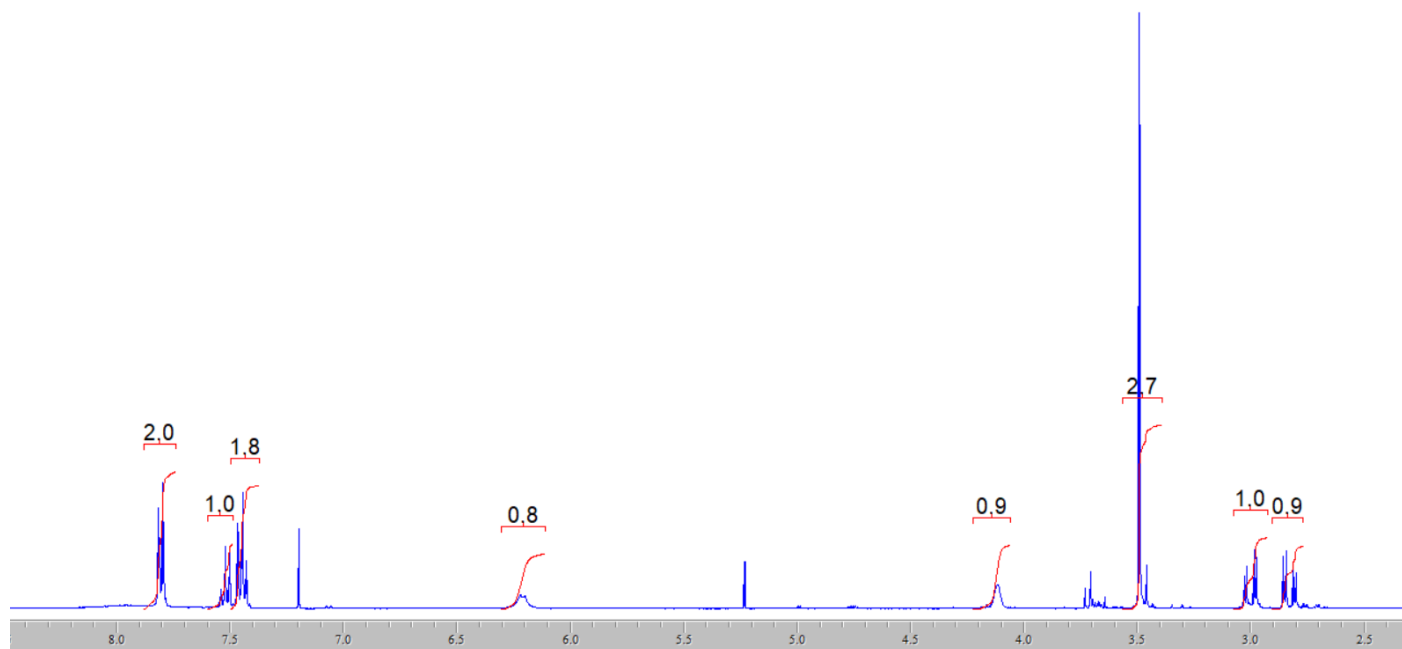
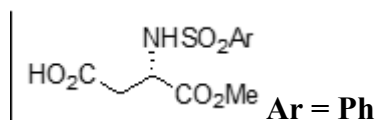
GRADIENT CHANNEL
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPNAM3 SINE.100
 GPE1 50.00 %
 GPE2 30.00 %
 GPE3 40.10 %
 F1C 1000.00 usec

F1 - Acquisition parameters
 MD0 2
 TD 128
 SFO1 100.6203 MHz
 FIDRES 130.208328 Hz
 SW 155.639 ppm
 F2MODE QF

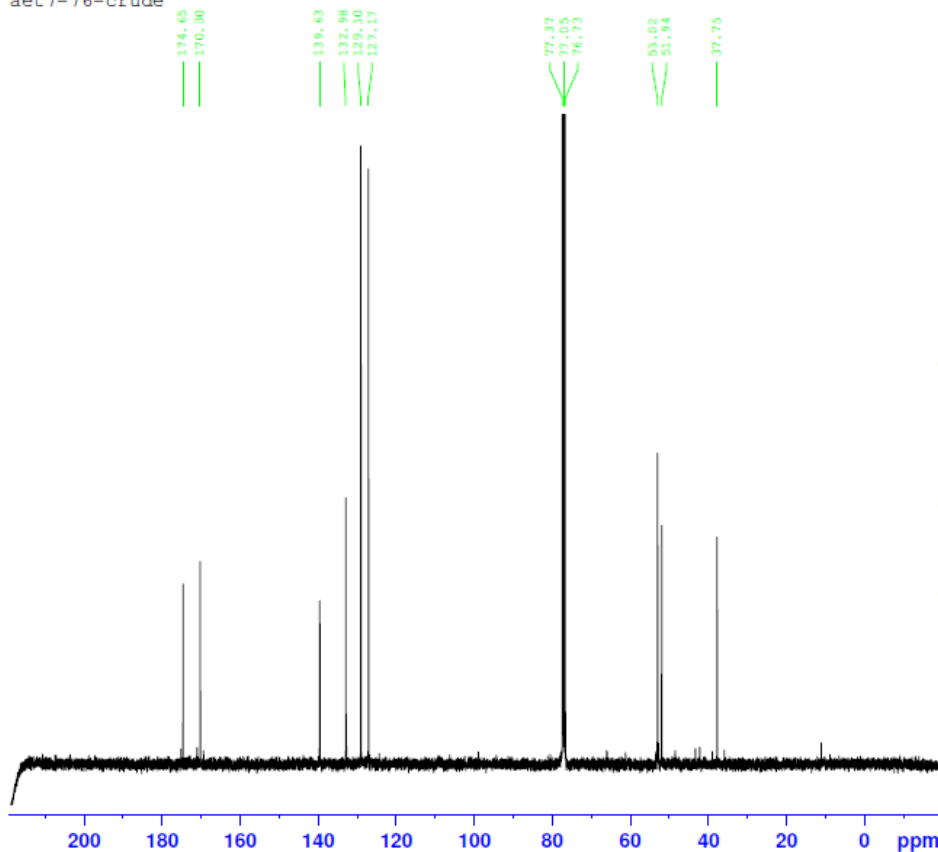
F2 - Processing parameters
 SI 1024
 SF 400.1300320 MHz
 WSW qSINE
 SSR 2
 LB 0.00 Hz
 GB 0
 FC 1.40

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 100.6127690 MHz
 WSW qSINE
 SSR 2
 LB 0.00 Hz
 GB 0

(S)-4-Methoxy-4-oxo-3-(phenylsulfonamido)butanoic acid [Compound 26]



aet7-76-crude



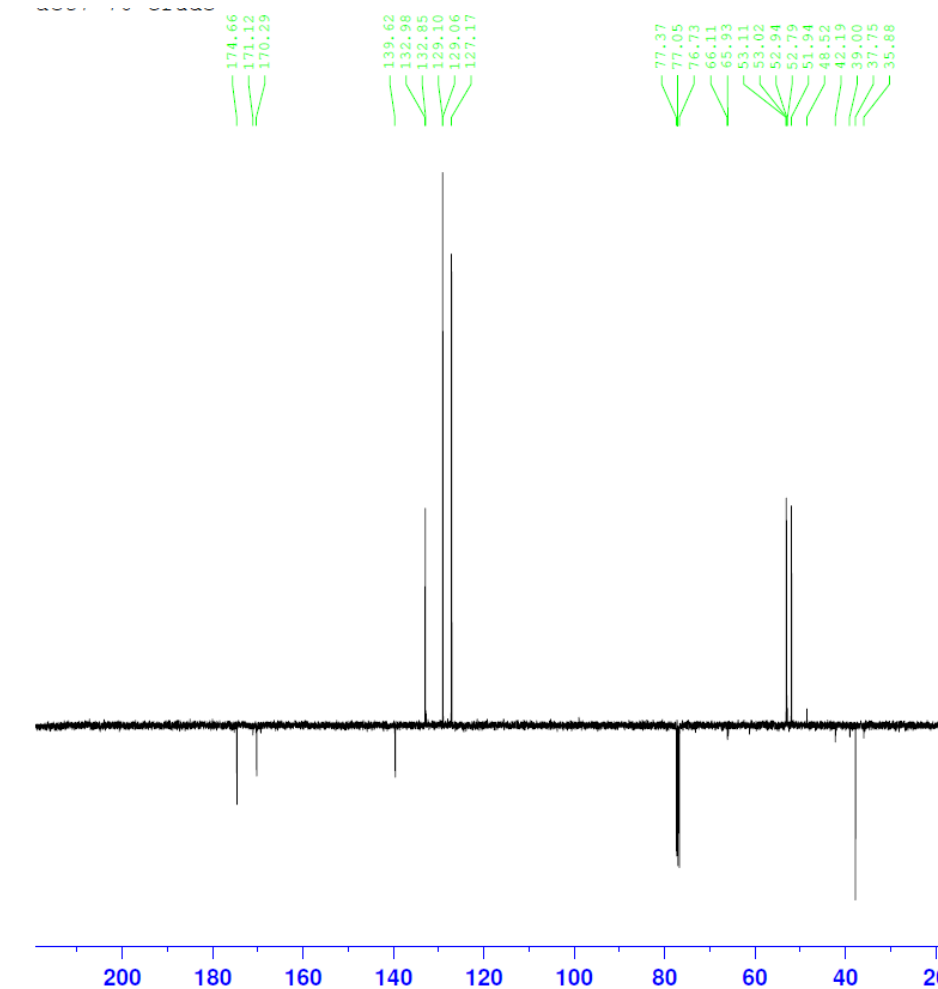
Current Data Parameters
 NAME aet7-76-crude
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120317
 Time 9.17
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 1024
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 724.1
 DW 20.850 usec
 DE 6.00 usec
 TE 295.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

----- CHANNEL f1 -----
 NUC1 13C
 P1 8.50 usec
 PL1 -2.60 dB
 SFO1 100.6228298 MHz

----- CHANNEL f2 -----
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 PL13 17.50 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 NWDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
 NAME aet7-76-crude
 EXPNO 12
 PROCNO 1

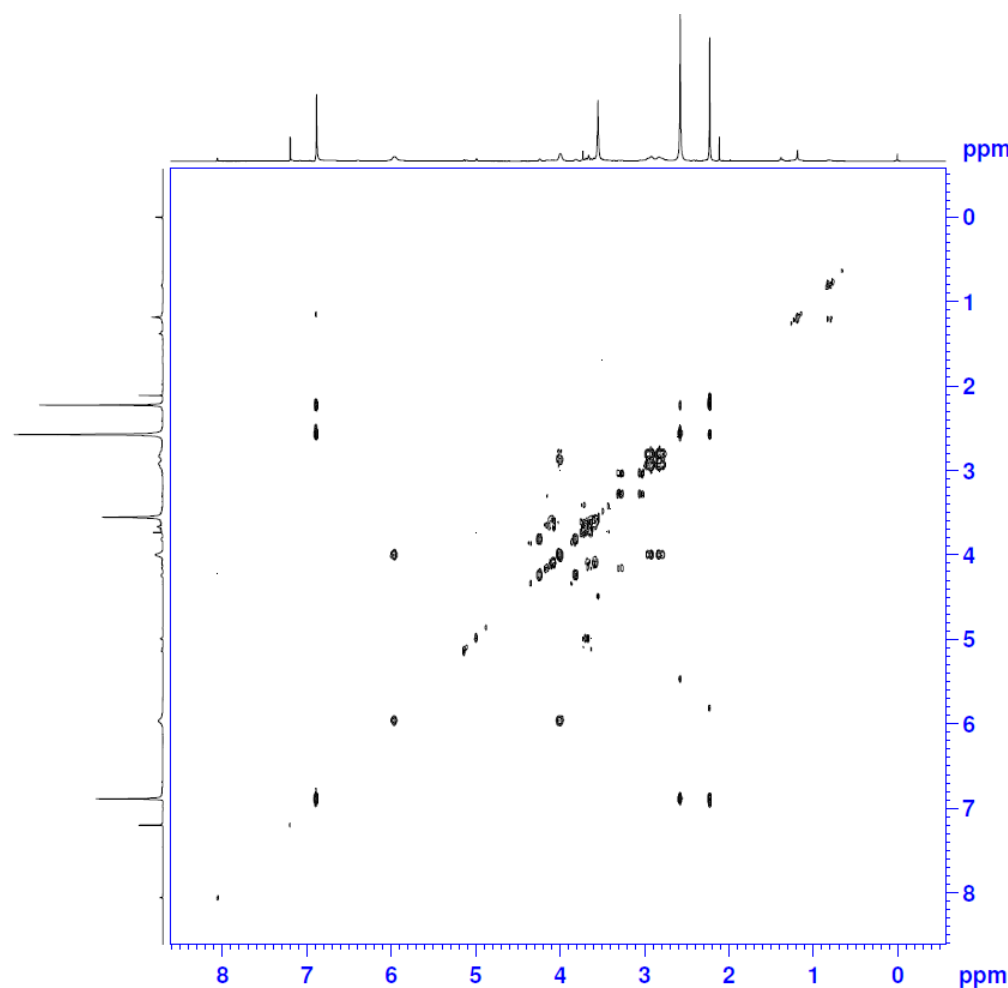
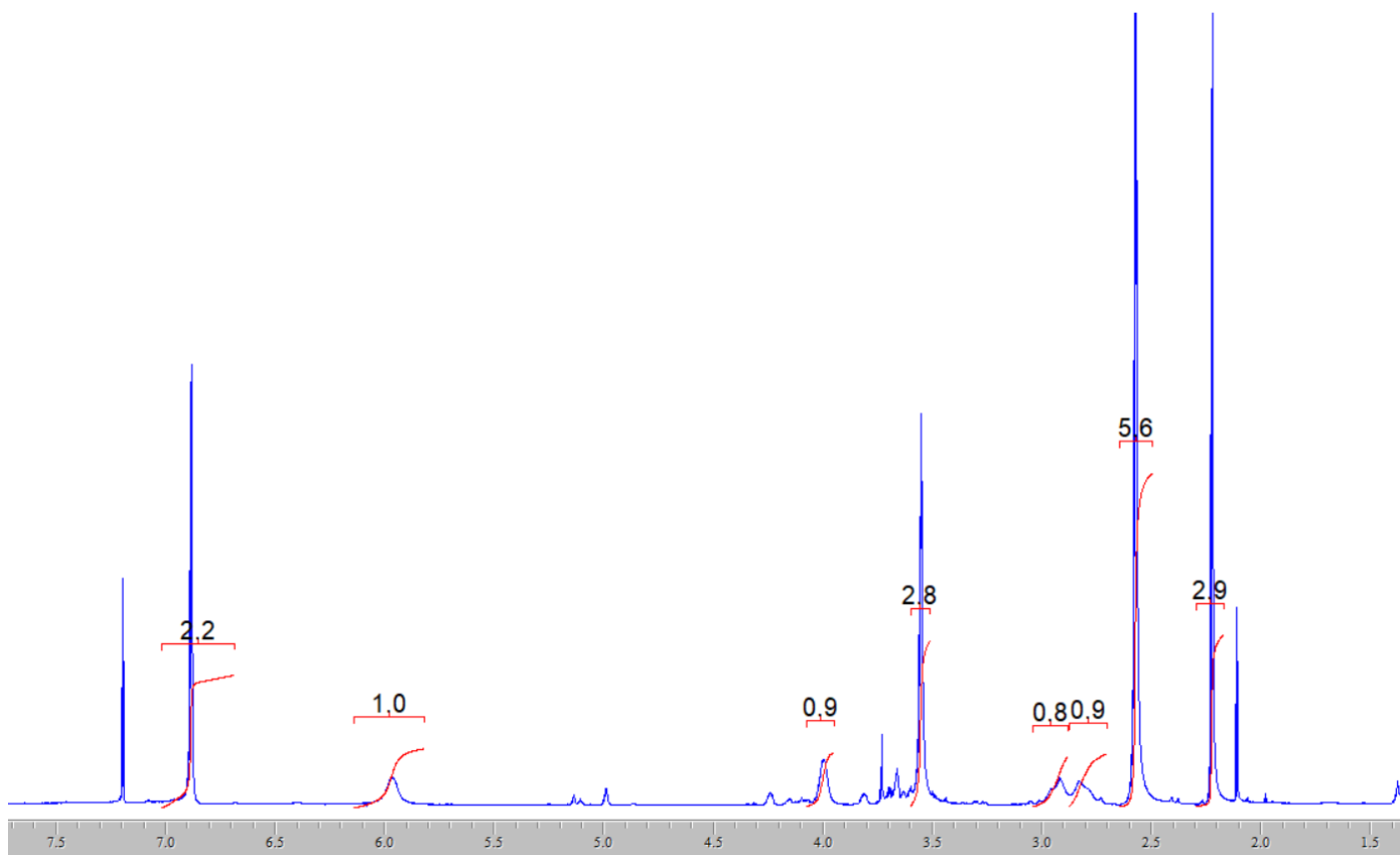
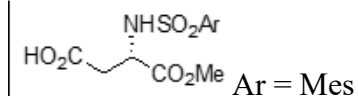
F2 - Acquisition Parameters
 Date_ 20120316
 Time 11.43
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG deptg_135
 TD 65536
 SOLVENT CDC13
 NS 512
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 11585.2
 DW 20.850 usec
 DE 6.00 usec
 TE 294.2 K
 CNST2 145.0000000
 D1 2.00000000 sec
 d2 0.00344828 sec
 D11 0.03000000 sec
 DELTA 0.00001082 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 P2 17.00 usec
 PL1 -2.60 dB
 SFO1 100.6228300 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 SFO2 400.1316000 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

(S)-4-Methoxy-4-oxo-3-(2,4,6-trimethylphenylsulfonamido)butanoic acid [Compound 27]



Current Data Parameters
NAME aet7-75-1
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120316
Time 3.39
INSTRUM dpx400
PROBHD 5 mm QNP 1H/13
PULPROG cosygmfgf
TD 2048
SOLVENT cdcl3
NS 4
DS 8
SWH 3676.471 Hz
FIDRES 1.795152 Hz
AQ 0.2785780 sec
RG 2580.3
DW 136.000 usec
DE 6.00 usec
TE 294.2 K
D0 0.0000300 sec
D1 1.91316497 sec
d13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00027200 sec

----- CHANNEL f1 -----
NUC1 1H
P1 10.00 usec
PL1 -1.50 dB
SFO1 400.1316438 MHz

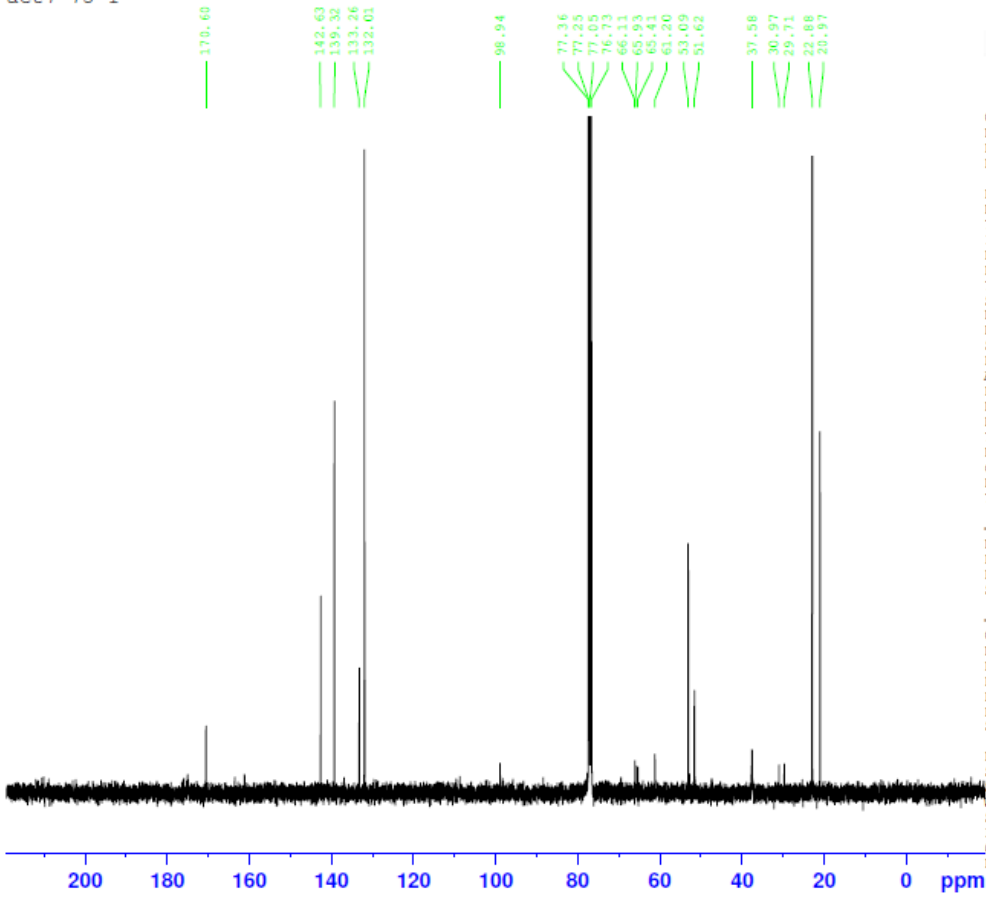
----- GRADIENT CHANNEL -----
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 16.00 %
GPZ2 12.00 %
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
ND0 1
TD 128
SFO1 400.1316 MHz
FIDRES 28.722427 Hz
SW 9.188 ppm
FMODE QF

F2 - Processing parameters
SI 1024
SF 400.1300353 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.1300353 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

aet7-75-1



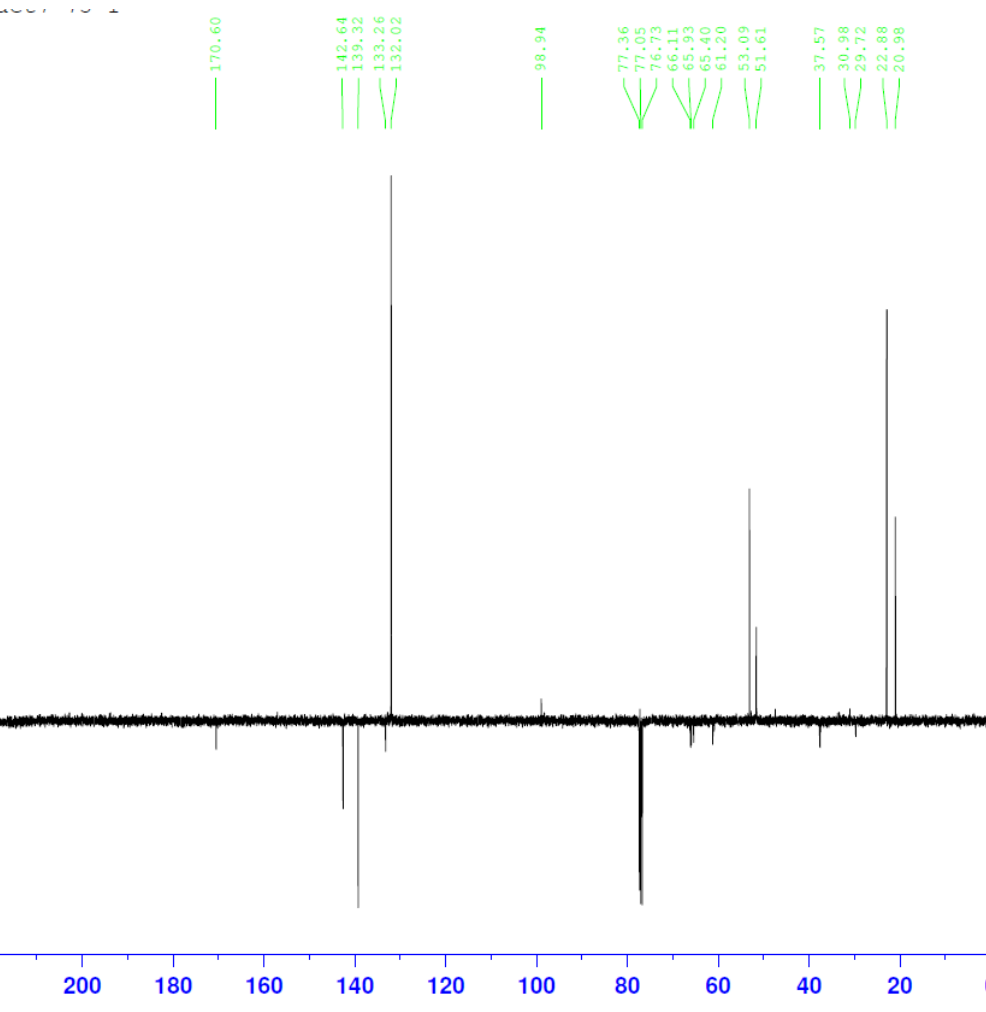
Current Data Parameters
 NAME aet7-75-1
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120316
 Time 3.25
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 1149.4
 DW 20.850 usec
 DE 6.00 usec
 TE 295.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

----- CHANNEL f1 -----
 NUC1 13C
 P1 8.50 usec
 PL1 -2.60 dB
 SFO1 100.6228298 MHz

----- CHANNEL f2 -----
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 PL13 17.50 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



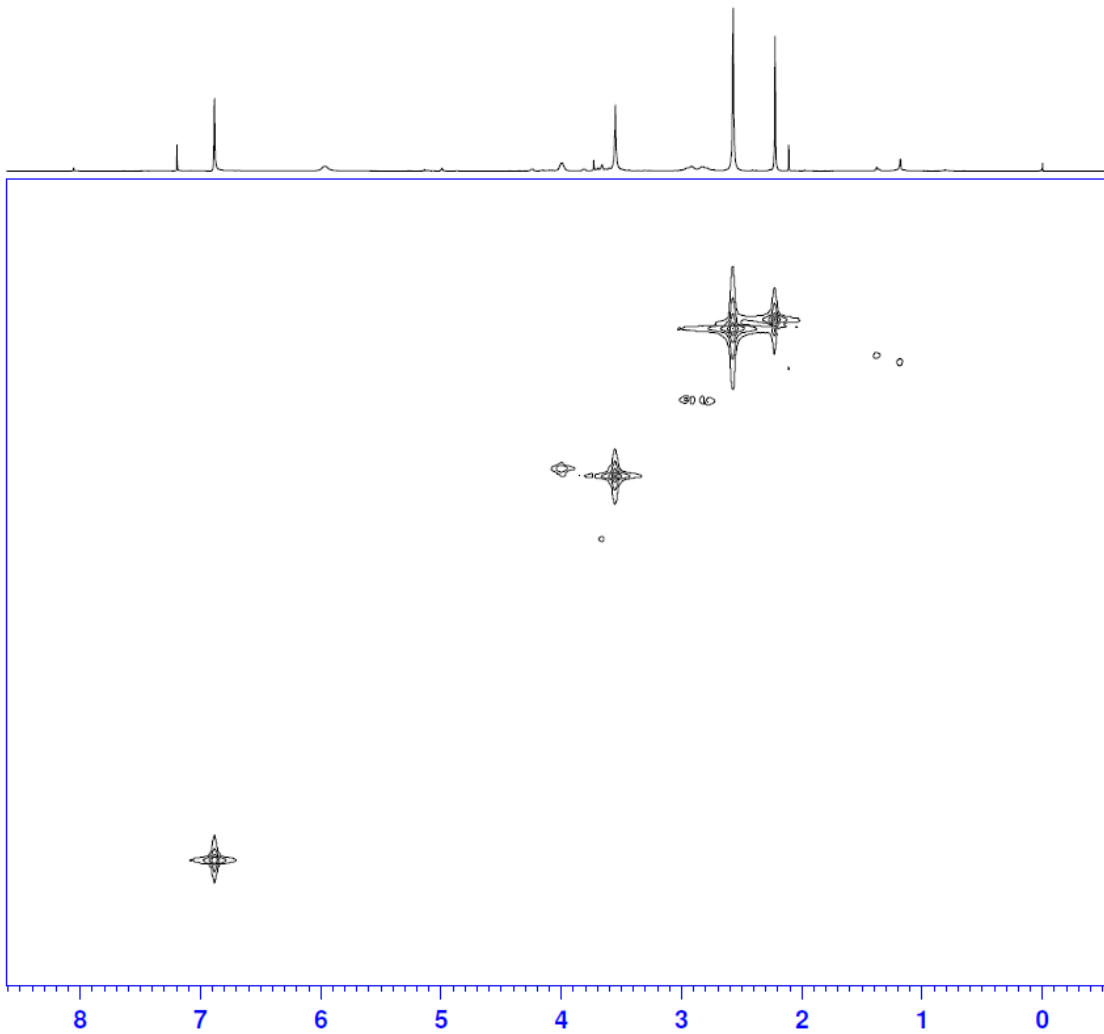
Current Data Parameters
 NAME aet7-75-1
 EXPNO 14
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120316
 Time 4.28
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG deptg_135
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 4096
 DW 20.850 usec
 DE 6.00 usec
 TE 294.2 K
 CNST2 145.0000000
 D1 2.00000000 sec
 d2 0.00344828 sec
 d11 0.03000000 sec
 DELTA 0.00001082 sec

----- CHANNEL f1 -----
 NUC1 13C
 P1 8.50 usec
 P2 17.00 usec
 PL1 -2.60 dB
 SFO1 100.6228300 MHz

----- CHANNEL f2 -----
 CPDPRG2 waltz16
 NUC2 1H
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 SFO2 400.1316000 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
NAME sat7-75-1
EXPTNO 15
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120314
Time 4.30
INSTRUM DPX400
PROBHD 5 mm QNP 1H/13
PULPROG hmqcpgpf
TD 1024
SOLVENT cdcl3
NS 4
DS 16
SWH 3676.471 Hz
FIDRES 3.590303 Hz
AQ 0.1393140 sec
RG 26008
DW 136.000 usec
DE 6.00 usec
TE 294.2 K
CNST2 145.0000000
d0 0.0000300 sec
d1 1.48771203 sec
d2 0.00344828 sec
d12 0.00002000 sec
d13 0.00000400 sec
d16 0.00020000 sec
DELTA1 0.00222428 sec
IN0 0.00003000 sec

==== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
p2 20.00 usec
PL1 -1.50 dB
SFO1 400.1316438 MHz

==== CHANNEL f2 =====
CPDPRG2 gapp
NUC2 13C
P3 8.00 usec
PCPD2 74.00 usec
PL2 -3.00 dB
PL12 18.00 dB
SFO2 100.6203140 MHz

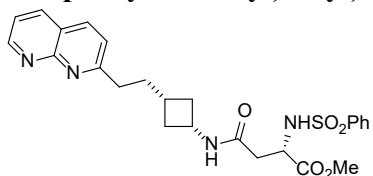
==== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
PI6 1000.00 usec

F1 - Acquisition parameters
ND0 2
TD 128
SFO1 100.6203 MHz
FIDRES 130.208328 Hz
SW 165.639 ppm
FRMODE QF

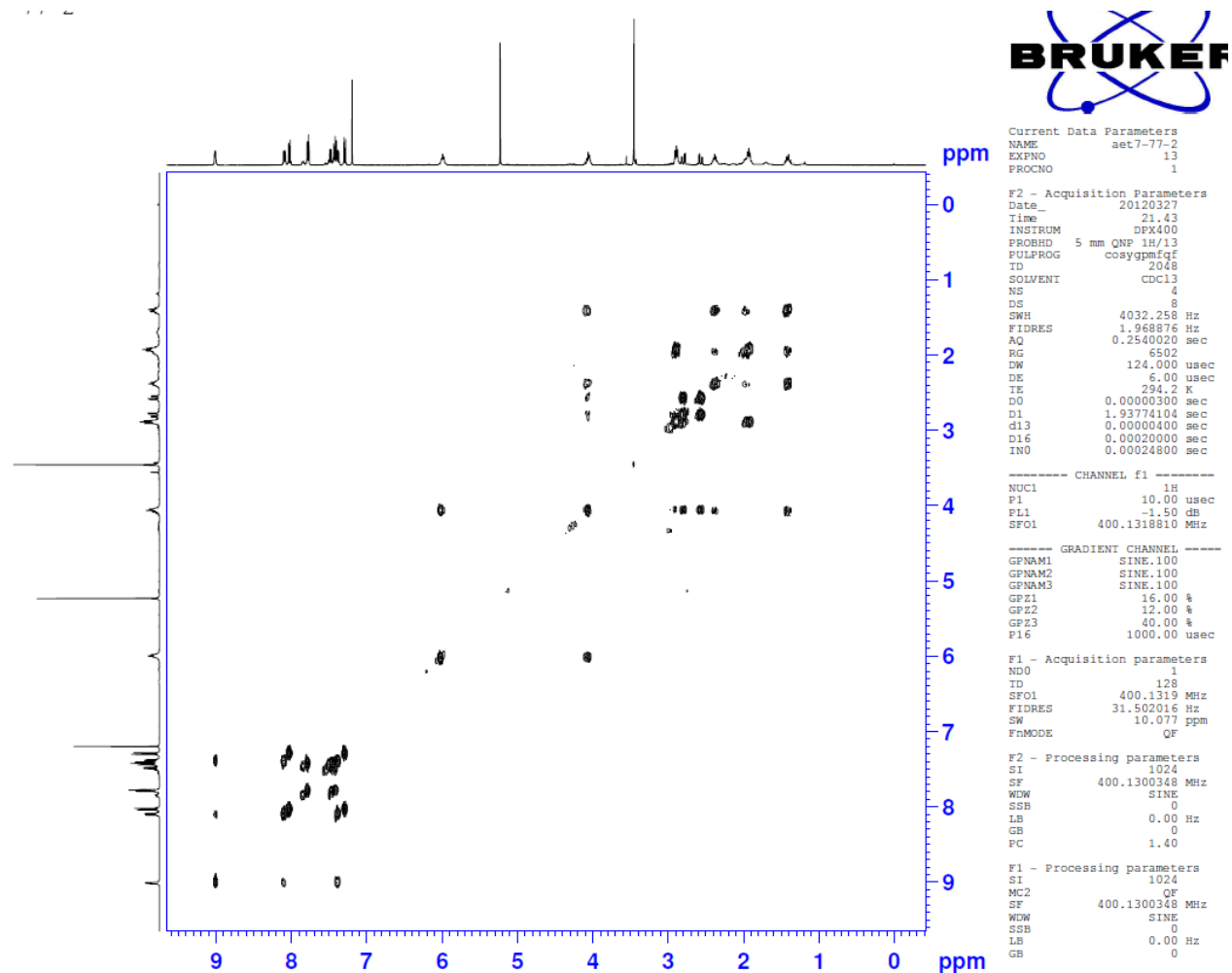
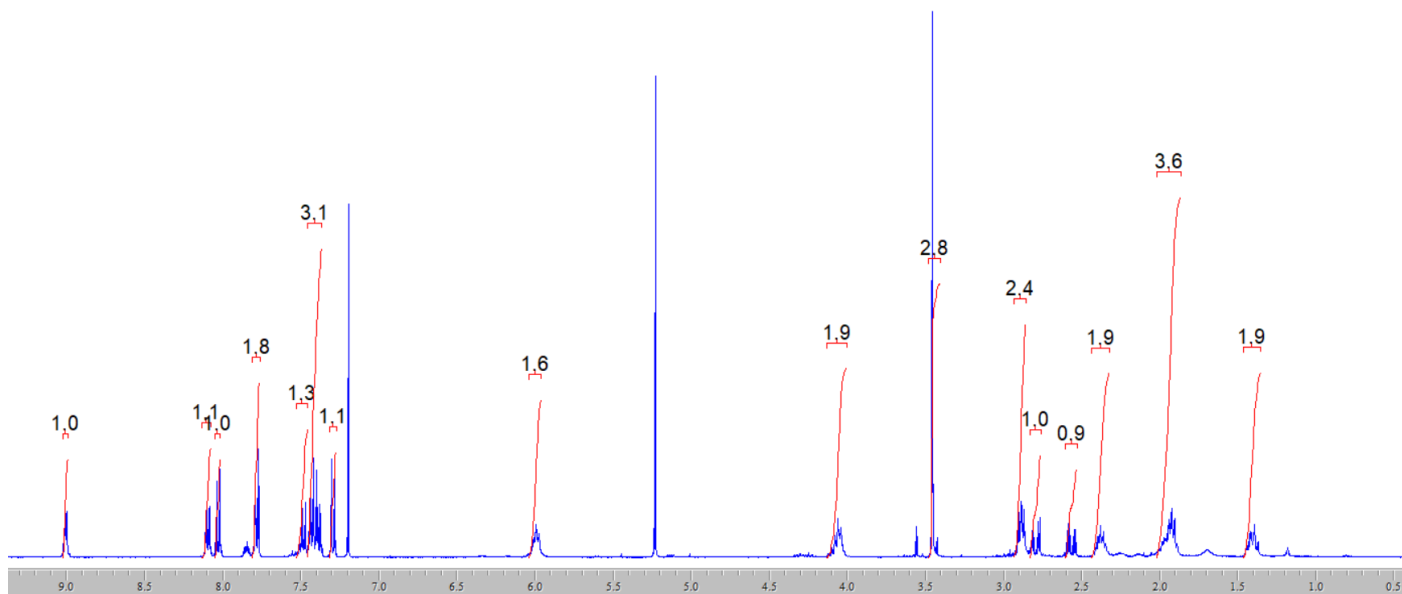
F2 - Processing parameters
SI 1024
SF 400.1300353 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 100.6127690 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

Methyl *N*⁴-((1*r**,3*R**)-3-(2-(1,8-naphthyridin-2-yl)ethyl)cyclobutyl)-*N*²-(phenylsulfonyl)-*L*-



asparaginate [Compound 28]



Current Data Parameters
 NAME set7-77-2
 EXPNO 13
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120327
 Time 21.43
 INSTRUM DFX400
 PROBHD 5 mm QNP 1H/13
 PULPROG cosygpmfqr
 TD 2048
 SOLVENT CDCl3
 NS 4
 DS 8
 SWH 4032.258 Hz
 FIDRES 1.968876 Hz
 AQ 0.2540020 sec
 RG 6502
 DW 124.000 usec
 DE 6.00 usec
 TE 294.2 K
 D0 0.00000300 sec
 D1 1.93774104 sec
 d13 0.00000400 sec
 D16 0.00020000 sec
 INO 0.00024800 sec

----- CHANNEL f1 -----
 NUC1 1H
 P1 10.00 usec
 PL1 -1.50 dB
 SFO1 400.1318810 MHz

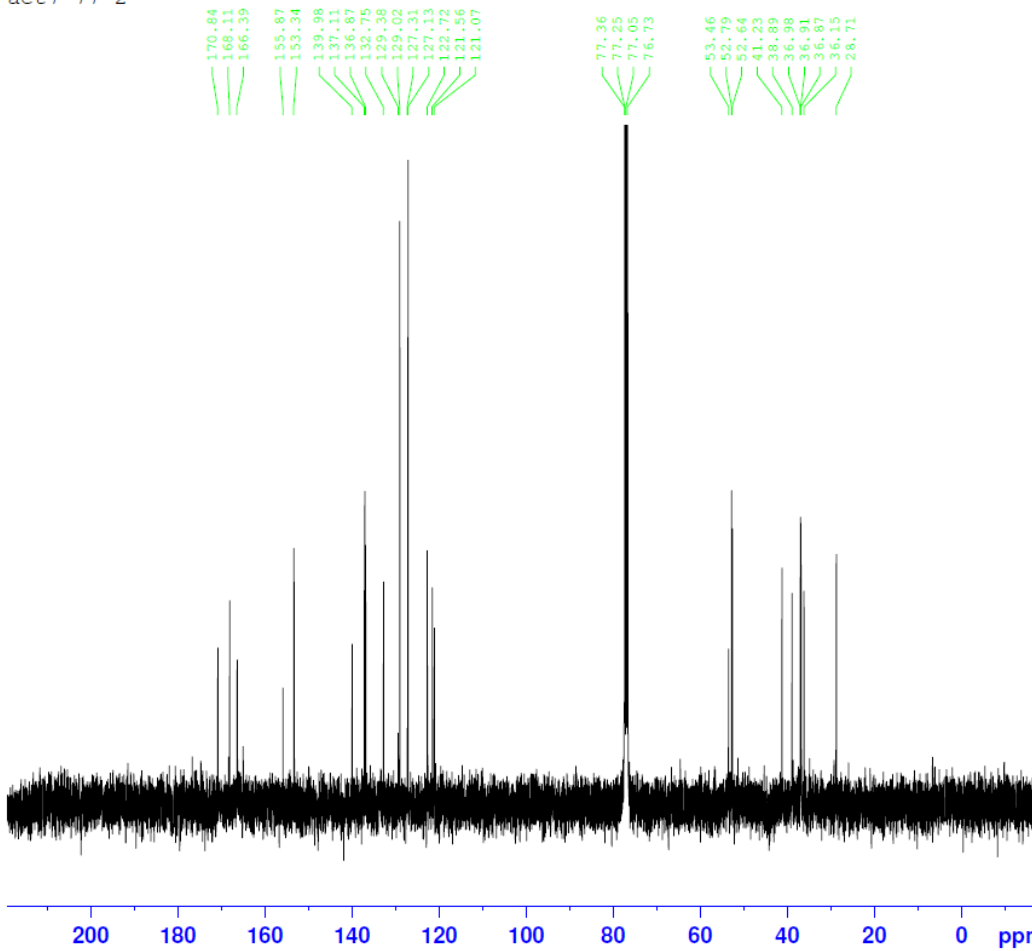
----- GRADIENT CHANNEL -----
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPNAM3 SINE.100
 GPZ1 16.00 %
 GPZ2 12.00 %
 GPZ3 40.00 %
 P16 1000.00 usec

F1 - Acquisition parameters
 ND0 1
 TD 128
 SFO1 400.1319 MHz
 FIDRES 31.502016 Hz
 SW 10.077 ppm
 FbMODE QF

F2 - Processing parameters
 SI 1024
 SF 400.1300348 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 400.1300348 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

aet7-77-2



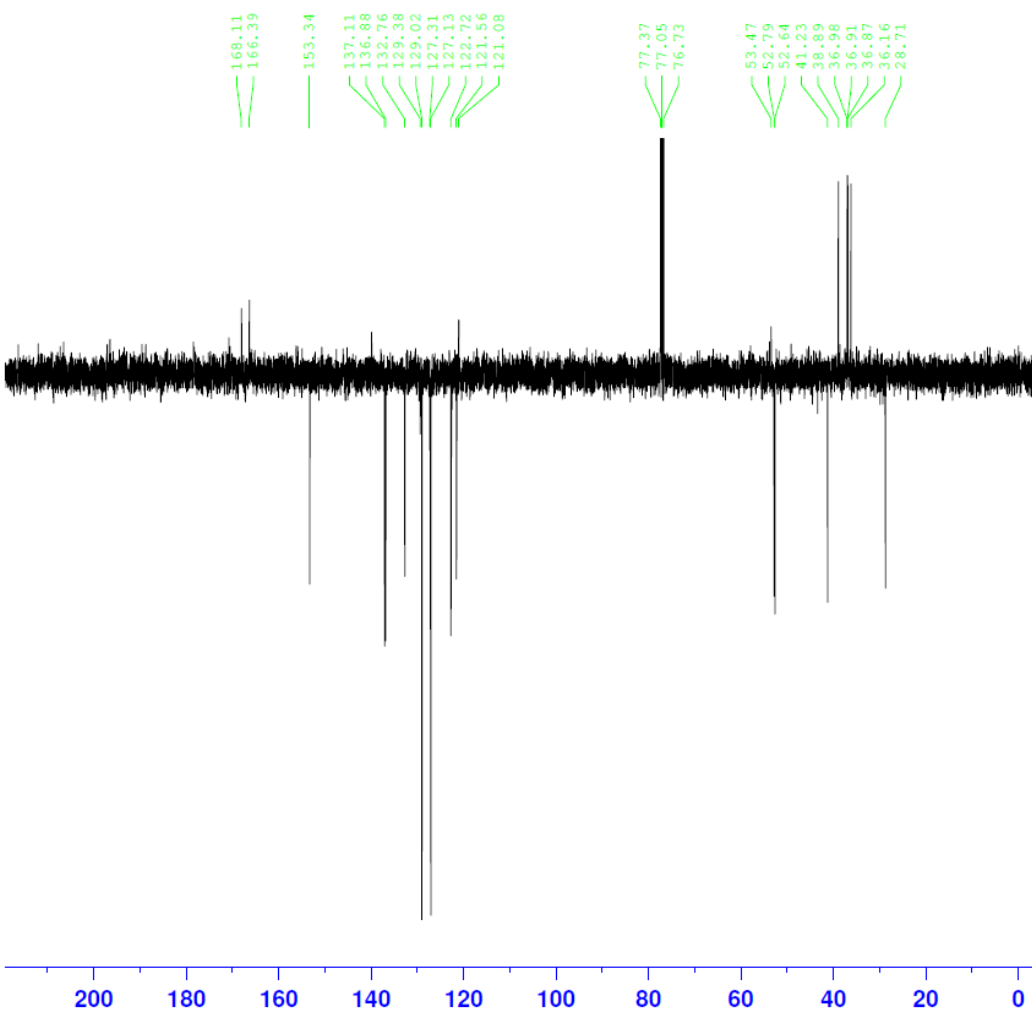
Current Data Parameters
 NAME aet7-77-2
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120327
 Time 21.12
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 724.1
 DW 20.850 usec
 DE 6.00 usec
 TE 294.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 PL1 -2.60 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 PL13 17.50 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



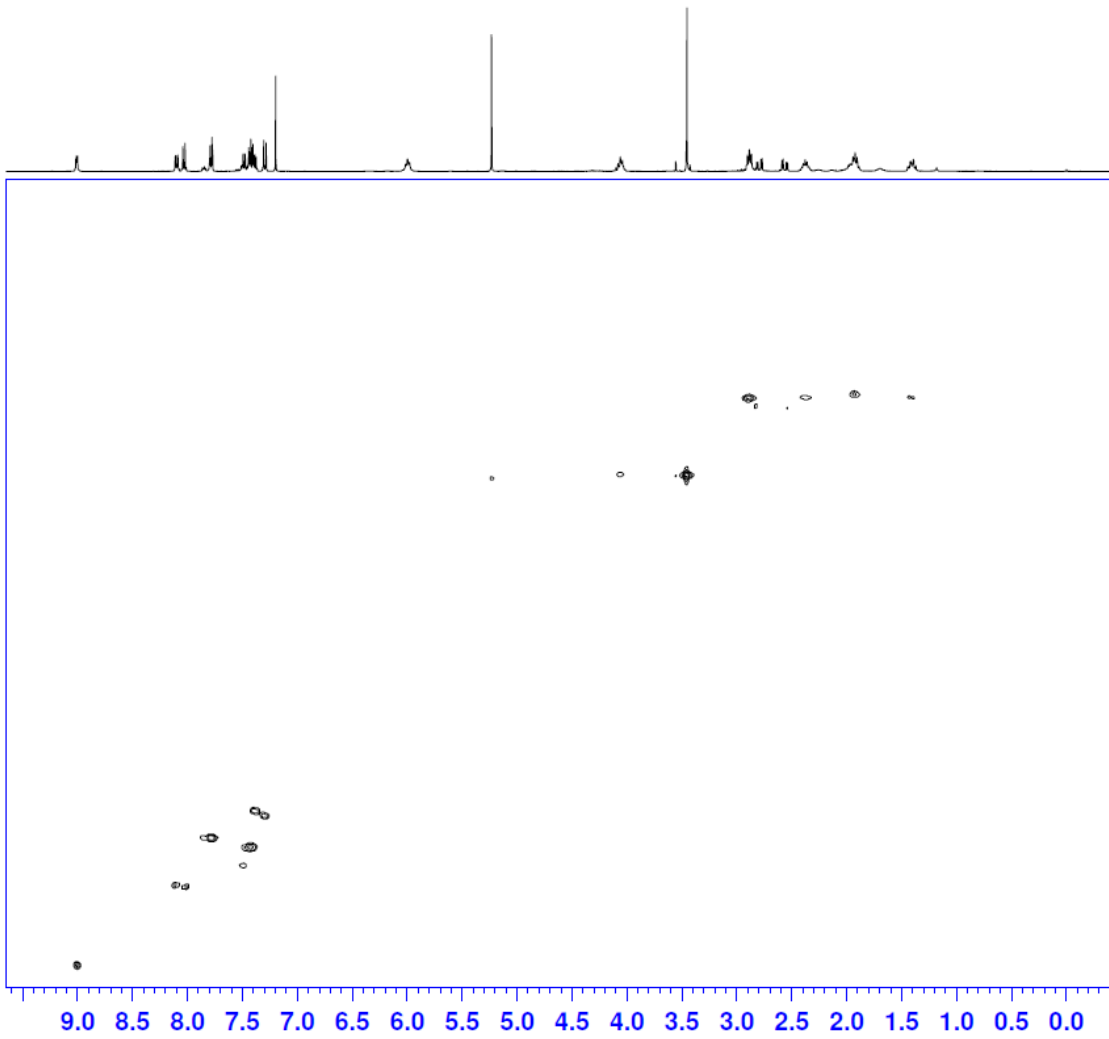
Current Data Parameters
 NAME aet7-77-2
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120327
 Time 21.42
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG deptq_135
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 11585.2
 DW 20.850 usec
 DE 6.00 usec
 TE 294.2 K
 CNST2 145.0000000
 D1 2.00000000 sec
 d2 0.00344828 sec
 D11 0.03000000 sec
 DELTA 0.00001082 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 P2 17.00 usec
 PL1 -2.60 dB
 SFO1 100.6228300 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 SFO2 400.1316000 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
NAME act7-77-2
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Data_ 20120327
Time 22.03
INSTRUM dpx400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 1024
SOLVENT cdcl3
NS 4
DS 16
SWH 4032.258 Hz
FIDRES 3.937752 Hz
AQ 0.1270260 sec
RG 9195.2
DW 124.000 usec
DE 6.00 usec
TE 294.2 K
CNS12 145.000000
d0 0.00000000 sec
d1 1.50000000 sec
d2 0.00344828 sec
d12 0.00020000 sec
d13 0.00000400 sec
d16 0.00020000 sec
DELTA1 0.00222428 sec
IN0 0.00030000 sec

==== CHANNEL F1 =====
NUC1 13
P1 10.00 usec
p2 20.00 usec
PL1 -1.50 dB
SFO1 400.1318810 MHz

==== CHANNEL F2 =====
CPDPRG2 gprp
NUC2 13
P3 8.00 usec
PCPD2 74.00 usec
PL2 -5.00 dB
PL12 18.00 dB
SFO2 100.6203140 MHz

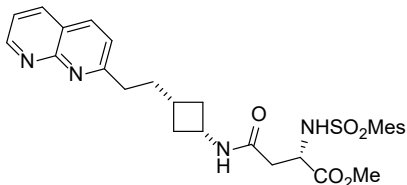
==== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
ND0 2
TD 128
SFO1 100.6203 MHz
FIDRES 130.208328 Hz
SW 165.639 ppm
FMODE QF

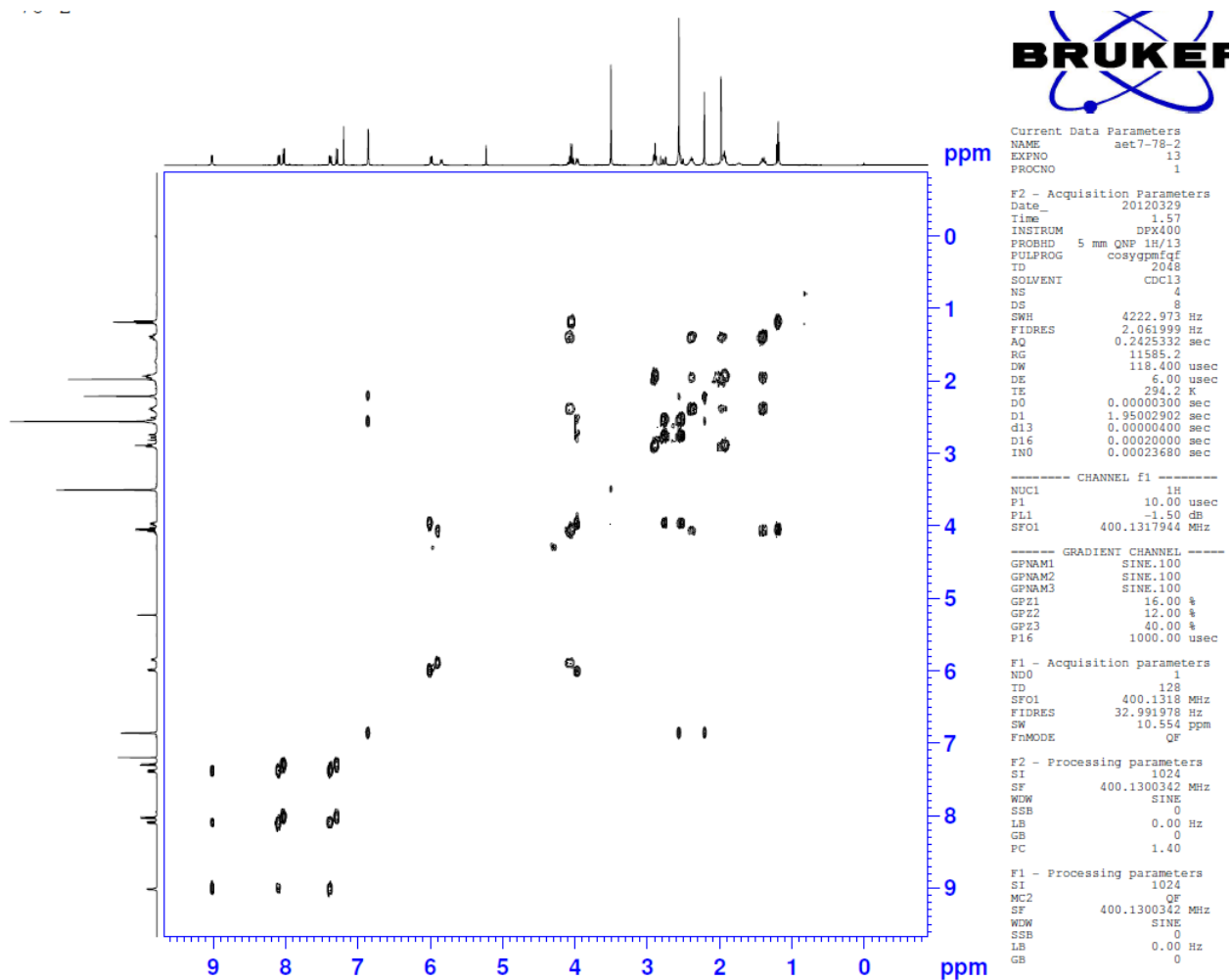
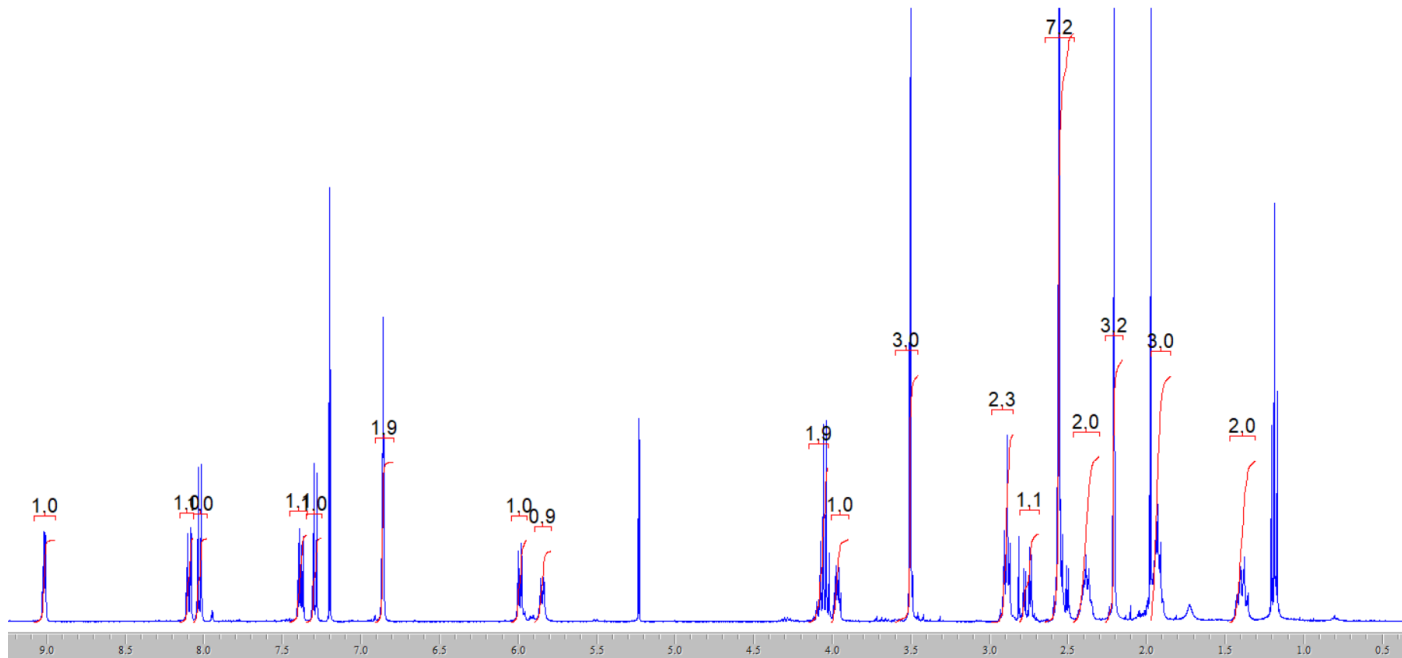
F2 - Processing parameters
SI 1024
SF 400.1300348 MHz
WFV QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 100.6127690 MHz
WFV QSINE
SSB 2
LB 0.00 Hz
GB 0

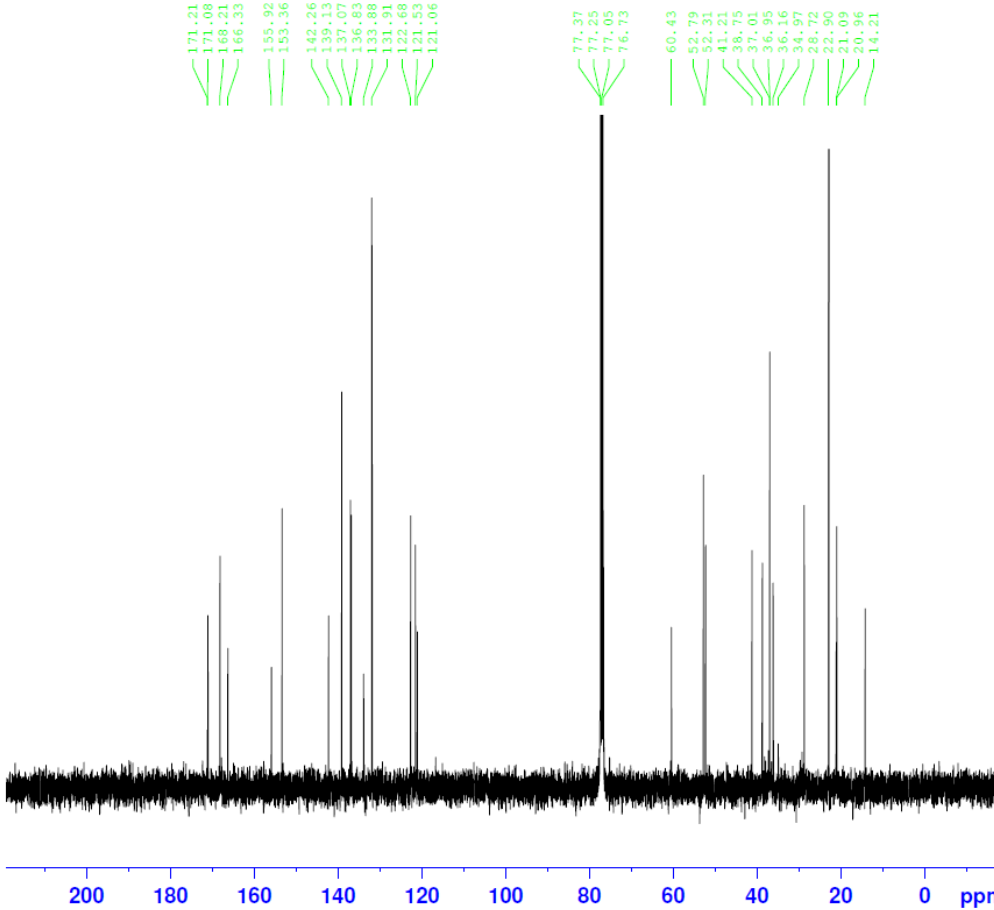
Methyl *N*⁴-((1*r**,3*R**)-3-(2-(1,8-naphthyridin-2-yl)ethyl)cyclobutyl)-*N*²-(mesitylsulfonyl)-*L*-



asparaginate [Compound 29]



aet7-78-2



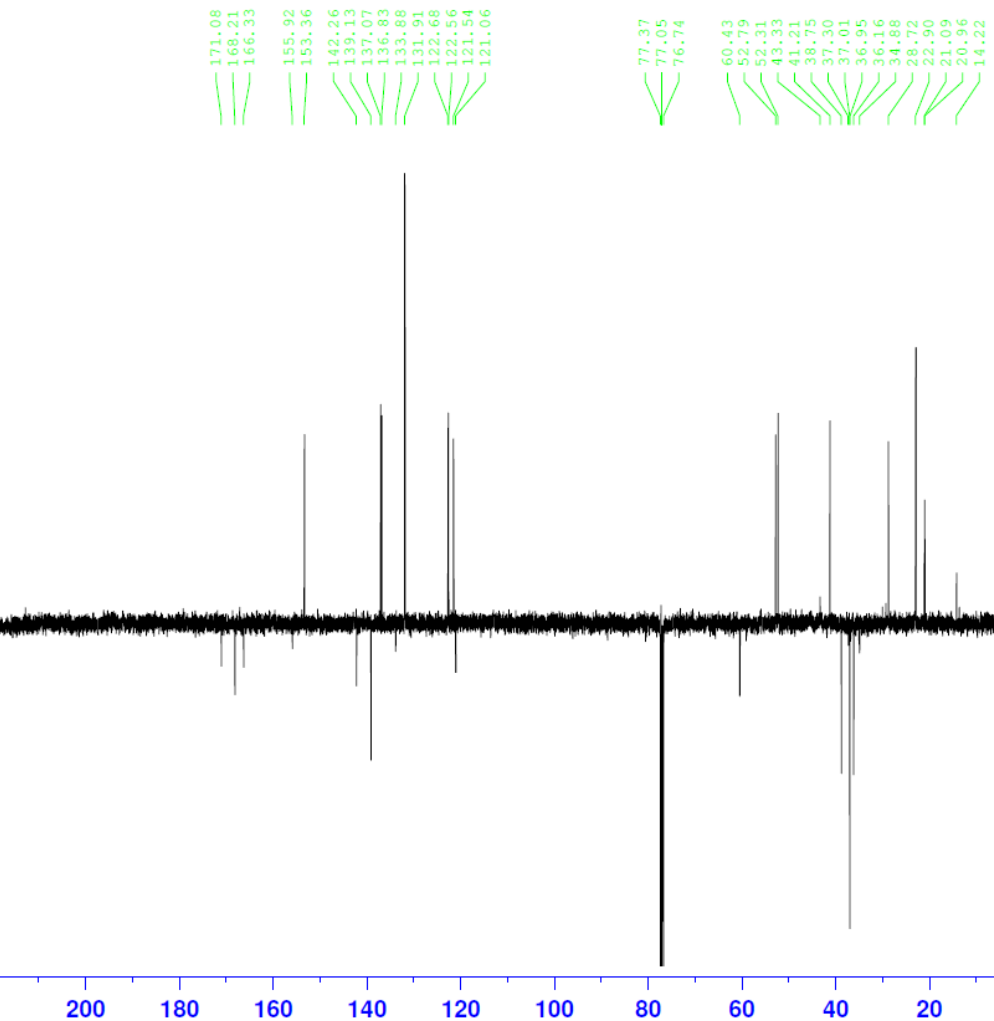
Current Data Parameters
 NAME aet7-78-2
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120329
 Time 1.26
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 1024
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 812.7
 DW 20.850 usec
 DE 6.00 usec
 TE 294.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999999 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 PL1 -2.60 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 PL13 17.50 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
 NAME aet7-78-2
 EXPNO 12
 PROCNO 1

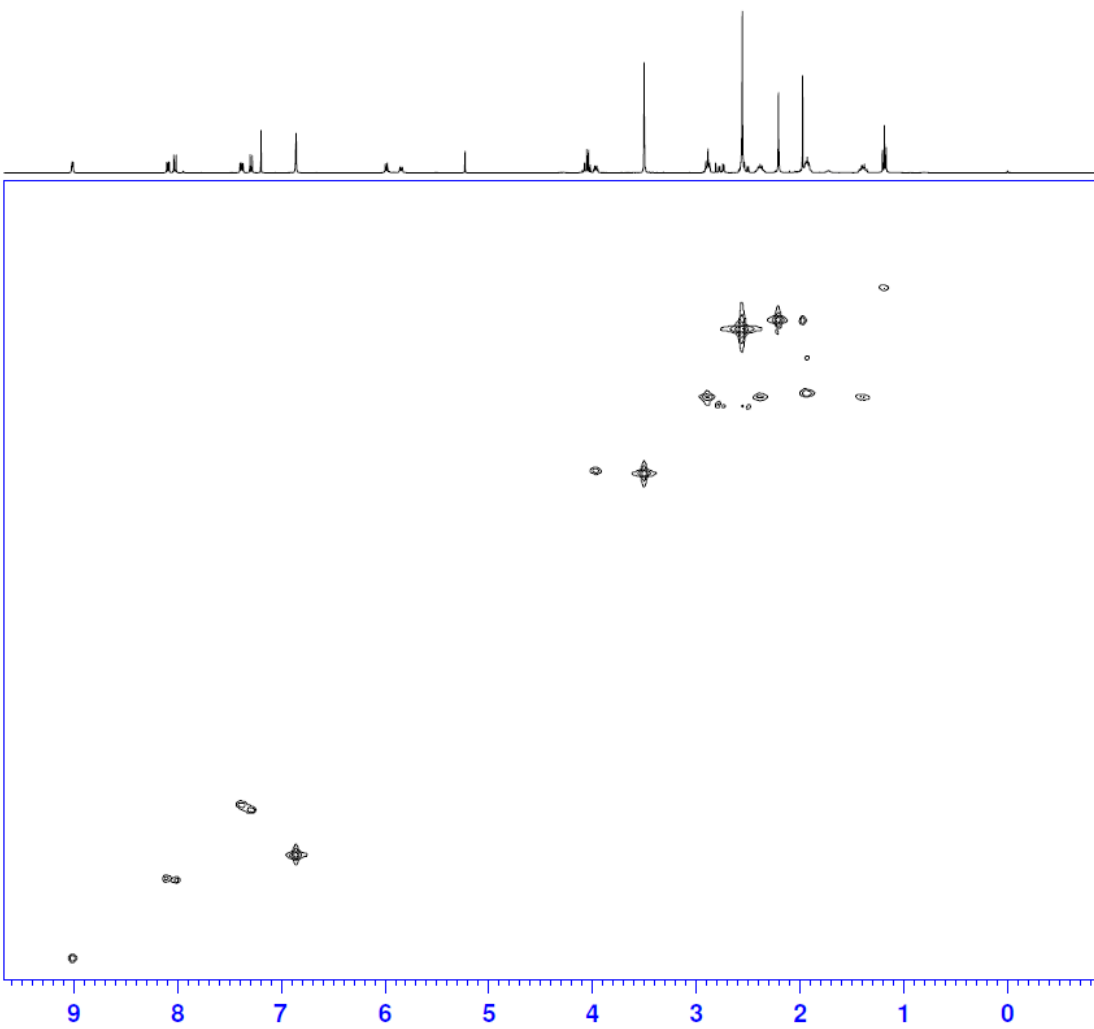
F2 - Acquisition Parameter:
 Date_ 20120329
 Time 1.56
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG deptq_135
 TD 65536
 SOLVENT CDC13
 NS 512
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 11585.2
 DW 20.850 usec
 DE 6.00 usec
 TE 294.2 K
 CNST2 145.0000000
 D1 2.00000000 sec
 d2 0.00344828 sec
 D11 0.03000000 sec
 DELTA 0.00001082 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 P2 17.00 usec
 PL1 -2.60 dB
 SFO1 100.6228300 MH:

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 SFO2 400.1316000 MH:

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MH:
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Current Data Parameters
 NAME act7-78-2
 EXPNO 14
 PROCNO 1



F2 - Acquisition Parameters
 Data 20120329
 Time 2.17
 INSTRUM DFX400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 ID 1024
 SOLVENT cdc13
 NS 4
 DS 16
 SWH 4222.973 Hz
 FIDRES 4.123997 Hz
 AQ 0.1212916 sec
 RG 5160.6
 DW 118.400 usec
 DE 6.00 usec
 TE 294.2 K
 CNST2 145.000000
 c0 0.0000300 sec
 D1 1.50614405 sec
 p2 0.00344828 sec
 d12 0.00002000 sec
 d13 0.00000400 sec
 D16 0.00020000 sec
 DELTAT1 0.0022423 sec
 INO 0.00003000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 p2 20.00 usec
 PL1 -1.50 dB
 SFO1 400.1317944 MHz

==== CHANNEL f2 =====
 CPDPRG2 garp
 NUC2 13C
 P3 8.00 usec
 PCPD2 74.00 usec
 PL2 -3.00 dB
 PL12 18.00 dB
 SFO2 100.6203140 MHz

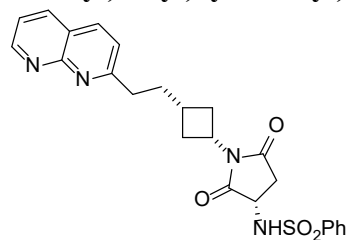
==== GRADIENT CHANNEL =====
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPNAM3 SINE.100
 GPZ1 50.00 %
 GPZ2 30.00 %
 GPZ3 40.10 %
 P16 1000.00 usec

F1 - Acquisition parameters
 ND0 2
 ID 128
 SFO1 100.6203 MHz
 FIDRES 130.208328 Hz
 SW 145.639 ppm
 PRMODE QF

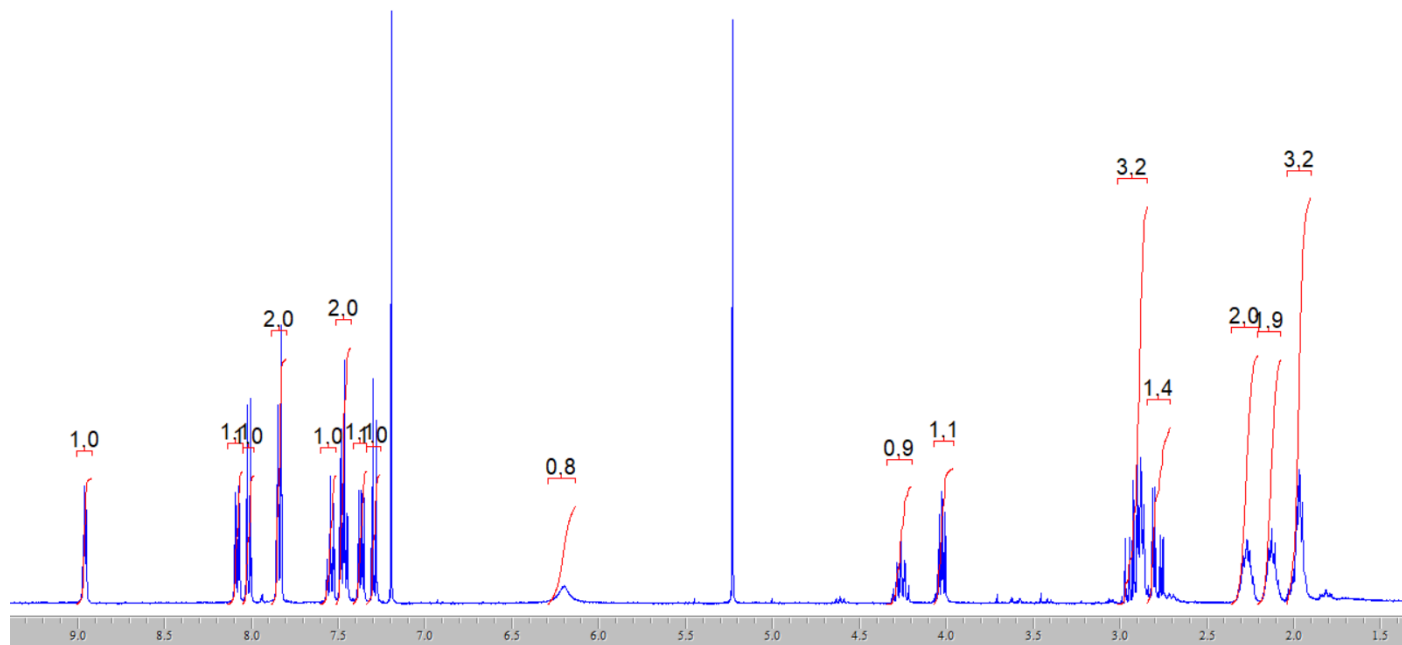
F2 - Processing parameters
 SI 1024
 SF 400.1300342 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 100.6127690 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

N-((*S*)-1-((1*r**,3*R**)-3-(2-(1,8-Naphthyridin-2-yl)ethyl)cyclobutyl)-2,5-dioxopyrrolidin-3-



yl)benzenesulfonamide [Compound 30]



Current Data Parameters
 NAME: acet7-77-1
 EXFNO: 13
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20120327
 Time: 19.34
 INSTRUM: DPX400
 PROBHD: 5 mm QNP 1H/13
 PULPROG: cosygmfzgpg
 TD: 2048
 SOLVENT: CDCl3
 NS: 4
 DS: 8
 SWH: 4222.973 Hz
 FIDRES: 2.061999 Hz
 AQ: 0.2425332 sec
 RG: 502
 DW: 118.400 usec
 DE: 5.00 usec
 TE: 294.2 K
 D0: 0.00000300 sec
 D1: 1.95002902 sec
 d12: 0.00009400 sec
 D15: 0.00020000 sec
 INU: 0.00023680 sec

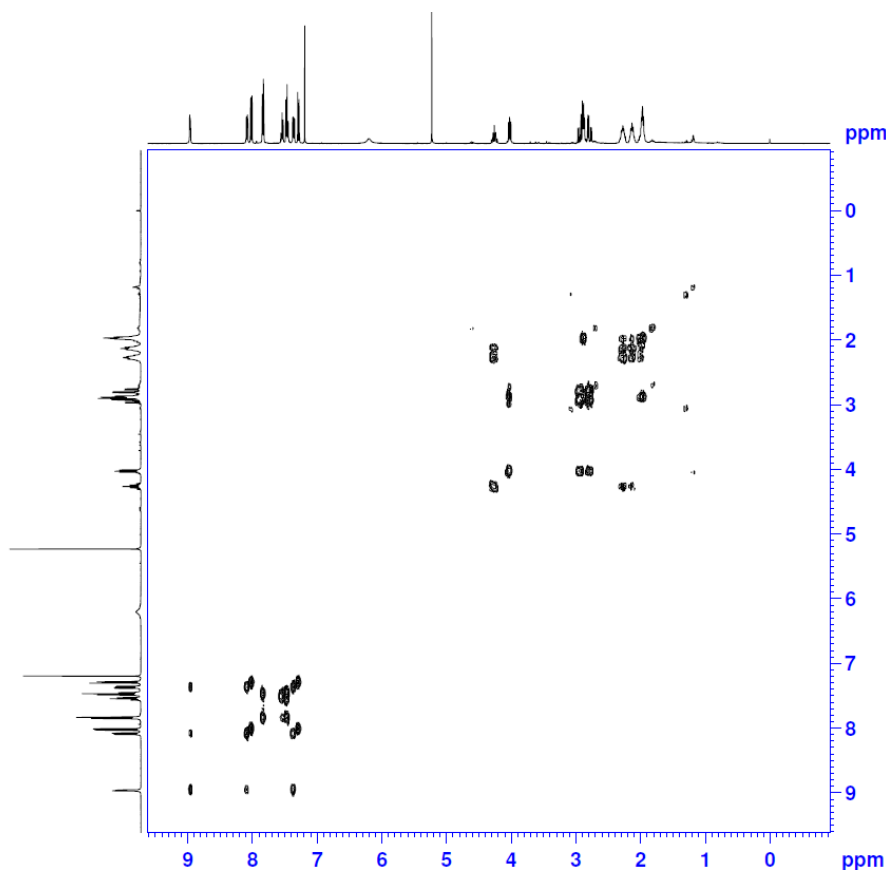
----- CHANNEL f1 -----
 NUC1: 1H
 P1: 10.00 usec
 PL1: -1.50 dB
 SF01: 400.1317724 MHz

----- GRADIENT CHANNEL -----
 GPMAM1: SINE.100
 GPMAM2: SINE.100
 GPMAM3: SINE.100
 GPZ1: 16.00 %
 GPZ2: 12.00 %
 GPZ3: 40.00 %
 P16: 1000.00 usec

F1 - Acquisition parameters
 NDO: 1
 TD: 128
 SF01: 400.1318 MHz
 FIDRES: 32.991978 Hz
 SW: 10.554 ppm
 FMODE: QF

F2 - Processing parameters
 SI: 1024
 SF: 400.1300350 MHz
 WDW: SINE
 SSB: 0
 LB: 0.00 Hz
 GB: 0
 PC: 1.40

F1 - Processing parameters
 SI: 1024
 MC2: QF
 SF: 400.1300350 MHz
 WDW: SINE
 SSB: 0
 LB: 0.00 Hz
 GB: 0



aet7-77-1



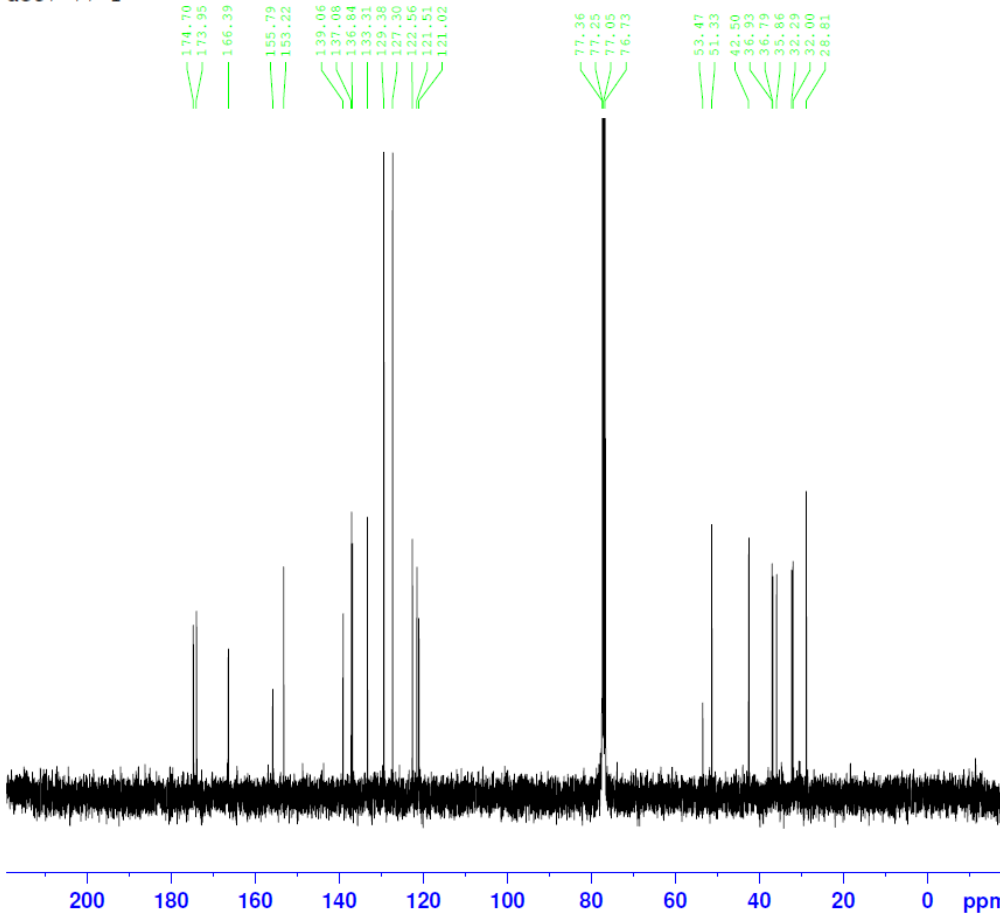
Current Data Parameters
NAME aet7-77-1
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120327
Time 19.03
INSTRUM DPX400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 724.1
DW 20.850 usec
DE 6.00 usec
TE 294.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 -2.60 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.50 dB
PL12 17.50 dB
PL13 17.50 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



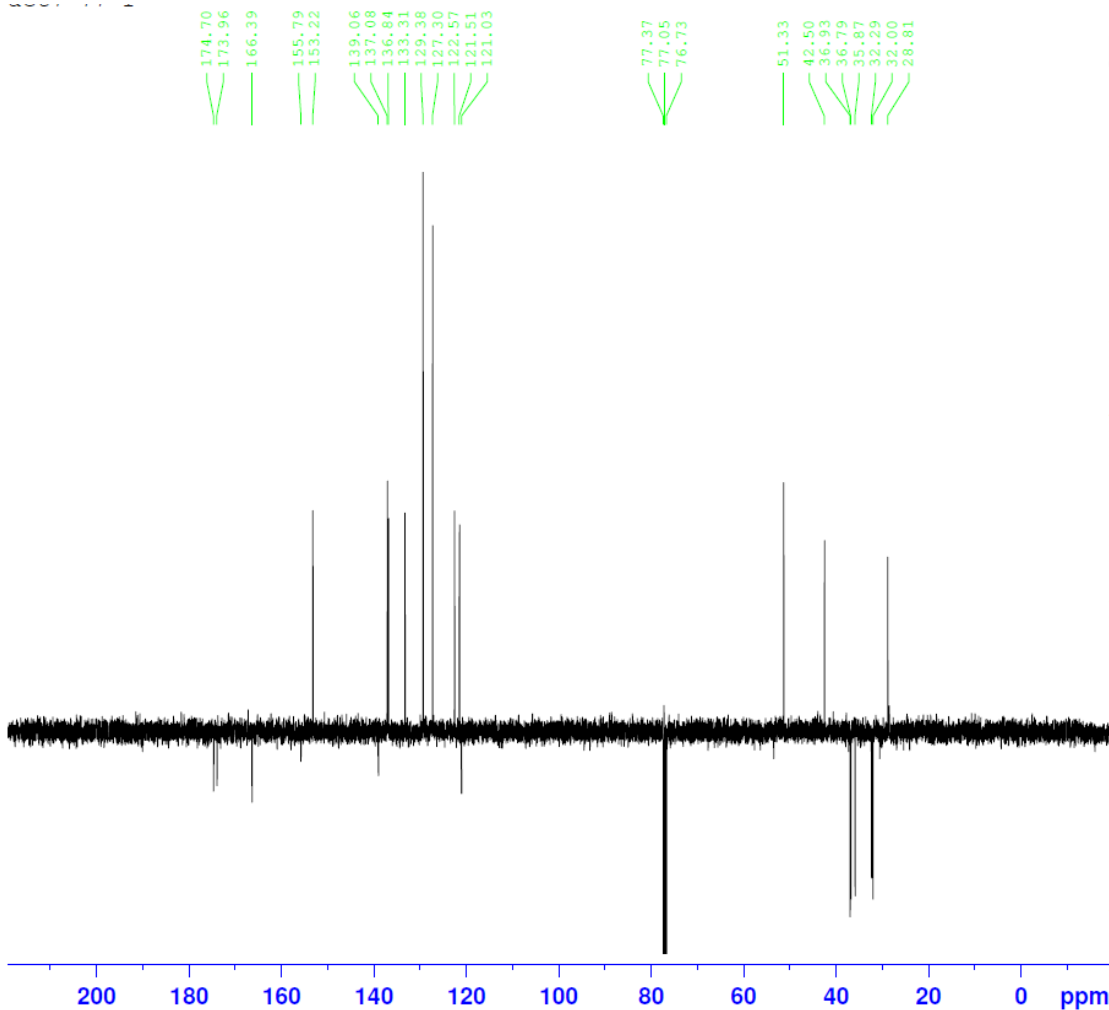
Current Data Parameters
NAME aet7-77-1
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120327
Time 19.33
INSTRUM DPX400
PROBHD 5 mm QNP 1H/13
PULPROG deptq_135
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 11585.2
DW 20.850 usec
DE 6.00 usec
TE 294.2 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
D11 0.03000000 sec
DELTA 0.00001082 sec

===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
P2 17.00 usec
PL1 -2.60 dB
SFO1 100.6228300 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 10.00 usec
P4 20.00 usec
PCPD2 80.00 usec
PL2 -1.50 dB
PL12 17.50 dB
SFO2 400.1316000 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





Current Data Parameters
NAME sat7-77-1
EXFNO 14
PROCNO 1

F2 - Acquisition Parameters
Date 20120327
Time 19.54

INSTRUM DFX400
PROBHD 5 mm QNP 1H/13
PULPROG hmqcpgpgf
TD 1024
SOLVENT ccc13
NS 4
DS 16
SWH 4222.973 Hz
FIDRES 4.123997 Hz
AQ 0.1212916 sec
RG 26008
RW 118.400 usec
DE 6.00 usec
TE 294.2 K
CNST2 145.000000
d0 0.0000300 sec
d1 1.50614405 sec
d2 0.00344828 sec
d12 0.00002000 sec
d13 0.00000400 sec
D16 0.00020000 sec
DELTA1 0.0023428 sec
IN0 0.00003000 sec

==== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
p2 20.00 usec
PL1 -1.50 dB
SFO1 400.1317724 MHz

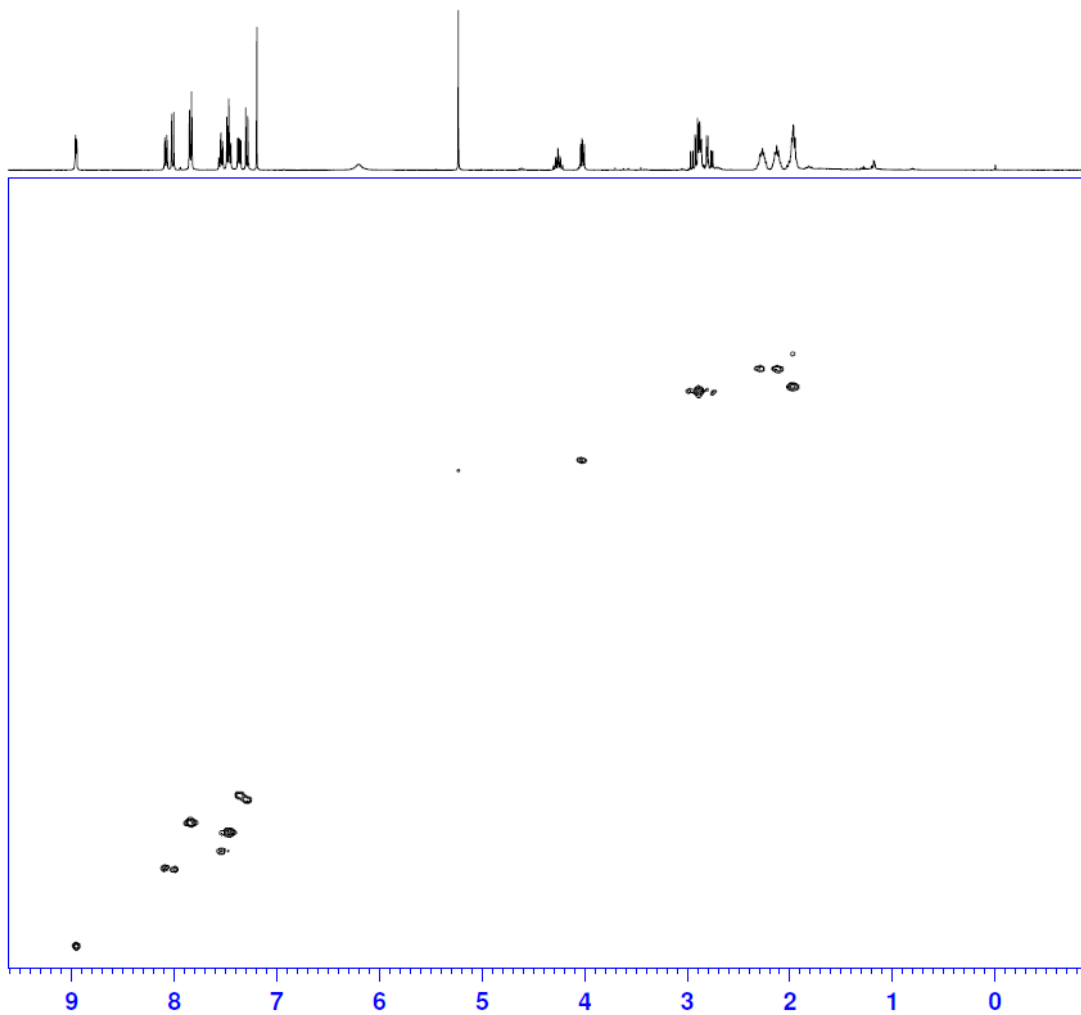
==== CHANNEL f2 =====
CPDPRG2 gqcp
NUC2 13C
P3 8.00 usec
PCPD2 74.00 usec
PL2 -3.00 dB
PL12 18.00 dB
SFO2 100.6203140 MHz

==== GRADIENT CHANNEL =====
GFNAME1 SINE.100
GFNAME2 SINE.100
GFNAME3 SINE.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

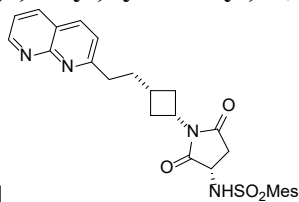
F1 - Acquisition parameters
ND0 2
TD 128
SFO1 100.6203 MHz
FIDRES 130.208328 Hz
SW 163.639 ppm
FMODE QF

F2 - Processing parameters
SI 1024
SF 400.1300350 MHz
WDW Q81NK
SFB 2
LB 0.00 Hz
GB 0
PC 1.40

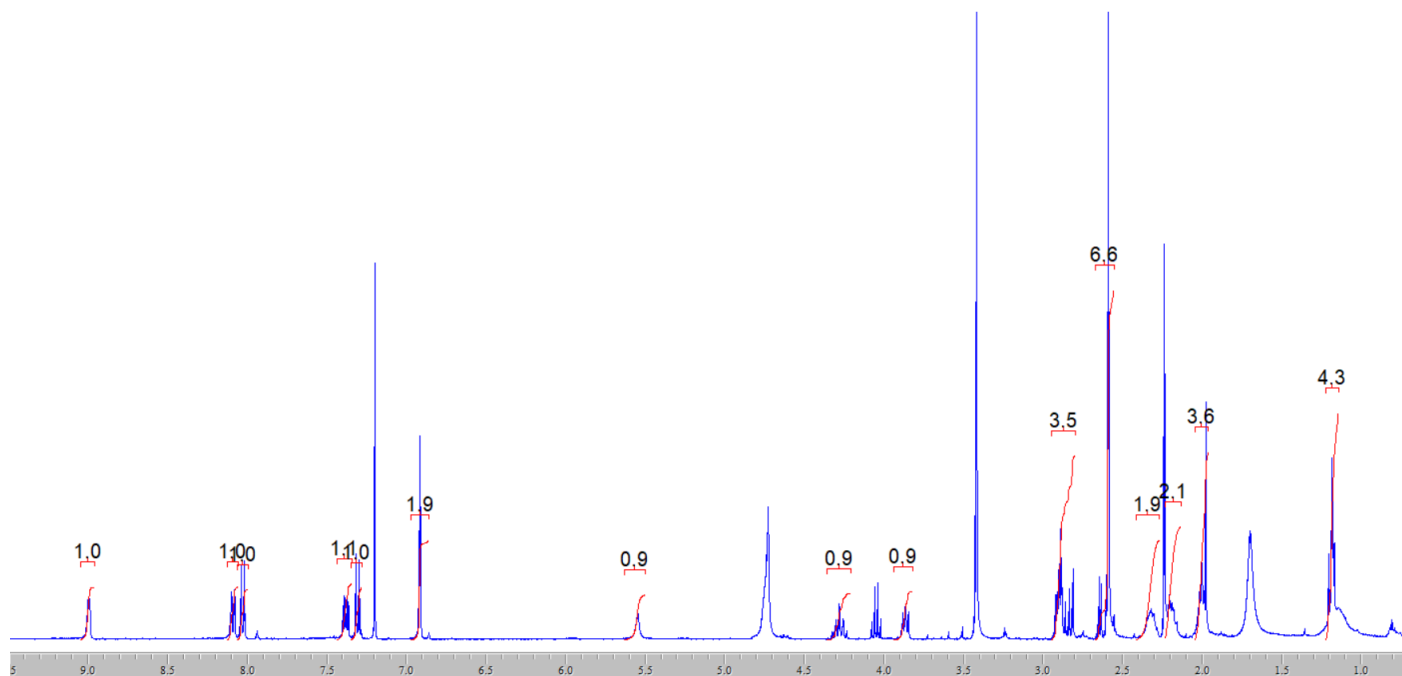
F1 - Processing parameters
SI 1024
MC2 QF
SF 100.6127690 MHz
WDW Q81NK
SFB 2
LB 0.00 Hz
GB 0



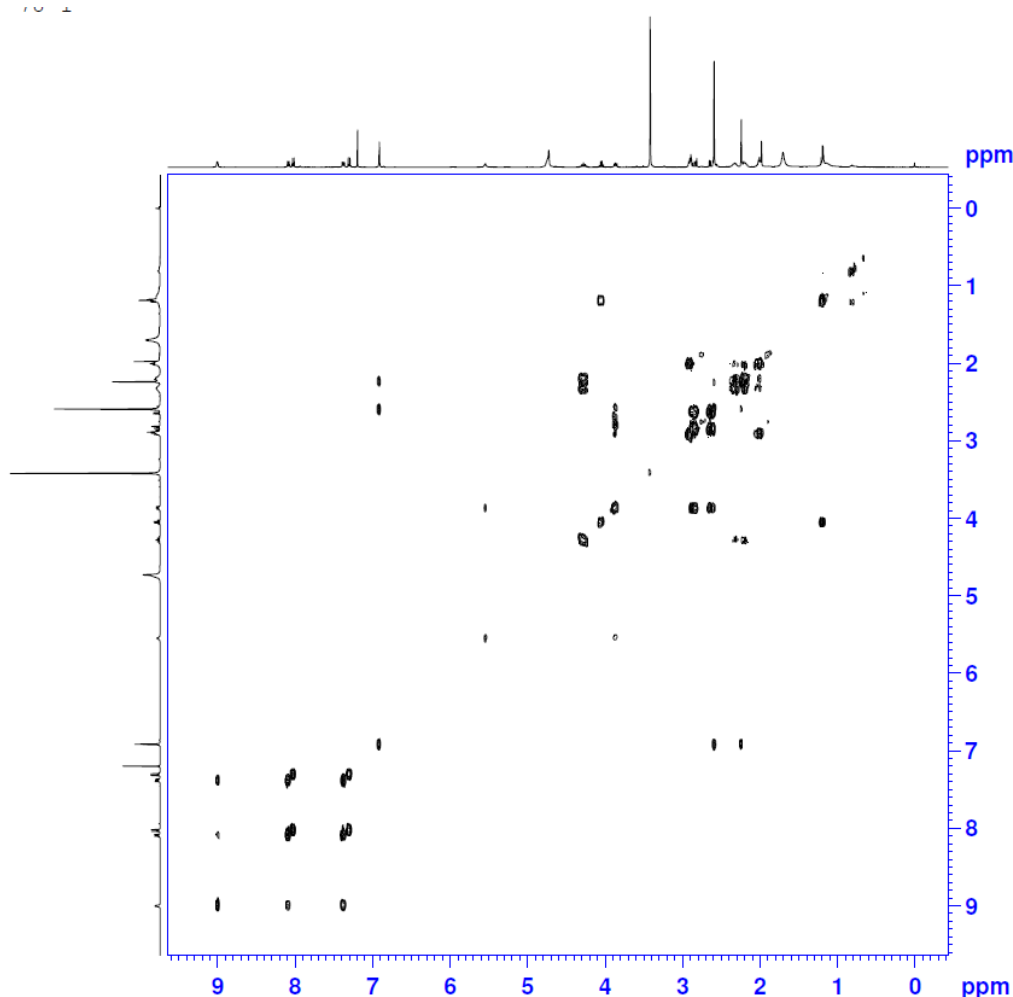
N-((*S*)-1-((1*r**,3*R**)-3-(2-(1,8-Naphthyridin-2-yl)ethyl)cyclobutyl)-2,5-dioxopyrrolidin-3-yl)-2,4,6-



trimethylbenzenesulfonamide [Compound 31]



0.7 0.1



Current Data Parameters
NAME set7-78-1
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120328
Time 23.49
INSTRUM DFX400
PROBHD 5 mm QNP 1H/13
PULPROG cosygpmzg5
ID 2048
SOLVENT CDCl3
NS 4
DS 8
SWH 4032.258 Hz
FIDRES 1.968876 Hz
AQ 0.2540020 sec
RG 8192
DW 124.000 usec
DE 6.00 usec
TE 294.2 K
D0 0.00000300 sec
D1 1.93774104 sec
d13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00024800 sec

----- CHANNEL f1 -----
NUC1 13
P1 10.00 usec
PL1 -1.50 dB
SF01 400.1318765 MHz

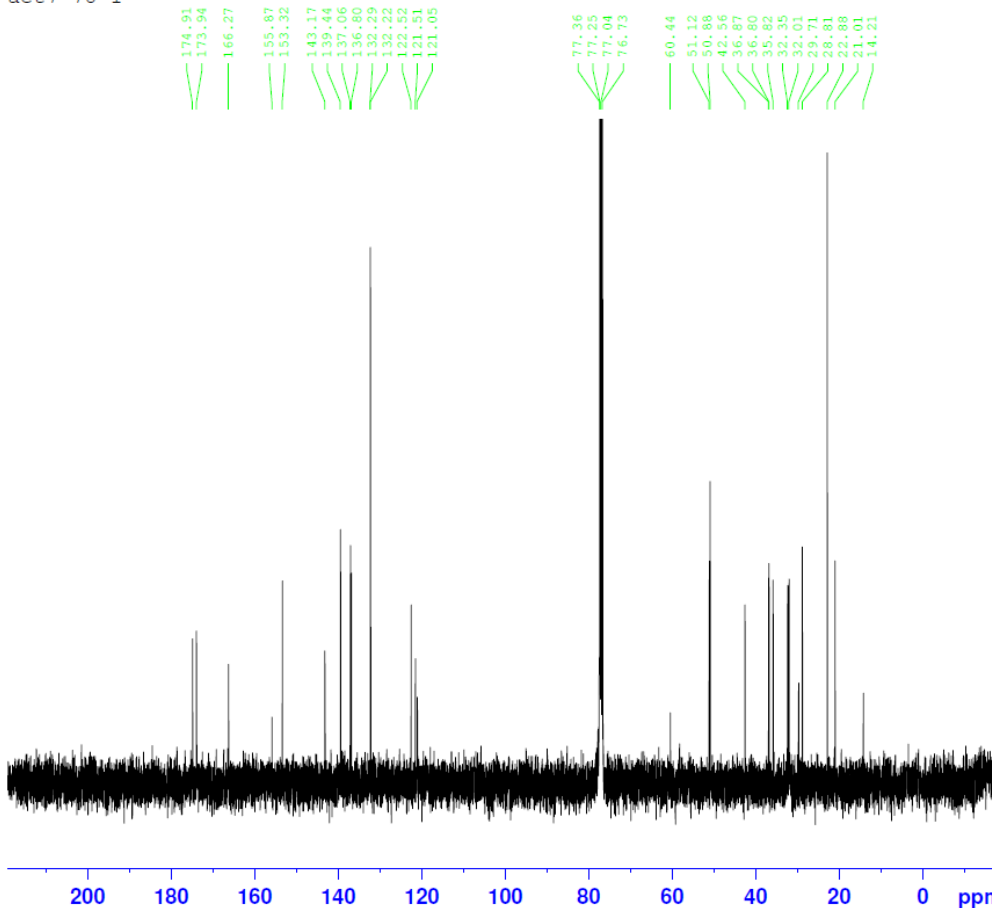
----- GRADIENT CHANNEL -----
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 16.00 %
GPZ2 12.00 %
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
ND0 1
ID 128
SF01 400.1319 MHz
FIDRES 31.502016 Hz
SW 10.077 ppm
F1MODE QF

F2 - Processing parameters
SI 1024
SF 400.1300339 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
FC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.1300339 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

aet7-78-1



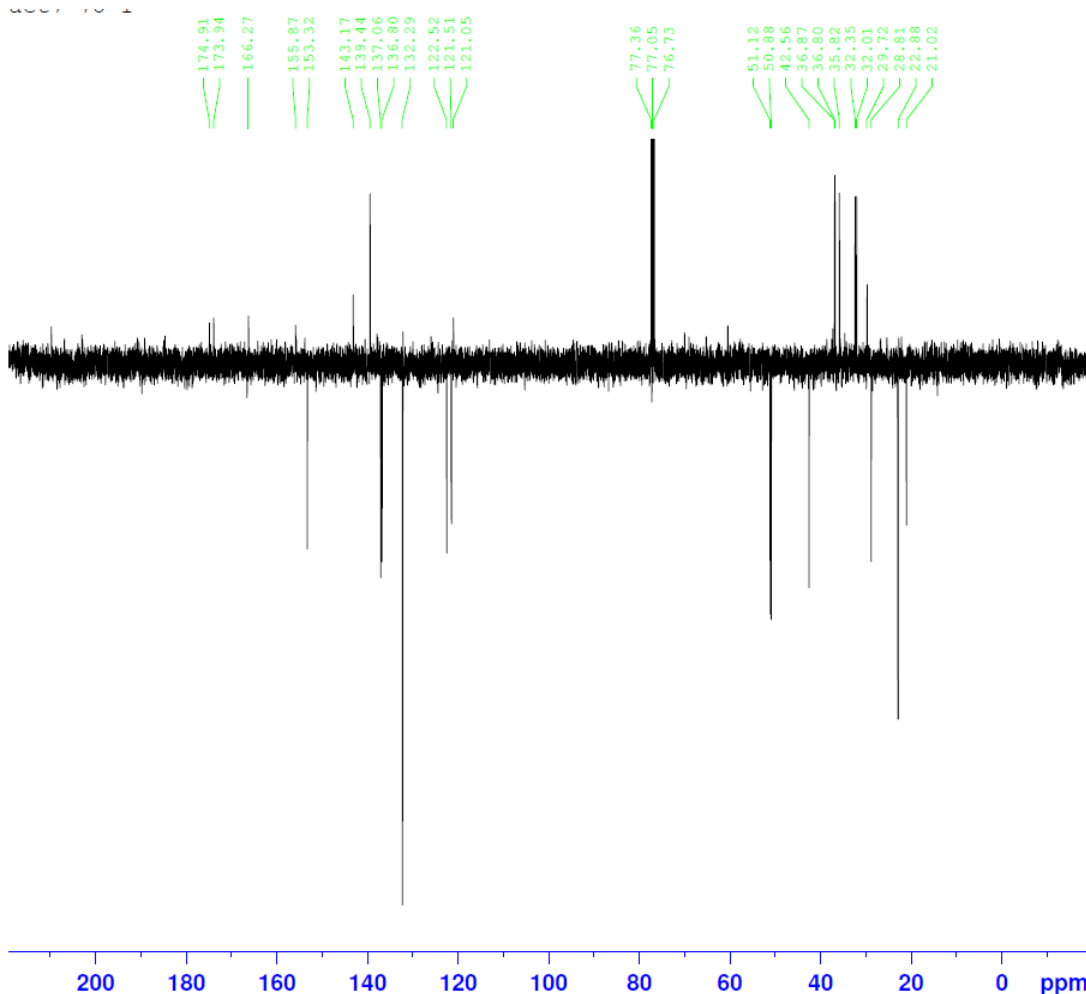
Current Data Parameters
 NAME aet7-78-1
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120328
 Time 23.18
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 724.1
 DW 20.850 usec
 DE 6.00 usec
 TE 295.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 PL1 -2.60 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 PL13 17.50 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



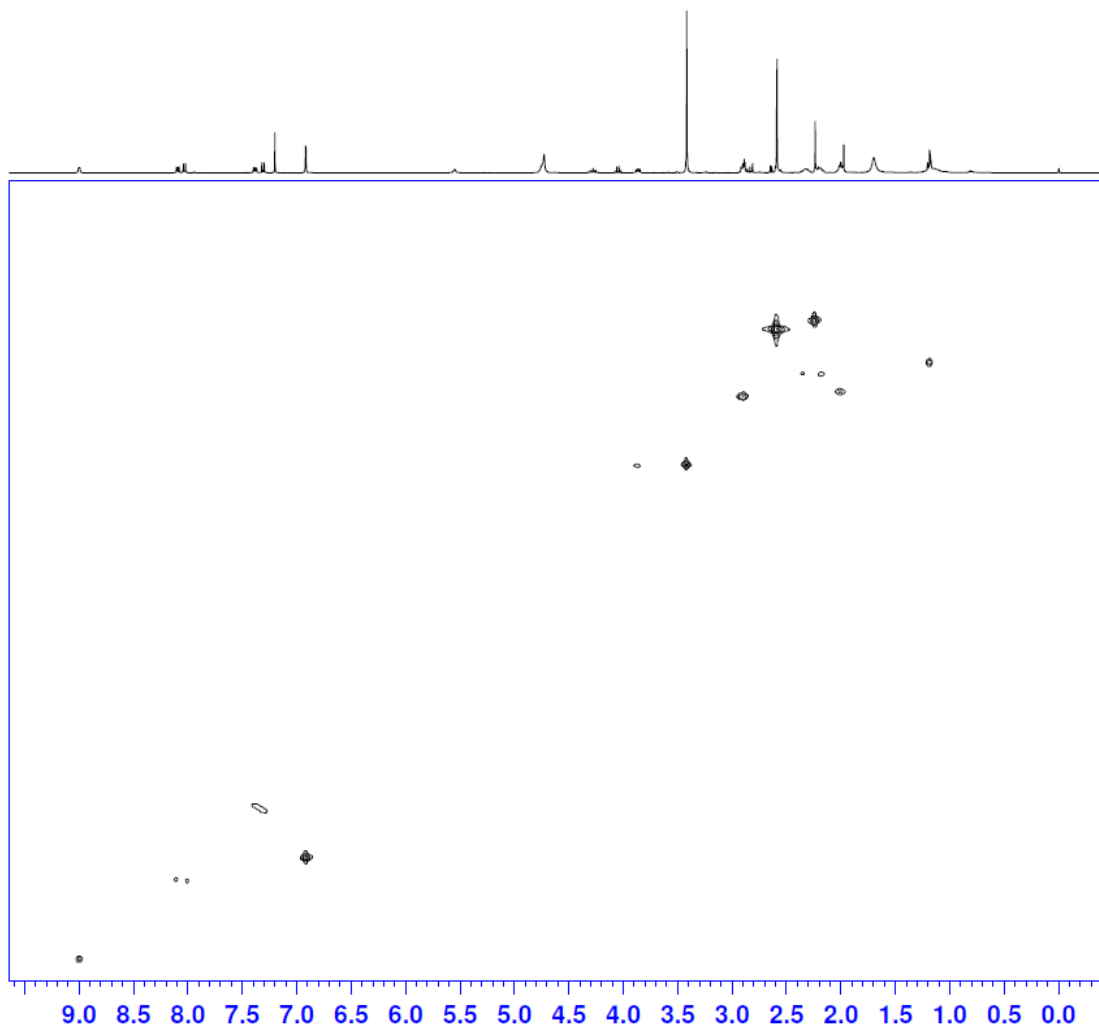
Current Data Parameters
 NAME aet7-78-1
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120328
 Time 23.48
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG deptq_135
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 11585.2
 DW 20.850 usec
 DE 6.00 usec
 TE 294.2 K
 CNST2 145.0000000
 D1 2.00000000 sec
 d2 0.00344828 sec
 D11 0.03000000 sec
 DELTA 0.00001082 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 P2 17.00 usec
 PL1 -2.60 dB
 SFO1 100.6228300 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 SFO2 400.1316000 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
NAME act7-78-1
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120329
Time 0.09
INSTRUM DRX400
PROBHD 5 mm QNP 1H/13
PULPROG hmqcpggf
TD 1024
SOLVENT CDCl3
NS 4
DS 16
SWH 4032.258 Hz
FIDRES 3.937752 Hz
AQ 0.1270260 sec
RG 26008
DW 124.000 usec
DE 6.00 usec
TE 294.2 K
CNS12 145.0000000 sec
d0 0.0000300 sec
d1 1.50000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
d13 0.00000400 sec
d14 0.00020000 sec
DELTA1 0.00222428 sec
IN0 0.00003000 sec

==== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
P2 20.00 usec
PL1 -1.50 dB
SFO1 400.1318765 MHz

==== CHANNEL f2 =====
CPDPRG2 garp
NUC2 13C
P3 8.00 usec
PCPD2 74.00 usec
PL2 -3.00 dB
PL12 18.00 dB
SFO2 100.6203140 MHz

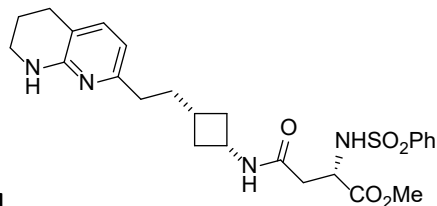
==== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 50.00 %
GPZ2 50.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
ND0 2
TD 128
SFO1 100.6203 MHz
FIDRES 130.208328 Hz
SW 165.639 ppm
FrMODE QF

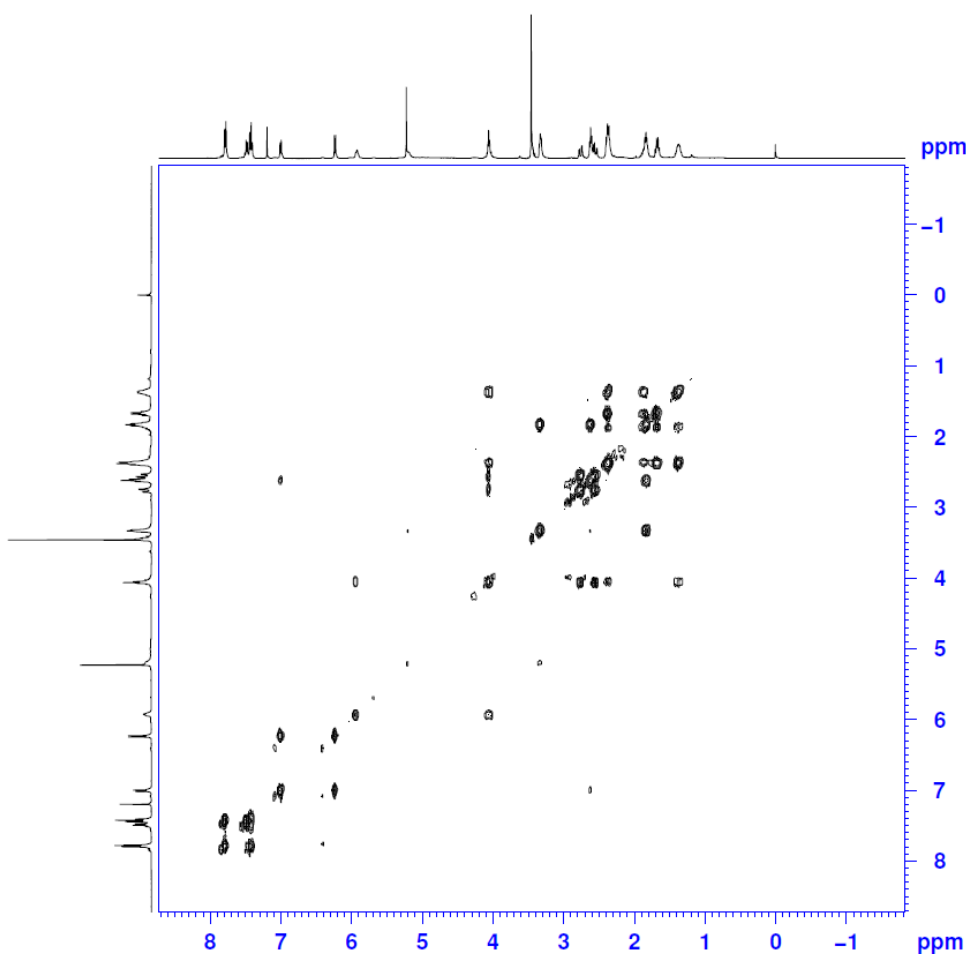
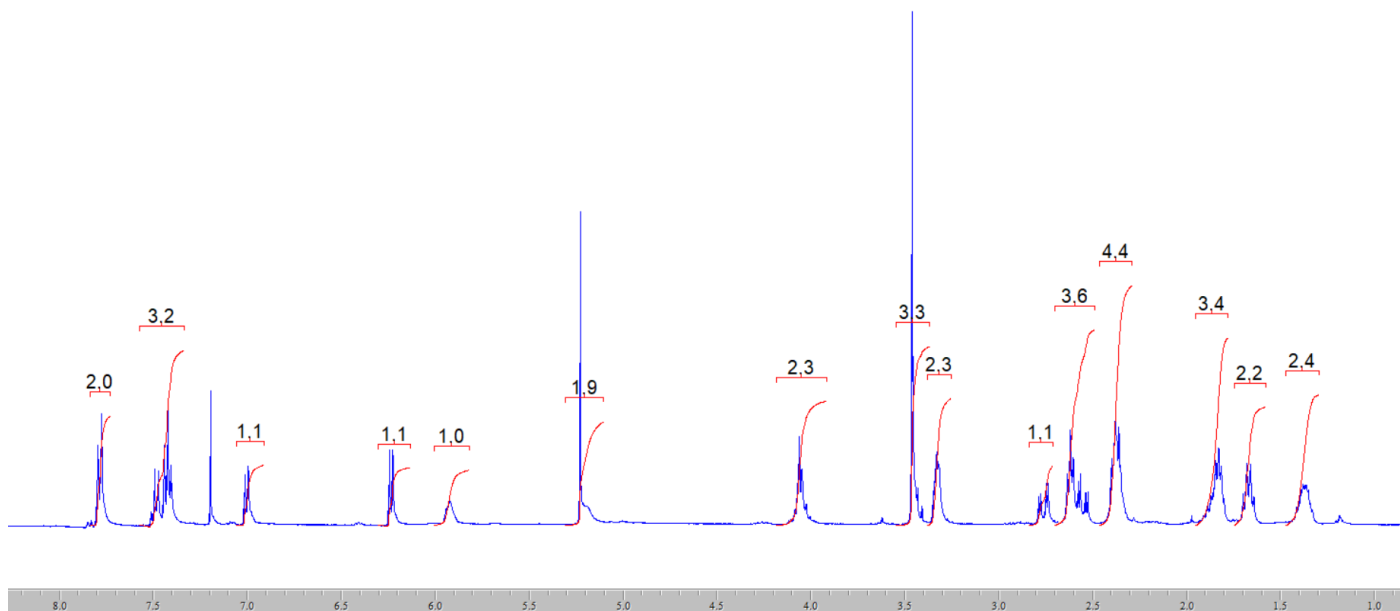
F2 - Processing parameters
SI 1024
SF 400.1300339 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 100.6127690 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

Methyl *N*²-(phenylsulfonyl)-*N*⁴-((1*r**,3*R**)-3-(2-(5,6,7,8-tetrahydro-1,8-naphthyridin-2-



yl)ethyl)cyclobutyl)-*L*-asparaginate [Compound 32]



Current Data Parameters
 NAME aet7-93-2
 EXPNO 13
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120608
 Time 22.11
 INSTRUM DFX400
 PROBHD 5 mm QNP 1H/13
 PULPROG cosygpmzgqf
 ID 2048
 SOLVENT CDCl3
 NS 4
 DS 8
 SWH 4222.973 Hz
 FIDRES 2.061999 Hz
 AQ 0.2425332 sec
 RG 5160.6
 DW 118.400 usec
 DE 6.00 usec
 TE 298.2 K
 D0 0.0000300 sec
 D1 1.95002902 sec
 d13 0.00000400 sec
 D16 0.00020000 sec
 INO 0.00023680 sec

----- CHANNEL f1 -----
 NUC1 13
 P1 10.00 usec
 PL1 -1.50 dB
 SFO1 400.1314144 MHz

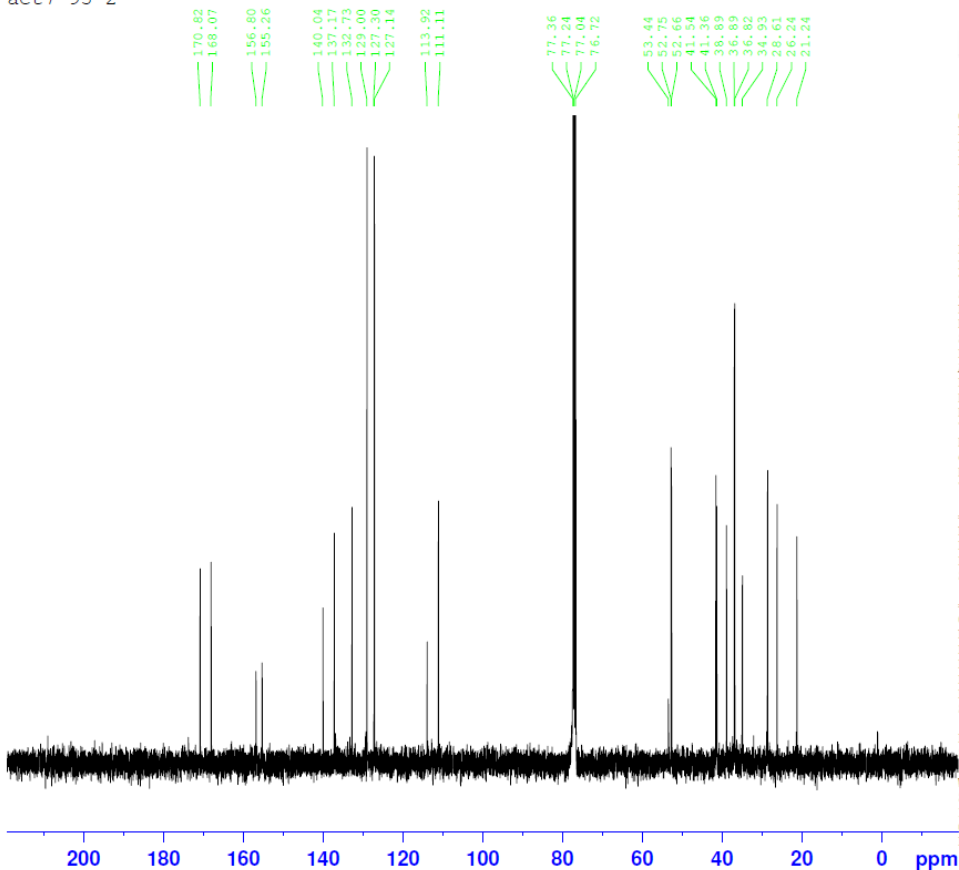
----- GRADIENT CHANNEL -----
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPNAM3 SINE.100
 GPZ1 16.00 %
 GPZ2 12.00 %
 GPZ3 40.00 %
 P16 1000.00 usec

F1 - Acquisition parameters
 NDO 1
 ID 128
 SFO1 400.1314 MHz
 FIDRES 32.991978 Hz
 SW 10.554 ppm
 FqMODE QF

F2 - Processing parameters
 SI 1024
 SF 400.1300344 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 400.1300344 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

aet7-93-2



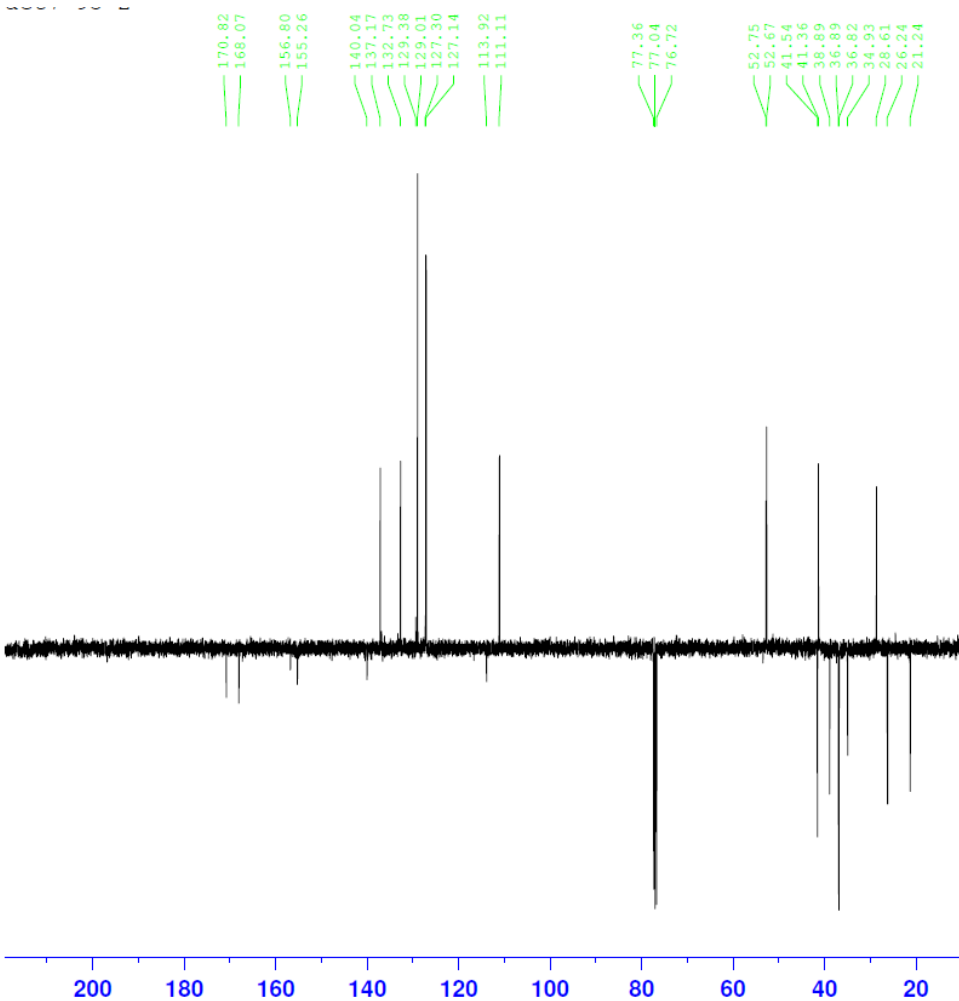
Current Data Parameters
 NAME aet7-93-2
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120608
 Time 21.40
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 812.7
 DW 20.850 usec
 DE 6.00 usec
 TE 298.2 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 PL1 -2.60 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 PL13 17.50 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



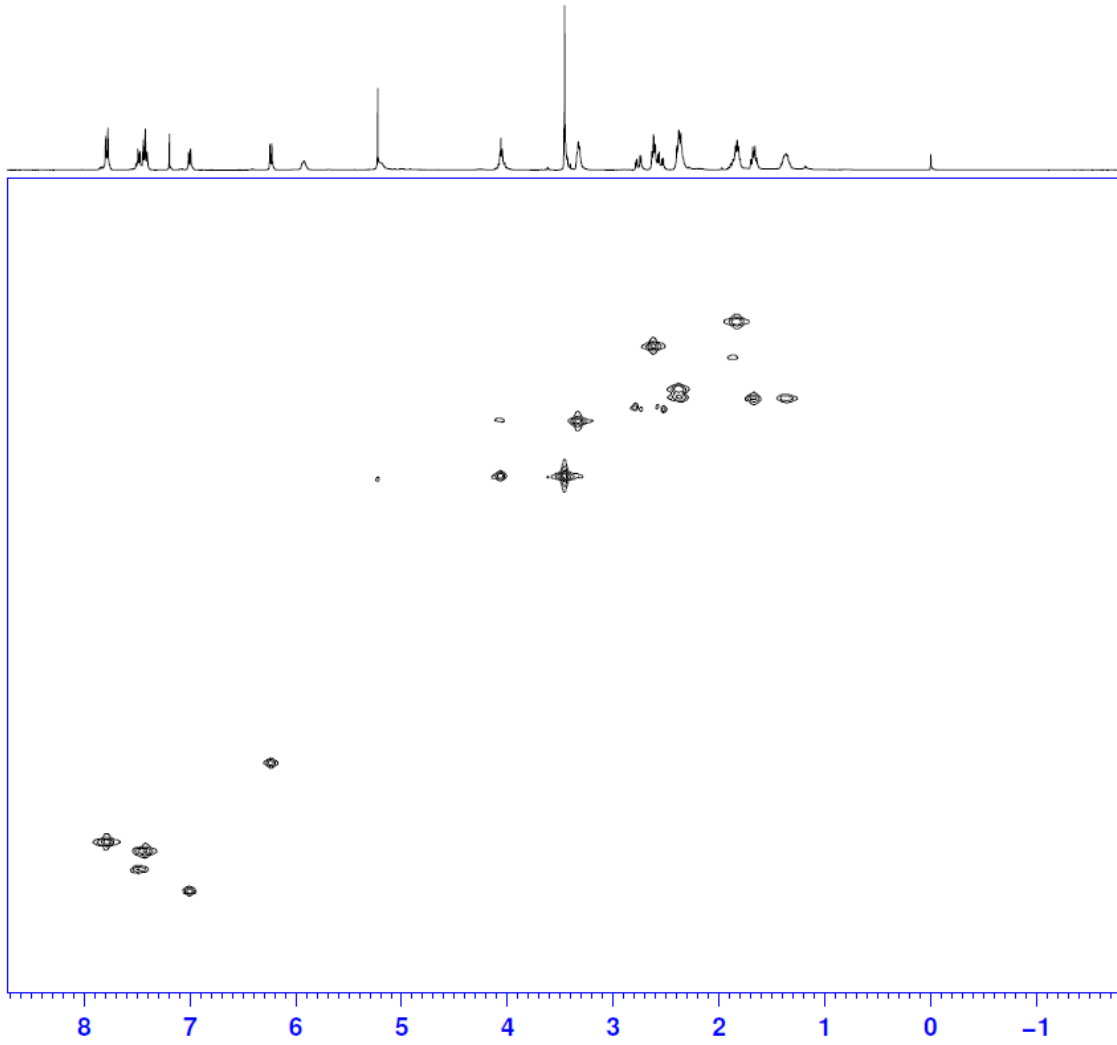
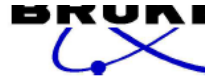
Current Data Parameters
 NAME aet7-93-2
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120608
 Time 22.10
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG deptq_135
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 18390.4
 DW 20.850 usec
 DE 6.00 usec
 TE 298.2 K
 CNST2 145.0000000
 D1 2.0000000 sec
 d2 0.00344828 sec
 D11 0.0300000 sec
 DELTA 0.00001082 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 P2 17.00 usec
 PL1 -2.60 dB
 SFO1 100.6228300 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 SFO2 400.1316000 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
NAME sat7-93-2
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120608
Time 22.31
INSTRUM DPK400
PROBHD 5 mm QNP 1H/13
PULPROG hmqcqpqf
TD 1024
SOLVENT CDCl3
NS 4
DS 16
SWH 4222.973 Hz
FIDRES 4.123997 Hz
AQ 0.1212916 sec
RG 8192
DW 118.400 usec
DE 6.00 usec
TE 298.2 K
CNST2 145.0000000
d0 0.0000300 sec
d1 1.50614405 sec
d2 0.00344828 sec
d12 0.00002000 sec
d13 0.00000400 sec
d16 0.00020000 sec
DELTA1 0.00222428 sec
IN0 0.00003000 sec

==== CHANNEL F1 ====
NUC1 1H
P1 10.00 usec
P2 20.00 usec
PL1 -1.50 dB
SFO1 400.1314144 MHz

==== CHANNEL F2 ====
CPDPRG2 gqcp
NUC2 13C
P3 8.00 usec
PCPD2 74.00 usec
PL2 -3.00 dB
PL12 18.00 dB
SFO2 100.6203140 MHz

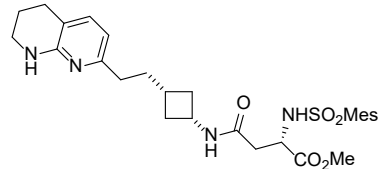
==== GRADIENT CHANNEL ====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
F16 1000.00 usec

F1 - Acquisition parameters
NDO 2
TD 128
SFO1 100.6203 MHz
FIDRES 130.208328 Hz
SW 165.639 ppm
FMODE QF

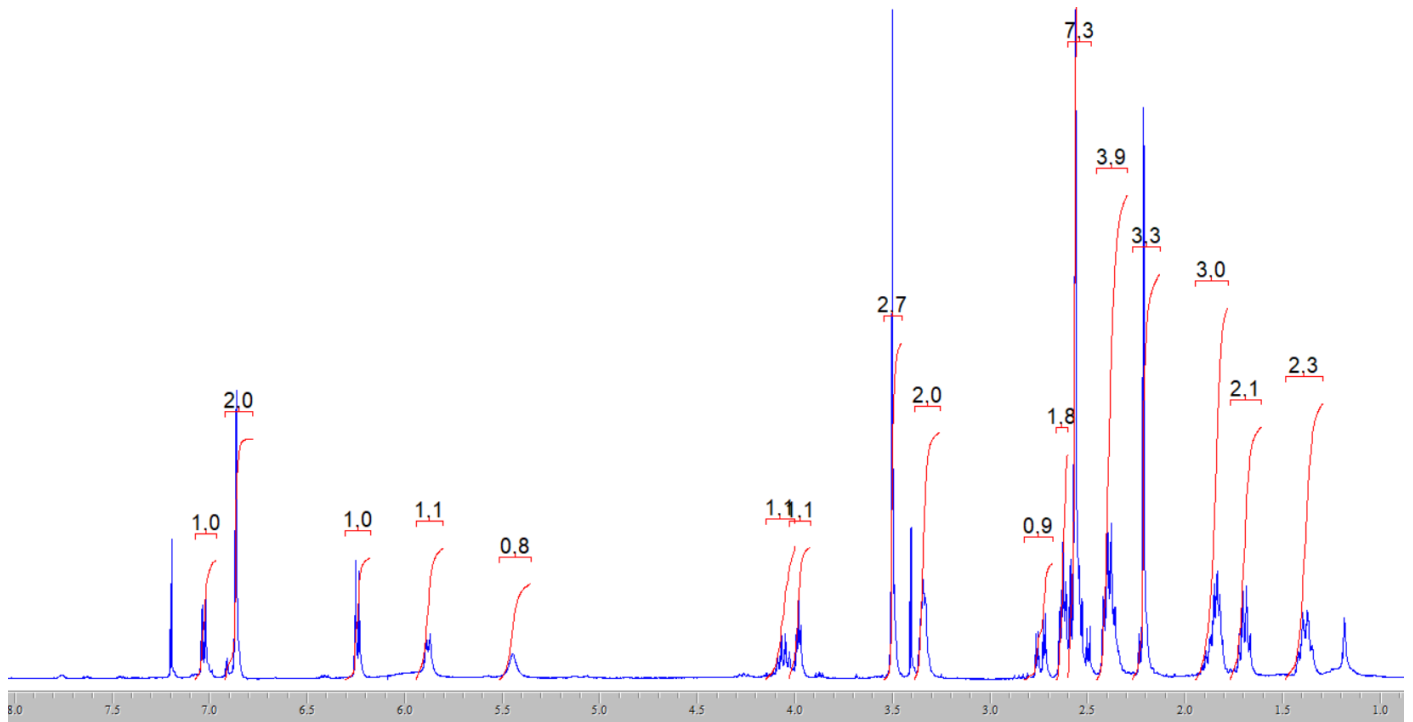
F2 - Processing parameters
SI 1024
SF 400.1300344 MHz
WDW QSSINE
SBB 2
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 100.6127690 MHz
WDW QSSINE
SBB 2
LB 0.00 Hz
GB 0

Methyl *N*²-(mesitylsulfonyl)-*N*⁴-((1*r**,3*R**)-3-(2-(5,6,7,8-tetrahydro-1,8-naphthyridin-2-



yl)ethyl)cyclobutyl)-*L*-asparaginate [Compound 33]



Current Data Parameters
 NAME set7-96-2a
 EXPNO 14
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120618
 Time 19.53
 INSTRUM dpx400
 PROBHD 5 mm QNP 1H/13
 PULPROG cosygmrgf
 ID 2048
 SOLVENT CDCl3
 NS 4
 DS 8
 SWH 3654.971 Hz
 FIDRES 1.784654 Hz
 AQ 0.2802164 sec
 RG 2896.3
 DW 136.900 usec
 DE 6.00 usec
 TE 298.2 K
 DO 0.00000300 sec
 D1 1.91111696 sec
 d13 0.00000400 sec
 D16 0.00020000 sec
 IN0 0.00027360 sec

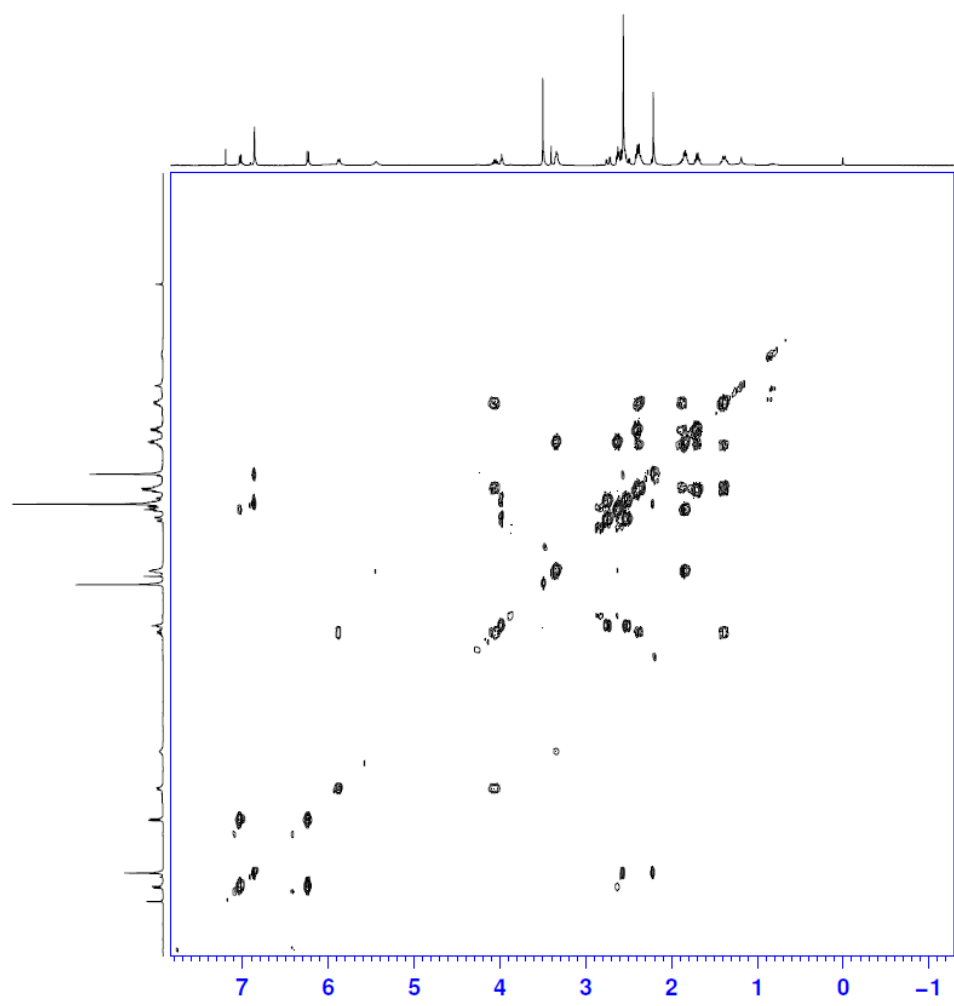
----- CHANNEL f1 -----
 NUC1 1H
 P1 10.00 usec
 PL1 -1.50 dB
 SFO1 400.1313427 MHz

----- GRADIENT CHANNEL -----
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPNAM3 SINE.100
 GPZ1 16.00 %
 GPZ2 12.00 %
 GPZ3 40.00 %
 P16 1000.00 usec

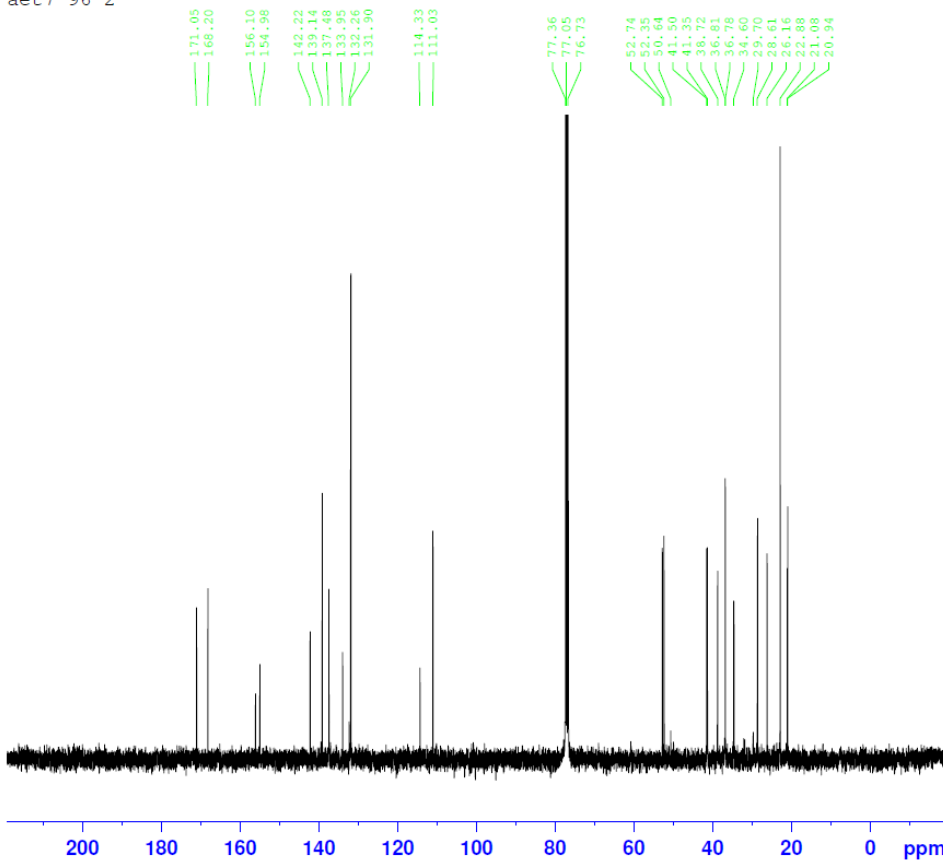
F1 - Acquisition parameters
 ND0 1
 ID 128
 SFO1 400.1313 MHz
 FIDRES 28.554459 Hz
 SW 9.134 ppm
 FMODE QF

F2 - Processing parameters
 SI 1024
 SF 400.1300342 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 FC 1.40

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 400.1300342 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0



aet7-96-2



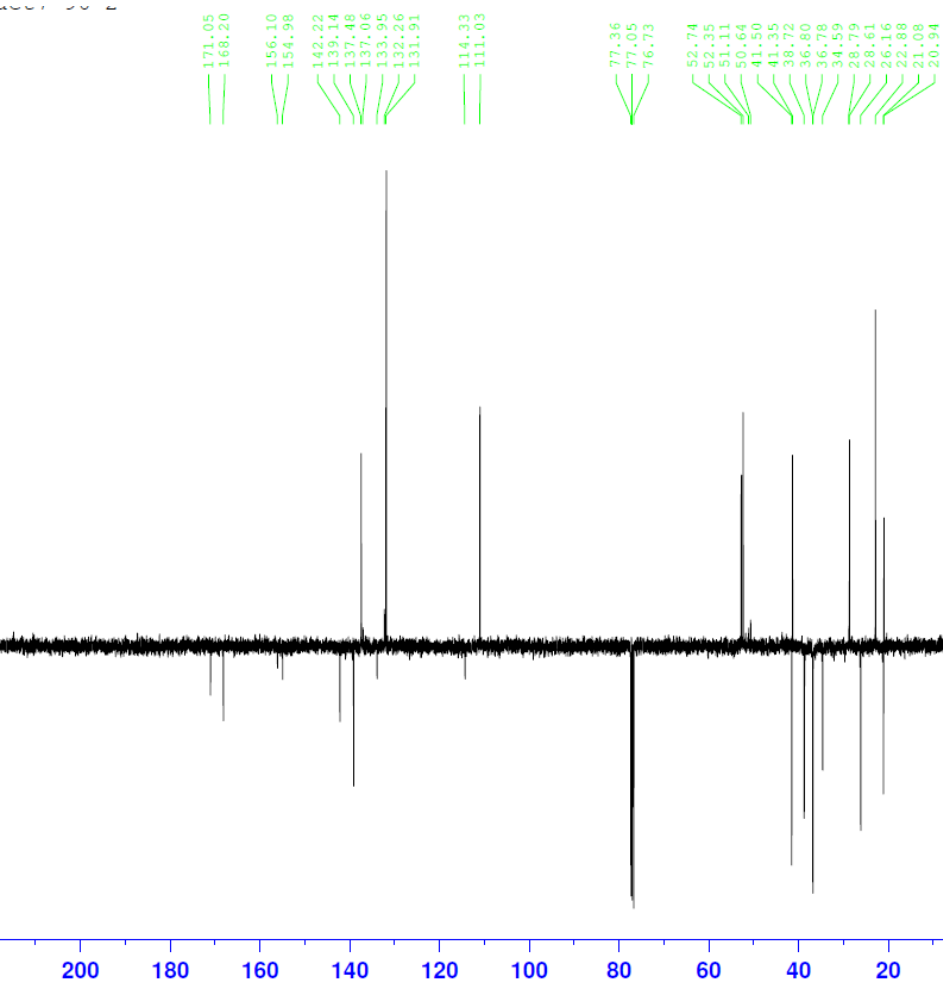
Current Data Parameters
 NAME aet7-96-2a
 EXPNO 20
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120618
 Time 19.06
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 1024
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 912.3
 DW 20.850 usec
 DE 6.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 PL1 -2.60 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 PL13 17.50 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
 NAME aet7-96-2a
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120618
 Time 19.36
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG deptq_135
 TD 65536
 SOLVENT CDC13
 NS 512
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 11585.2
 DW 20.850 usec
 DE 6.00 usec
 TE 298.2 K
 CNST2 145.0000000
 D1 2.00000000 sec
 d2 0.00344828 sec
 D11 0.03000000 sec
 DELTA 0.00001082 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 P2 17.00 usec
 PL1 -2.60 dB
 SFO1 100.6228300 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 SFO2 400.1316000 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Current Data Parameters
 NAME ast7-96-2a
 EXPNO 13
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120618
 Time 19:38
 INSTRUM DFX400
 PROBHD 5 mm QNP 1H/13
 PULPROG hmqcpgpgf
 TD 1024
 SOLVENT CDCl3
 NS 4
 DS 16
 SWH 3654.971 Hz
 FIDRES 3.569307 Hz
 AQ 0.1401332 sec
 RG 26008
 DW 136.800 usec
 DE 6.00 usec
 TE 298.2 K
 C12 145.0000000 sec
 d0 0.000003000 sec
 d1 1.48668802 sec
 d2 0.0034828 sec
 d12 0.00002000 sec
 d13 0.00000400 sec
 D16 0.00020000 sec
 DELTA1 0.00222428 sec
 INO 0.00003000 sec

==== CHANNEL F1 =====
 NUC1 1H
 P1 10.00 usec
 p2 20.00 usec
 PL1 -1.50 dB
 SFO1 400.1313427 MHz

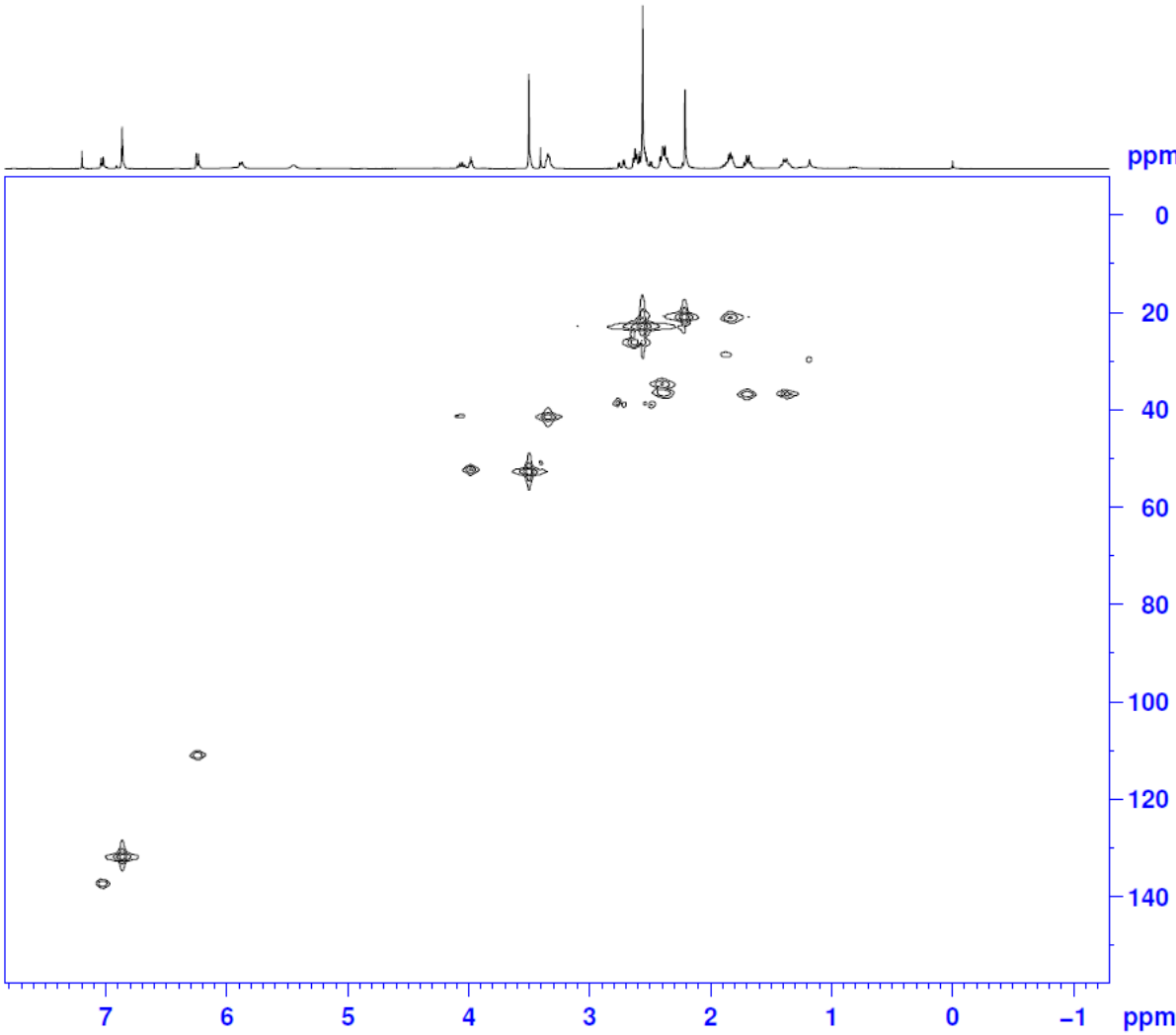
==== CHANNEL F2 =====
 CPDPRG2 gcp
 NUC2 13C
 P3 8.00 usec
 PCPD2 74.00 usec
 PL2 -3.00 dB
 PL12 18.00 dB
 SFO2 100.6203140 MHz

==== GRADIENT CHANNEL =====
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPNAM3 SINE.100
 GPZ1 50.00 %
 GPZ2 30.00 %
 GPZ3 40.10 %
 P16 1000.00 usec

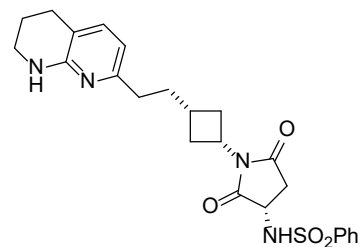
F1 - Acquisition parameters
 ND0 2
 TD 128
 SFO1 100.6203 MHz
 FIDRES 130.208328 Hz
 SW 165.639 ppm
 F1MODE QF

F2 - Processing parameters
 SI 1024
 SF 400.1300342 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 FC 1.40

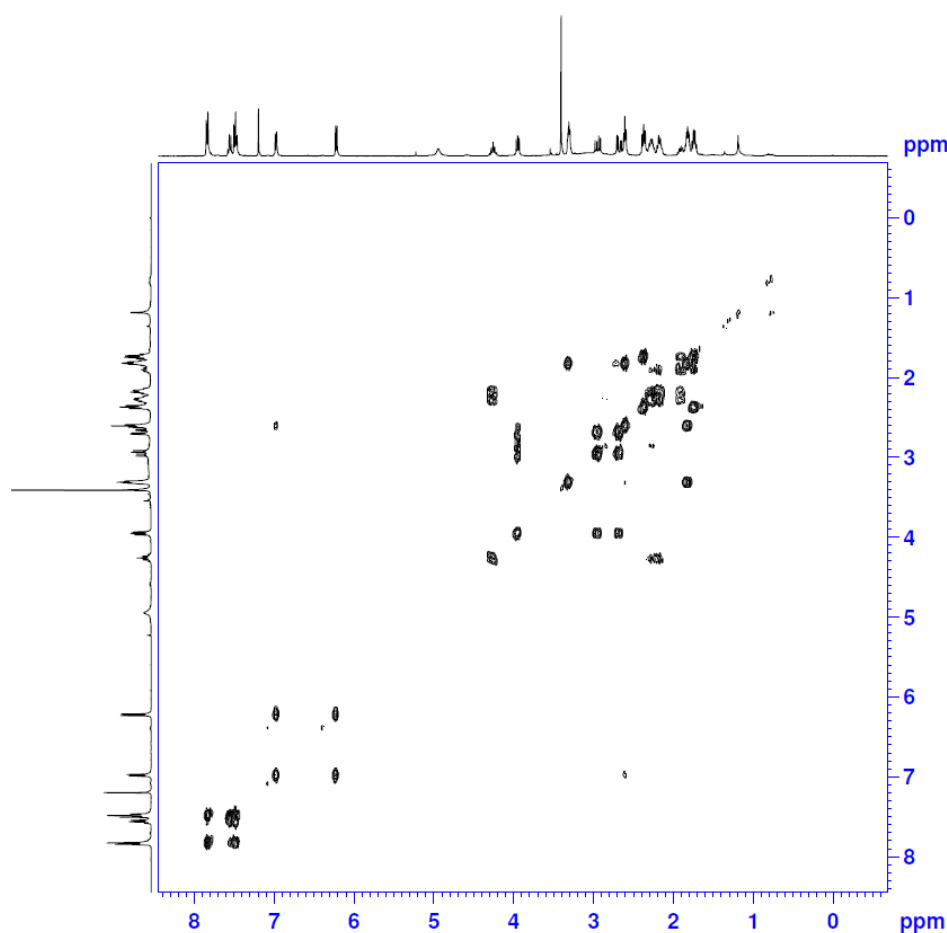
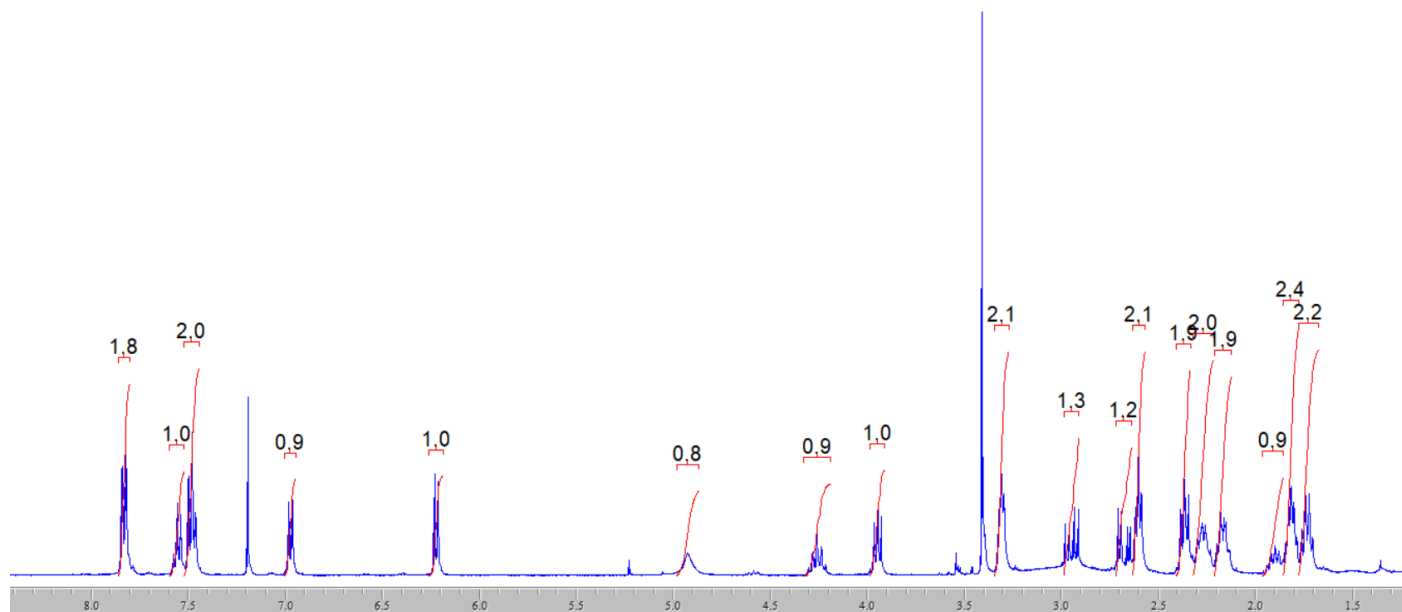
F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 100.6127690 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0



N-((*S*)-2,5-dioxo-1-((1*r**,3*R**)-3-(2-(5,6,7,8-tetrahydro-1,8-naphthyridin-2-



yl)ethyl)cyclobutyl)pyrrolidin-3-yl)benzenesulfonamide [Compound 34]



Current Data Parameters
NAME aet9-1-2
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120623
Time 2.35
INSTRUM spect400
PROBHD 5 mm QNP 1H/13
PULPROG cosygmfzf
TD 2048
SOLVENT cdcl3
NS 4
DS 8
SWH 3654.971 Hz
FIDRES 1.784654 Hz
AQ 0.2802164 sec
RG 4096
DW 136.800 usec
DE 6.00 usec
TE 298.2 K
D0 0.0000300 sec
D1 1.9111696 sec
d13 0.0000400 sec
D16 0.0002000 sec
IN0 0.00027360 sec

CHANNEL f1
NUC1 13C
P1 10.00 usec
PL1 -1.50 dB
SFO1 400.1315885 MHz

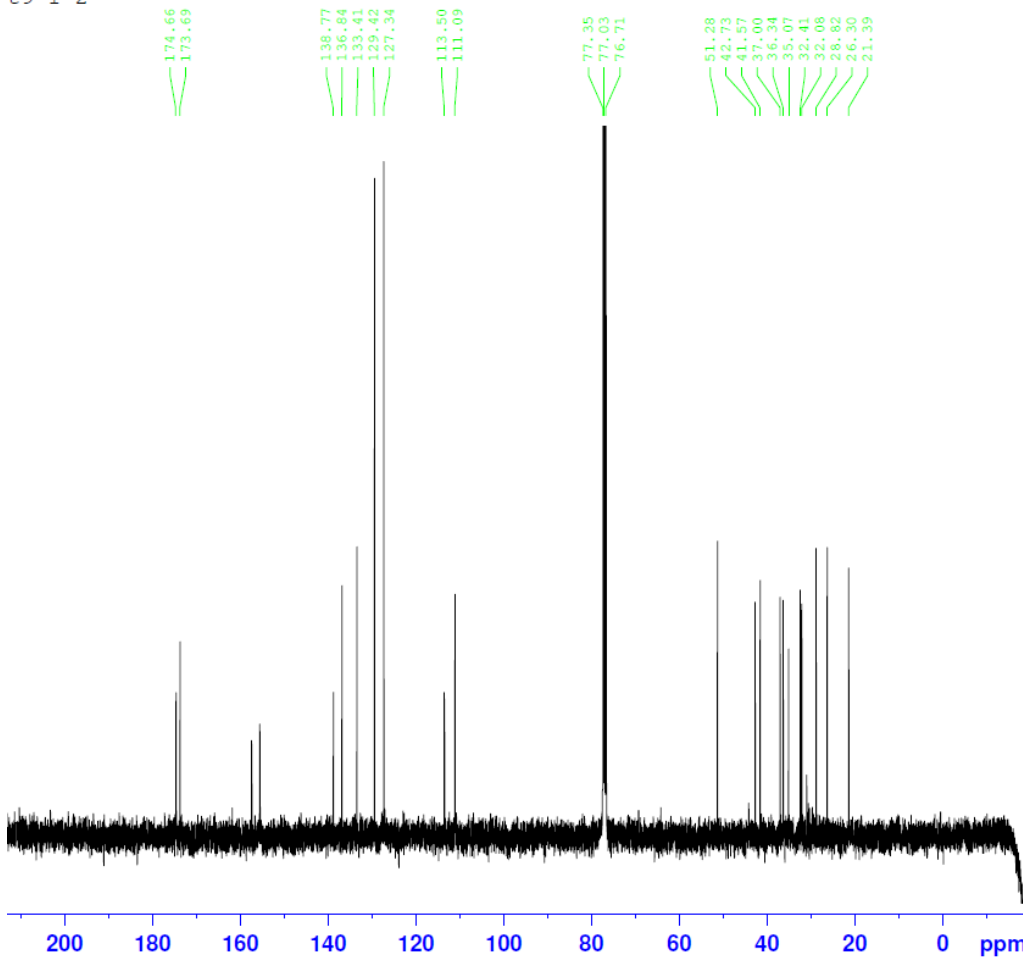
GRADIENT CHANNEL
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 15.00 %
GPZ2 12.00 %
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
ND0 1
TD 128
SFO1 400.1316 MHz
FIDRES 28.554459 Hz
SW 9.134 ppm
FMODE QF

F2 - Processing parameters
SI 1024
SF 400.1300355 MHz
WVW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.1300355 MHz
WVW SINE
SSB 0
LB 0.00 Hz
GB 0

t9-1-2



Current Data Parameters
 NAME aet9-1-2
 EXPNO 30
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120705
 Time 20.26
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 1024
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 912.3
 DW 20.850 usec
 DE 6.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 PL1 -2.60 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 PL13 17.50 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
 NAME aet9-1-2
 EXPNO 13
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120705
 Time 20.59
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG hmqcgpuf
 TD 1024
 SOLVENT CDC13
 NS 16
 DS 4
 SWH 4166.667 Hz
 FIDRES 4.069010 Hz
 AQ 0.1229300 sec
 RG 7298.2
 DW 120.000 usec
 DE 6.00 usec
 TE 298.2 K
 CNST2 145.0000000
 d0 0.0000300 sec
 D1 1.50409603 sec
 d2 0.00344828 sec
 d12 0.00002000 sec
 d13 0.00000400 sec
 D16 0.00020000 sec
 DELTA1 0.00222428 sec
 INO 0.00003000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 P2 20.00 usec
 PL1 -1.50 dB
 SFO1 400.1313712 MHz

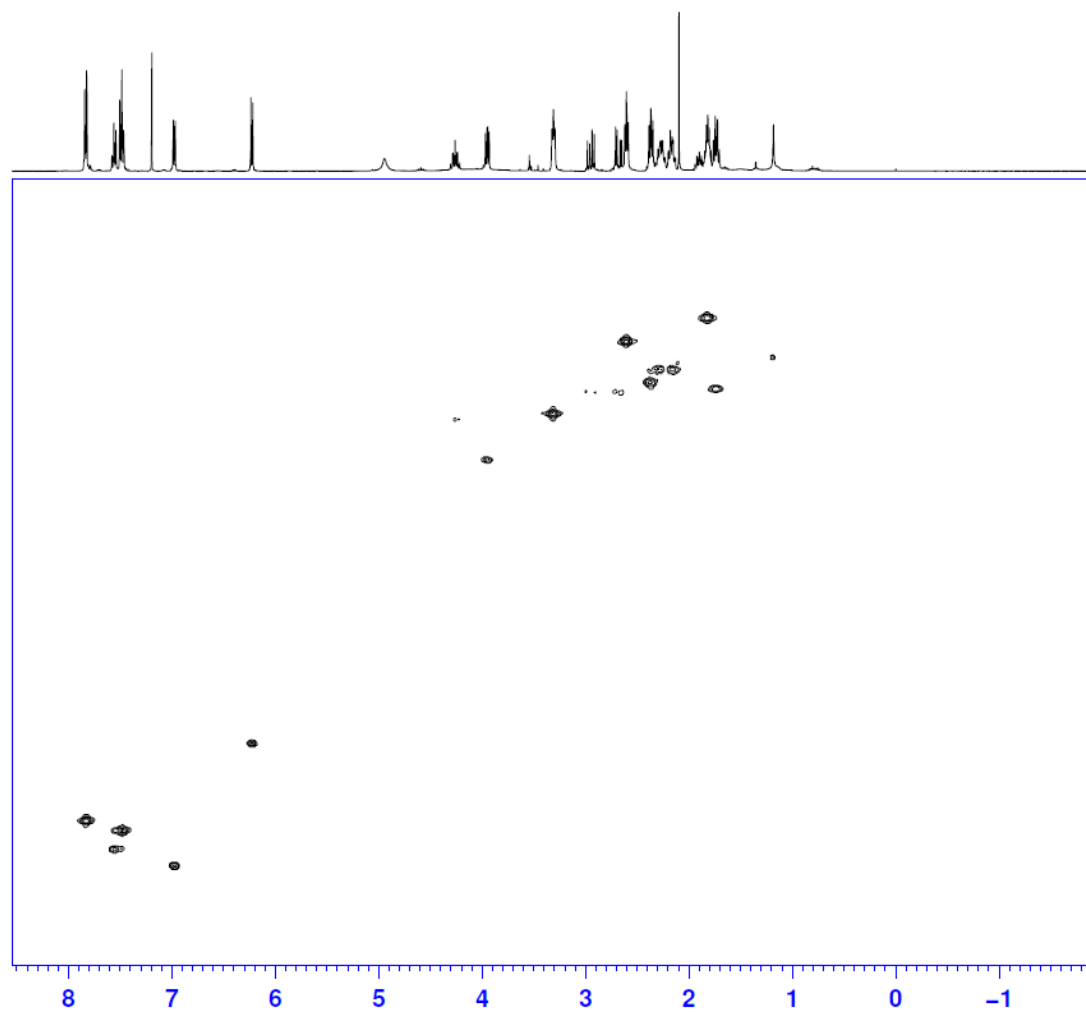
===== CHANNEL f2 =====
 CPDPRG2 gprp
 NUC2 13C
 P3 8.00 usec
 PCPD2 74.00 usec
 PL2 -3.00 dB
 PL12 18.00 dB
 SFO2 100.6203140 MHz

===== GRADIENT CHANNEL =====
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPNAM3 SINE.100
 GPZ1 50.00 %
 GPZ2 30.00 %
 GPZ3 40.10 %
 P16 1000.00 usec

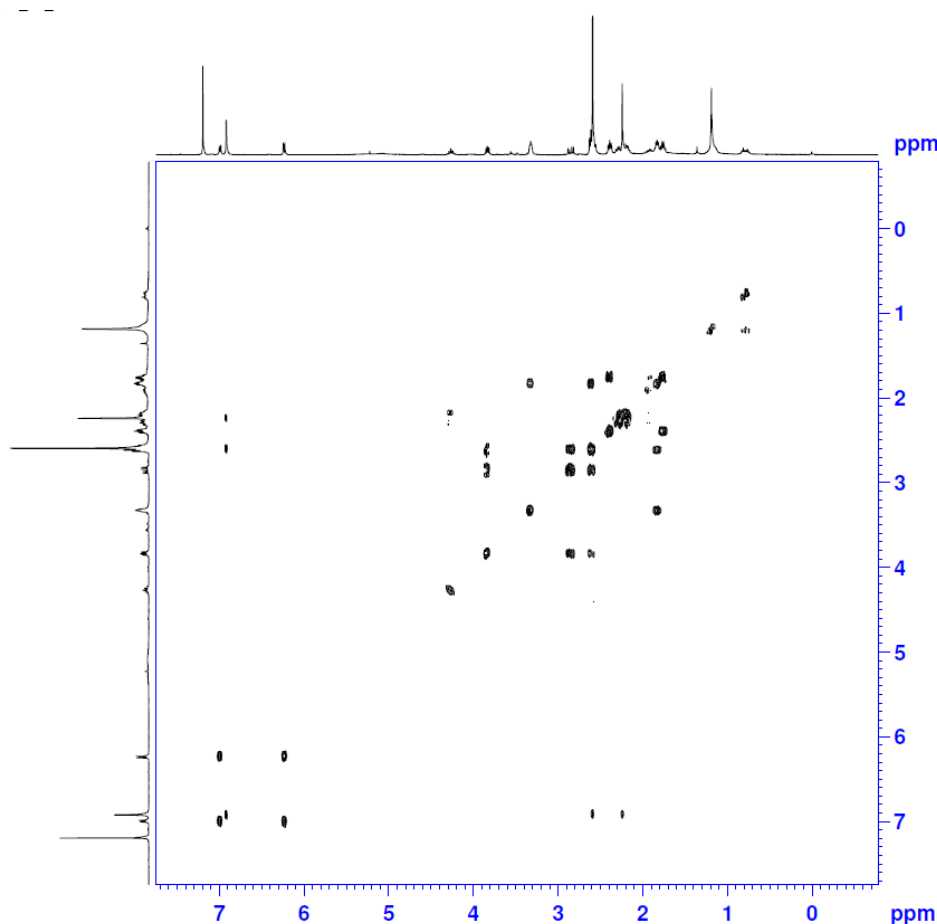
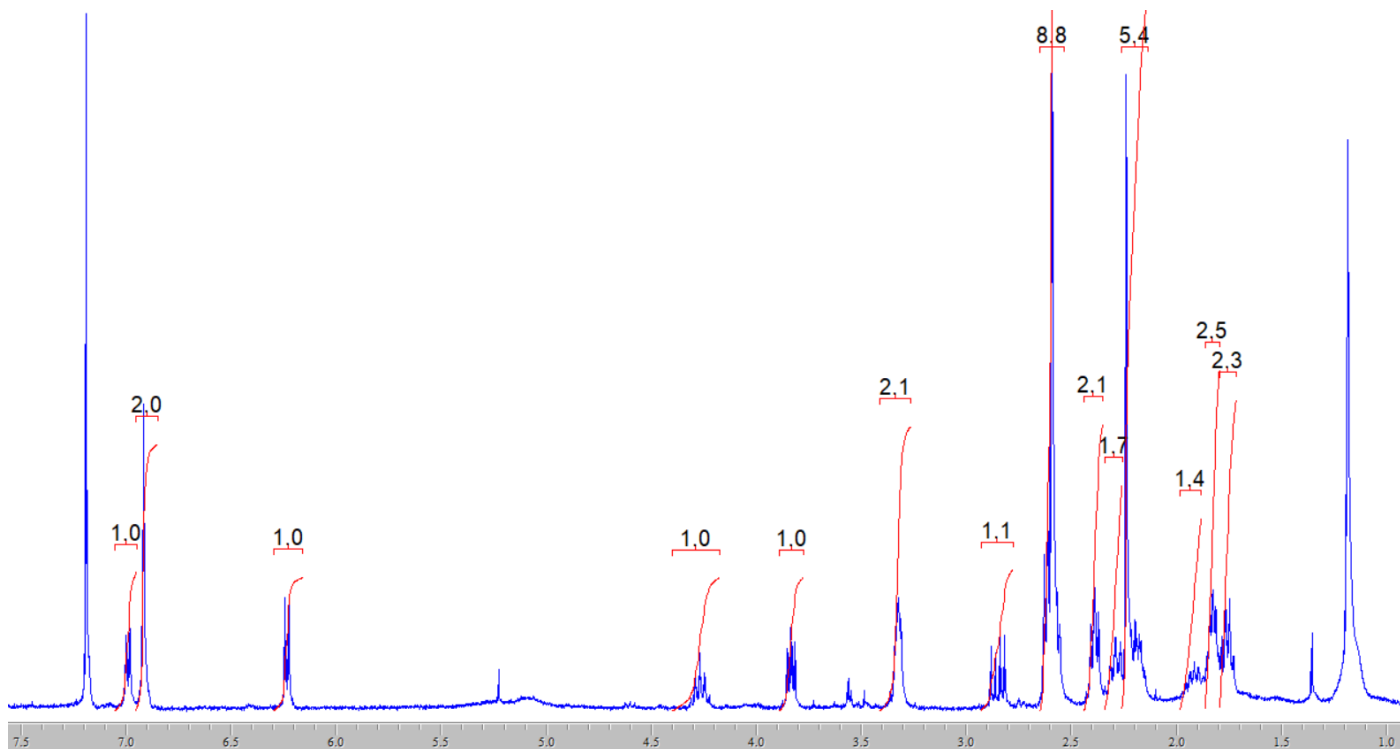
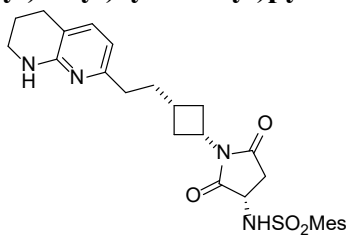
F1 - Acquisition parameters
 ND0 2
 TD 128
 SFO1 100.6203 MHz
 FIDRES 130.208328 Hz
 SW 165.639 ppm
 FMODE QF

F2 - Processing parameters
 SI 1024
 SF 400.1300358 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 100.6127690 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0



***N*-((*S*)-2,5-Dioxo-1-((1*r**,3*R**)-3-(2-(5,6,7,8-tetrahydro-1,8-naphthyridin-2-yl)ethyl)cyclobutyl)pyrrolidin-3-yl)-2,4,6-trimethylbenzenesulfonamide [Compound 35]**



```

Current Data Parameters
NAME          act9-2-2
EXPNO        13
PROCNO       1

F2 - Acquisition Parameters
Date_        20120623
Time         4.29
INSTRUM      DPX400
PROBHD       5 mm QNP 1H/13
PULPROG      cosygmfgf
TD           2048
SOLVENT      CDCl3
NS           4
DS           8
SWH          3415.301 Hz
FIDRES       1.667627 Hz
AQ           0.2998772 sec
RG           6502
DW           146.400 usec
DE           6.00 usec
TE           298.2 K
D0           0.0000300 sec
D1           1.89268506 sec
d13          0.00000400 sec
D16          0.00020000 sec
IN0          0.00029280 sec

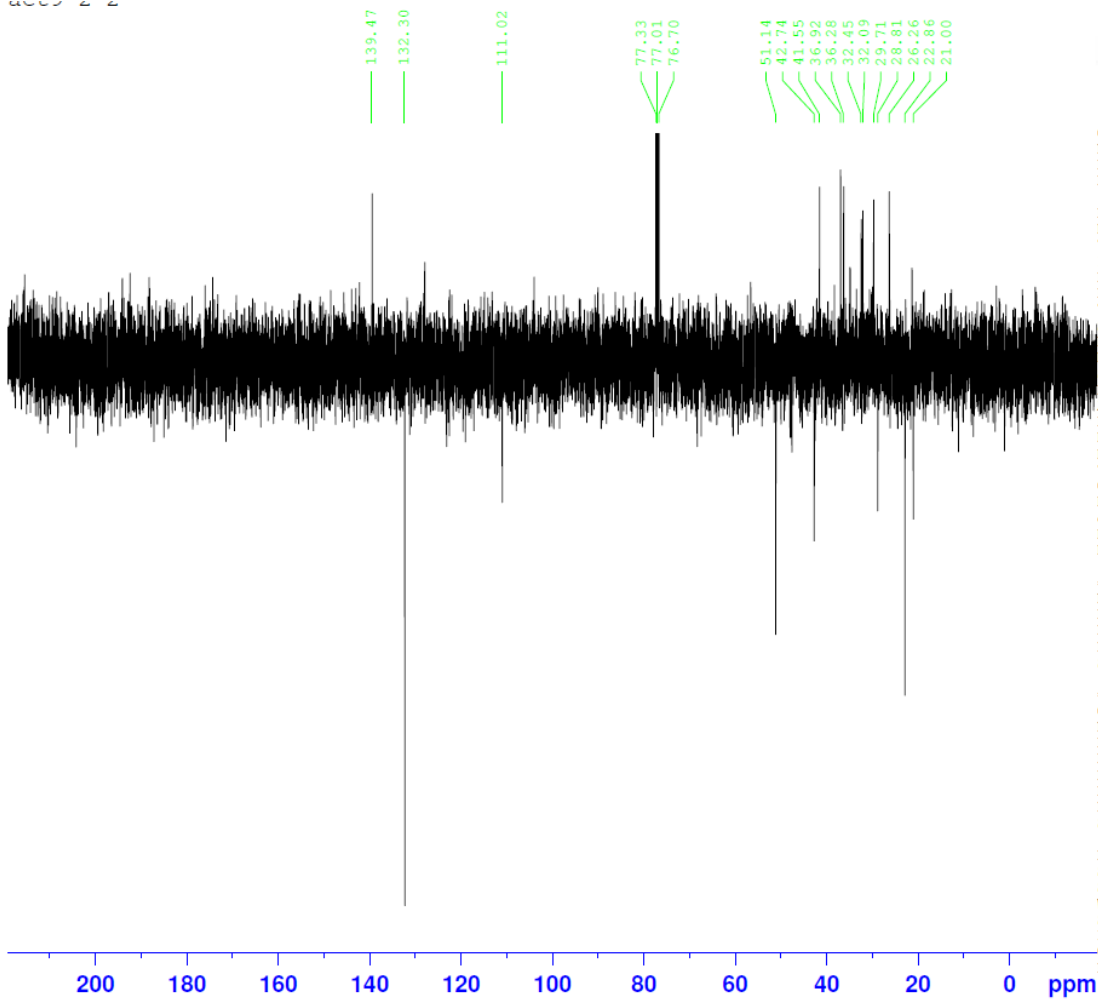
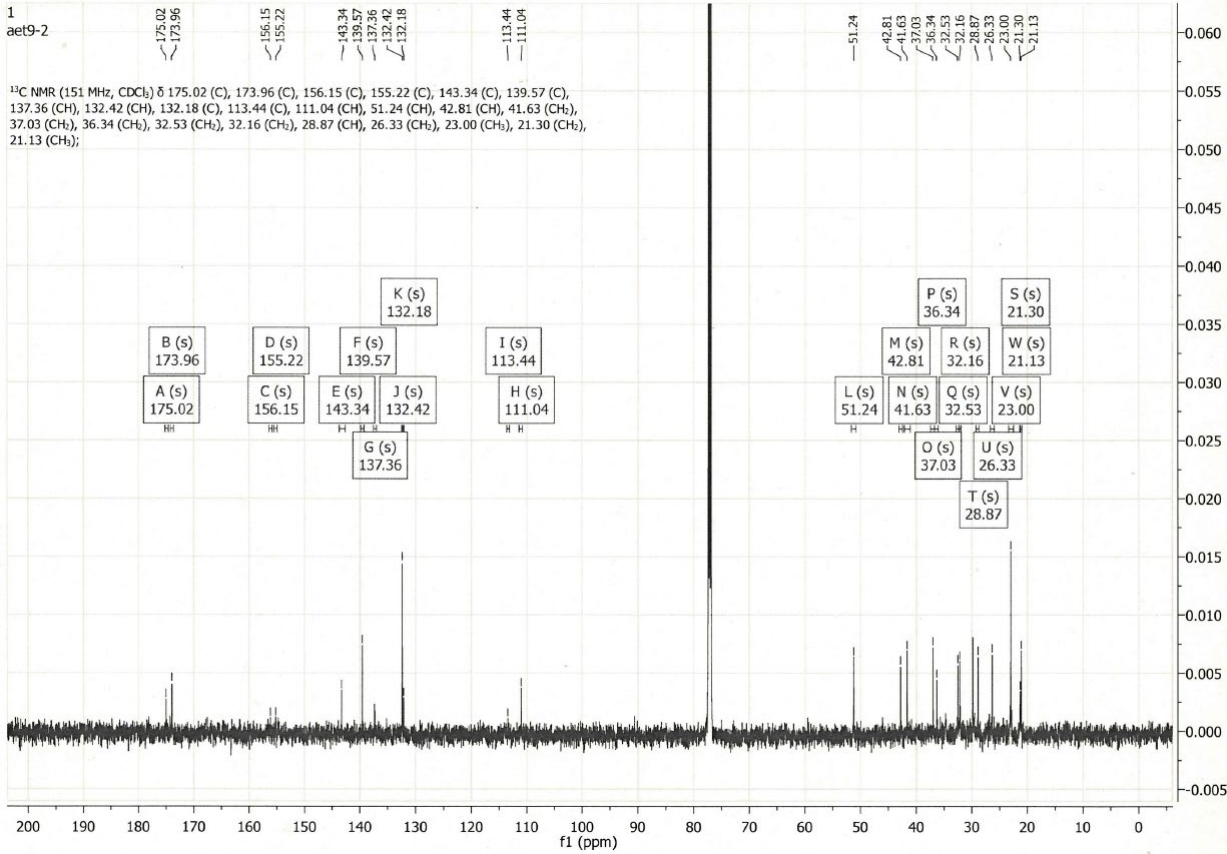
----- CHANNEL f1 -----
NUC1         13
P1           10.00 usec
PL1          -1.50 dB
SF01         400.1314298 MHz

----- GRADIENT CHANNEL -----
GPNAM1      SINE.100
GPNAM2      SINE.100
GPNAM3      SINE.100
GPZ1        16.00 %
GPZ2        12.00 %
GPZ3        40.00 %
P16         1000.00 usec

F1 - Acquisition parameters
ND0          1
TD           128
SF01         400.1314 MHz
FIDRES       26.682035 Hz
SW           8.535 ppm
FMODE        QF

F2 - Processing parameters
SI           1024
SF           400.1300373 MHz
WDW          SINE
SSB          0
LB           0.00 Hz
GB           0
PC           1.40

F1 - Processing parameters
SI           1024
MC2          QF
SF           400.1300373 MHz
WDW          SINE
SSB          0
LB           0.00 Hz
GB           0
    
```



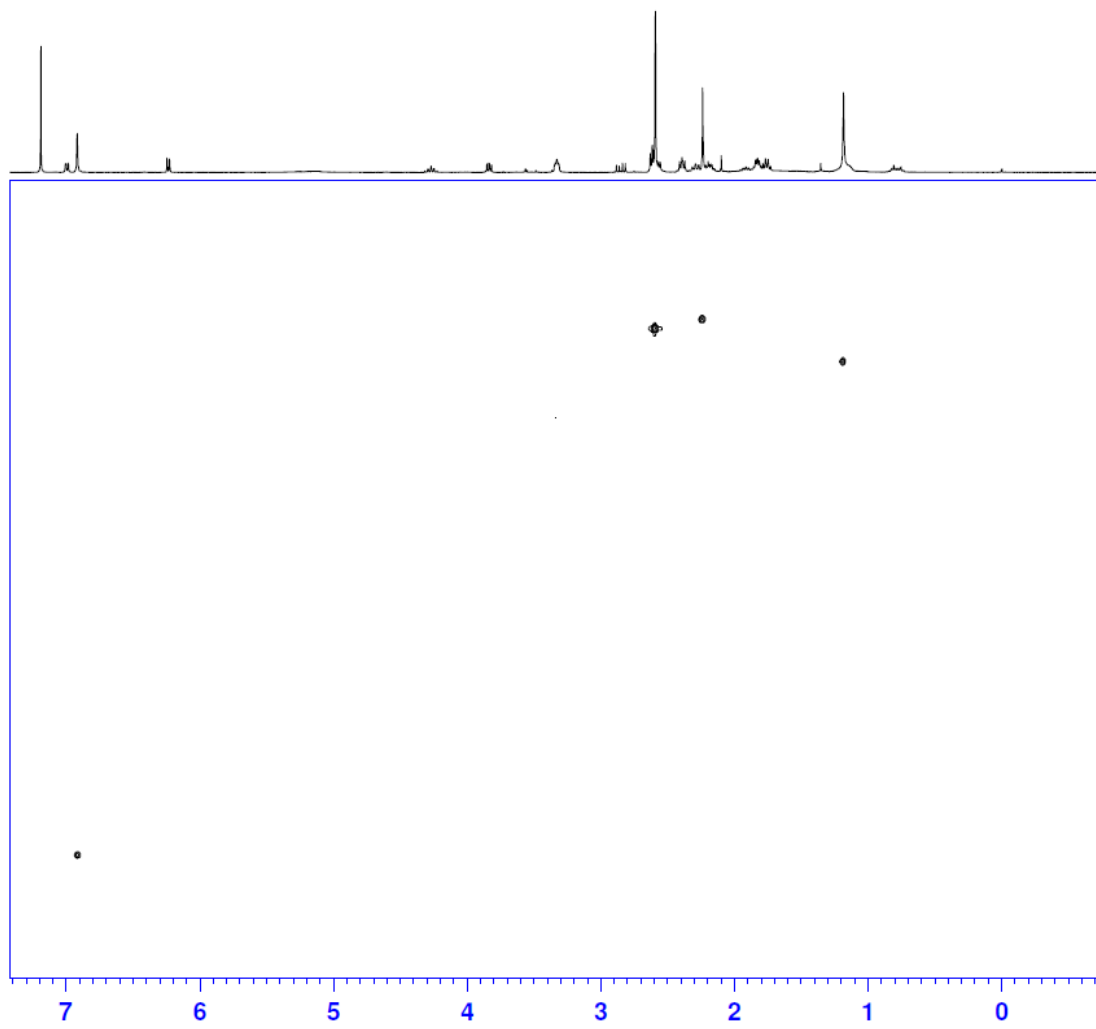
Current Data Parameters
NAME aet9-2-2
EXPNO 30
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120705
Time 22.46
INSTRUM DPX400
PROBHD 5 mm QNP 1H/13
PULPROG deptg_135
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 13004
DW 20.850 usec
DE 6.00 usec
TE 298.2 K
CNST2 145.000000
D1 2.0000000 sec
d2 0.00344828 sec
D11 0.0300000 sec
DELTA 0.00001082 sec

===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
P2 17.00 usec
PL1 -2.60 dB
SFO1 100.6228300 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 10.00 usec
P4 20.00 usec
PCPD2 80.00 usec
PL2 -1.50 dB
PL12 17.50 dB
SFO2 400.1316000 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
 NAME act9-2-2
 EXNO 41
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120705
 Time 22.49
 INSTRUM DPX400
 PROBRD 5 mm QNP 1H/13
 PULPROG hmqcpgf
 TD 1024
 SOLVENT cdcl3
 NS 4
 DS 16
 SWH 3272.251 Hz
 FIDRES 3.195558 Hz
 AQ 0.1565172 sec
 RG 4096
 DW 152.800 usec
 DE 6.00 usec
 TE 298.2 K
 CNST2 145.000000
 d0 0.0000300 sec
 d1 1.47030401 sec
 d2 0.00344828 sec
 d12 0.00020000 sec
 d13 0.00000400 sec
 D16 0.00020000 sec
 DELTA1 0.00222428 sec
 INO 0.00003000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 p2 20.00 usec
 PL1 -1.50 dB
 SFO1 400.1313712 MHz

==== CHANNEL f2 =====
 CPDPRG2 qasp
 NUC2 13C
 P3 8.00 usec
 PCPD2 74.00 usec
 PL2 -3.00 dB
 PL12 18.00 dB
 SFO2 100.6203140 MHz

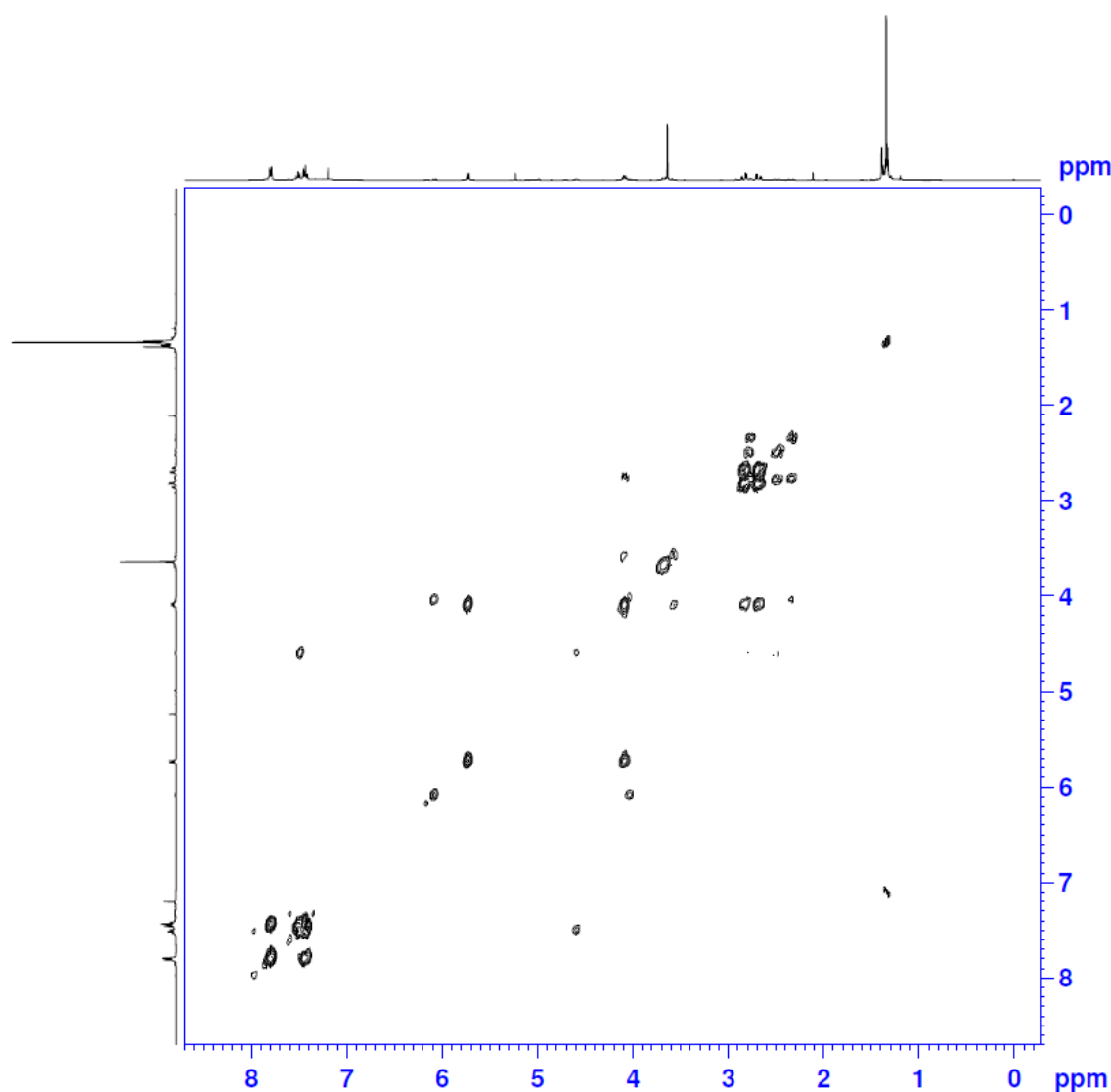
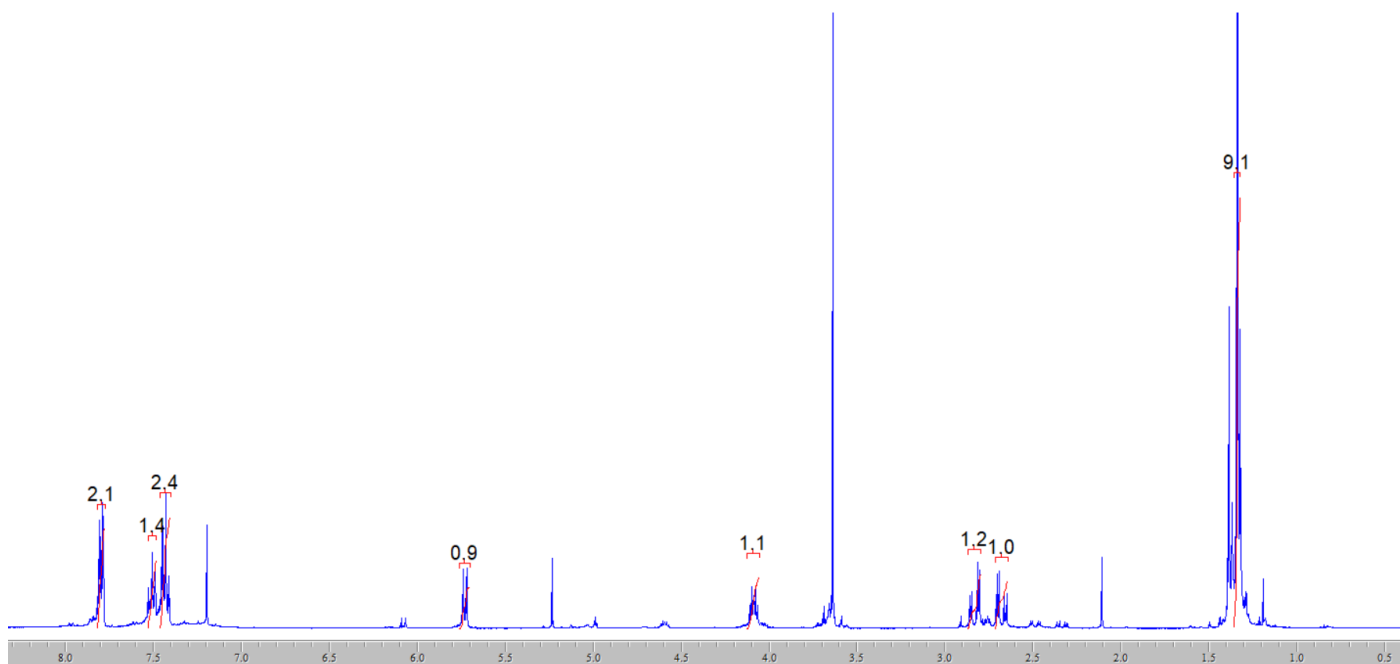
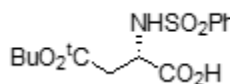
==== GRADIENT CHANNEL =====
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPNAM3 SINE.100
 GPZ1 50.00 %
 GPZ2 30.00 %
 GPZ3 40.10 %
 P16 1000.00 usec

F1 - Acquisition parameters
 ND0 2
 TD 128
 SFO1 100.6203 MHz
 FIDRES 130.208328 Hz
 SW 165.639 ppm
 FmMODE QF

F2 - Processing parameters
 SI 1024
 SF 400.1300372 MHz
 WW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 100.6127650 MHz
 WW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

(S)-4-(*tert*-butoxy)-4-oxo-2-(phenylsulfonamido)butanoic acid [Compound 36]



Current Data Parameters
NAME aet9-6
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121003
Time 0.24
INSTRUM DPX400
PROBHD 5 mm QNP 1H/13
PULPROG cosygpmfzf
ID 2048
SOLVENT CDCl3
NS 4
DS 8
SWH 3591.954 Hz
FIDRES 1.753884 Hz
AQ 0.2851316 sec
RG 9195.2
DW 139.200 usec
DE 6.00 usec
TE 292.2 K
D0 0.00000300 sec
D1 1.90702105 sec
d13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00027840 sec

----- CHANNEL f1 -----
NUC1 1H
P1 10.00 usec
PL1 -1.50 dB
SFO1 400.1317199 MHz

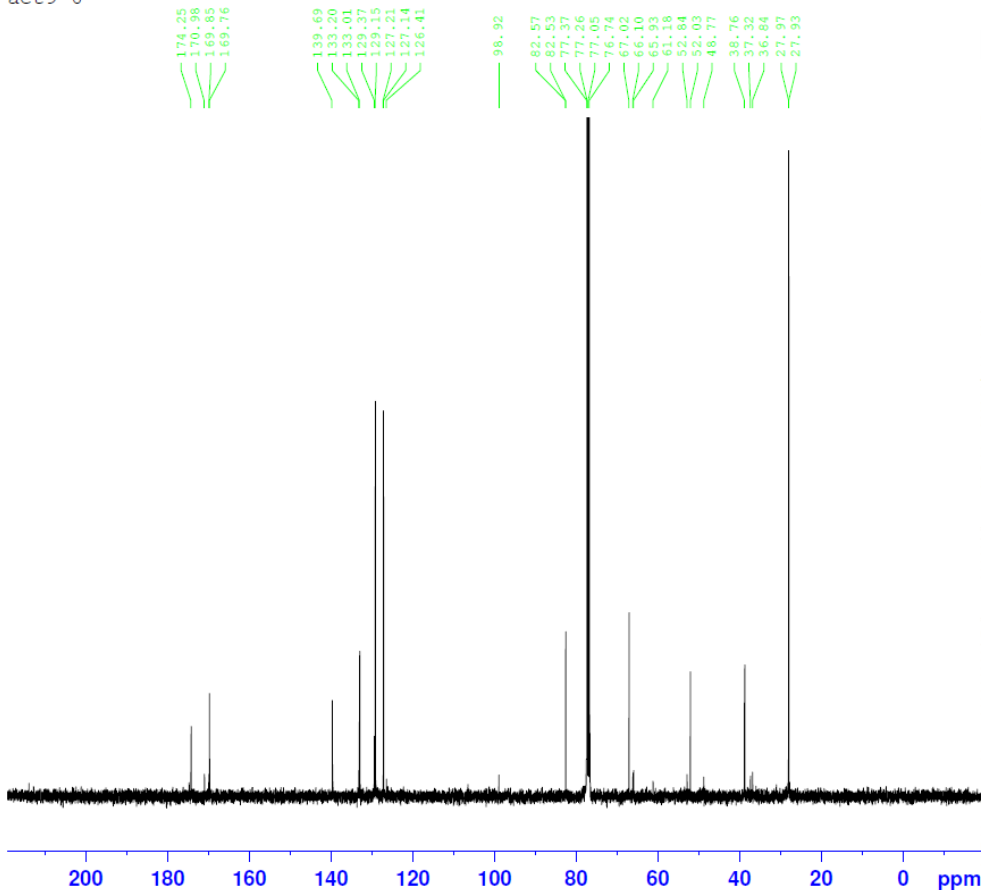
----- GRADIENT CHANNEL -----
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 16.00 %
GPZ2 12.00 %
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
ND0 1
ID 128
SFO1 400.1317 MHz
FIDRES 28.062141 Hz
SW 8.977 ppm
FMODE QF

F2 - Processing parameters
SI 1024
SF 400.1300341 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.1300341 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

aet9-6

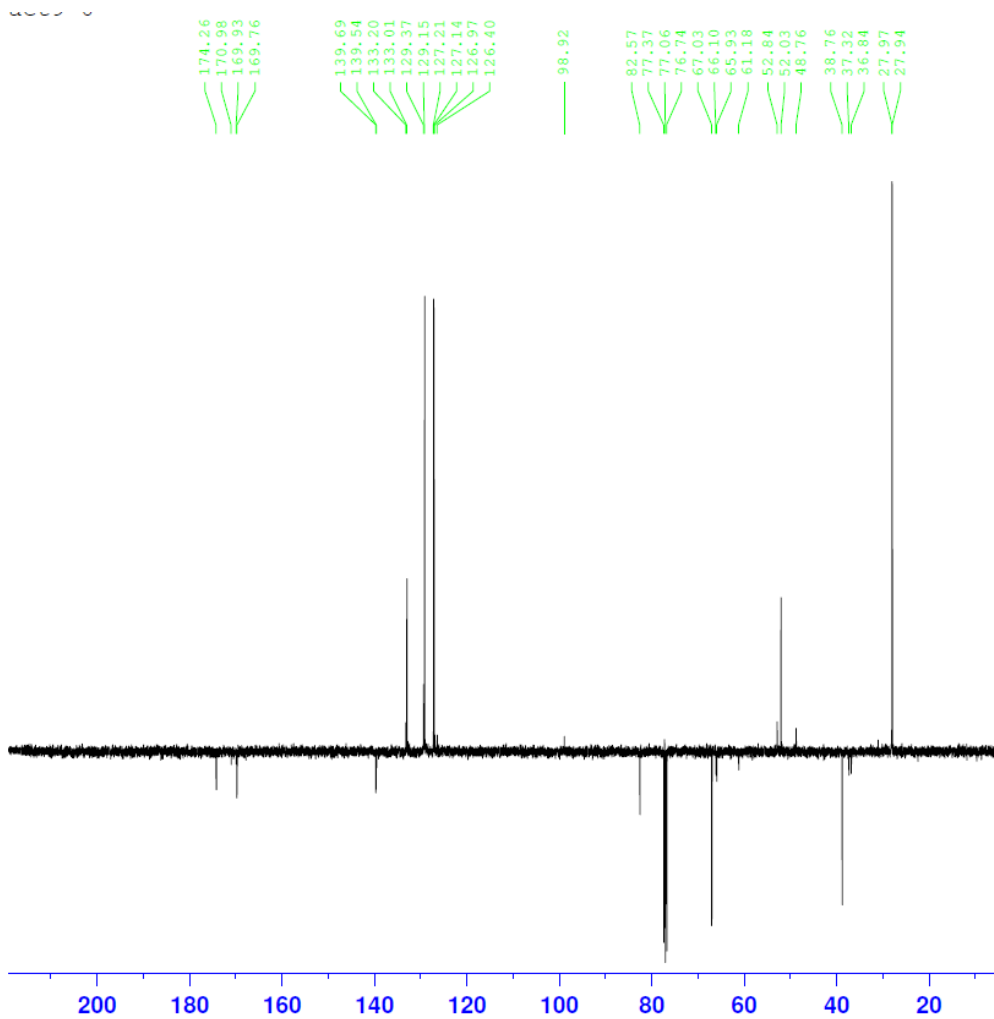


Current Data Parameters
 NAME aet9-6
 EXPNO 11
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20121002
 Time 23.53
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 912.3
 DW 20.850 usec
 DE 6.00 usec
 TE 293.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 PL1 -2.60 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 PL13 17.50 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

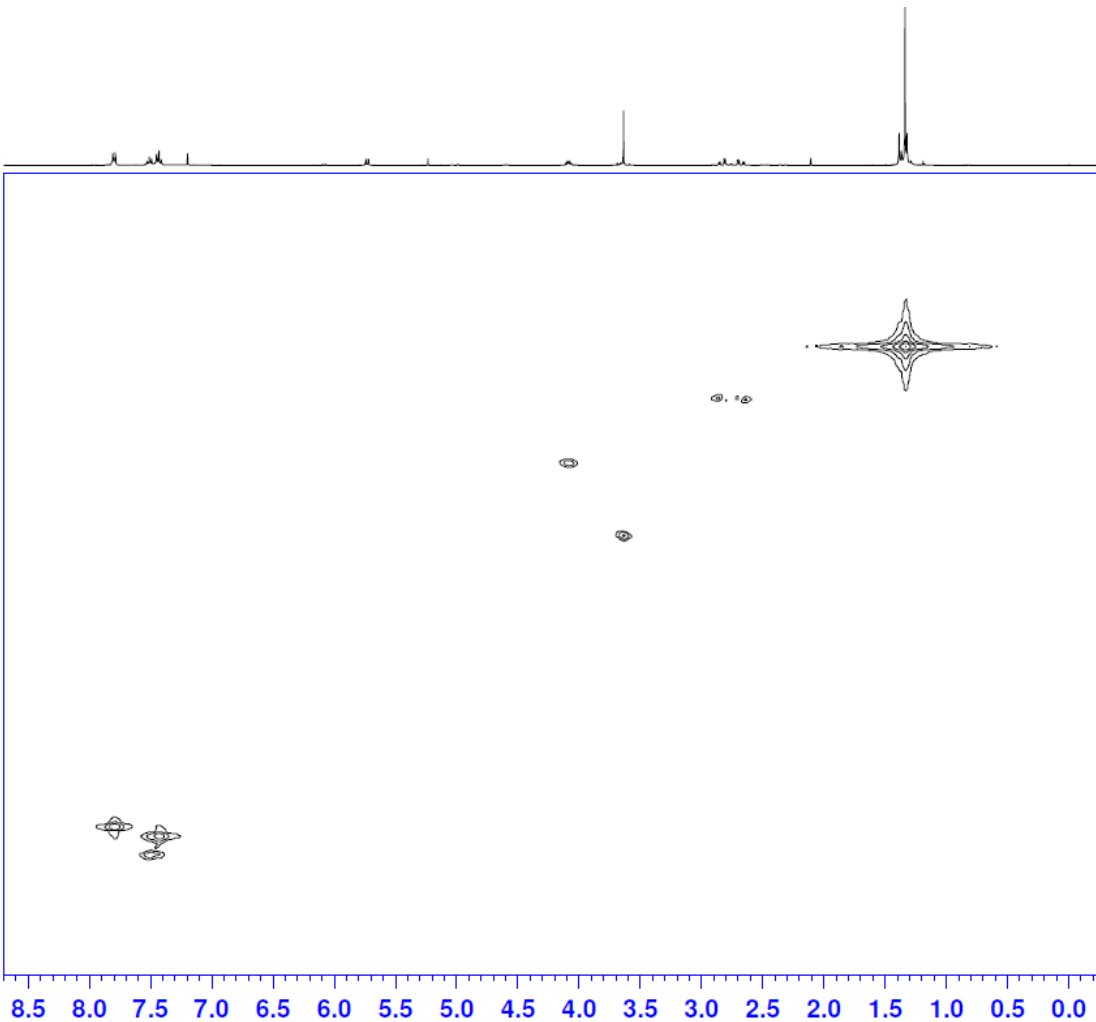


Current Data Parameters
 NAME aet9-6
 EXPNO 12
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20121003
 Time 0.23
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG deptg_135
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 18390.4
 DW 20.850 usec
 DE 6.00 usec
 TE 292.2 K
 CNST2 145.0000000
 D1 2.00000000 sec
 d2 0.00344828 sec
 D11 0.03000000 sec
 DELTA 0.00001082 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 P2 17.00 usec
 PL1 -2.60 dB
 SFO1 100.6228300 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 SFO2 400.1316000 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
 NAME set9-6
 EXPNO 14
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121003
 Time 0.44
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG hmcgpgpf
 TD 1024
 SOLVENT CDCl3
 NS 4
 DS 16
 SWH 3591.954 Hz
 FIDRES 3.507768 Hz
 AQ 0.1425908 sec
 RG 26008
 DW 139.200 usec
 DE 6.00 usec
 TE 292.2 K
 CMBT2 145.000000
 d0 0.0000300 sec
 d1 1.48464000 sec
 d2 0.00344828 sec
 d12 0.00020000 sec
 d13 0.00004000 sec
 D16 0.00020000 sec
 DELTA1 0.00222428 sec
 IN0 0.00030000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 p2 20.00 usec
 PL1 -1.50 dB
 SFO1 400.1317199 MHz

==== CHANNEL f2 =====
 CPDPRG2 gairp
 NUC2 13C
 P3 8.00 usec
 PCPD2 74.00 usec
 PL2 -3.00 dB
 PL12 18.00 dB
 SFO2 100.6203140 MHz

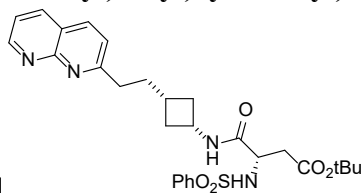
==== GRADIENT CHANNEL =====
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPNAM3 SINE.100
 GPZ1 50.00 %
 GPZ2 30.00 %
 GPZ3 40.10 %
 P16 1000.00 usec

F1 - Acquisition parameters
 ND0 2
 TD 128
 SFO1 100.6203 MHz
 FIDRES 130.208328 Hz
 SW 165.639 ppm
 FMODE QF

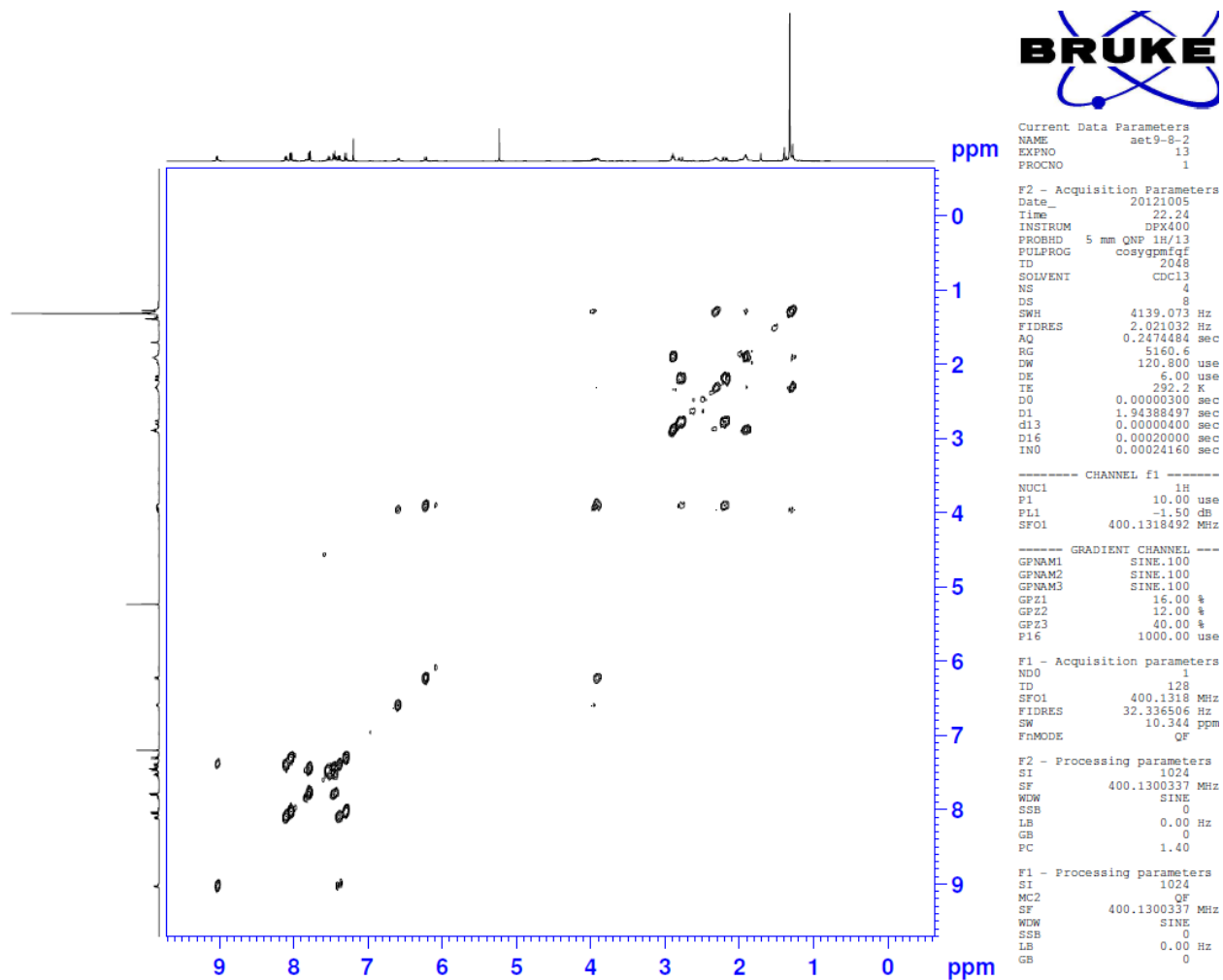
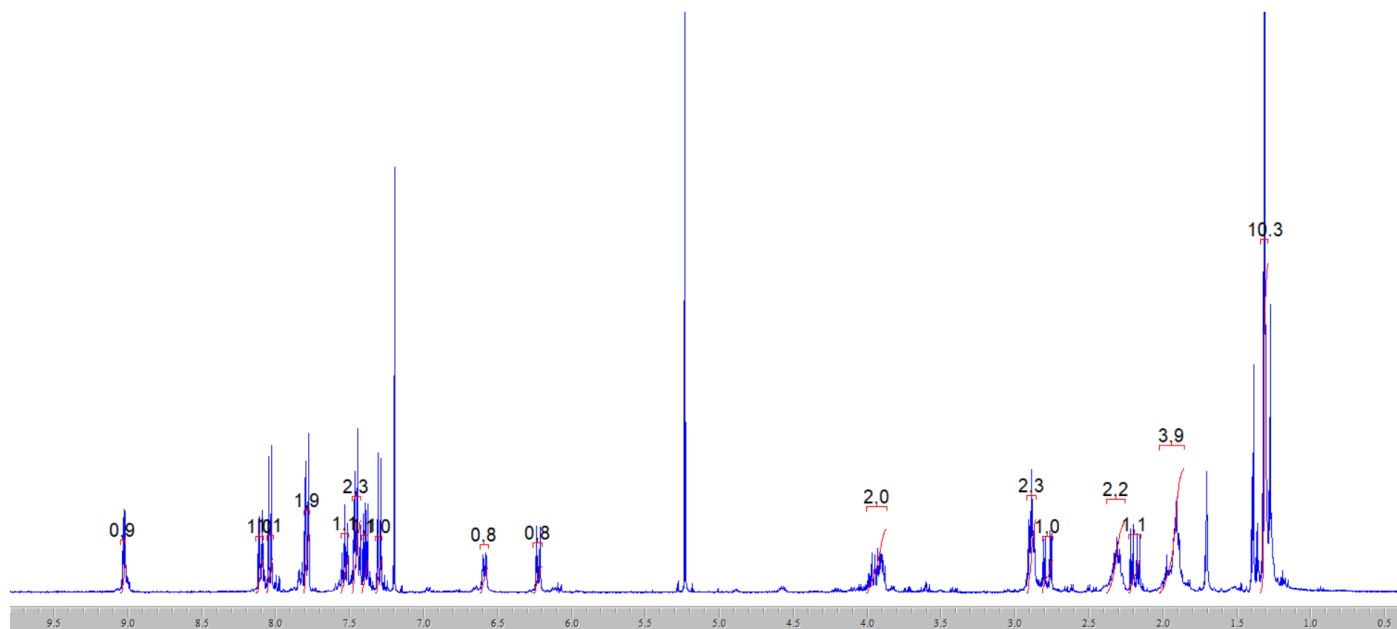
F2 - Processing parameters
 SI 1024
 SF 400.1300341 MHz
 WW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 100.6127690 MHz
 WW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

tert-butyl (S)-4-(((1*r**,3*R**)-3-(2-(1,8-naphthyridin-2-yl)ethyl)cyclobutyl)amino)-4-oxo-3-



(phenylsulfonamido)butanoate [Compound 37]



Current Data Parameters
 NAME act9-8-2
 EXPNO 13
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121005
 Time 22.24
 INSTRUM DFX400
 PROBHD 5 mm QNP 1H/13
 PULPROG cosygmrgf2
 TD 2048
 SOLVENT CDCl3
 NS 4
 DS 8
 SWH 4139.073 Hz
 FIDRES 2.021032 Hz
 AQ 0.2474484 sec
 RG 5160.6
 DW 120.800 use
 DE 6.00 use
 TE 292.2 K
 D0 0.00000300 sec
 D1 1.94388497 sec
 d13 0.00000400 sec
 D16 0.00020000 sec
 IN0 0.00024160 sec

----- CHANNEL f1 -----
 NUC1 1H
 P1 10.00 use
 PL1 -1.50 dB
 SFO1 400.1318492 MHz

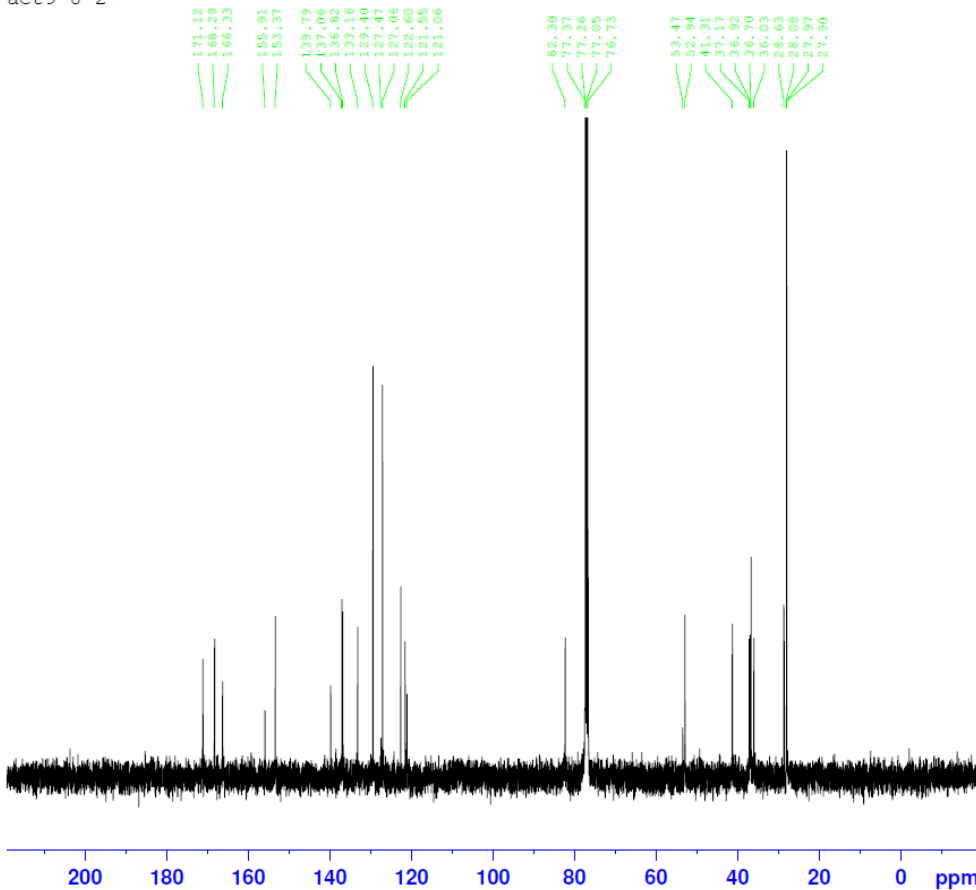
----- GRADIENT CHANNEL -----
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPNAM3 SINE.100
 GPZ1 16.00 %
 GPZ2 12.00 %
 GPZ3 40.00 %
 P16 1000.00 use

F1 - Acquisition parameters
 ND0 1
 TD 128
 SFO1 400.1318 MHz
 FIDRES 32.336506 Hz
 SW 10.344 ppm
 F1MODE QF

F2 - Processing parameters
 SI 1024
 SF 400.1300337 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 400.1300337 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

aet9-8-2



Current Data Parameters
 NAME aet9-8-2
 EXPNO 11
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20121005
 Time 21.53
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 724.1
 DW 20.850 usec
 DE 6.00 usec
 TE 293.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 PL1 -2.60 dB
 SFO1 100.6228298 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 PL13 17.50 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



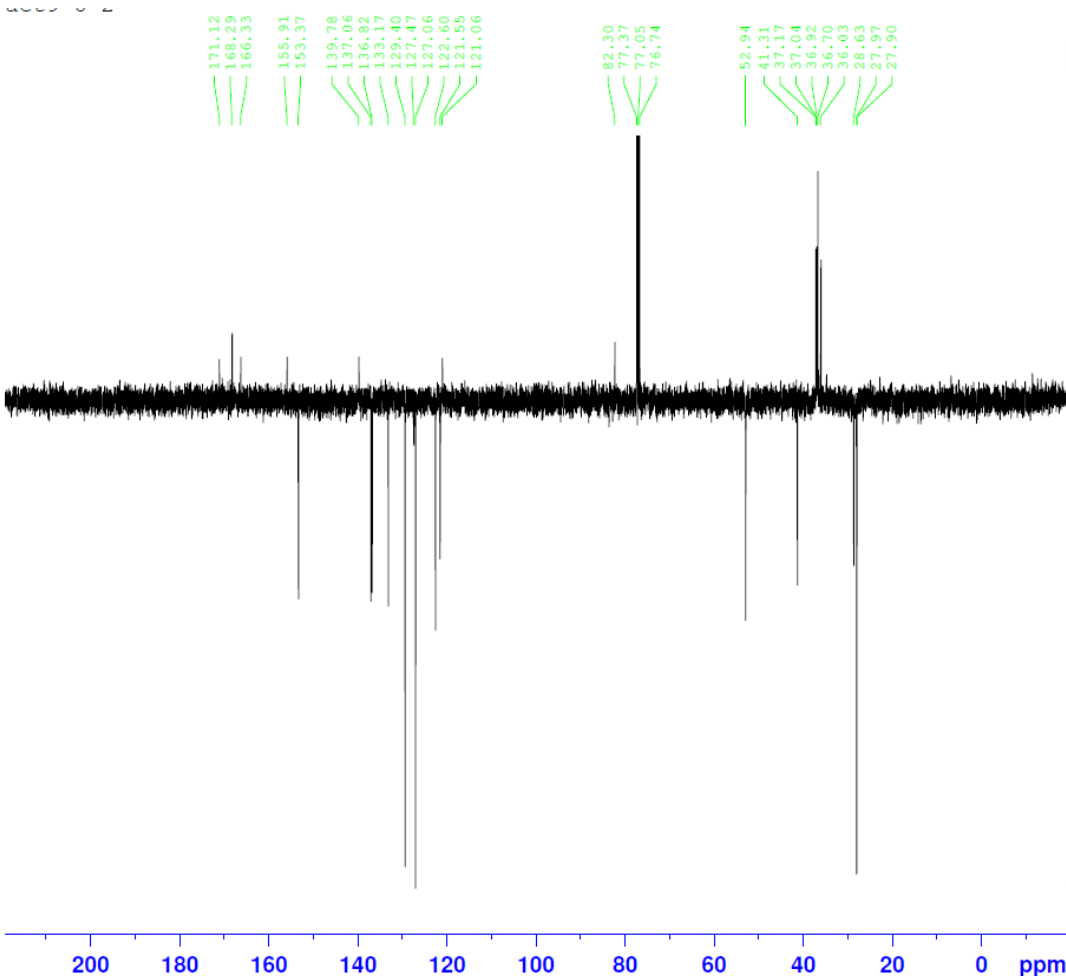
Current Data Parameters
 NAME aet9-8-2
 EXPNO 12
 PROCNO 1

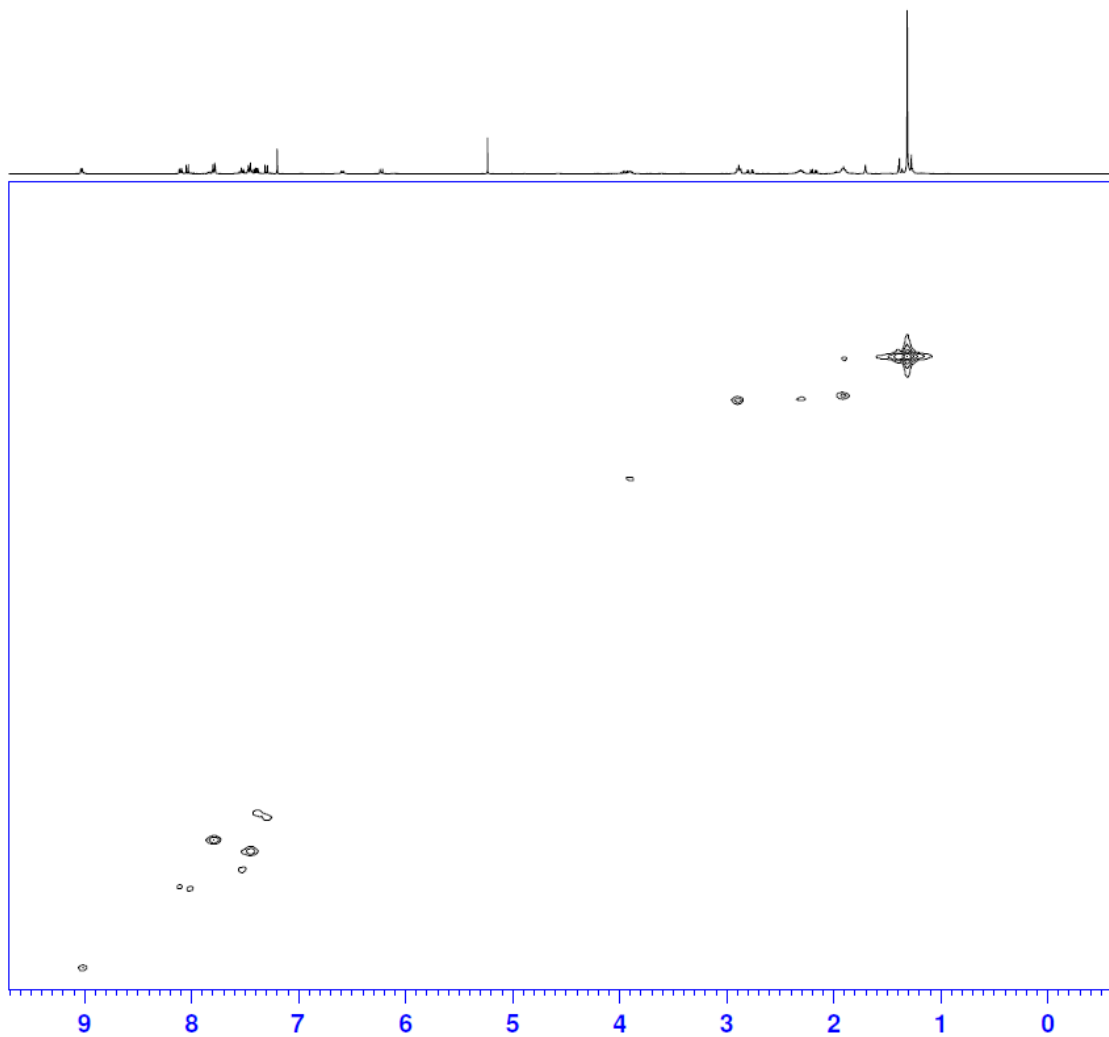
F2 - Acquisition Parameters
 Date_ 20121005
 Time 22.24
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG deptq_135
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 20642.5
 DW 20.850 usec
 DE 6.00 usec
 TE 292.2 K
 CNST2 145.0000000
 D1 2.00000000 sec
 d2 0.00344828 sec
 D11 0.03000000 sec
 DELTA 0.00001082 sec

==== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 P2 17.00 usec
 PL1 -2.60 dB
 SFO1 100.6228300 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 SFO2 400.1316000 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40





Current Data Parameters
NAME act9-8-2
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121005
Time 22.44
INSTRUM BRX400
PROBHD 5 mm QNP 1H/13
PULPROG hmqcpgpgf
TD 1024
SOLVENT cdc13
NS 4
DS 16
SWH 4139.073 Hz
FIDRES 4.042063 Hz
AQ 0.1237492 sec
RG 26008
DW 120.800 usec
DE 6.00 usec
TE 292.2 K
CNST2 145.000000
d0 0.0000300 sec
D1 1.50307202 sec
d2 0.00344828 sec
d12 0.0002000 sec
d13 0.0000400 sec
D16 0.0002000 sec
DELTA1 0.00222428 sec
IND 0.0000300 sec

==== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
p2 20.00 usec
PL1 -1.50 dB
SFO1 400.1318492 MHz

==== CHANNEL f2 =====
PCPDRC2 gspg
NUC2 13C
P3 8.00 usec
PCPD2 74.00 usec
PL2 -3.00 dB
PL12 18.00 dB
SFO2 100.6203140 MHz

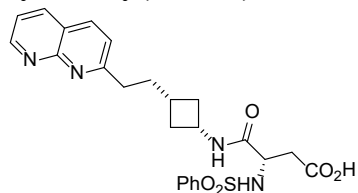
==== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
ND0 2
TD 128
SFO1 100.6203 MHz
FIDRES 130.208328 Hz
SW 165.639 ppm
FmMODE QF

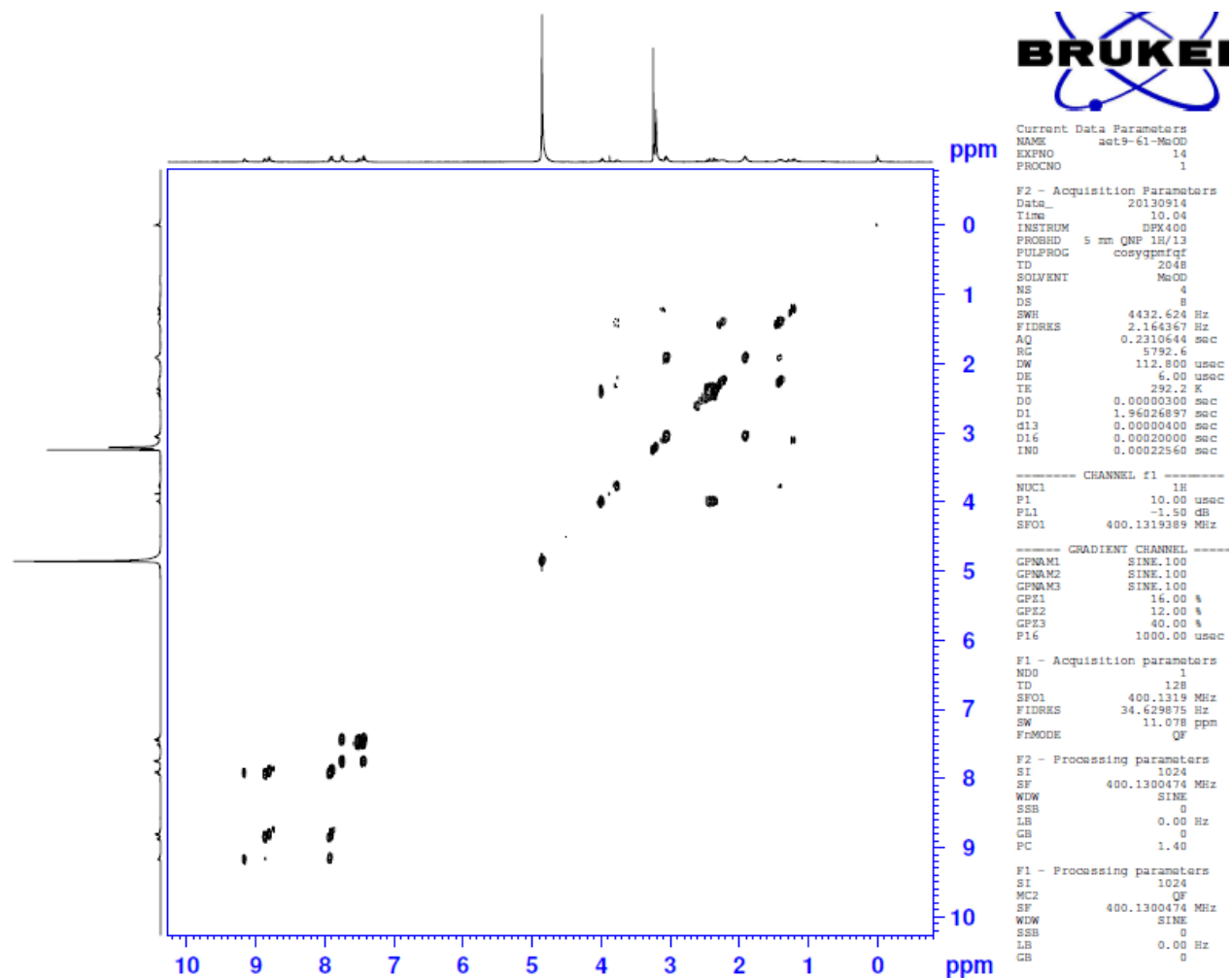
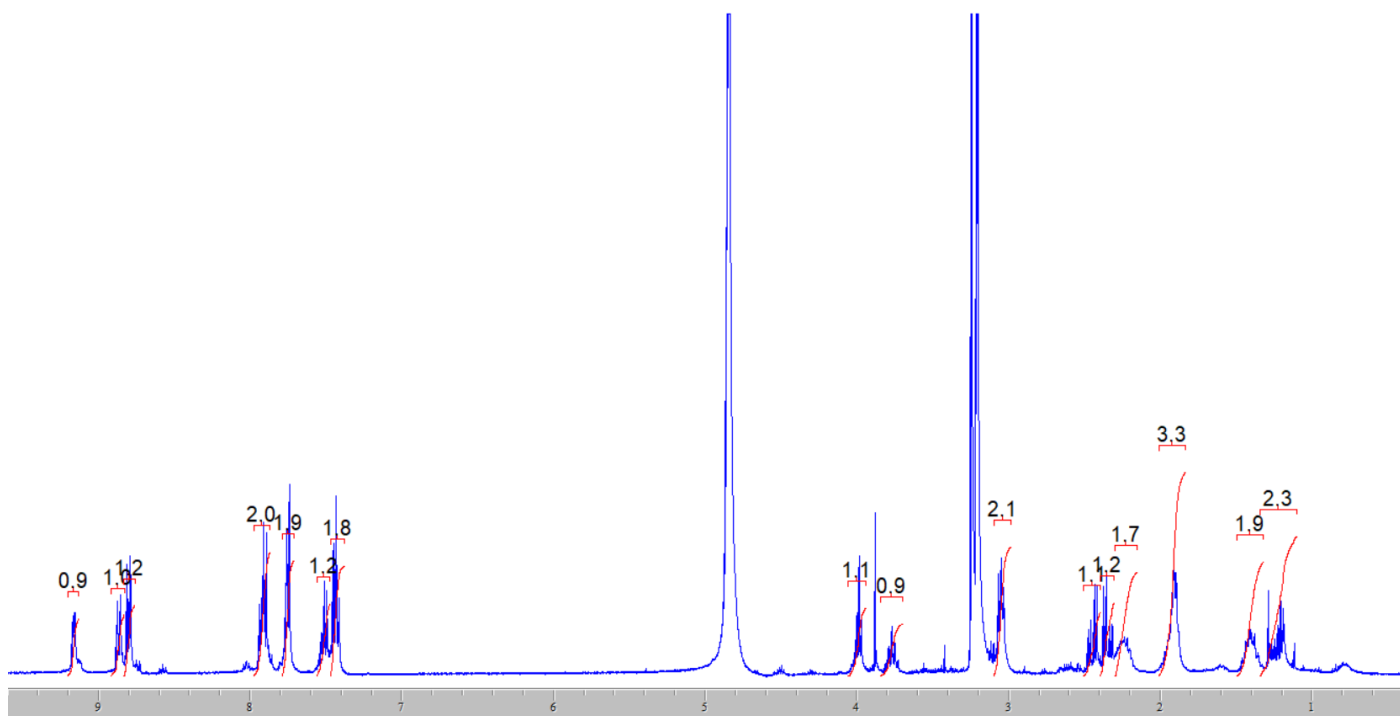
F2 - Processing parameters
SI 1024
SF 400.1300337 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 100.6127690 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

(S)-4-(((1R*,3R*)-3-(2-(1,8-naphthyridin-2-yl)ethyl)cyclobutyl)amino)-4-oxo-3-



(phenylsulfonamido)butanoic acid [Compound 38]



aet9-61-MeOD

153.48
144.19
144.07
133.91
130.22
128.19
126.08
124.96

54.61
49.87
49.66
49.54
49.23
48.02
48.81
48.39
42.37
37.93
37.12
36.98
36.85
35.80
29.71



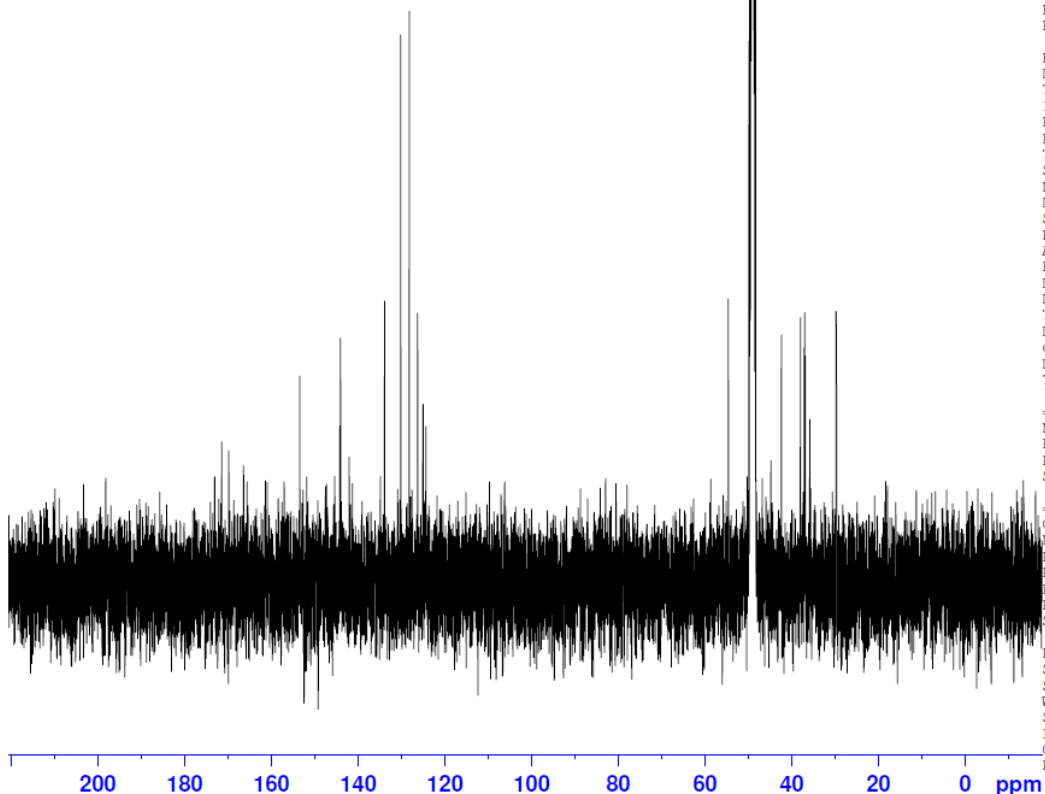
Current Data Parameters
NAME aet9-61-MeOD
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130914
Time 9.20
INSTRUM DPX400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 1024
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 2896.3
DW 20.850 usec
DE 6.00 usec
TE 293.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -2.60 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.50 dB
PL12 17.50 dB
PL13 17.50 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6126261 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



153.50
144.23
144.06
133.91
130.22
128.19
126.28
125.05

54.60
49.87
49.73
49.66
49.52
49.45
49.30
49.23
49.02
48.81
48.59
48.38
42.35
37.93
37.13
36.98
36.84
29.71



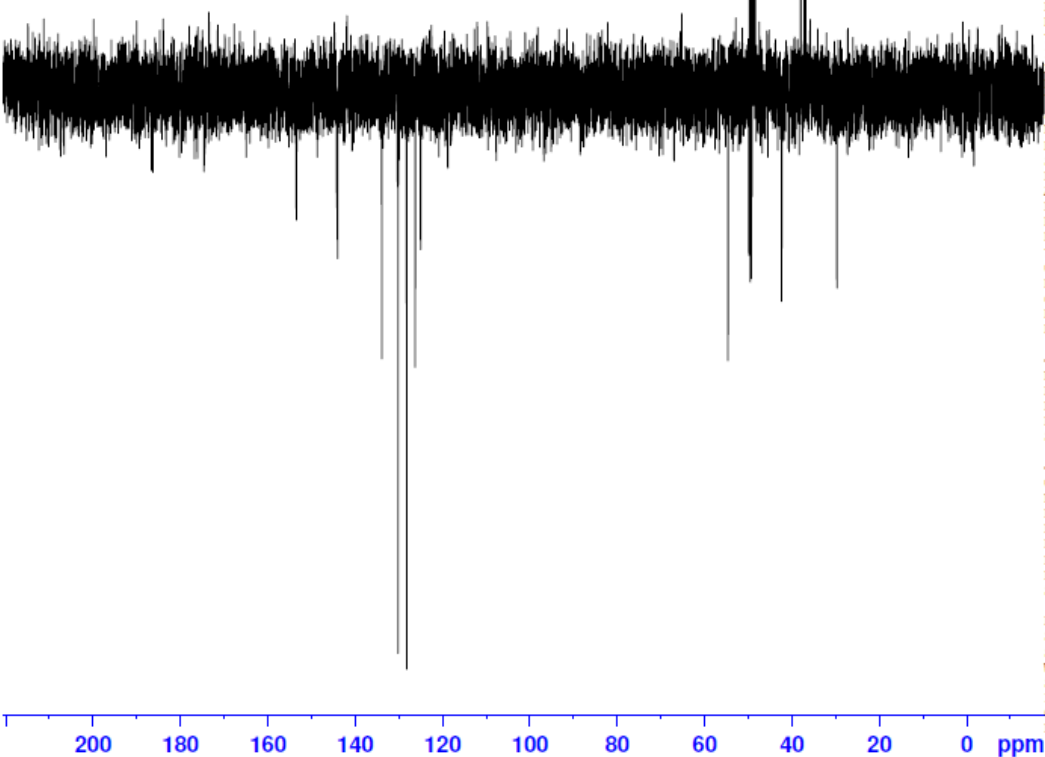
Current Data Parameters
NAME aet9-61-MeOD
EXPNO 12
PROCNO 1

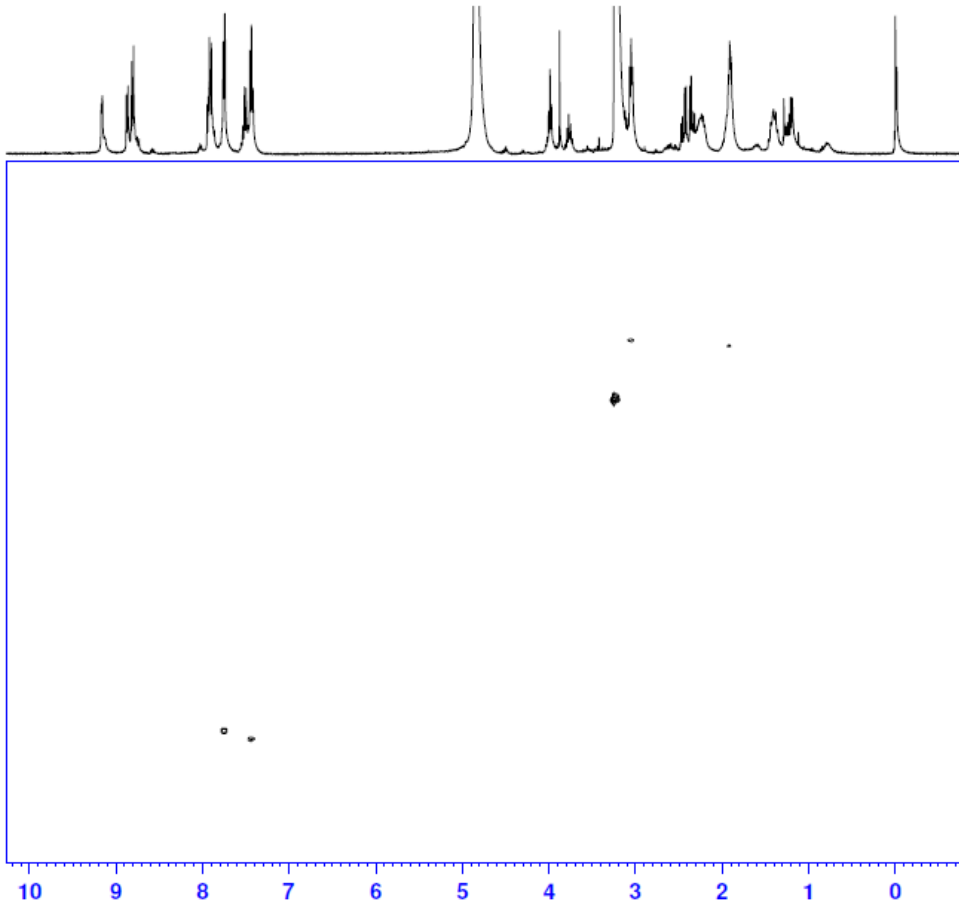
F2 - Acquisition Parameters
Date_ 20130914
Time 9.50
INSTRUM DPX400
PROBHD 5 mm QNP 1H/13
PULPROG deptq_135
TD 65536
SOLVENT MeOD
NS 512
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 11585.2
DW 20.850 usec
DE 6.00 usec
TE 293.2 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d11 0.03000000 sec
DELTA 0.00001146 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
P2 18.00 usec
PL1 -2.60 dB
SFO1 100.6228300 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 10.00 usec
P4 20.00 usec
PCPD2 80.00 usec
PL2 -1.50 dB
PL12 17.50 dB
SFO2 400.1316000 MHz

F2 - Processing parameters
SI 32768
SF 100.6126261 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





Current Data Parameters
NAME me3-Ci-MeCO
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130914
Time 10.24
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 1024
SOLVENT MeCO
NS 4
DS 16
SWH 4432.624 Hz
FIDRES 4.328734 Hz
AQ 0.1155572 sec
RG 7398.2
SM 112.800
DE 6.00 usec
TE 292.2 K
CHST2 145.0000000
d0 0.00000300 usec
d1 1.5136397 usec
d2 0.00344828 usec
d12 0.00002000 usec
d13 0.00000400 usec
d16 0.00020000 usec
DELTA1 0.00224258 usec
IN0 0.00000300 usec

----- CHANNEL F1 -----
NUC1 13C
P1 10.00 usec
PL 0.00 dB
PL1 -1.50 dB
SFO1 400.1319389 MHz

----- CHANNEL F2 -----
CPDPRG2 9MTE
NUC2 13C
P2 8.00 usec
PL2 74.00 usec
PL12 -3.00 dB
PL13 18.00 dB
SFO2 100.6203140 MHz

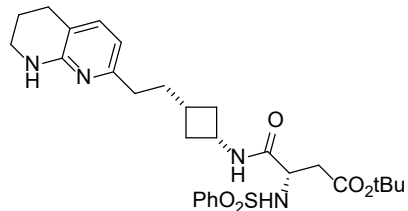
----- GRADIENT CHANNEL -----
GPMAM1 SINE.100
GPMAM2 SINE.100
GPMAM3 SINE.100
GPE1 50.00 %
GPE2 30.00 %
GPE3 40.10 %
PLG 1000.00 usec

F1 - Acquisition parameters
MD0 2
TD 128
SFO1 100.6203 MHz
FIDRES 130.208328 Hz
SM 165.639 ppm
P0MODE QF

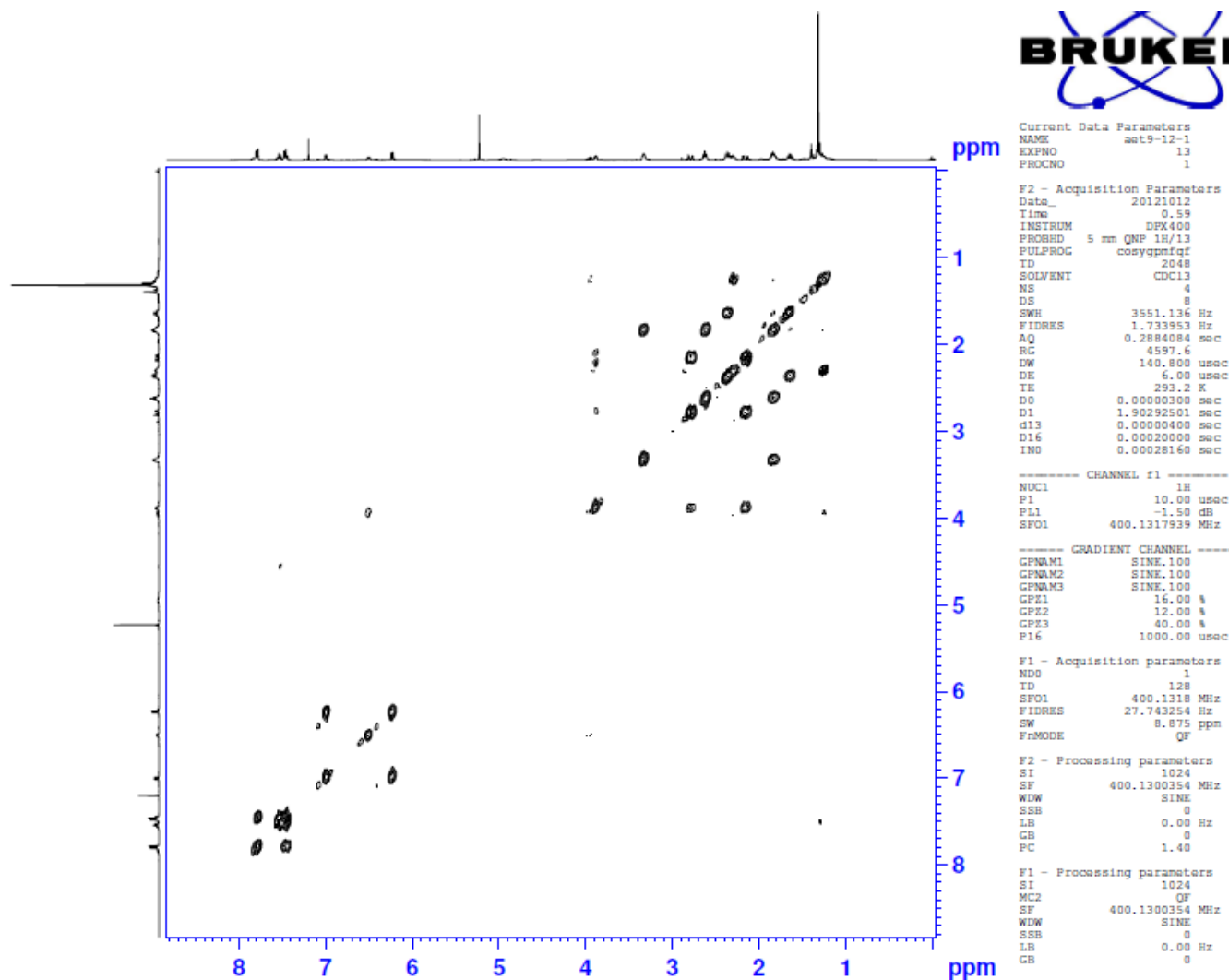
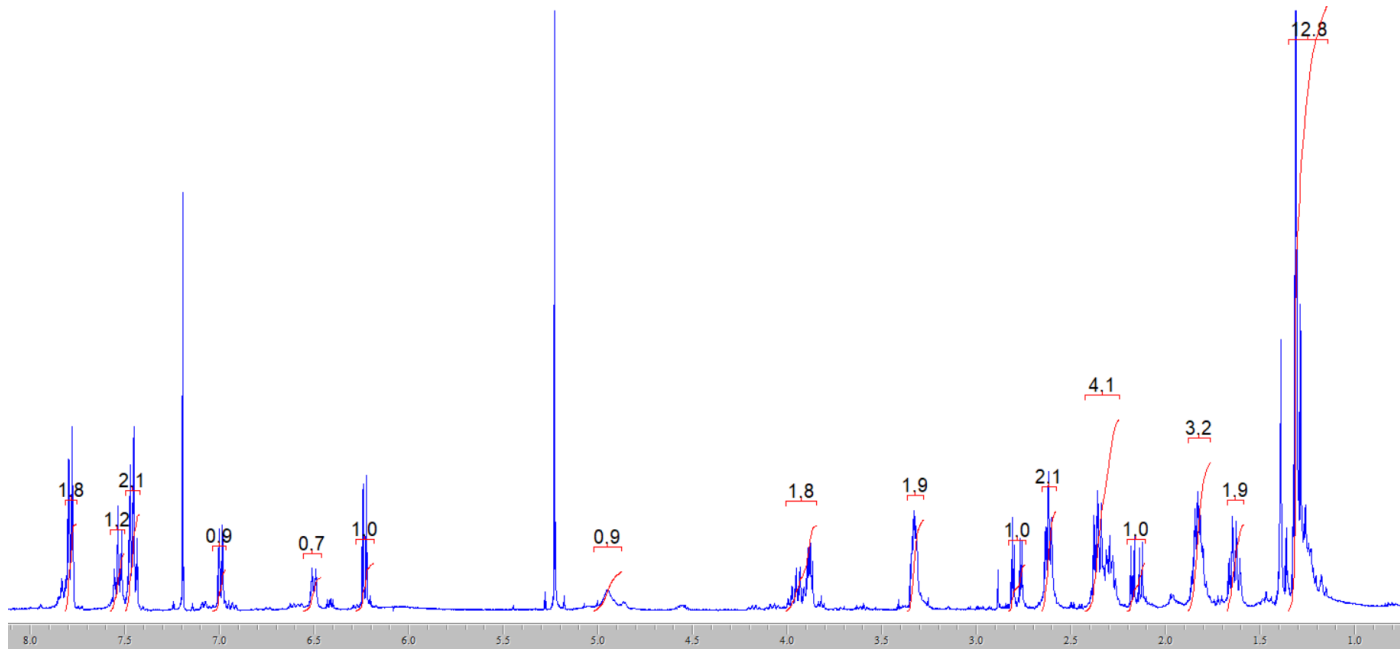
F2 - Processing parameters
SI 1024
SF 400.1300474 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 100.627650 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

tert-butyl (S)-4-oxo-3-(phenylsulfonamido)-4-(((1*r**,3*R**)-3-(2-(5,6,7,8-tetrahydro-1,8-naphthyridin-2-



yl)ethyl)cyclobutyl)amino)butanoate [Compound 39]



BRUKER

Current Data Parameters
NAME set9-12-1
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121012
Time 0.59
INSTRUM DPX400
PROBHD 5 mm QNP 1H/13
PULPROG cosygpcmgf
TD 2048
SOLVENT CDCl3
NS 4
DS 8
SWH 3551.136 Hz
FIDRES 1.733953 Hz
AQ 0.284084 sec
RG 4597.6
DW 140.800 usec
DE 6.00 usec
TE 293.2 K
D0 0.00000300 sec
D1 1.90292501 sec
d13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00028160 sec

----- CHANNEL f1 -----
NUC1 1H
P1 10.00 usec
PL1 -1.50 dB
SF01 400.1317939 MHz

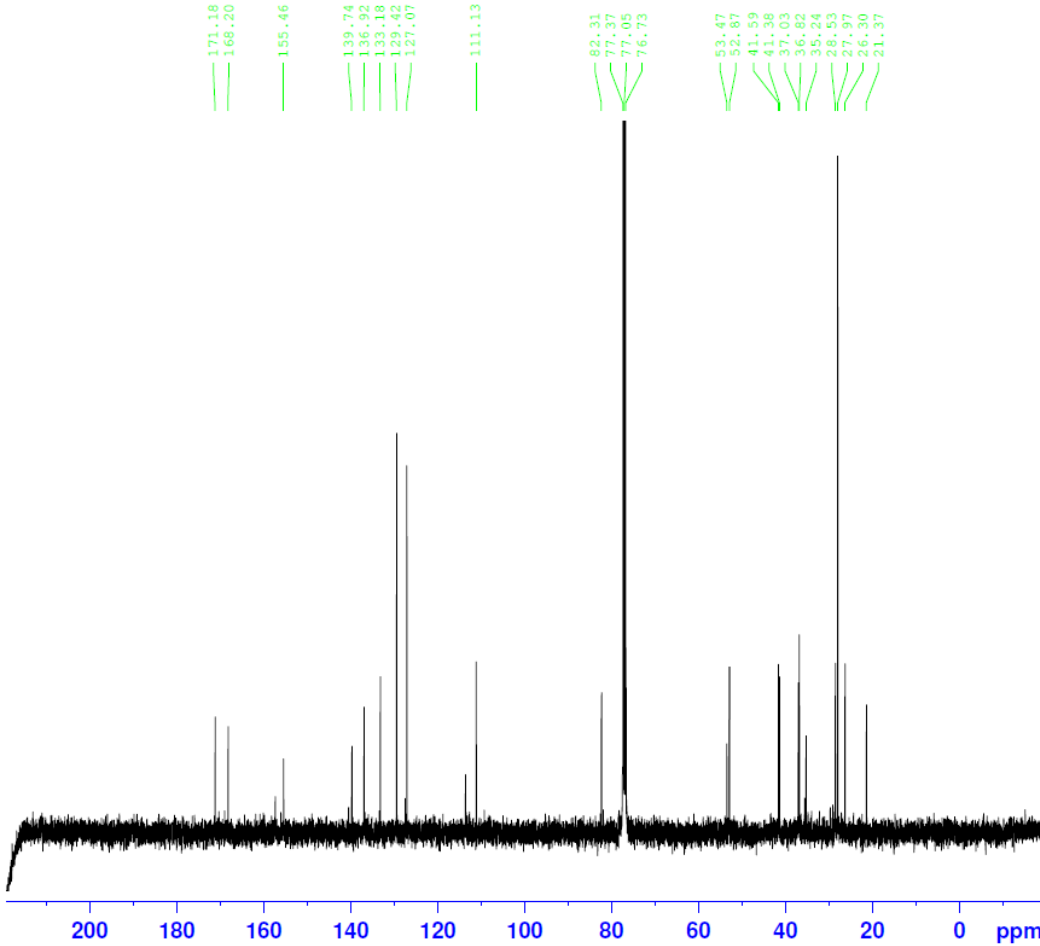
----- GRADIENT CHANNEL -----
GPNM1 SINE.100
GPNM2 SINE.100
GPNM3 SINE.100
GPE1 16.00 %
GPE2 12.00 %
GPE3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
ND0 1
TD 128
SF01 400.1318 MHz
FIDRES 27.743254 Hz
SW 8.875 ppm
FMODE QF

F2 - Processing parameters
SI 1024
SF 400.1300354 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.1300354 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

aet9-12-1



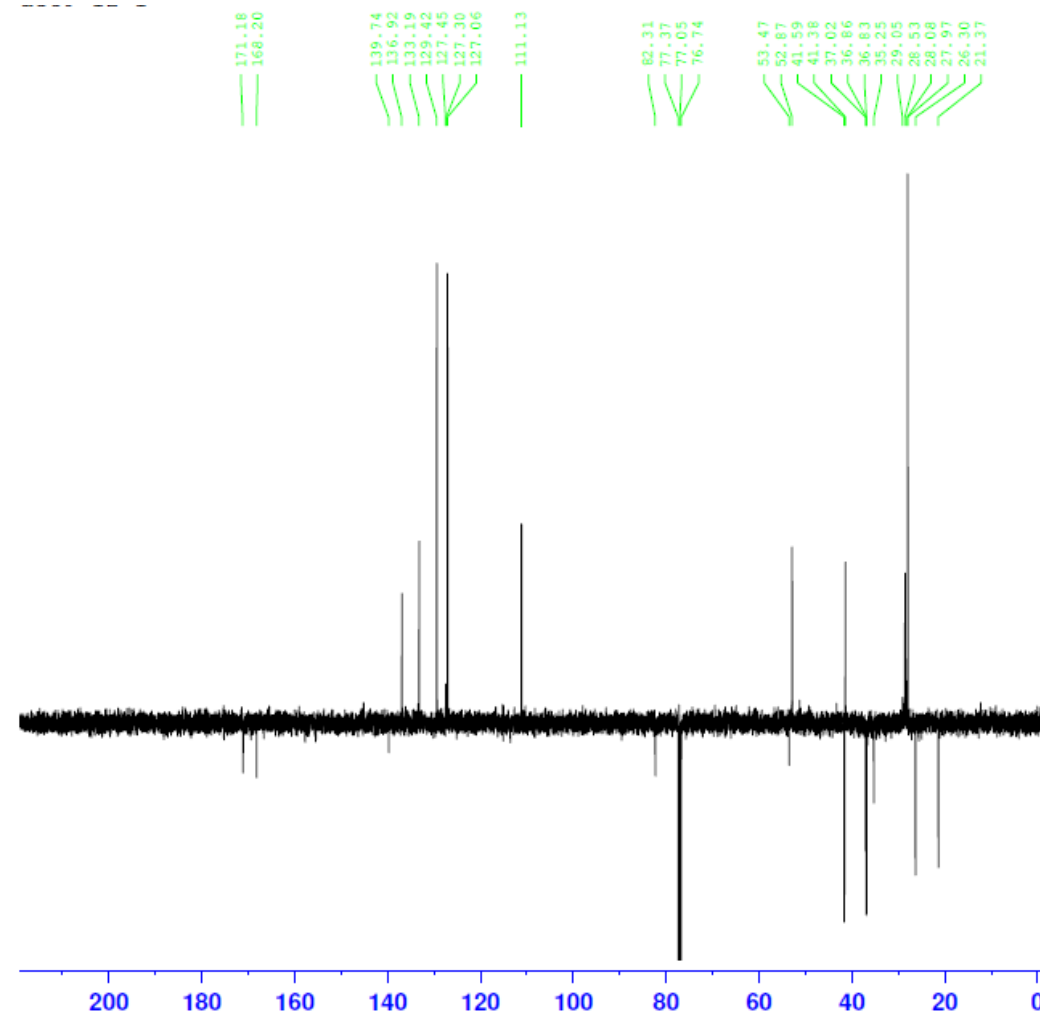
Current Data Parameters
 NAME aet9-12-1
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121012
 Time 0.28
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 812.7
 DW 20.850 usec
 DE 6.00 usec
 TE 293.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999999 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 PL1 -2.60 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 PL13 17.50 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
 NAME aet9-12-1
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121012
 Time 0.59
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG deptg_135
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 18390.4
 DW 20.850 usec
 DE 6.00 usec
 TE 292.2 K
 CNST2 145.0000000
 D1 2.00000000 sec
 d2 0.00344828 sec
 D11 0.03000000 sec
 DELTA 0.00001082 sec

----- CHANNEL f1 -----
 NUC1 13C
 P1 8.50 usec
 P2 17.00 usec
 PL1 -2.60 dB
 SFO1 100.6228300 MHz

----- CHANNEL f2 -----
 CPDPRG2 waltz16
 NUC2 1H
 F3 10.00 usec
 F4 20.00 usec
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 SFO2 400.1316000 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Current Data Parameters
 NAME: smt9-12-1
 EXPNO: 14
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20121012
 Time: 1.20

INSTRUM: DPX400
 PROBHD: 5 mm QNP 1H/13
 PULPROG: hmgpporf
 TD: 1024
 SOLVENT: CDCl3
 NS: 4
 DS: 16
 SWH: 3551.134 Hz
 FIDRES: 3.467907 Hz
 AQ: 0.1442292 sec
 RG: 5792.0
 SW: 140.800 us/c
 DE: 6.00 us/c
 TE: 292.2 K
 CHST2: 145.000000 sec
 d0: 0.0000300 sec
 d1: 1.48259199 sec
 d2: 0.00244628 sec
 d12: 0.00020000 sec
 d13: 0.00004000 sec
 d16: 0.00020000 sec
 DELTA1: 0.00224428 sec
 IN0: 0.00003000 sec

CHANNEL F1
 NUC1: 1H
 P1: 10.00 us/c
 P2: 20.00 us/c
 PL1: -1.50 dB
 SFO1: 400.1317939 MHz

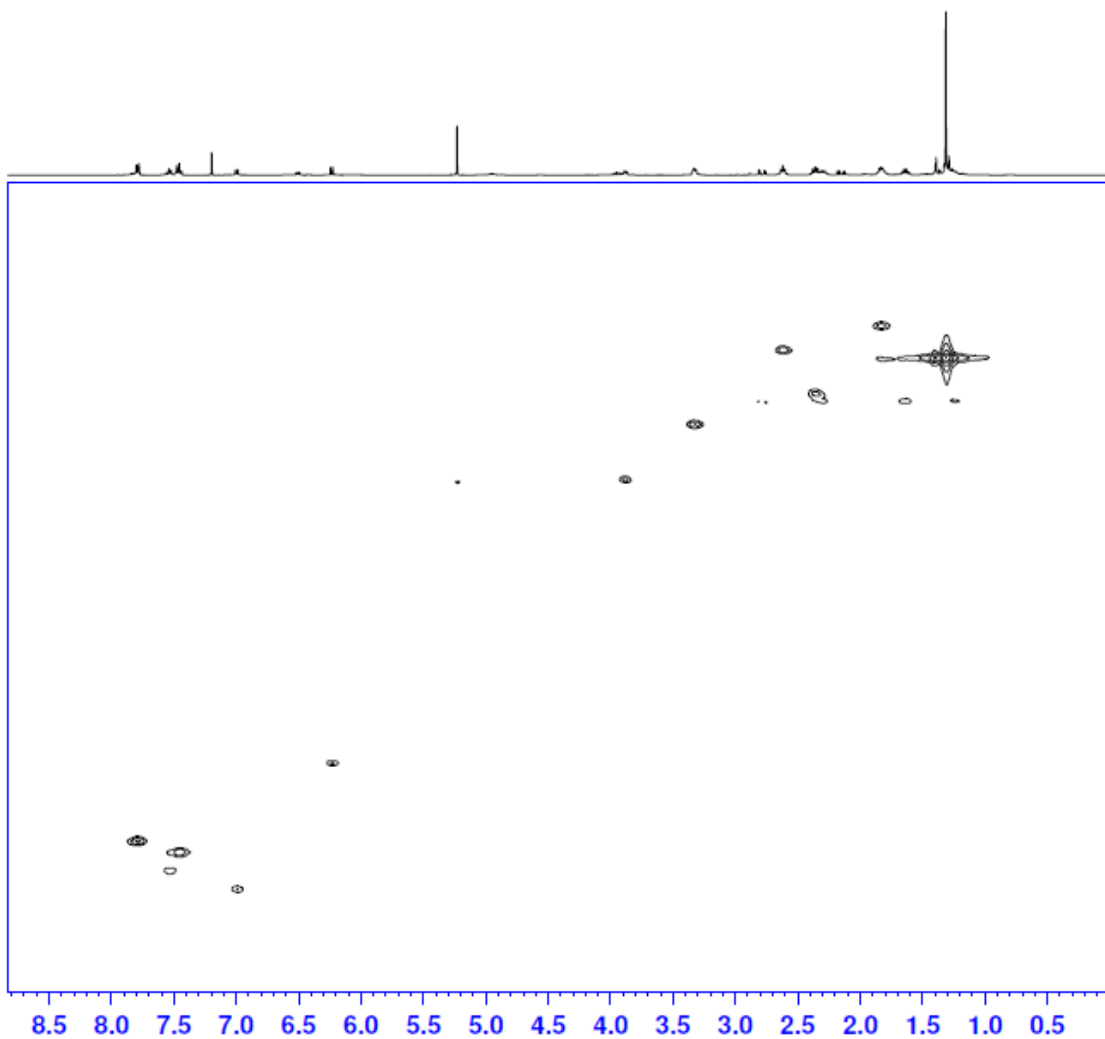
CHANNEL F2
 CPDPRG2: gmsf2
 NUC2: 13C
 P3: 8.00 us/c
 PCPD2: 74.00 us/c
 PL2: -3.00 dB
 PL12: 18.00 dB
 SFO2: 100.6203140 MHz

GRADIENT CHANNEL
 GPARAM1: SINE.100
 GPARAM2: SINE.100
 GPARAM3: SINE.100
 GPX1: 50.00 %
 GPX2: 30.00 %
 GPX3: 40.10 %
 P1G: 1000.00 us/c

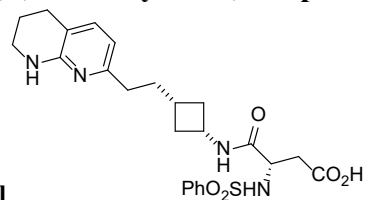
F1 - Acquisition parameters
 MD0: 2
 TD: 128
 SFO1: 100.6203 MHz
 FIDRES: 130.208328 Hz
 SW: 165.639 ppm
 FWHMDE: 0

F2 - Processing parameters
 SI: 1024
 SF: 400.1300354 MHz
 WDW: QSIWV
 SSB: 2
 LB: 0.00 Hz
 GB: 0
 PC: 1.40

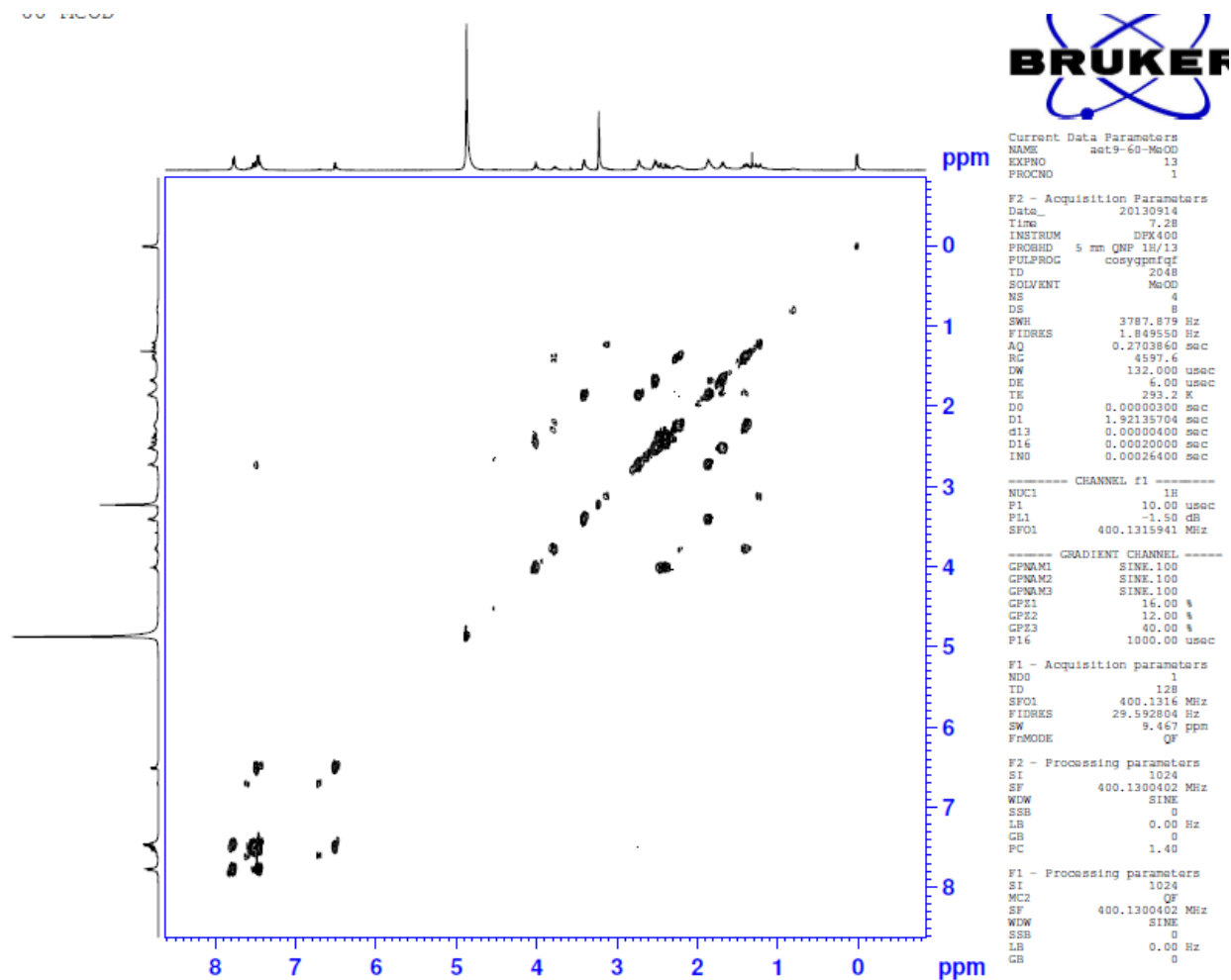
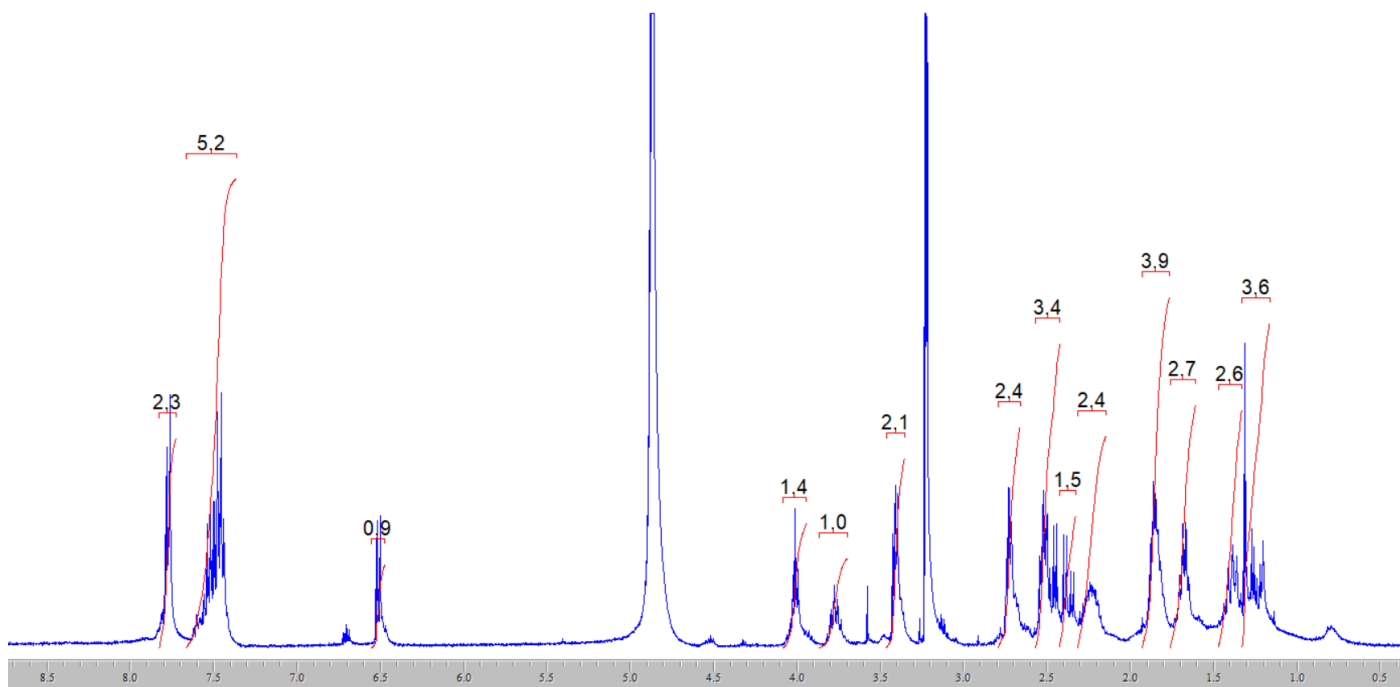
F1 - Processing parameters
 SI: 1024
 WC2: 0
 SF: 100.6127690 MHz
 WDW: QSIWV
 SSB: 2
 LB: 0.00 Hz
 GB: 0



(S)-4-oxo-3-(phenylsulfonamido)-4-(((1*r,3*R**)-3-(2-(5,6,7,8-tetrahydro-1,8-naphthyridin-2-**



yl)ethyl)cyclobutyl)amino)butanoic acid [Compound 40]



Current Data Parameters
 NAME act9-60-MeOD
 EXPNO 13
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130914
 Time 7.28
 INSTRUM DFX400
 PROBRD 5 mm QNP 1H/13
 PULPROG coesyppmgf
 TD 2048
 SOLVENT MeOD
 NS 4
 DS 8
 SWH 3787.879 Hz
 FIDRES 1.849550 Hz
 AQ 0.2703860 sec
 RG 4597.6
 DW 132.000 usec
 DE 6.00 usec
 TE 293.2 K
 D0 0.00000300 sec
 D1 1.92135704 sec
 d12 0.0000400 sec
 D16 0.0002000 sec
 IN0 0.00026400 sec

----- CHANNEL f1 -----
 NUC1 1H
 P1 10.00 usec
 PL1 -1.50 dB
 SFO1 400.1315941 MHz

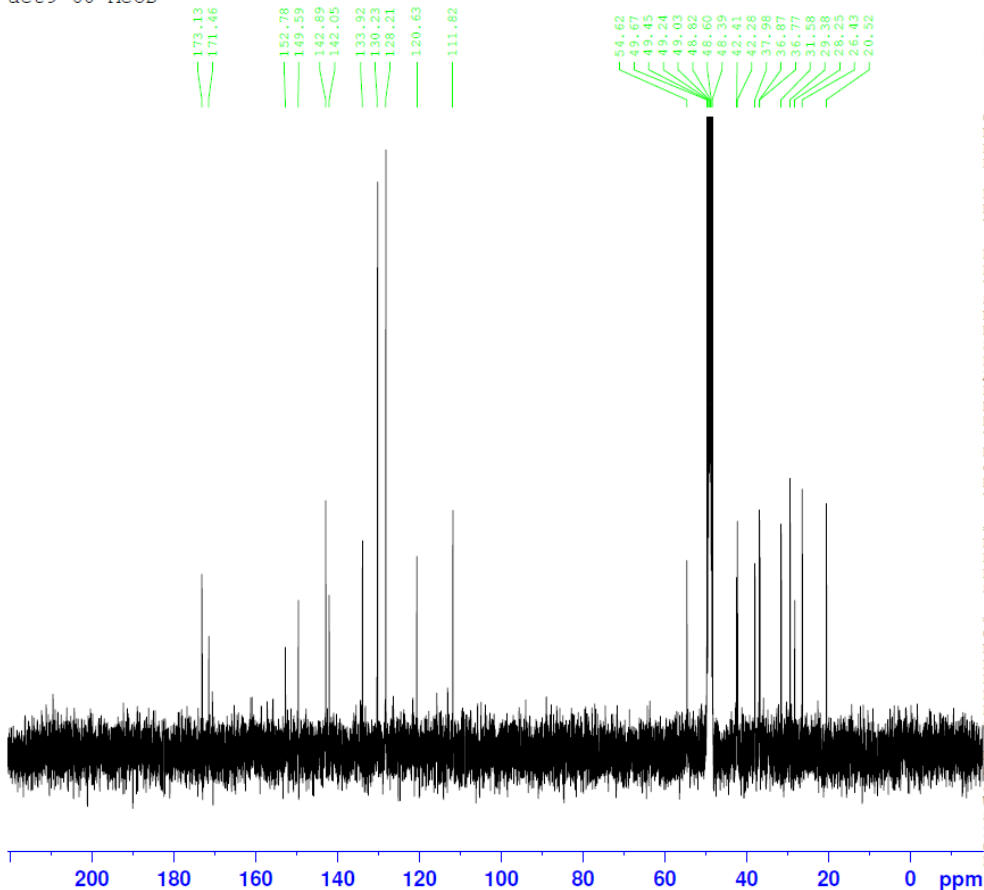
----- GRADIENT CHANNEL -----
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPNAM3 SINE.100
 GPE1 16.00 %
 GPE2 12.00 %
 GPE3 40.00 %
 P16 1000.00 usec

F1 - Acquisition parameters
 NDO 1
 TD 128
 SFO1 400.1316 MHz
 FIDRES 29.592804 Hz
 SW 9.467 ppm
 FhMODE QF

F2 - Processing parameters
 SI 1024
 SF 400.1300402 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 400.1300402 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

aet9-60-MeOD



Current Data Parameters
 NAME aet9-60-MeOD
 EXPNO 11
 PROCNO 1

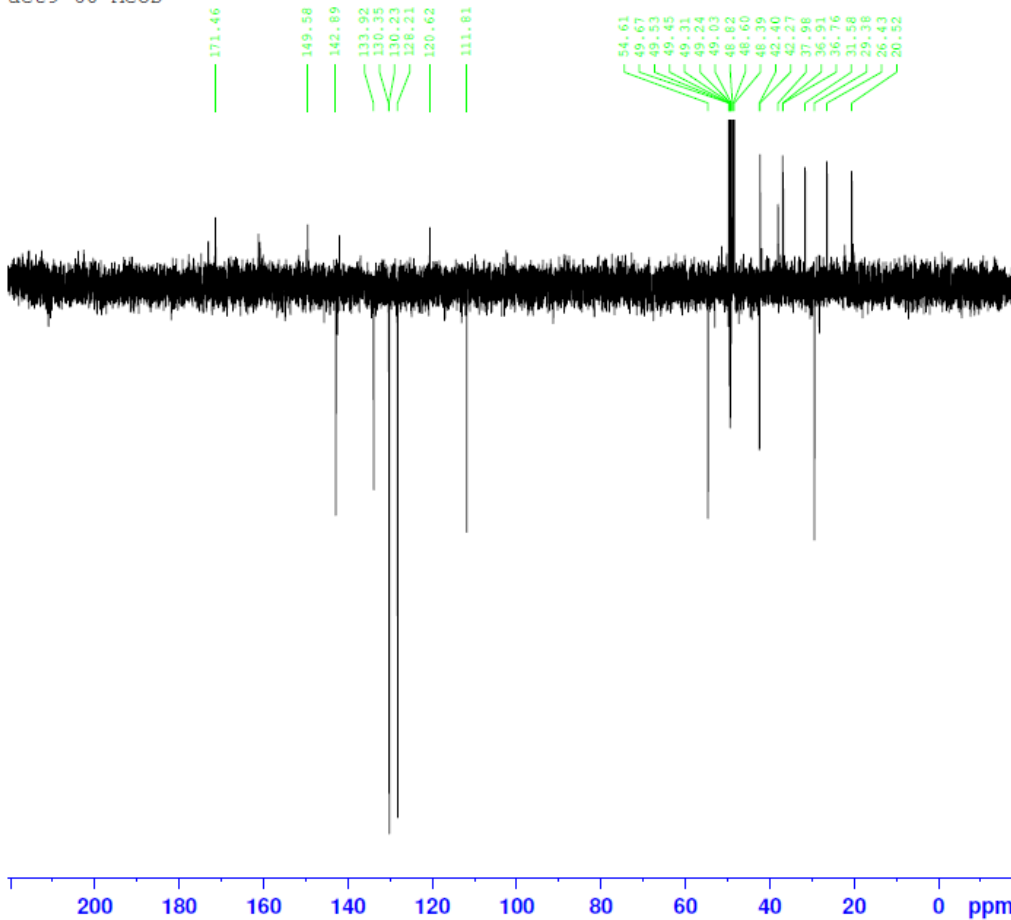
F2 - Acquisition Parameters
 Date_ 20130914
 Time 6.57
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT MeOD
 NS 1024
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 2580.3
 DW 20.850 usec
 DE 6.00 usec
 TE 293.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.00 usec
 PL1 -2.60 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 PL13 17.50 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6126261 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

aet9-60-MeOD



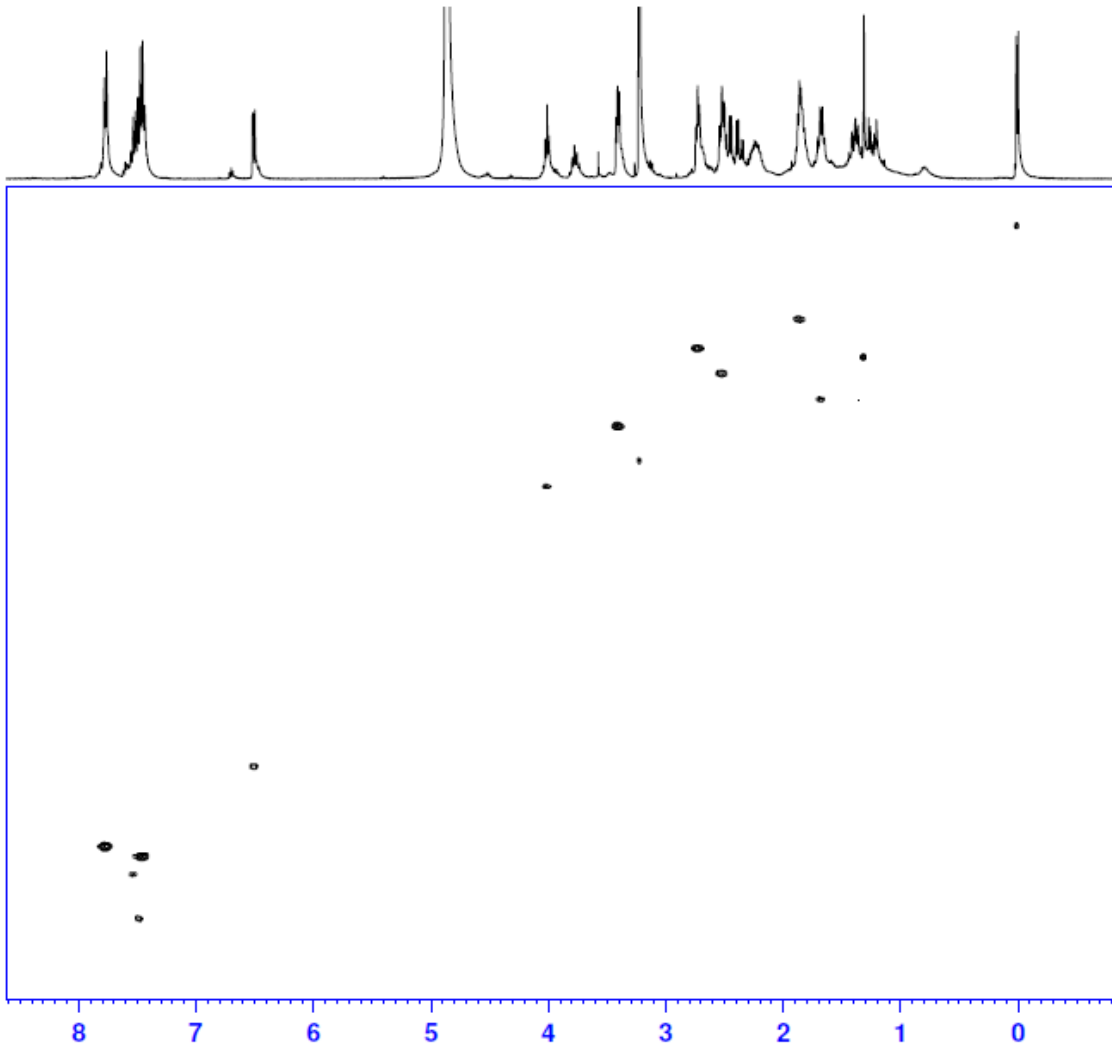
Current Data Parameters
 NAME aet9-60-MeOD
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130914
 Time 7.27
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG deptc135
 TD 65536
 SOLVENT MeOD
 NS 512
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 11585.2
 DW 20.850 usec
 DE 6.00 usec
 TE 293.2 K
 CNST2 145.0000000 sec
 D1 2.00000000 sec
 d2 0.00344828 sec
 D11 0.03000000 sec
 DELTA 0.00001146 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.00 usec
 P2 18.00 usec
 PL1 -2.60 dB
 SFO1 100.6228300 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 SFO2 400.1316000 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6126261 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



```

Current Data Parameters
NAME          acet9-CD-MeCD
EXPNO         14
PROCNO        1

F2 - Acquisition Parameters
Data_         20130914
Time          7.48
INSTRUM       spect
PROBHD        5 mm QNP 1H/13
PULPROG       zgpg30
TD             1024
SOLVENT       MeCD
NS             4
DS             16
SWH           3787.879 Hz
FIDRES        3.699100 Hz
AQ            0.1352180 sec
RG            5160.6
DW            132.000 usec
DE            6.00 usec
TE            292.2 K
CMST2         145.0000000
d0            0.00000300 usec
d1            1.49198906 usec
d2            0.00344828 usec
d12           0.00002000 usec
d13           0.00000400 usec
d16           0.00020000 usec
DELTA1        0.00222428 usec
IN0           0.00003000 usec

----- CHANNEL f1 -----
NUC1           1H
P1            10.00 usec
PL1           -1.50 dB
SFO1          400.1315941 MHz

----- CHANNEL f2 -----
CPDPRG2       gssp
NUC2           13C
P2            8.00 usec
PCPD2         74.00 usec
PL2           -3.00 dB
PL12          18.00 dB
SFO2          100.6203140 MHz

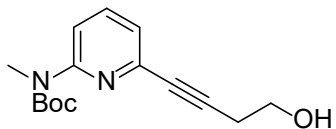
----- GRADIENT CHANNEL -----
GPNAM1        SINE.100
GPNAM2        SINE.100
GPNAM3        SINE.100
GPE1          50.00 %
GPE2          30.00 %
GPE3          40.10 %
PLG           1000.00 usec

F1 - Acquisition parameters
ND0            2
TD             128
SFO1          100.6203 MHz
FIDRES        130.208328 Hz
SW            165.639 ppm
F0MODE        QF

F2 - Processing parameters
SI             1024
SF            400.1300462 MHz
WDW           COSINE
SSB           0
LB            0.00 Hz
GB            0
PC            1.40

F1 - Processing parameters
SI             1024
MC2           QF
SF            100.6127690 MHz
WDW           COSINE
SSB           0
LB            0.00 Hz
GB            0
  
```

tert-butyl (6-(4-hydroxy-but-1-yn-1-yl)-pyridin-2-yl)(methyl)carbamate [Compound 46]



hms15-108-a



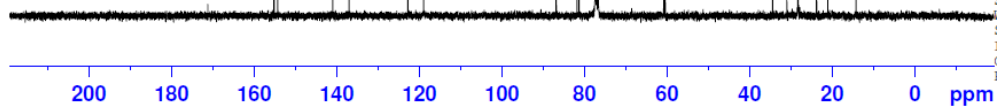
Current Data Parameters
 NAME HMS151202
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20151202
 Time 21.24
 INSTRUM DFX400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 1024
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 512
 DW 20.850 usec
 DE 6.00 usec
 TE 294.2 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.8999999 sec
 TD0 1

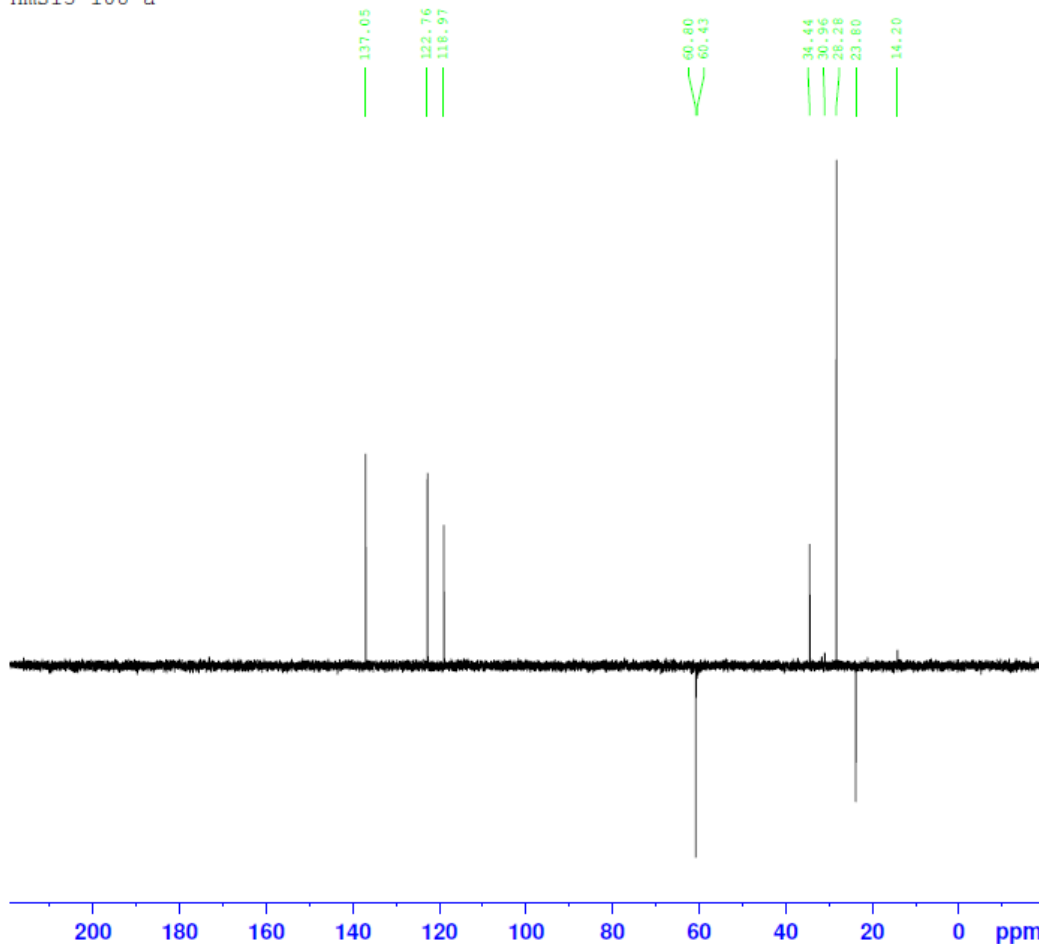
===== CHANNEL f1 =====
 NUC1 13C
 P1 9.00 usec
 PL1 -2.60 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 PL13 17.50 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



HMS151202



Current Data Parameters
NAME HMS151202
EXPNO 12
PROCNO 1

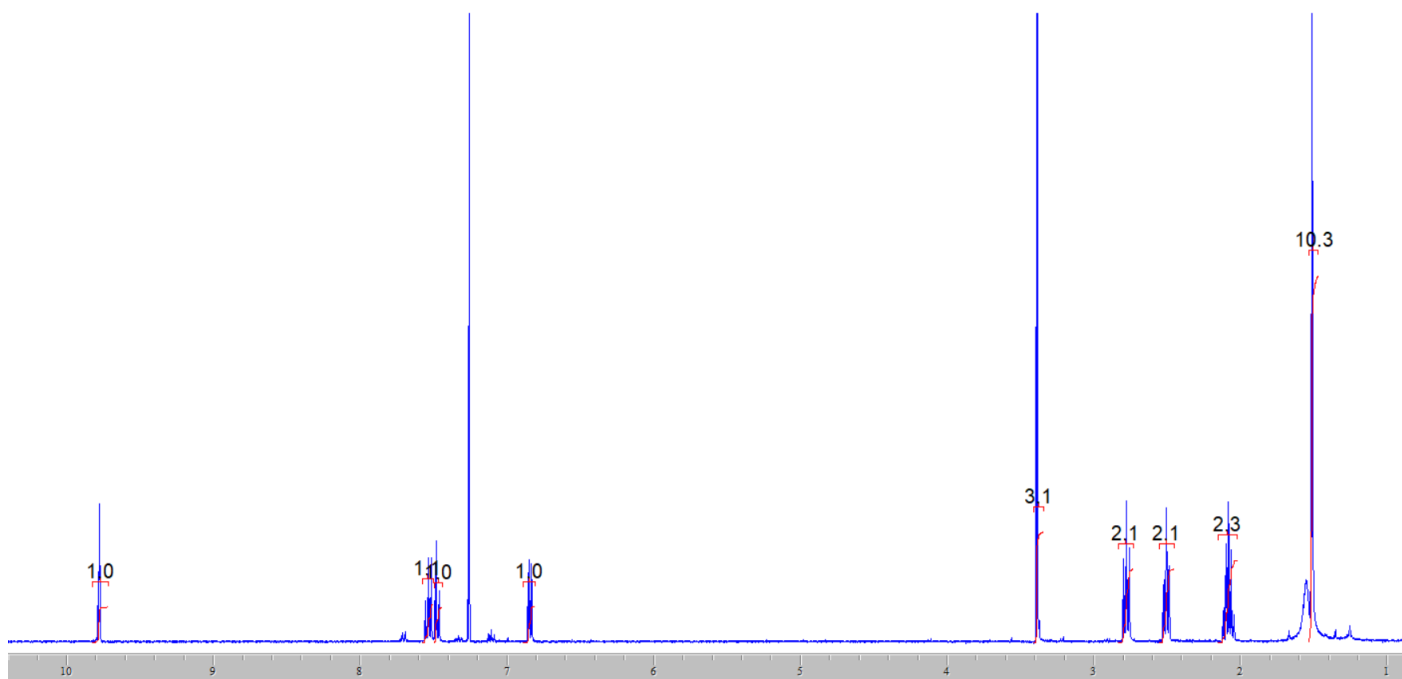
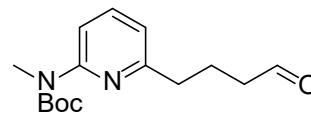
F2 - Acquisition Parameters
Date_ 20151202
Time 21.39
INSTRUM DPX400
PROBHD 5 mm QNP 1H/13
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 7298.2
DW 20.850 usec
DE 6.00 usec
TE 294.2 K
CNST2 145.0000000
D1 2.0000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00001146 sec
TD0 1

----- CHANNEL f1 -----
NUC1 13C
P1 9.00 usec
p2 18.00 usec
PL1 -2.60 dB
SFO1 100.6228298 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
P3 10.00 usec
P4 20.00 usec
PCPD2 80.00 usec
PL2 -1.50 dB
PL12 17.50 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

tert-butyl methyl(6-(4-oxobutyl)pyridin-2-yl)carbamate [Compound 43]



ppm

Current Data Parameters
 NAME: aat7-9-f4_6
 EXPNO: 13
 PROCNO: 1

F2 - Acquisition Parameters
 Data_: 20111015
 Time: 0.41
 INSTRUM: DFX400
 PROBHD: 5 mm QNP 1H/13
 PULPROG: cosygpsfgf
 TD: 2048
 SOLVENT: CDCl3
 NS: 4
 DS: 8
 SWH: 4280.822 Hz
 FIDRES: 2.090245 Hz
 AQ: 0.2392564 sec
 RG: 4096
 LW: 116.800 usec
 DE: 6.00 usec
 TE: 298.2 K
 D0: 0.00000300 sec
 D1: 1.95207703 sec
 d13: 0.00000400 sec
 D16: 0.00020000 sec
 IN0: 0.00023360 sec

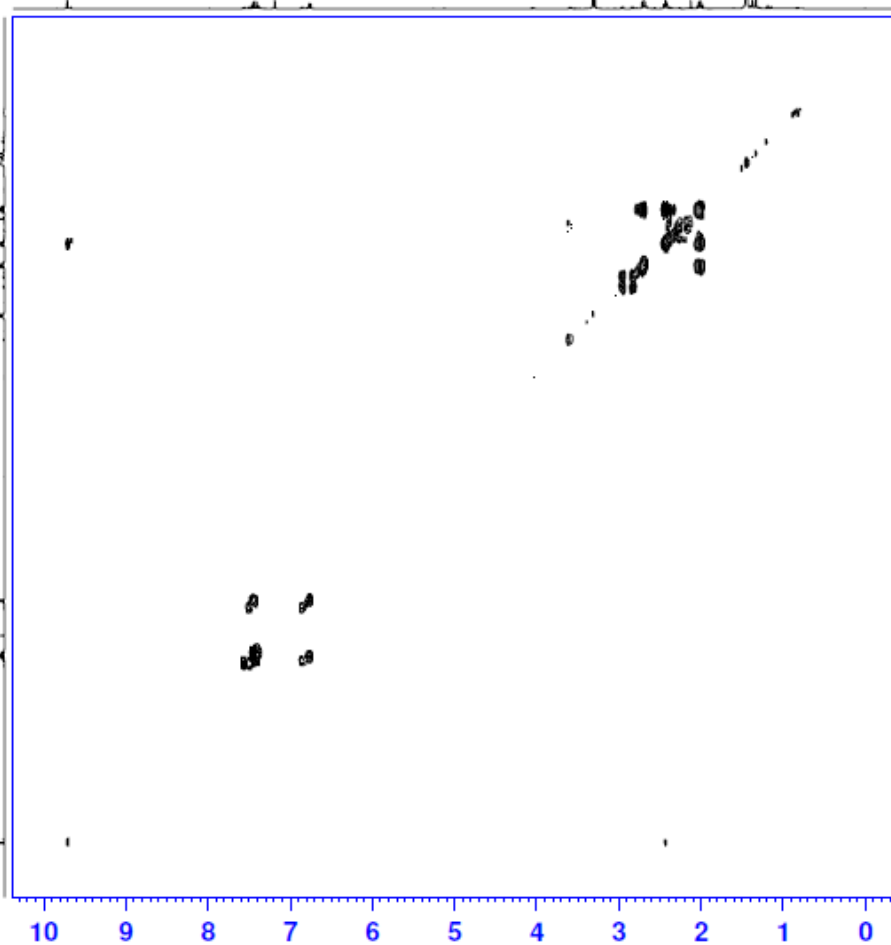
----- CHANNEL f1 -----
 NUC1: 1H
 P1: 10.00 usec
 PL1: -1.50 dB
 SFO1: 400.1320448 MHz

----- GRADIENT CHANNEL -----
 GPNAM1: SINE.100
 GPNAM2: SINE.100
 GPNAM3: SINE.100
 GPE1: 16.00 %
 GPE2: 12.00 %
 GPE3: 40.00 %
 P16: 1000.00 usec

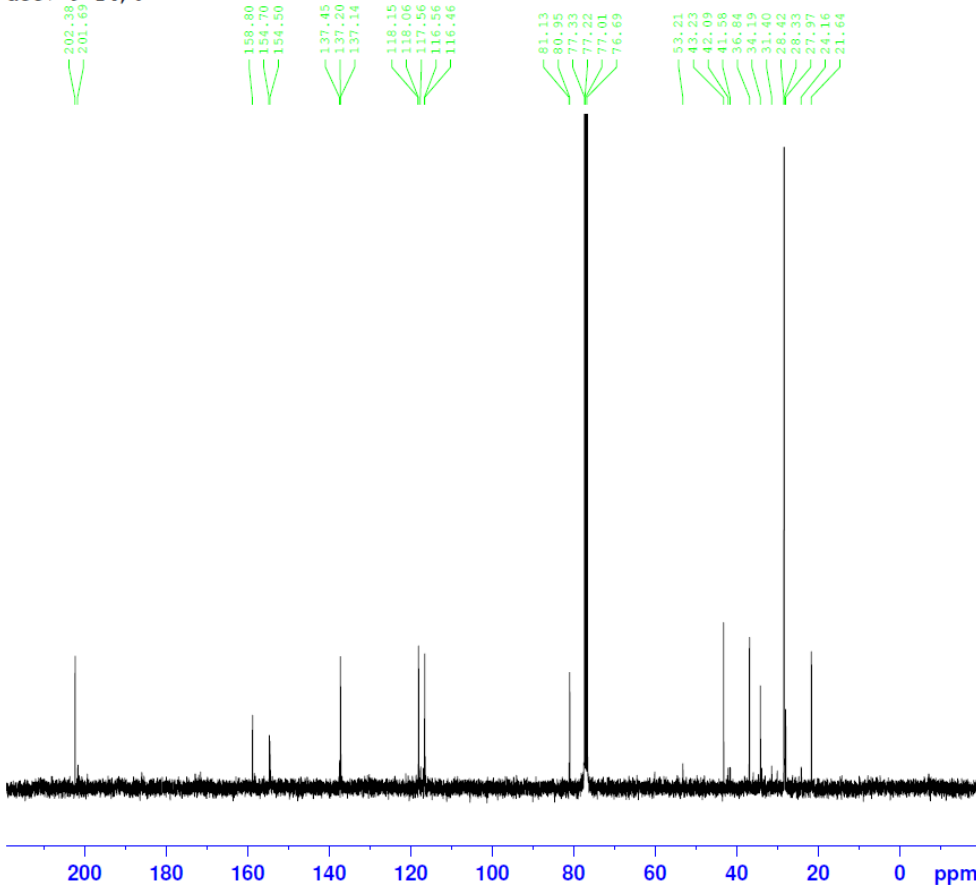
F1 - Acquisition parameters
 NDD: 1
 TD: 128
 SFO1: 400.132 MHz
 FIDRES: 33.443920 Hz
 SW: 10.699 ppm
 FrMODE: QF

F2 - Processing parameters
 SI: 1024
 SF: 400.1300365 MHz
 WDW: SINE
 SSB: 0
 LB: 0.00 Hz
 GB: 0
 PC: 1.40

F1 - Processing parameters
 SI: 1024
 MC2: QF
 SF: 400.1300365 MHz
 WDW: SINE
 SSB: 0
 LB: 0.00 Hz
 GB: 0



aet7-9-f4,6



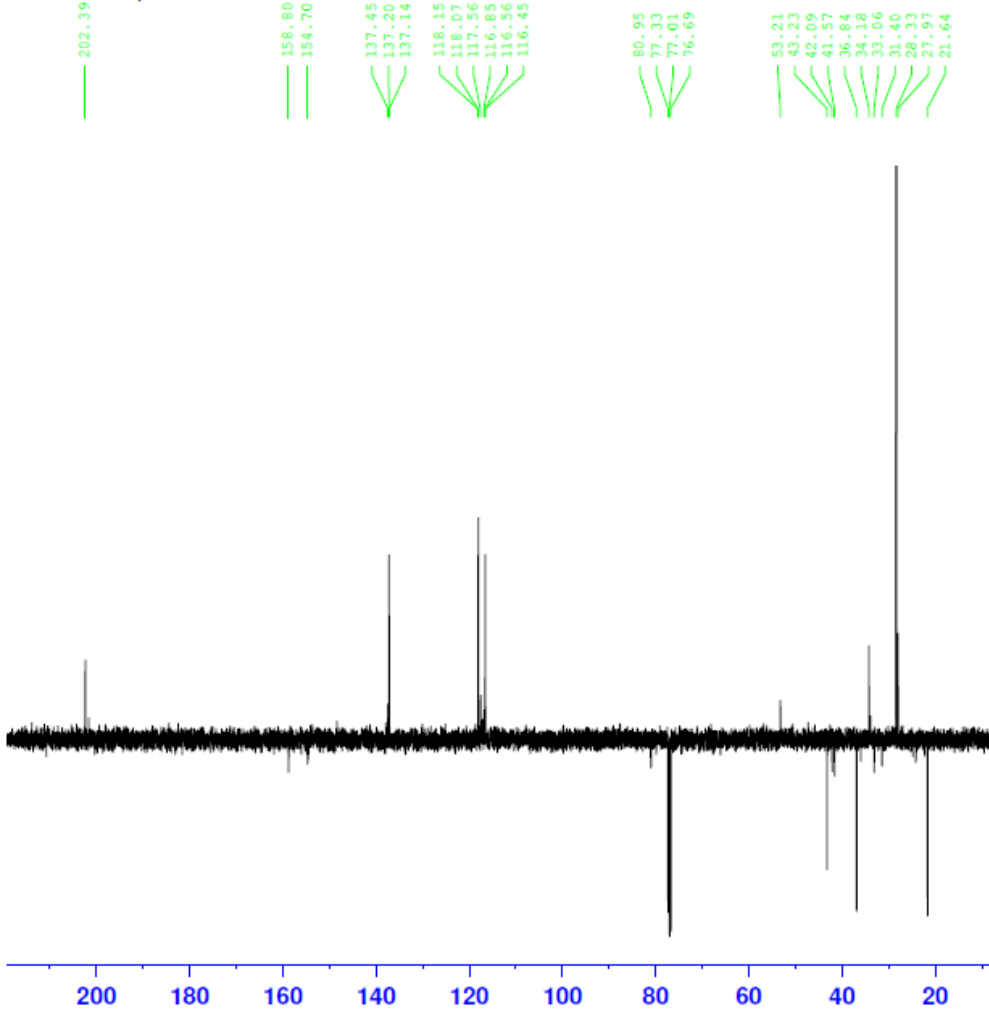
Current Data Parameters
 NAME aet7-9-f4,6
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20111015
 Time 0.10
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 1448.2
 DW 20.850 usec
 DE 6.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.00 usec
 PL1 -2.60 dB
 SFO1 100.6228298 MHz
 ===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 PL13 17.50 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

aet7-9-f4,6



Current Data Parameters
 NAME aet7-9-f4,6
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20111015
 Time 0.40
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG deptq_135
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 18390.4
 DW 20.850 usec
 DE 6.00 usec
 TE 298.2 K
 CNST2 145.0000000
 D1 2.00000000 sec
 d2 0.00344828 sec
 D11 0.03000000 sec
 DELTA 0.00001019 sec

----- CHANNEL f1 -----
 NUC1 13C
 P1 8.00 usec
 P2 16.00 usec
 PL1 -2.60 dB
 SFO1 100.6228300 MHz

----- CHANNEL f2 -----
 CPDPRG2 waltz16
 NUC2 1H
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 SFO2 400.1316000 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Current Data Parameters
 NAME met7-9-f4_c
 EXPNO 14
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 2011015
 Time 1.01

INSTRUM spect
 PROBRD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 1024
 SOLVENT cdcl3
 NS 4
 DS 16
 SWH 4280.822 Hz
 FIDRES 4.186490 Hz
 AQ 0.1196530 sec
 RG 4096
 DW 116.800 usec
 DE 6.00 usec
 TE 298.2 K
 CMST2 145.0000000
 d0 0.0000300 sec
 d1 1.5716805 sec
 d2 0.00344828 sec
 d12 0.0002000 sec
 d13 0.0000400 sec
 d16 0.0002000 sec
 DELTA1 0.00222428 sec
 IN0 0.00003000 sec

CHANNEL F1
 NUC1 1H
 P1 10.00 usec
 P2 20.00 usec
 PL1 -1.50 dB
 SFO1 400.1320448 MHz

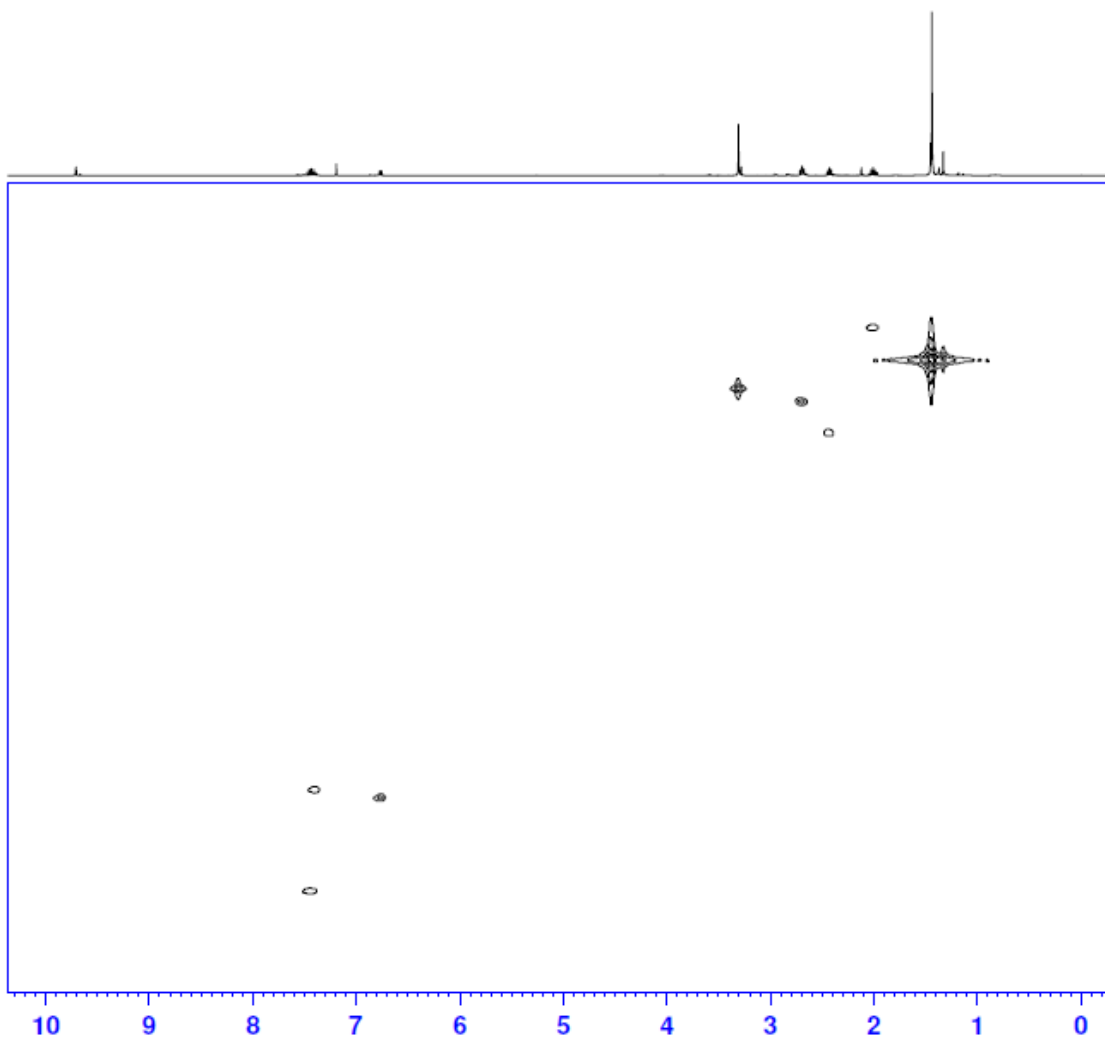
CHANNEL F2
 CPDPRG2 gqzgpg
 NUC2 13C
 P3 8.00 usec
 PCPD2 74.00 usec
 PL2 -2.00 dB
 PL12 18.00 dB
 SFO2 100.6203140 MHz

GRADIENT CHANNEL
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPNAM3 SINE.100
 GPF1 50.00 %
 GPF2 30.00 %
 GPF3 40.10 %
 P16 1000.00 usec

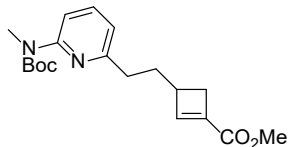
F1 - Acquisition parameters
 NS0 2
 TD 128
 SFO1 100.6203 MHz
 FIDRES 130.208328 Hz
 SW 165.439 ppm
 FWHM 0.9

F2 - Processing parameters
 SI 1024
 SF 400.1300365 MHz
 MW 0.00 Hz
 LB 0.00 Hz
 GB 0
 PC 1.40

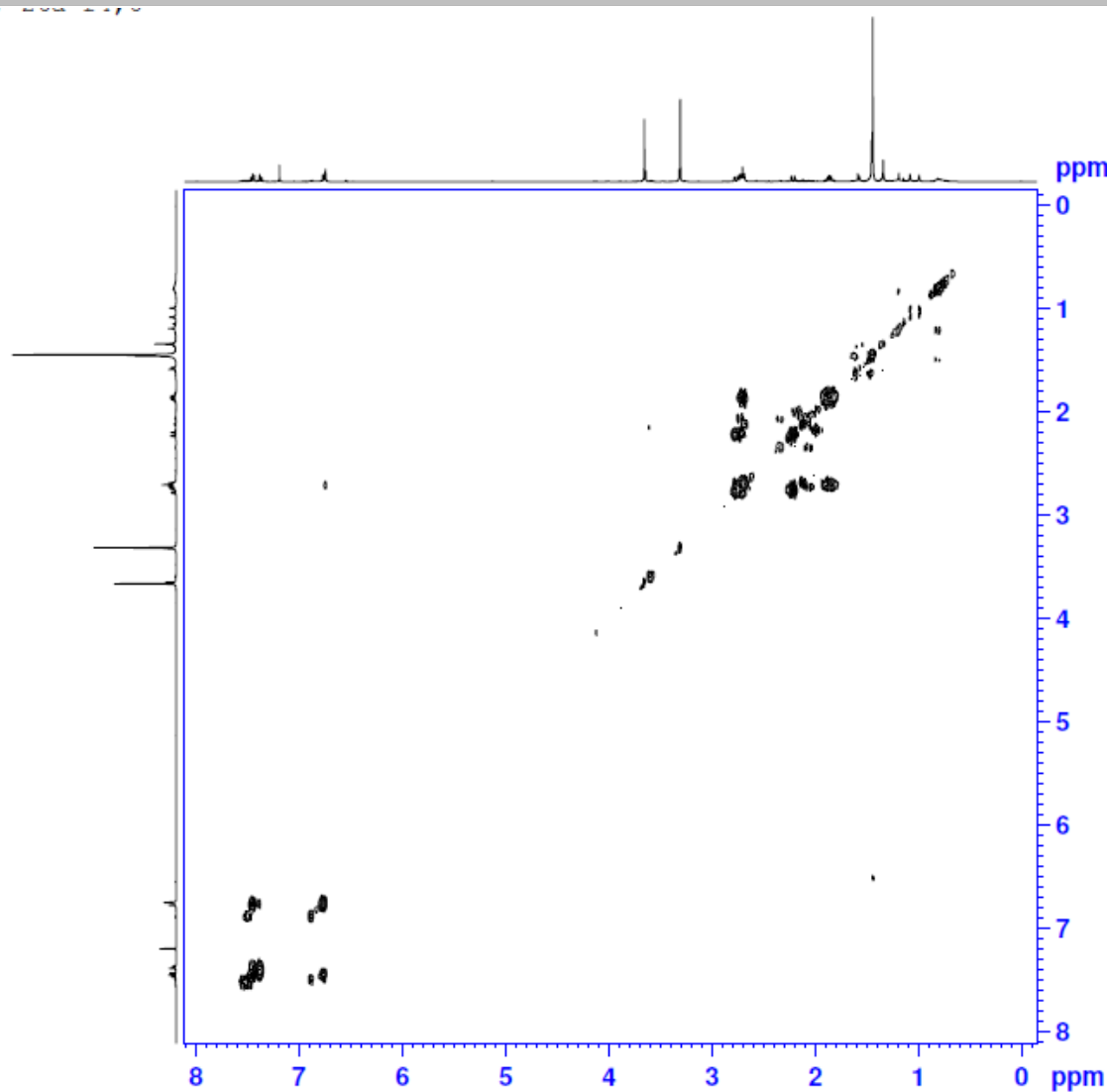
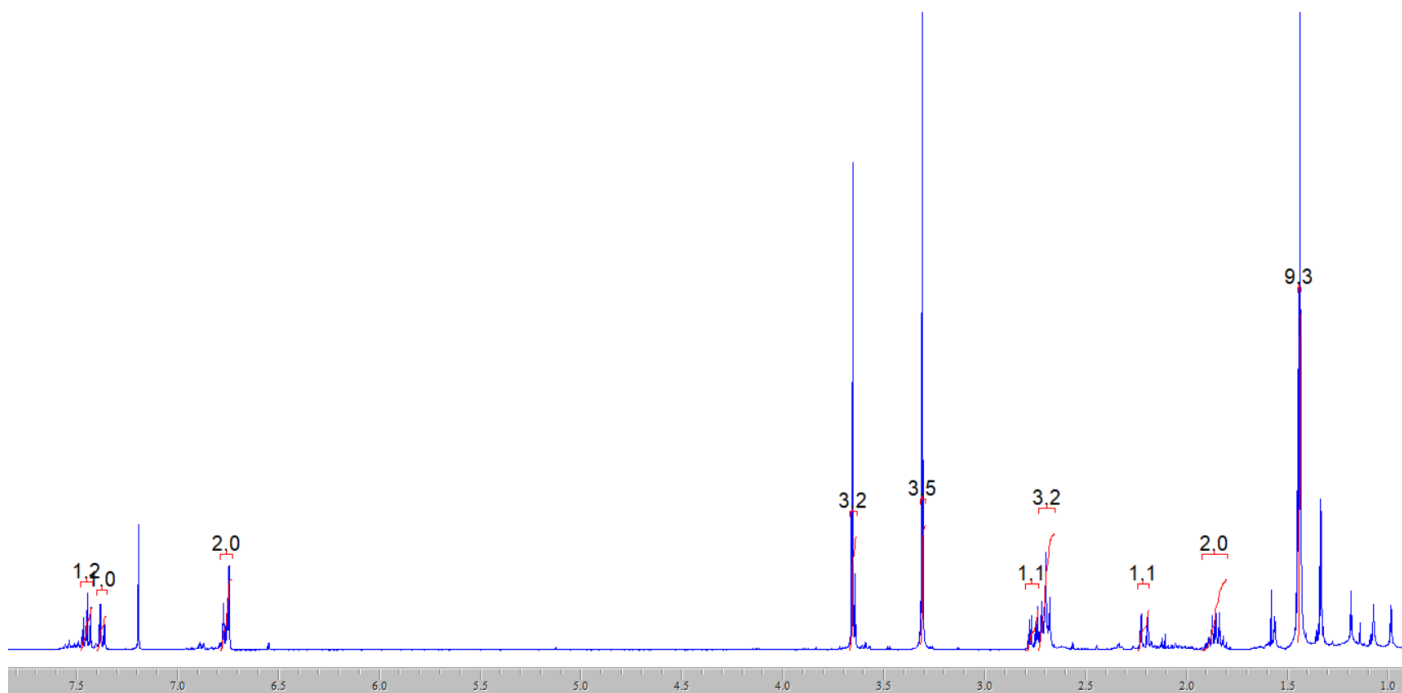
F1 - Processing parameters
 SI 1024
 MC2 0.9
 SF 100.6127690 MHz
 MW 0.00 Hz
 LB 0
 GB 0



Methyl 3-(2-(6-((*tert*-butoxycarbonyl)(methyl)amino)pyridin-2-yl)ethyl)cyclobut-1-ene-1-carboxylate



[Compound 47]



Current Data Parameters
NAME ast7-26a-f4,6
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111117
Time 1.49
INSTRUM DFX400
PROBHD 5 mm QNP 1H/13
PULPROG cosygmfzf
TD 2048
SOLVENT CDCl3
NS 4
DS 8
SWH 3306.878 Hz
FIDRES 1.614687 Hz
AQ 0.3097076 sec
RG 10321.3
DW 151.200 usec
DE 6.00 usec
TE 294.2 K
D0 0.00000300 sec
D1 1.88244498 sec
d13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00030240 sec

----- CHANNEL f1 -----
NUC1 1H
P1 10.00 usec
PL1 -1.50 dB
SF01 400.1316264 MHz

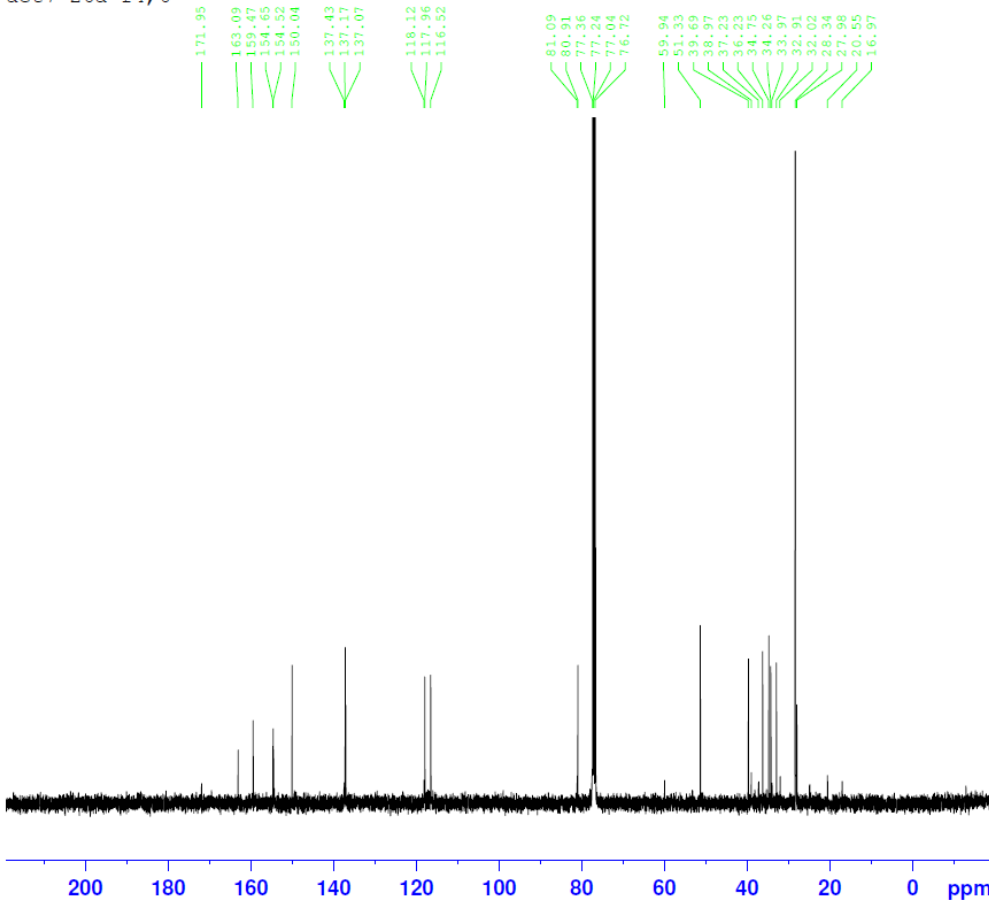
----- GRADIENT CHANNEL -----
CPNAM1 SINE.100
CPNAM2 SINE.100
CPNAM3 SINE.100
GPZ1 16.00 %
GPZ2 12.00 %
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
ND0 1
TD 128
SF01 400.1316 MHz
FIDRES 25.834988 Hz
SW 8.264 ppm
FrMODE QF

F2 - Processing parameters
SI 1024
SF 400.1300355 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.1300355 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

aet7-26a-f4, 6



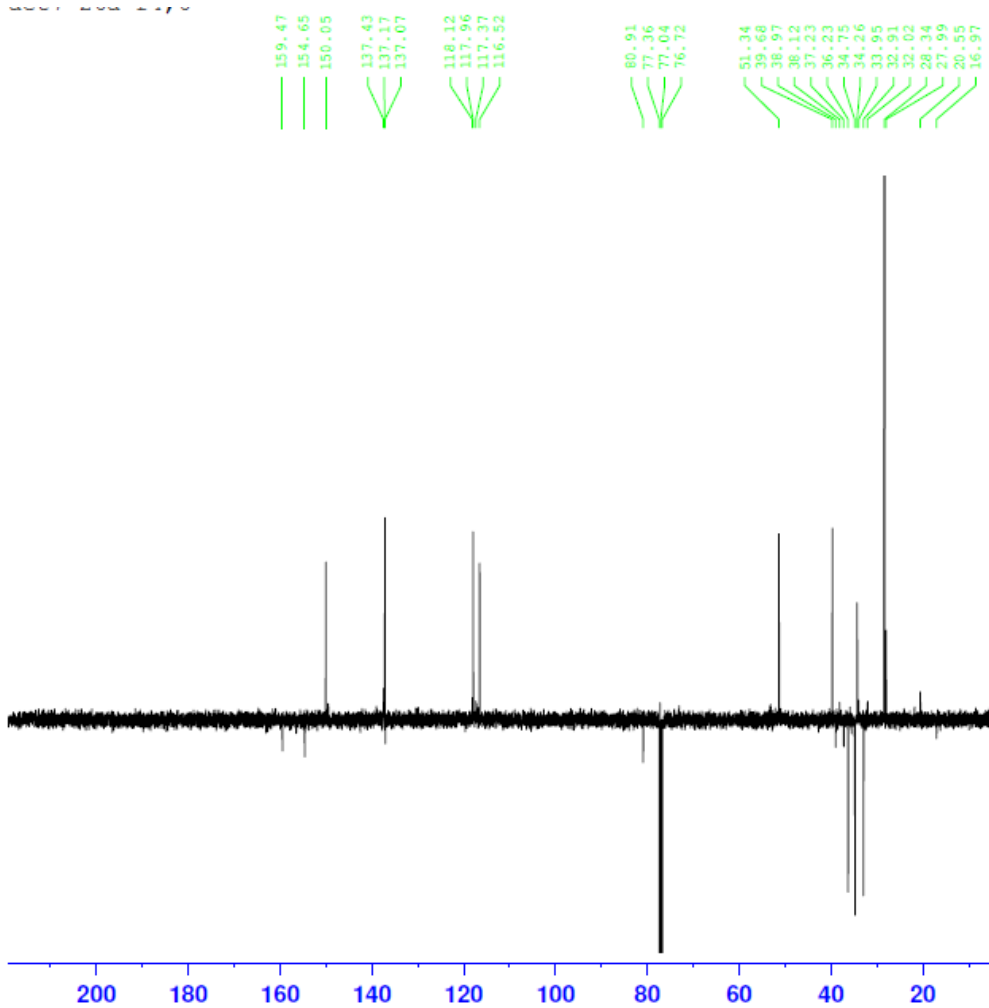
Current Data Parameters
 NAME aet7-26a-f4, 6
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 2011117
 Time 1.18
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 1824.6
 DW 20.850 usec
 DE 6.00 usec
 TE 295.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.00 usec
 PL1 -2.60 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 PL13 17.50 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
 NAME aet7-26a-f4, 6
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 2011117
 Time 1.48
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG deptq_135
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 16384
 DW 20.850 usec
 DE 6.00 usec
 TE 294.2 K
 CNST2 145.0000000
 D1 2.00000000 sec
 d2 0.00344828 sec
 D11 0.03000000 sec
 DELTA 0.00001019 sec

----- CHANNEL f1 -----
 NUC1 13C
 P1 8.00 usec
 P2 16.00 usec
 PL1 -2.60 dB
 SFO1 100.6228300 MHz

----- CHANNEL f2 -----
 CPDPRG2 waltz16
 NUC2 1H
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 SFO2 400.1316000 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Current Data Parameters
 NAME: act7-26a-14_C
 EXPNO: 14
 PROCNO: 1

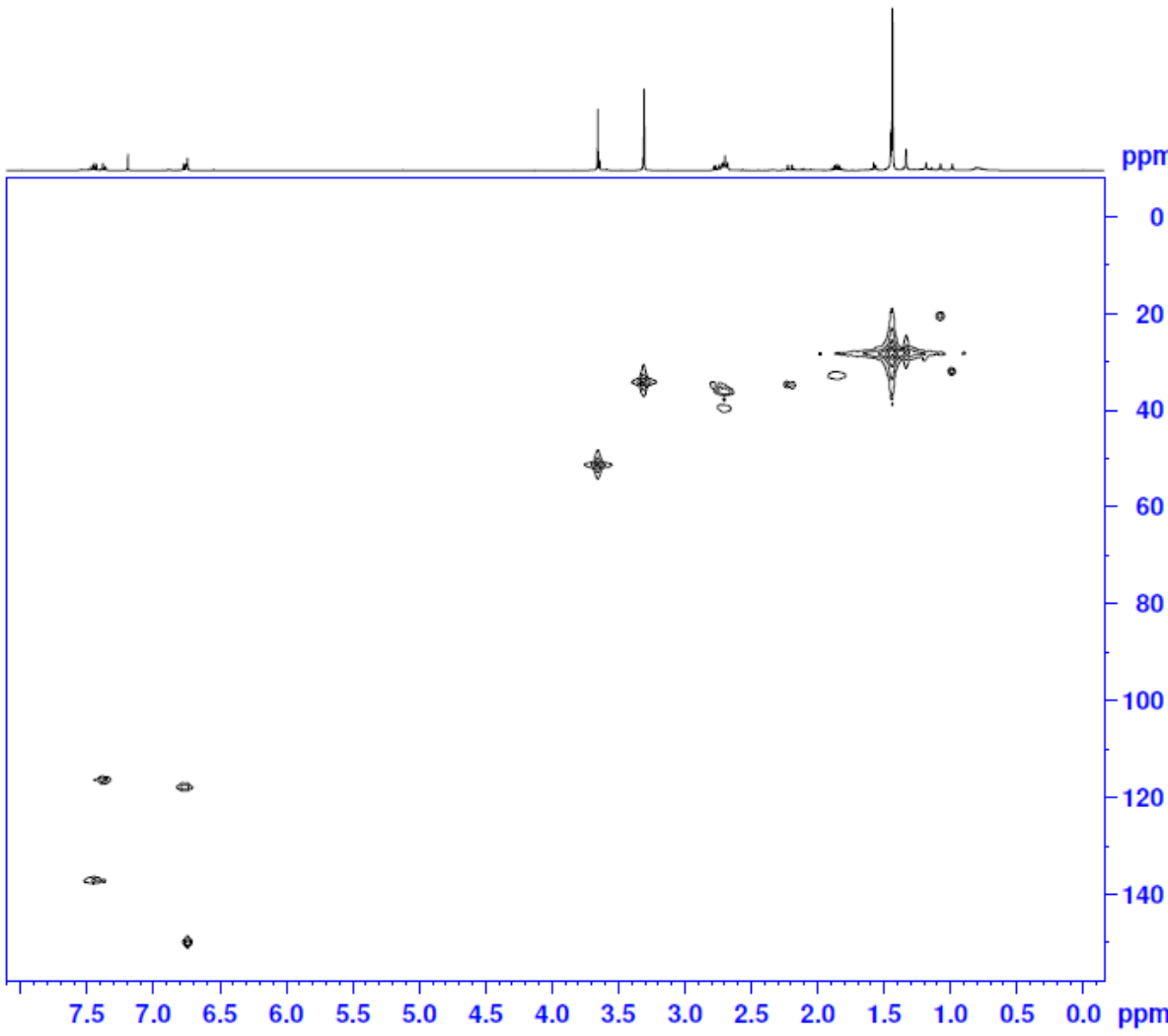
F2 - Acquisition Parameters
 Date_: 20111117
 Time: 2.09
 INSTRUM: spect
 PULPROG: zgpg30
 TD: 1024
 SOLVENT: cdcl3
 NS: 4
 DS: 16
 SWH: 3306.878 Hz
 FIDRES: 3.229373 Hz
 AQ: 0.1548788 sec
 RG: 5120.6
 DW: 151.200 usec
 DE: 6.00 usec
 TE: 294.2 K
 CMT2: 145.0000000
 d0: 0.000003000 sec
 d1: 1.47235203 sec
 d2: 0.00344828 sec
 d12: 0.00002000 sec
 d13: 0.00000400 sec
 d16: 0.00020000 sec
 DELTA1: 0.00222428 sec
 TNO: 0.00003000 sec

CHANNEL F1
 NUC1: 1H
 P1: 10.00 usec
 P2: 20.00 usec
 PL1: -1.50 dB
 SFO1: 400.1316264 MHz
 CHANNEL F2
 CPDPRG2: gpg3
 NUC2: 13C
 P3: 8.00 usec
 PCPD2: 74.00 usec
 PL2: -3.00 dB
 PL12: 18.00 dB
 SFO2: 100.6203140 MHz
 GRADIENT CHANNEL
 GPMAM1: SINE.100
 GPMAM2: SINE.100
 GPMAM3: SINE.100
 GPF1: 50.00 %
 GPF2: 30.00 %
 GPF3: 40.10 %
 P16: 1000.00 usec

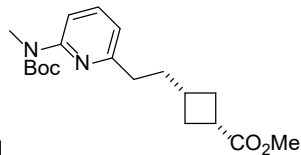
F1 - Acquisition parameters
 MD: 2
 TD: 128
 SFO1: 100.6203 MHz
 FIDRES: 130.208328 Hz
 SW: 165.639 ppm
 FMODE: CF

F2 - Processing parameters
 SI: 1024
 SF: 400.1300355 MHz
 WDW: QSINE
 SSB: 2
 LB: 0.00 Hz
 GB: 0
 PC: 1.40

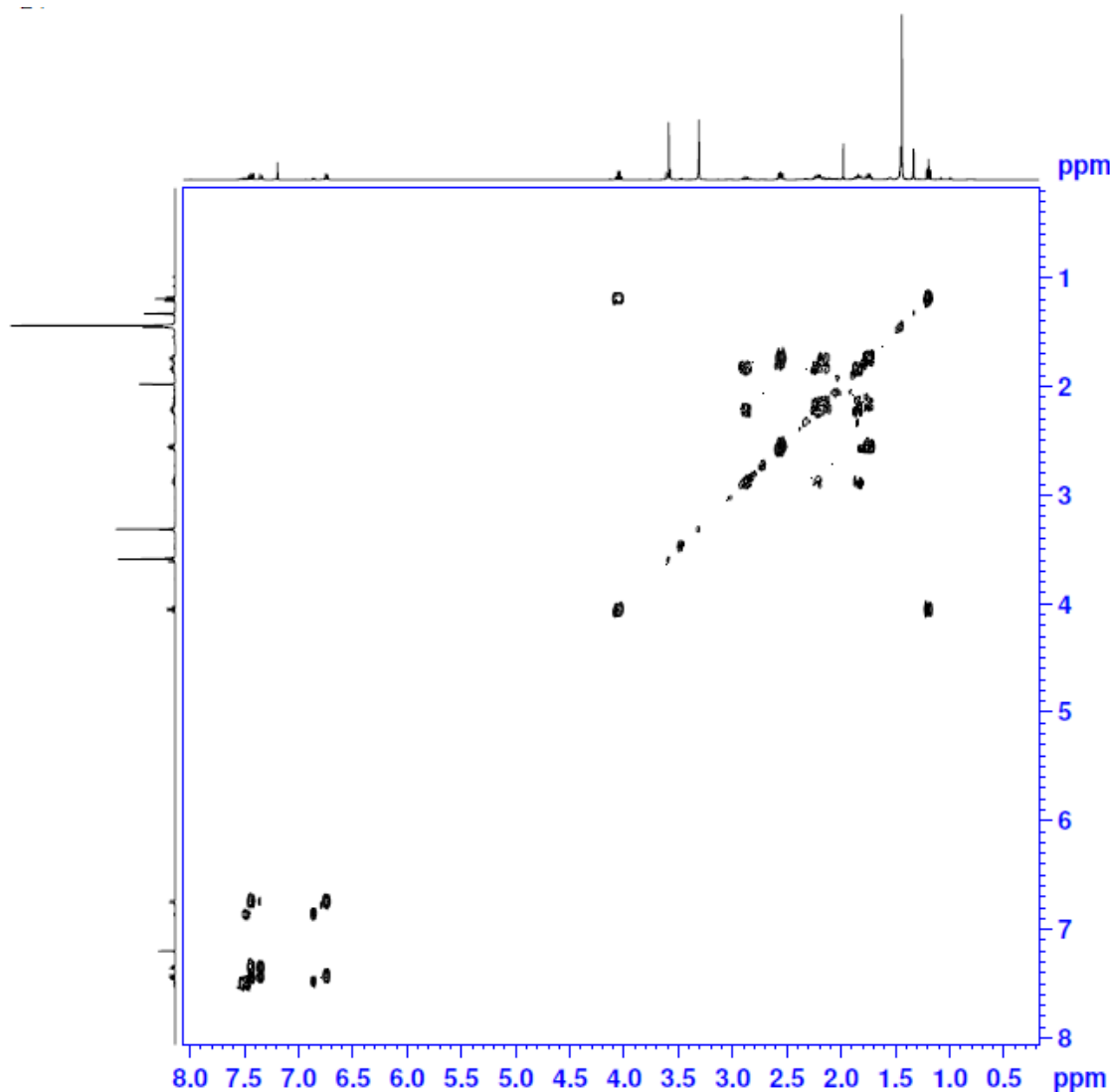
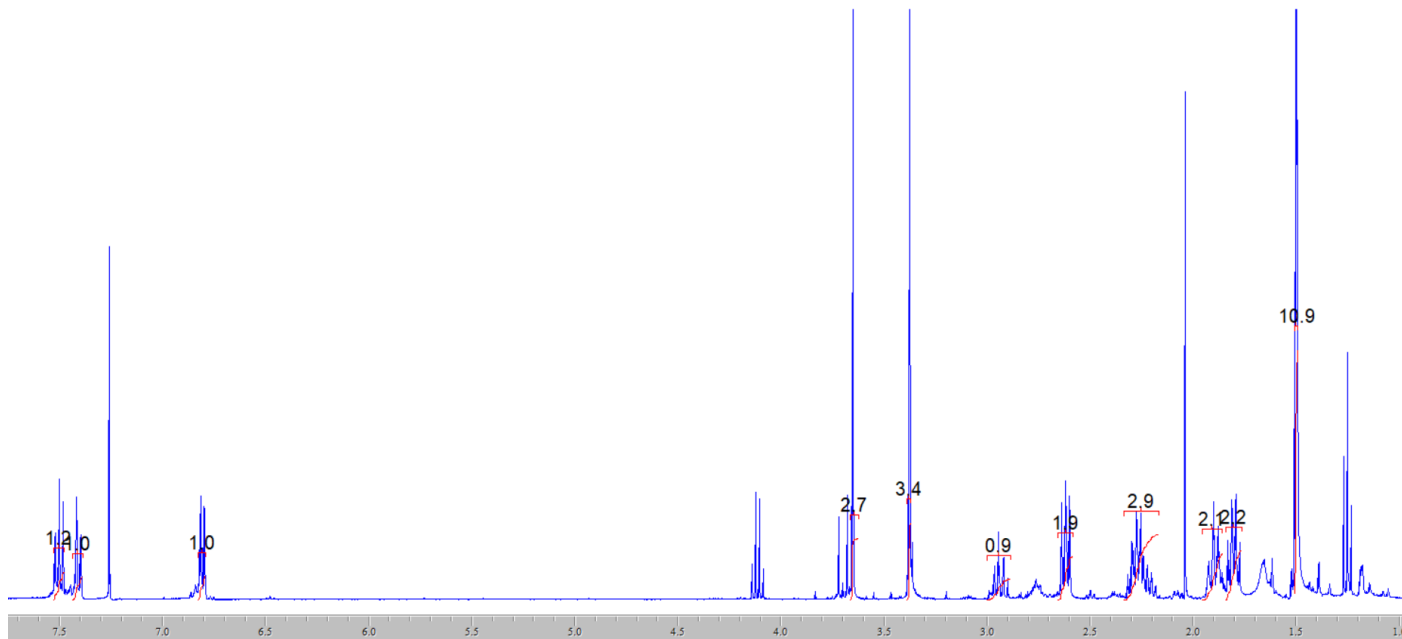
F1 - Processing parameters
 SI: 1024
 MC: CF
 SF: 100.6127690 MHz
 WDW: QSINE
 SSB: 2
 LB: 0.00 Hz
 GB: 0



Methyl (1*r**,3*s**)-3-(2-(6-((tert-butoxycarbonyl)(methyl)amino)pyridin-2-yl)ethyl) cyclobutane-1-



carboxylate [Compound 48]



Current Data Parameters
 NAME set7-27
 EXPNO 15
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20111123
 Time 19.51
 INSTRUM DPX400
 PROBRD 5 mm QNP 1H/13
 PULPROG cosygpsmfgf
 TD 2048
 SOLVENT CDCl3
 NS 4
 DS 8
 SWH 3156.566 Hz
 FIDRES 1.541292 Hz
 AQ 0.3244532 sec
 RG 11585.2
 DW 158.400 usec
 DE 6.00 usec
 TE 294.2 K
 D0 0.00000300 sec
 D1 1.86810899 sec
 d13 0.00000400 sec
 D16 0.00020000 sec
 INO 0.00031680 sec

----- CHANNEL f1 -----
 MUC1 1H
 P1 10.00 usec
 PL1 -1.50 dB
 SFO1 400.1316815 MHz

----- GRADIENT CHANNEL -----
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPNAM3 SINE.100
 GPZ1 16.00 %
 GPZ2 12.00 %
 GPZ3 40.00 %
 P16 1000.00 usec

F1 - Acquisition parameters
 MD0 1
 TD 128
 SFO1 400.1317 MHz
 FIDRES 24.660669 Hz
 SW 7.889 ppm
 FrMODE QF

F2 - Processing parameters
 SI 1024
 SF 400.1300351 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 FC 1.40

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 400.1300351 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

aet7-27



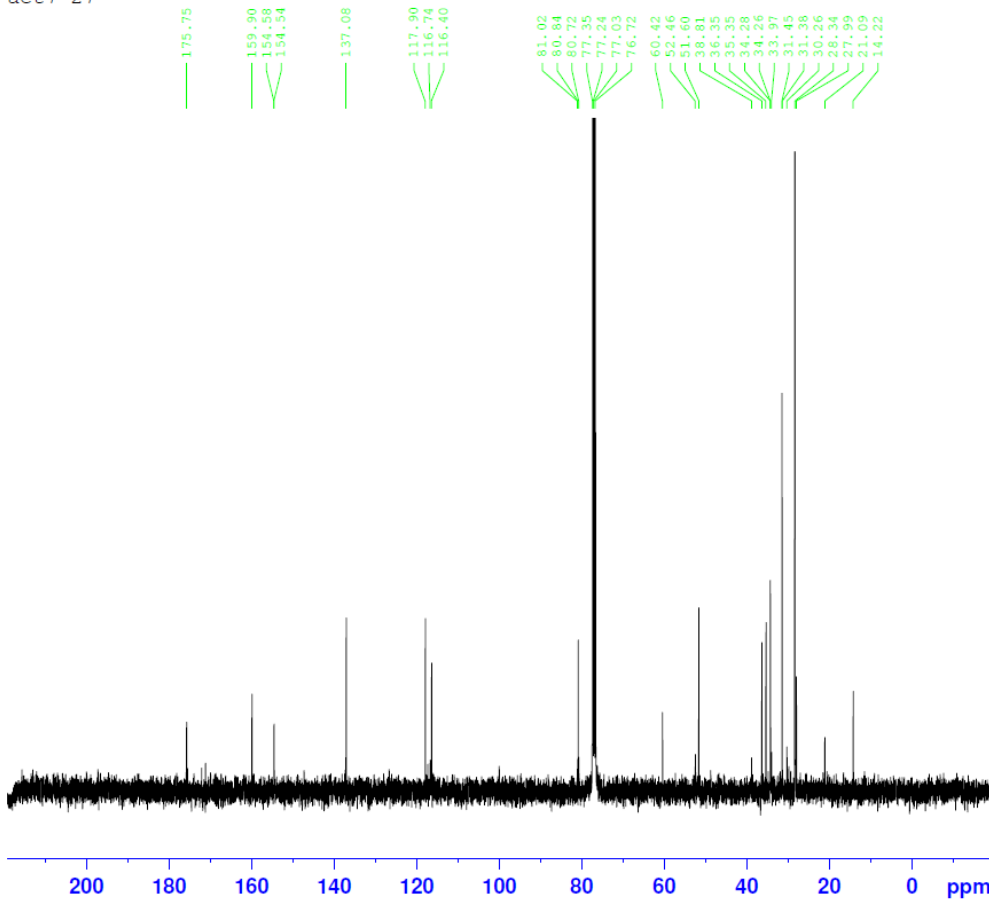
Current Data Parameters
 NAME aet7-27
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20111123
 Time 19.03
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 1024
 DW 20.850 usec
 DE 6.00 usec
 TE 294.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.00 usec
 PL1 -2.60 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 PL13 17.50 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



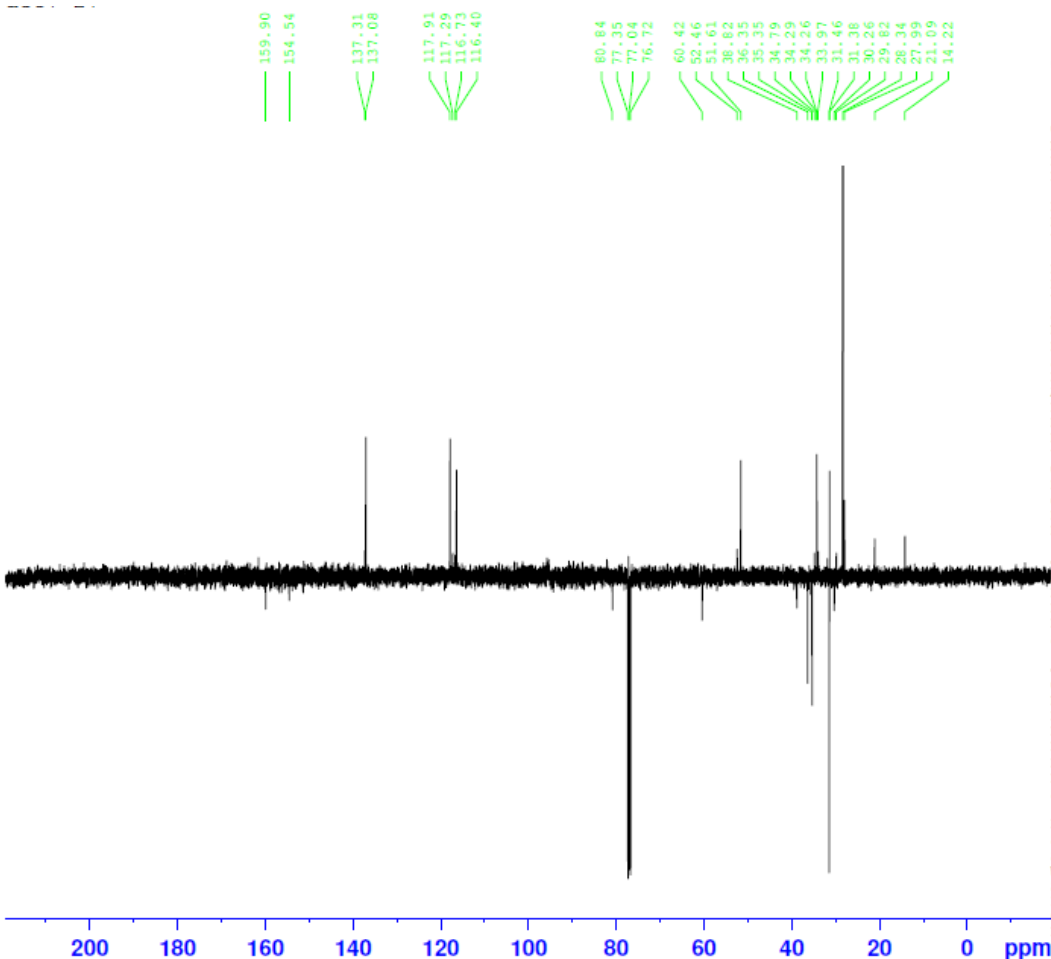
Current Data Parameters
 NAME aet7-27
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20111123
 Time 19.33
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG deptq 135
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 11585.2
 DW 20.850 usec
 DE 6.00 usec
 TE 294.2 K
 CNST2 145.0000000
 D1 2.00000000 sec
 d2 0.00344828 sec
 D11 0.03000000 sec
 DELTA 0.00001019 sec

----- CHANNEL f1 -----
 NUC1 13C
 P1 8.00 usec
 P2 16.00 usec
 PL1 -2.60 dB
 SFO1 100.6228300 MHz

----- CHANNEL f2 -----
 CPDPRG2 waltz16
 NUC2 1H
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 SFO2 400.1316000 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40





Current Data Parameters
NAME ac7-27
EXFNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 2011123
Time 19.36
INSTRUM DFX400
PROBHD 5 mm QNP 1H/13
PULPROG hmqcpgpgf
TD 1024
SOLVENT CDCl3
NS 4
DS 16
SWH 3156.566 Hz
FIDRES 3.082584 Hz
AQ 0.1622516 sec
RG 5120.6
SW 158.400 usec
DE 6.00 usec
TE 294.2 K
CMT2 145.000000 sec
d0 0.00003000 sec
d1 1.46518397 sec
d2 0.00344828 sec
d12 0.00002000 sec
d13 0.00004000 sec
d16 0.00020000 sec
DELTA1 0.0022428 sec
IND 0.00003000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 10.00 usec
P2 20.00 usec
PL1 -1.50 dB
SFO1 400.1316815 MHz

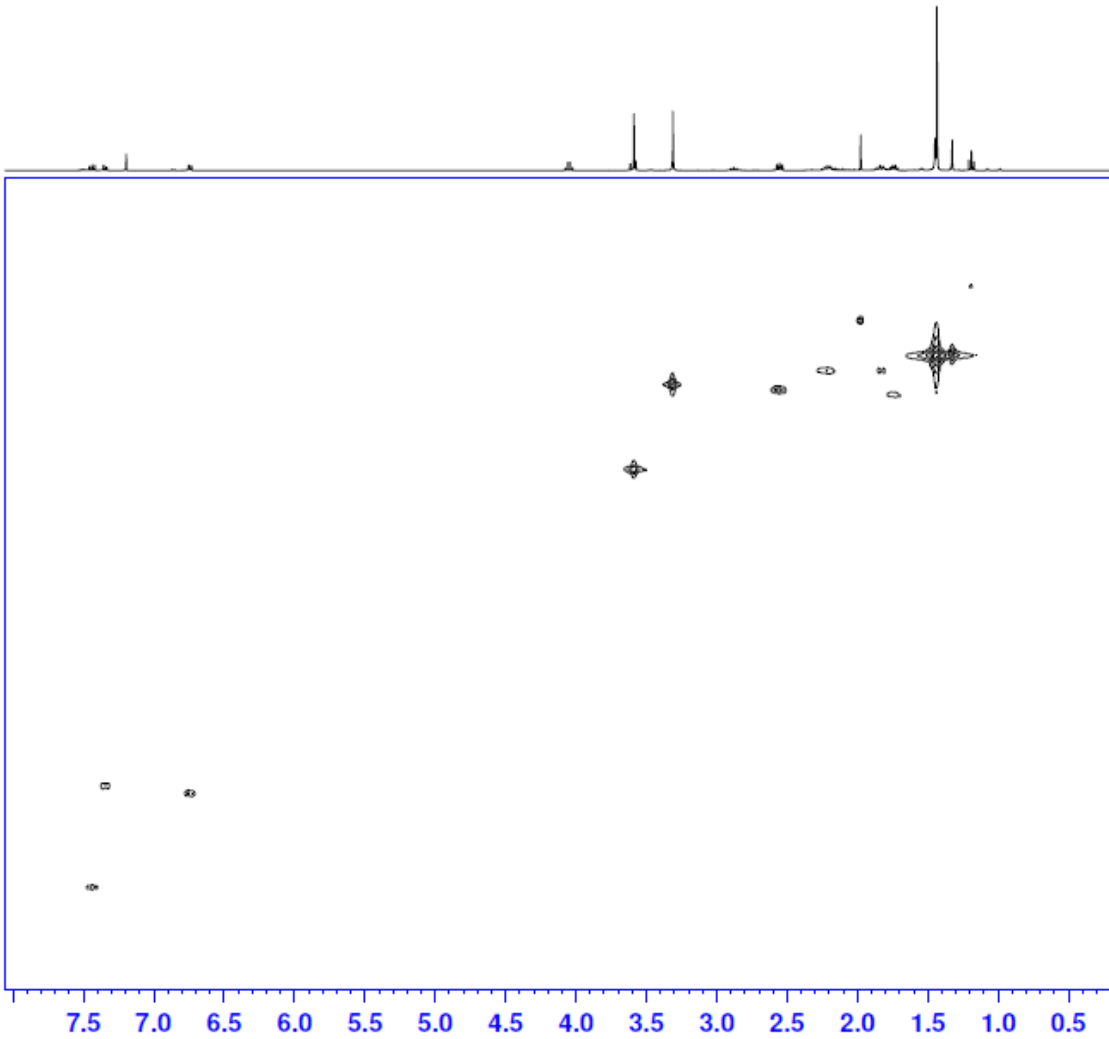
----- CHANNEL f2 -----
CPDPRG2 gwhf
NUC2 13C
P3 9.00 usec
PCPD2 74.00 usec
PL2 -3.00 dB
PL12 18.00 dB
SFO2 100.6203140 MHz

----- GRADIENT CHANNEL -----
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPE1 50.00 %
GPE2 30.00 %
GPE3 40.10 %
P16 1000.00 usec

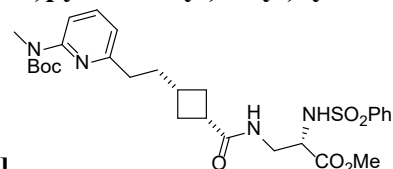
F1 - Acquisition parameters
ND0 2
TD 128
SFO1 100.6203 MHz
FIDRES 130.208328 Hz
SW 165.639 ppm
FrMODE QF

F2 - Processing parameters
SI 1024
SF 400.1300351 MHz
WDW GCINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

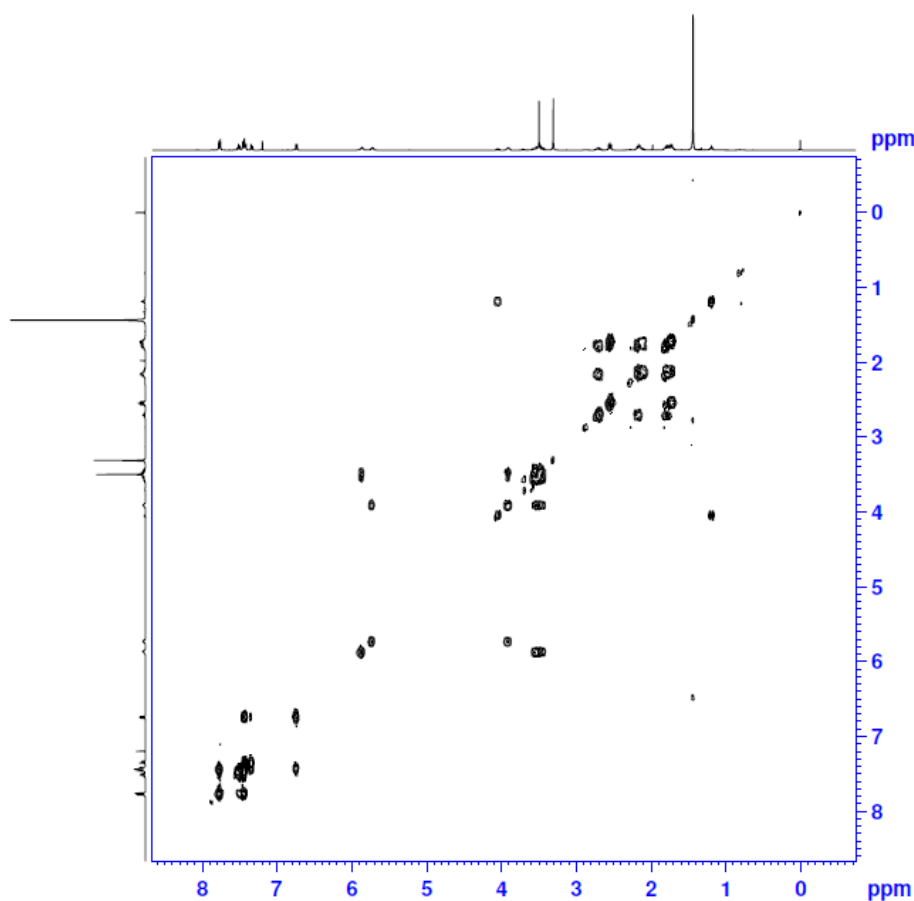
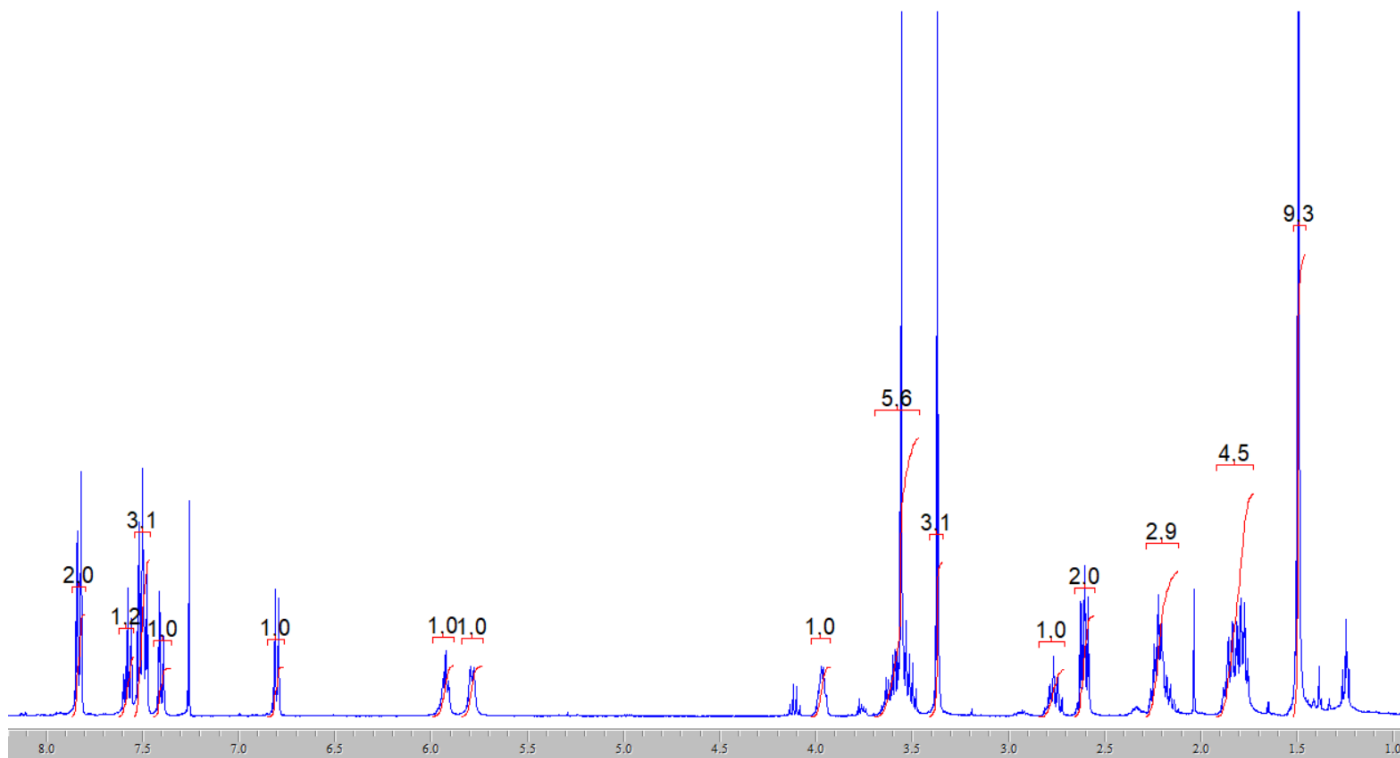
F1 - Processing parameters
SI 1024
MC2 QF
SF 100.6127690 MHz
WDW GCINE
SSB 2
LB 0.00 Hz
GB 0



Methyl (*S*)-3-((1*r**,3*R**)-3-(2-(6-((*tert*-butoxycarbonyl)(methyl)amino)pyridin-2-yl)ethyl)cyclobutane-



1-carboxamido)-2-(phenylsulfonamido)propanoate [Compound 51]



Current Data Parameters
NAME ast7-39-2
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 2011209
Time 19.36
INSTRUM DPK400
PROBHD 5 mm QNP 1H/13
PULPROG cosygpmpfgf
TD 2048
SOLVENT CDCl3
NS 4
DS 8
SWH 2765.060 Hz
FIDRES 1.938408 Hz
AQ 0.2720244 sec
RG 8192
DW 132.800 usec
DE 6.00 usec
TE 294.2 K
D0 0.00000300 sec
D1 1.91930902 sec
d13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00026560 sec

CHANNEL f1
NUC1 1H
P1 10.00 usec
PL1 -1.50 dB
SFO1 400.1316186 MHz

GRADIENT CHANNEL
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPE1 16.00 %
GPE2 12.00 %
GPE3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
ND0 1
TD 128
SFO1 400.1316 MHz
FIDRES 29.41534 Hz
SW 9.410 ppm
FRMODE QF

F2 - Processing parameters
SI 1024
SF 400.1300340 MHz
WVW SINE
SSB 0
LB 0.00 Hz
GB 0
FC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.1300340 MHz
WVW SINE
SSB 0
LB 0.00 Hz
GB 0

aet7-39-2



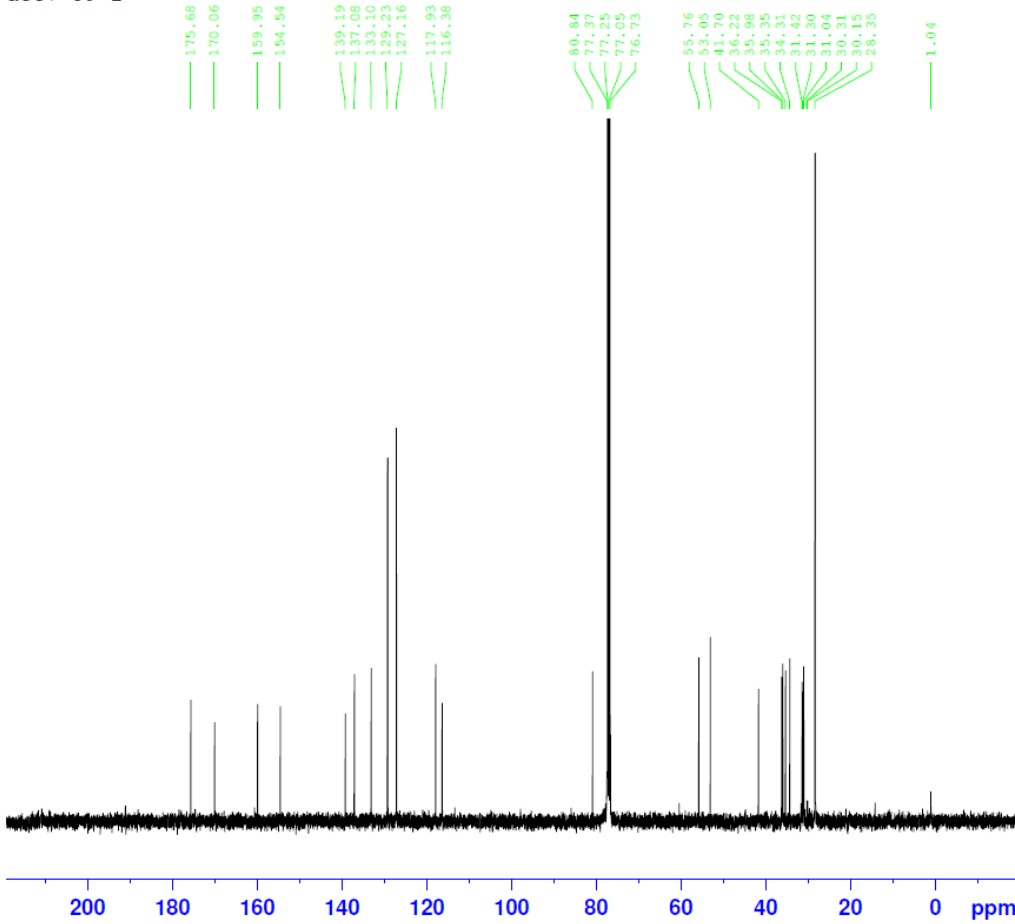
Current Data Parameters
 NAME aet7-39-2
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20111209
 Time 19.04
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 1024
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 1290.2
 DW 20.850 usec
 DE 6.00 usec
 TE 294.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

----- CHANNEL f1 -----
 NUC1 13C
 P1 8.00 usec
 PL1 -2.60 dB
 SFO1 100.6228298 MHz

----- CHANNEL f2 -----
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 PL13 17.50 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



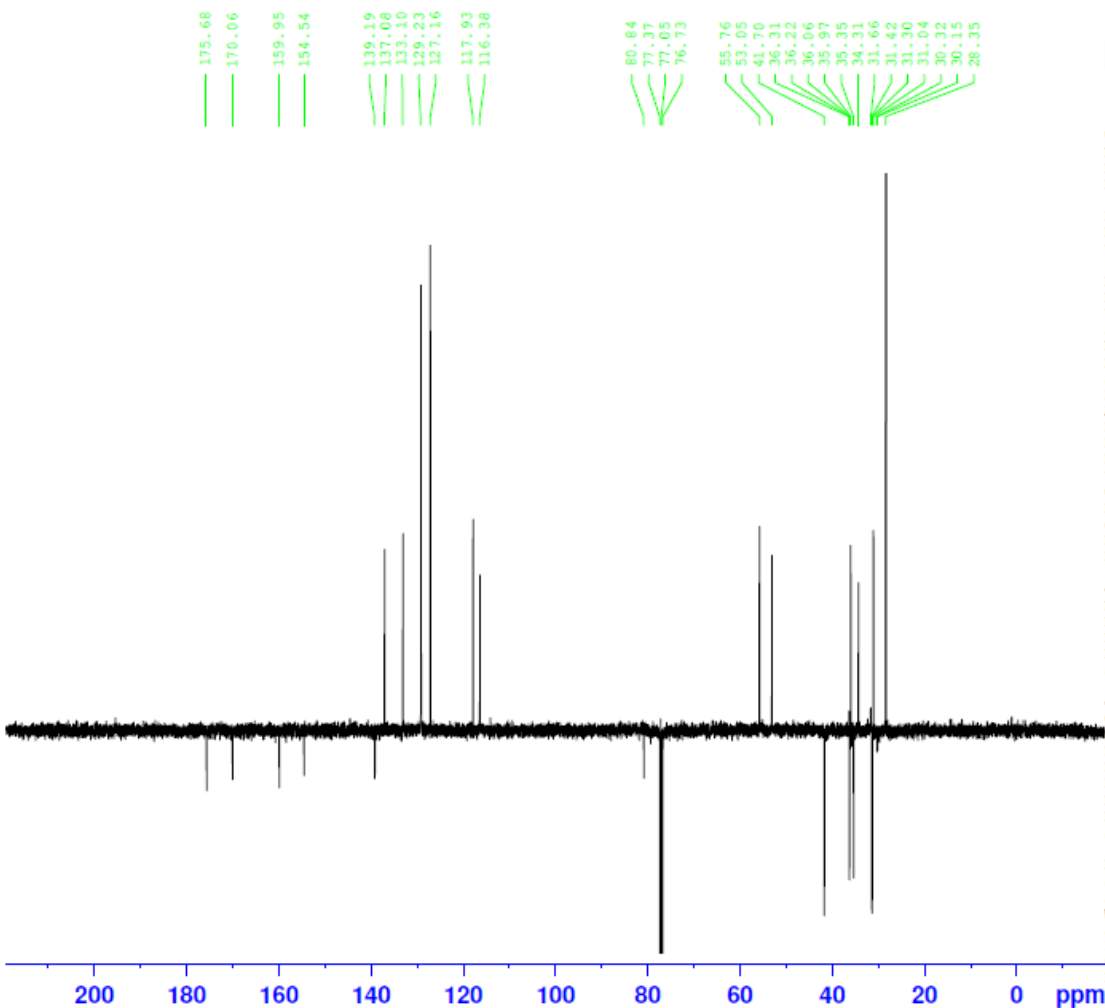
Current Data Parameters
 NAME aet7-39-2
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20111209
 Time 19.35
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG deptq 135
 ID 65536
 SOLVENT CDC13
 NS 512
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 18390.4
 DW 20.850 usec
 DE 6.00 usec
 TE 294.2 K
 CNST2 145.0000000
 D1 2.00000000 sec
 d2 0.00344828 sec
 D11 0.03000000 sec
 DELTA 0.00001019 sec

----- CHANNEL f1 -----
 NUC1 13C
 P1 8.00 usec
 P2 16.00 usec
 PL1 -2.60 dB
 SFO1 100.6228300 MHz

----- CHANNEL f2 -----
 CPDPRG2 waltz16
 NUC2 1H
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 SFO2 400.1316000 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
 NAME ant7-39-2
 EXPNO 14
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 2011209
 Time 19.56
 INSTRUM dpk400
 PULPROG 5 mm CWP 1M/13
 FULPROG hmcgpgpf
 TD 1024
 SOLVENT cdcl3
 NS 4
 DS 16
 SWH 3765.060 Hz
 FIDRES 3.676817 Hz
 AQ 0.1360372 sec
 RG 5160.6
 DW 132.800 usec
 DE 6.00 usec
 TE 294.2 K
 CMST2 145.000000
 d0 0.0000300 sec
 d1 1.4907940 sec
 d2 0.00344828 sec
 d12 0.0002000 sec
 d13 0.0000400 sec
 d16 0.0002000 sec
 DELTA1 0.0022428 sec
 IN0 0.0000300 sec

CHANNEL F1
 NUC1 1H
 P1 10.00 usec
 P2 20.00 usec
 PL1 -1.50 dB
 SFO1 400.1316186 MHz

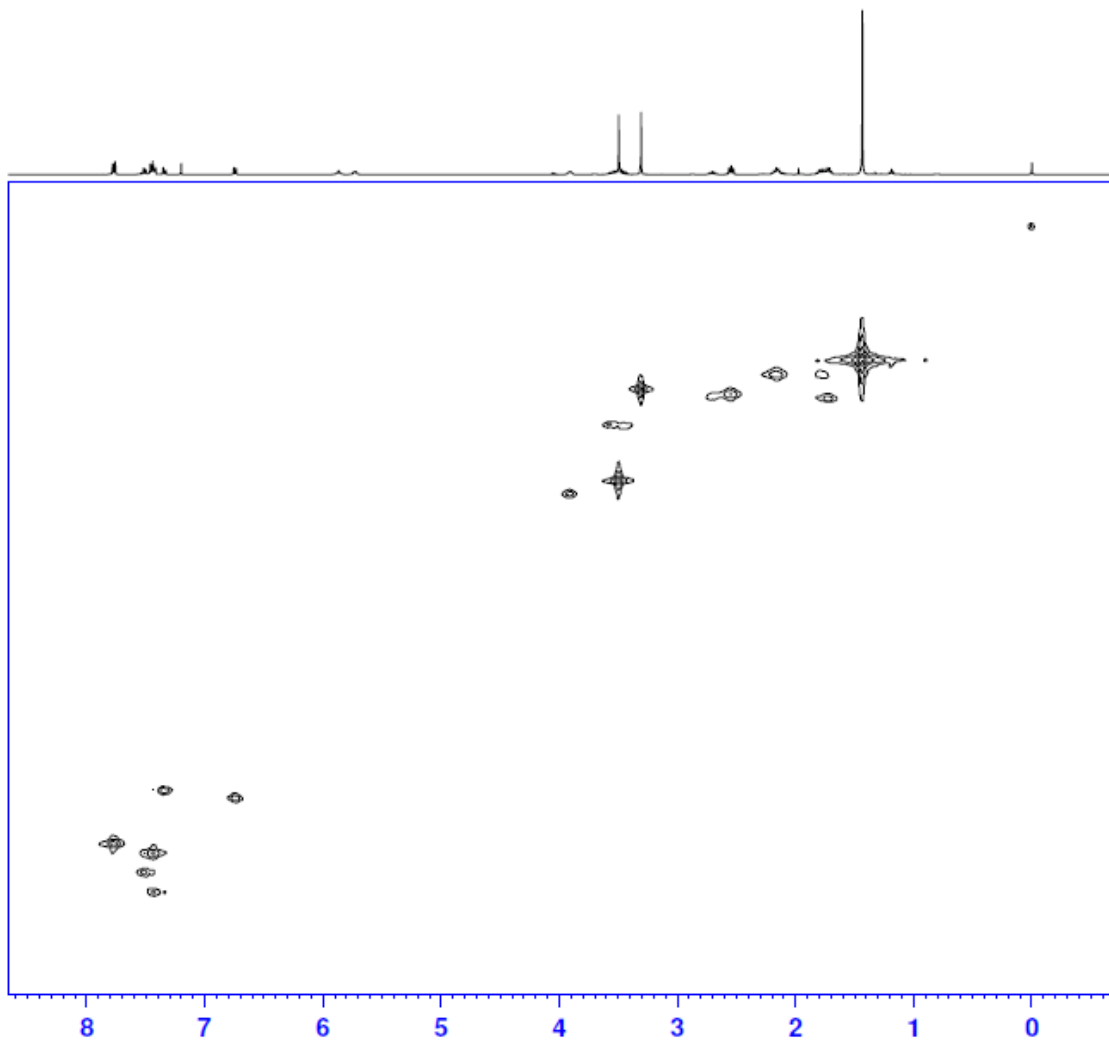
CHANNEL F2
 CPDPRG2 9atp
 NUC2 13C
 P3 8.00 usec
 PCPD2 74.00 usec
 PL2 -3.00 dB
 PL12 18.00 dB
 SFO2 100.6203140 MHz

GRADIENT CHANNEL
 GFNAM1 SINE.100
 GFNAM2 SINE.100
 GFNAM3 SINE.100
 GFE1 50.00 t
 GFE2 30.00 t
 GFE3 40.10 t
 F1G 1000.00 usec

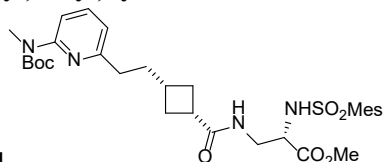
F1 - Acquisition parameters
 MD0 2
 TD 128
 SFO1 100.6203 MHz
 FIDRES 130.208328 Hz
 SW 165.639 ppm
 F2MODE qf

F2 - Processing parameters
 SI 1024
 SF 400.1300340 MHz
 WDM QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

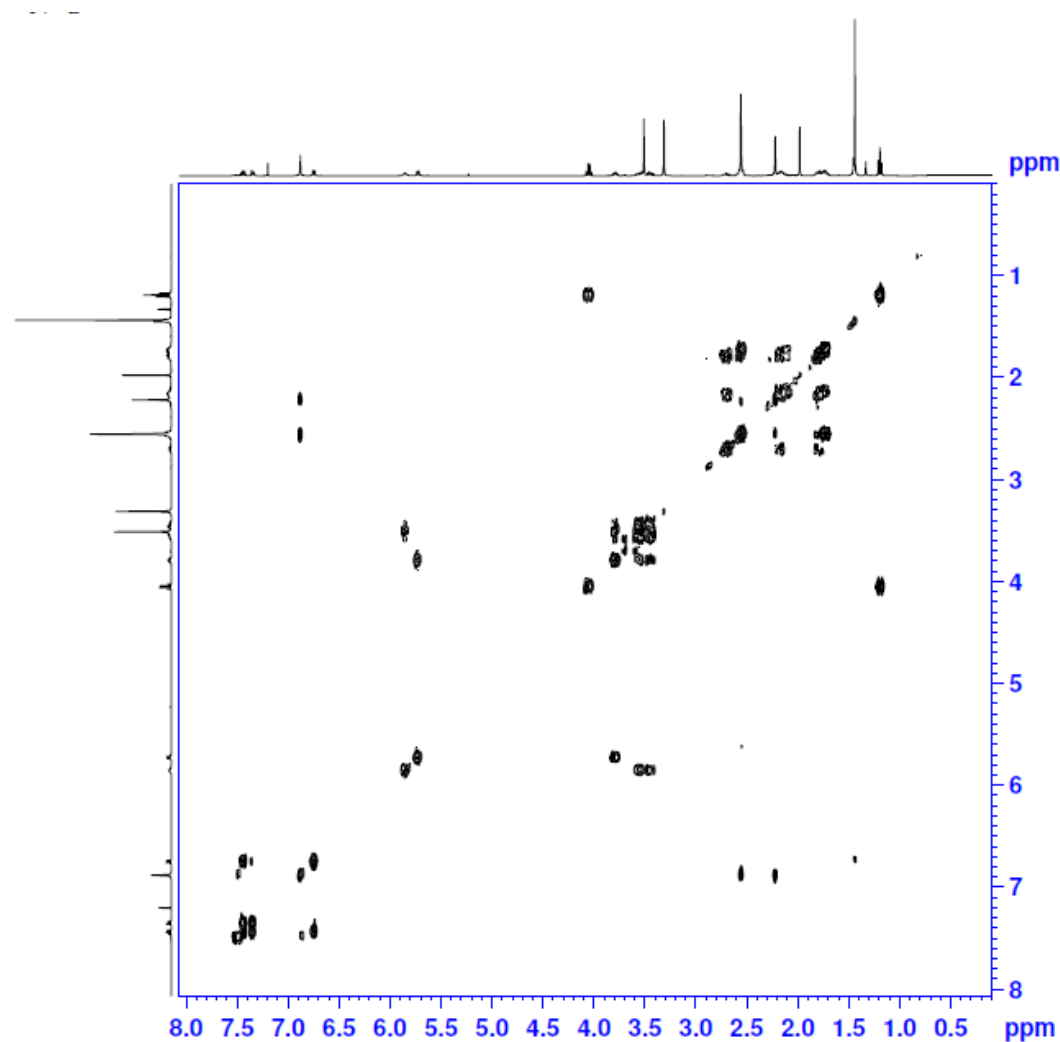
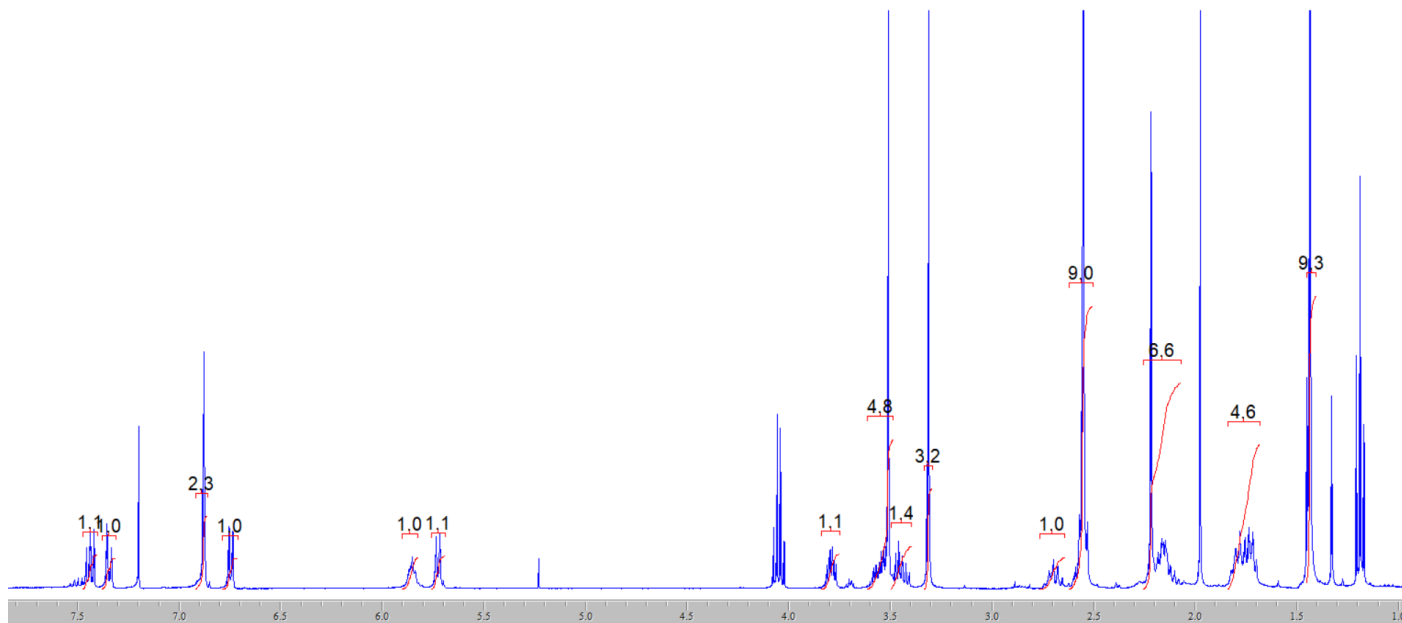
F1 - Processing parameters
 SI 1024
 SF 100.6127690 MHz
 WDM QSINE
 SSB 0
 LB 0.00 Hz
 GB 0



Methyl (S)-3-((1*r**,3*R**)-3-(2-(6-((tert-butoxycarbonyl)(methyl)amino)pyridin-2-yl)ethyl)cyclobutane-1-



carboxamido)-2-(2,4,6-trimethylphenylsulfonamido)propanoate [Compound 52]



Current Data Parameters
NAME set7-47-2
EXPNO 23
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111221
Time 19.40
INSTRUM DFX400
PROBHD 5 mm QNP 1H/13
PULPROG cosygpsifzf
TD 2048
SOLVENT CDCl3
NS 4
DS 8
SWH 3188.775 Hz
FIDRES 1.557019 Hz
AQ 0.3211764 sec
RG 5160.6
DW 156.800 usec
DE 6.00 usec
TE 294.2 K
D0 0.00000300 sec
D1 1.87015700 sec
d13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00031360 sec

----- CHANNEL f1 -----
NUC1 1H
P1 10.00 usec
PL1 -1.50 dB
SFO1 400.1316663 MHz

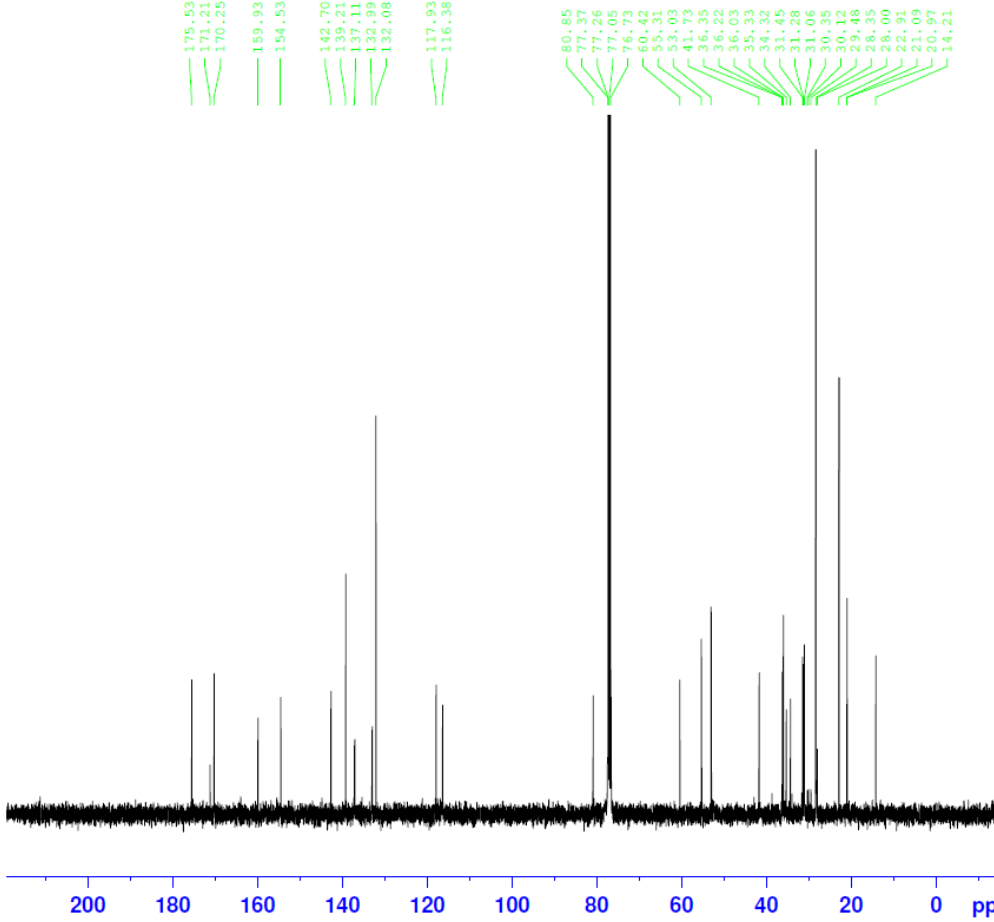
----- GRADIENT CHANNEL -----
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPE1 16.00 %
GPE2 12.00 %
GPE3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
ND0 1
TD 128
SFO1 400.1317 MHz
FIDRES 24.912308 Hz
SW 7.969 ppm
FRMODE QF

F2 - Processing parameters
SI 1024
SF 400.1300336 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.1300336 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

aet7-47-2



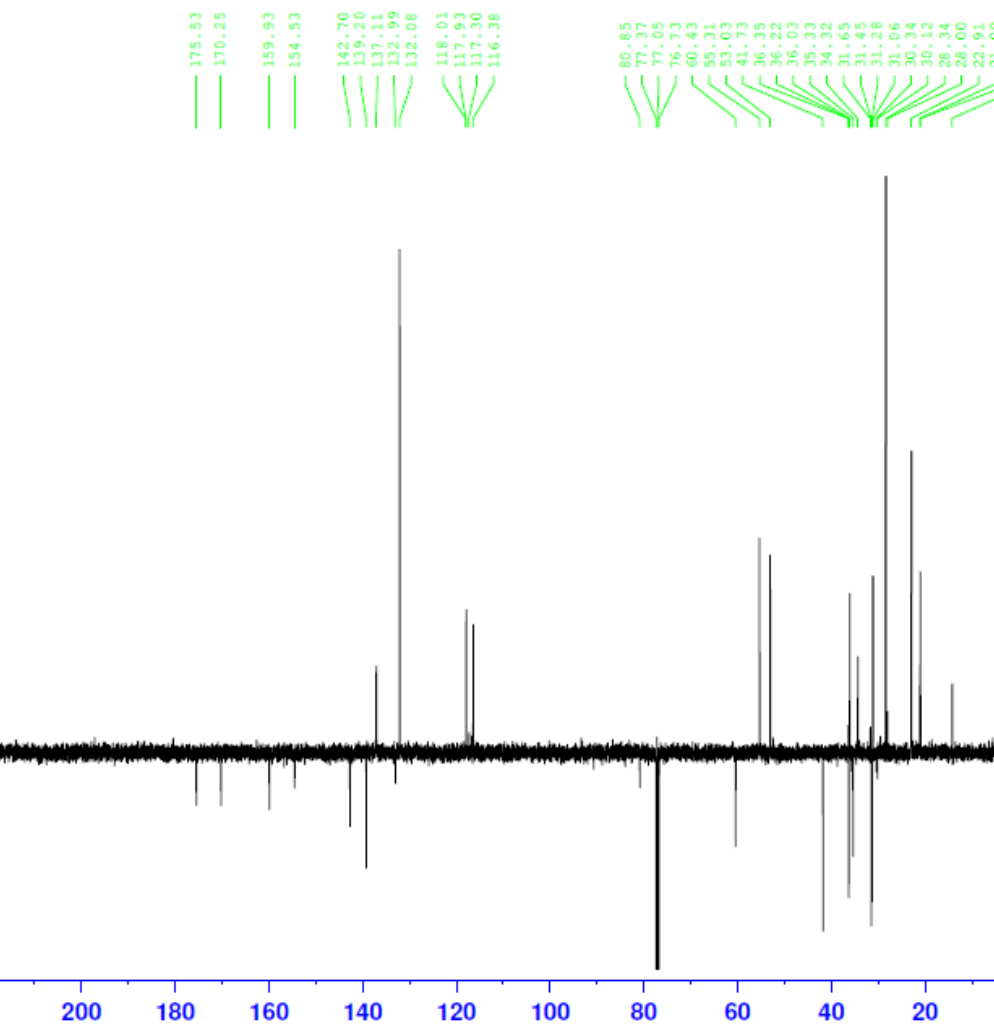
Current Data Parameters
 NAME aet7-47-2
 EXPNO 21
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20111221
 Time 19.09
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 1024
 DW 20.850 usec
 DE 6.00 usec
 TE 294.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.00 usec
 PL1 -2.60 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 PL13 17.50 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
 NAME aet7-47-2
 EXPNO 22
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20111221
 Time 19.39
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG deptq_135
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 16384
 DW 20.850 usec
 DE 6.00 usec
 TE 294.2 K
 CNST2 145.0000000
 D1 2.00000000 sec
 d2 0.00344828 sec
 d11 0.03000000 sec
 DELTA 0.00001019 sec

----- CHANNEL f1 -----
 NUC1 13C
 P1 8.00 usec
 P2 16.00 usec
 PL1 -2.60 dB
 SFO1 100.6228300 MHz

----- CHANNEL f2 -----
 CPDPRG2 waltz16
 NUC2 1H
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 SFO2 400.1316000 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Current Data Parameters
 NAME ant7-47-2
 EXPNO 24
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20111221
 Time 20.00

INSTRUM spect
 PROBRD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 1024
 SOLVENT cdc13
 NS 4
 DS 16
 SWH 3188.775 Hz
 FIDRES 3.114038 Hz
 AQ 0.1606132 sec
 RG 4096
 SW 156.800 usec
 DE 6.00 usec
 TE 294.2 K
 CNST2 145.000000
 d0 0.0000300 sec
 d1 1.4620798 sec
 d2 0.00344828 sec
 d12 0.0002000 sec
 d13 0.0000400 sec
 d16 0.0002000 sec
 DELTA1 0.0022428 sec
 INO 0.0003000 sec

CHANNEL F1
 NUC1 1H
 P1 10.00 usec
 P2 20.00 usec
 PL1 -1.50 dB
 SFO1 400.1316663 MHz

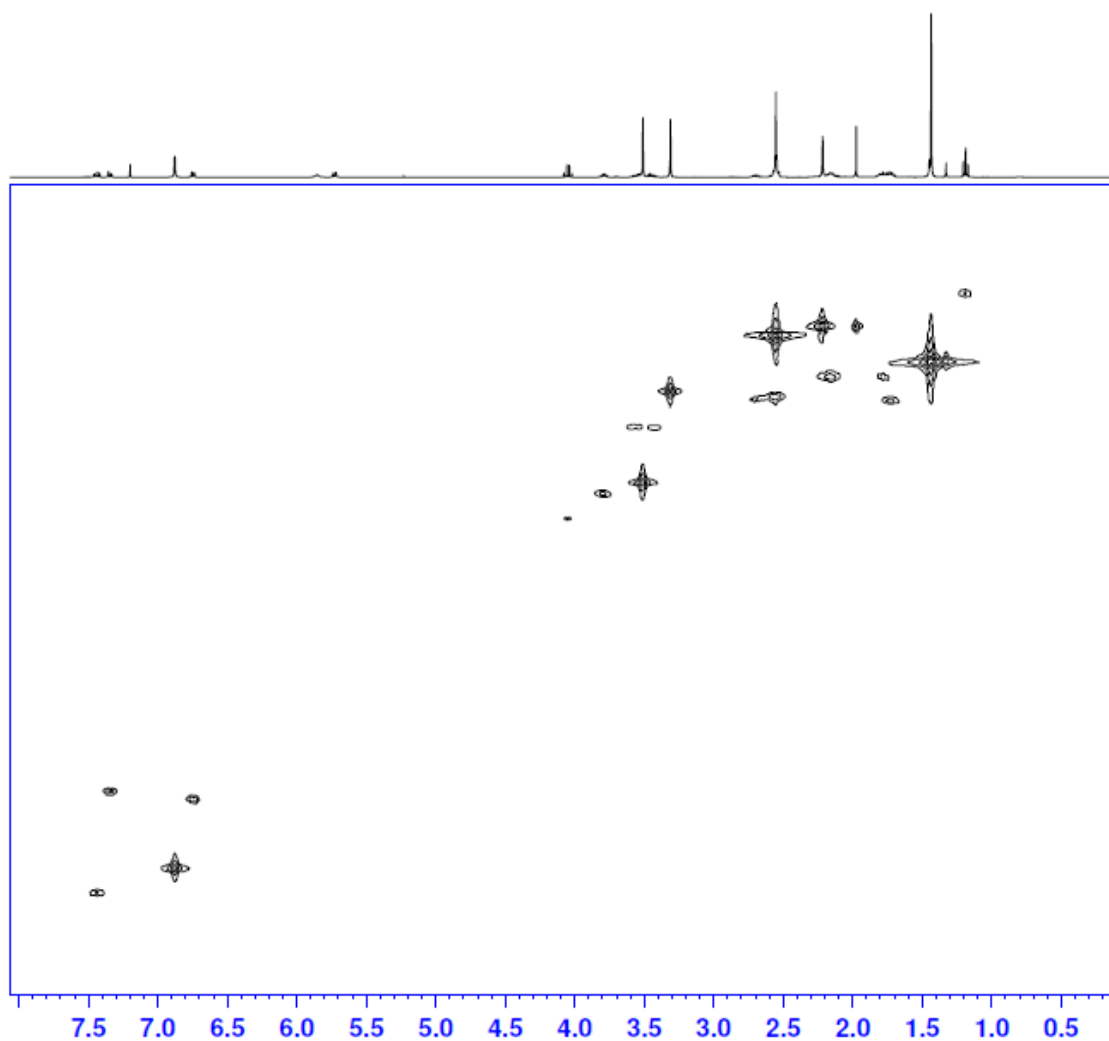
CHANNEL F2
 CPDPRG2 gpgp
 NUC2 13C
 P3 8.00 usec
 PCPD2 74.00 usec
 PL2 -3.00 dB
 PL12 18.00 dB
 SFO2 100.6203140 MHz

GRADIENT CHANNEL
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPNAM3 SINE.100
 GPE1 50.00 %
 GPE2 30.00 %
 GPE3 40.10 %
 F16 1000.00 usec

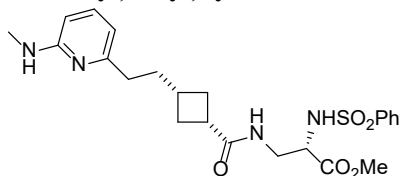
F1 - Acquisition parameters
 ND0 2
 TD 128
 SFO1 100.6203 MHz
 FIDRES 130.208228 Hz
 SW 145.439 ppm
 PRMODE QF

F2 - Processing parameters
 SI 1024
 SF 400.1300336 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

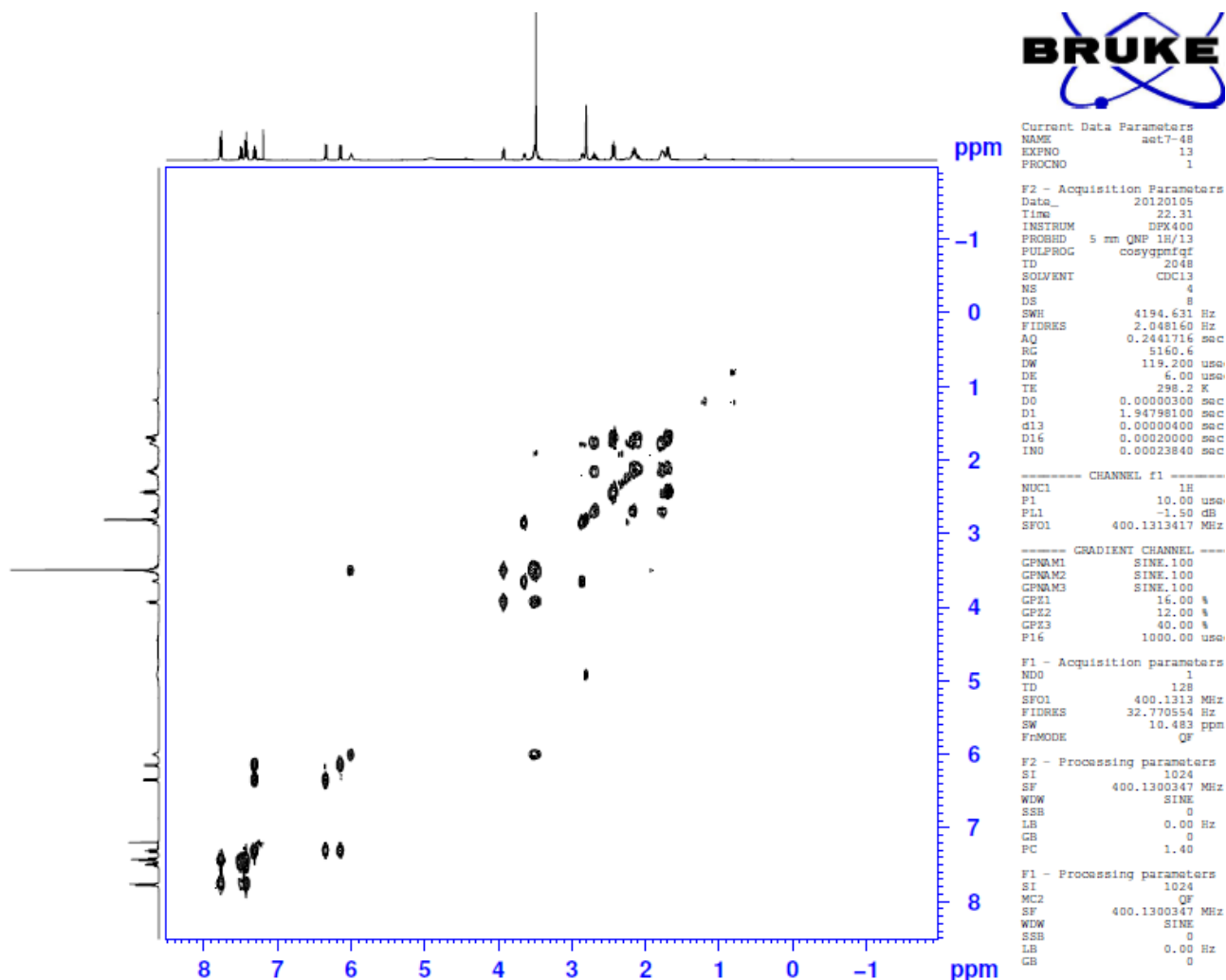
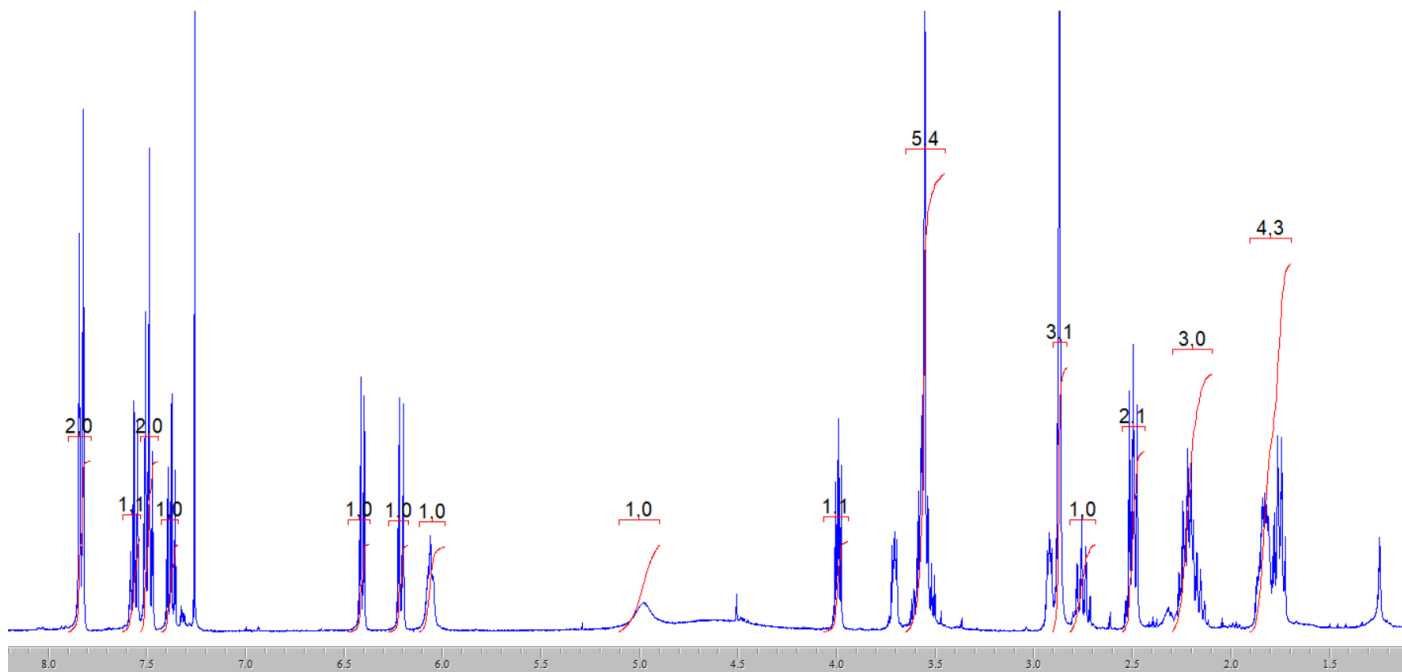
F1 - Processing parameters
 SI 1024
 WC2 QF
 SF 100.6127690 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0



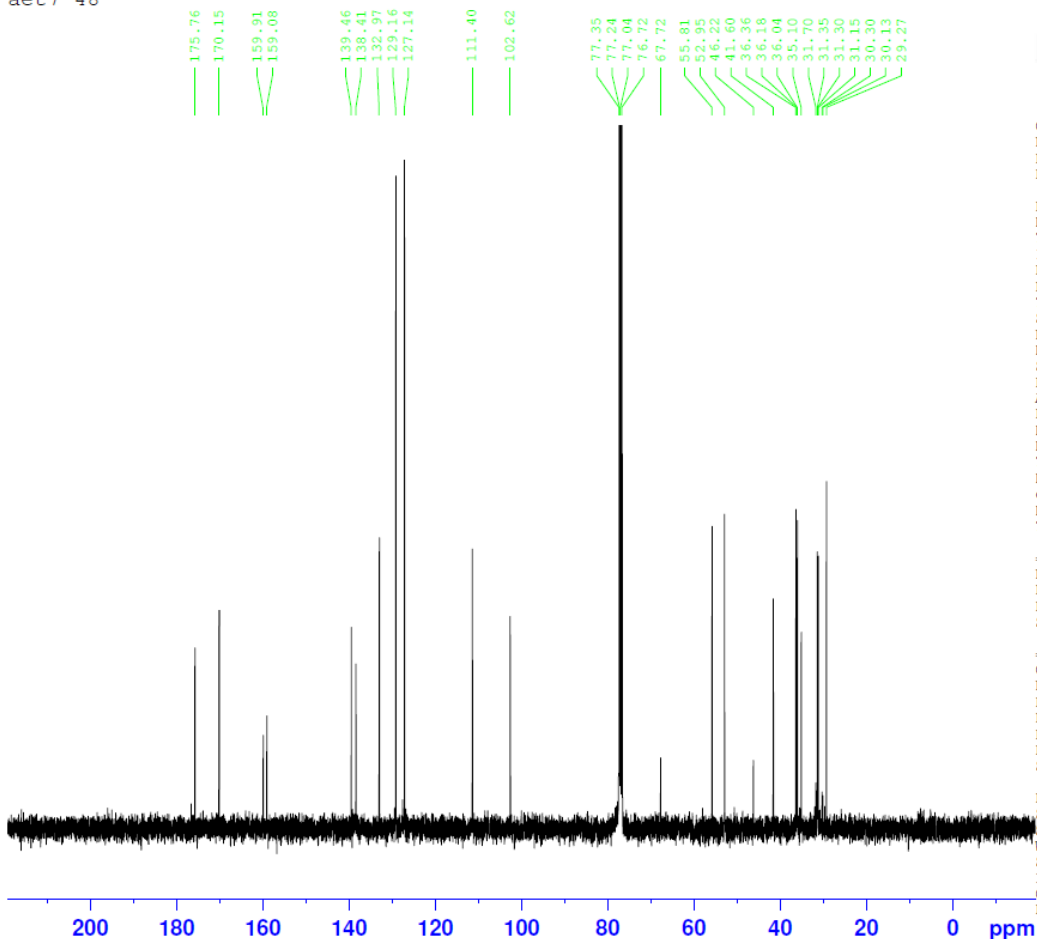
Methyl (S)-3-((1*r**,3*R**)-3-(2-(6-(methylamino)pyridin-2-yl)ethyl)cyclobutane-1-carboxamido)-2-



(phenylsulfonamido)propanoate [Compound 53]



aet7-48



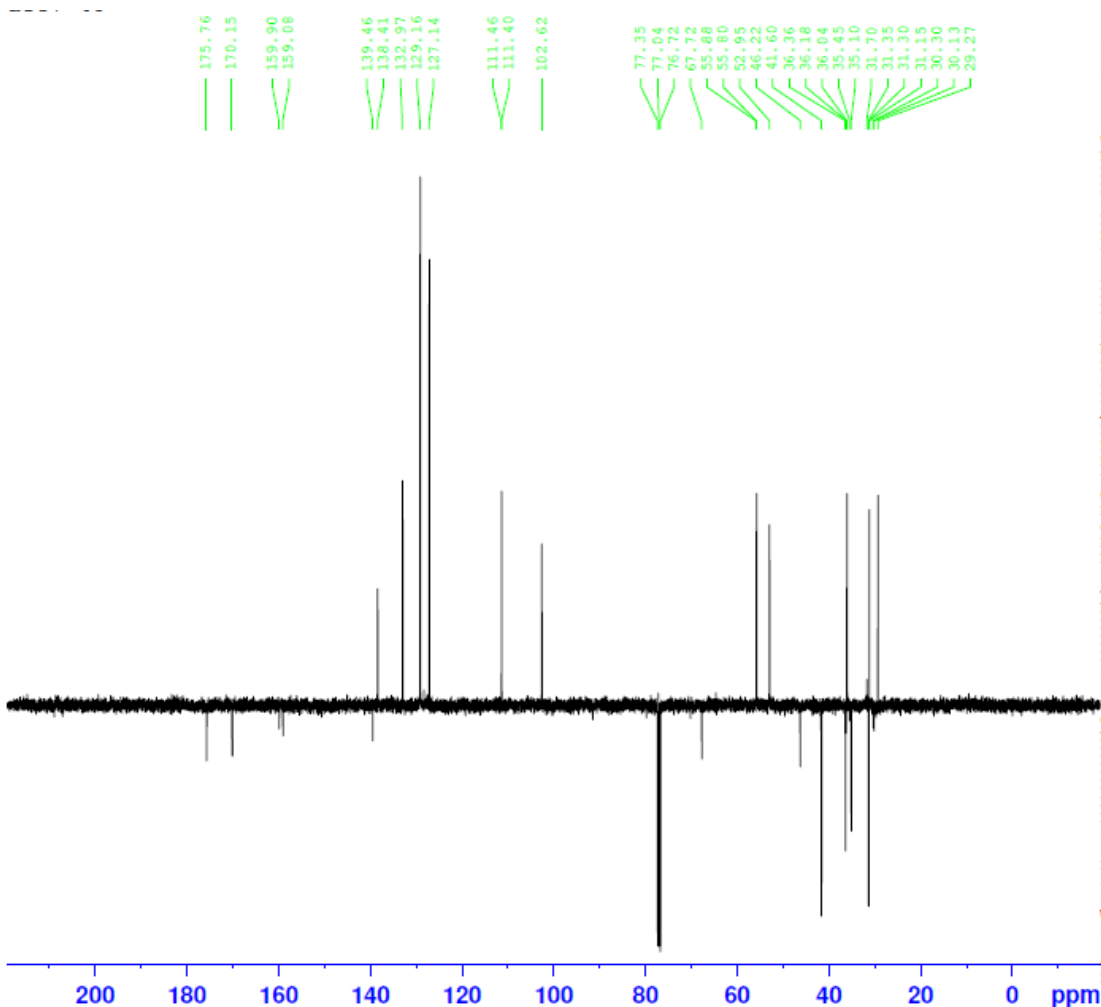
Current Data Parameters
 NAME aet7-48
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120105
 Time 22.00
 INSTRUM DFX400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 912.3
 DW 20.850 usec
 DE 6.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

==== CHANNEL f1 =====
 NUC1 13C
 P1 8.00 usec
 PL1 -2.60 dB
 SFO1 100.6228298 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 PL13 17.50 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
 NAME aet7-48
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120105
 Time 22.30
 INSTRUM DFX400
 PROBHD 5 mm QNP 1H/13
 PULPROG deptq_135
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 18390.4
 DW 20.850 usec
 DE 6.00 usec
 TE 298.2 K
 CNST2 145.00000000
 D1 2.00000000 sec
 d2 0.00344828 sec
 D11 0.03000000 sec
 DELTA 0.00001019 sec

==== CHANNEL f1 =====
 NUC1 13C
 P1 8.00 usec
 P2 16.00 usec
 PL1 -2.60 dB
 SFO1 100.6228300 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 SFO2 400.1316000 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Current Data Parameters
 NAME test7-48
 EXPRNO 14
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120105
 Time 22.51

INSTRUM spect
 PULPROG zgpg30
 TD 1024
 SOLVENT cdc13
 NS 4
 DS 16
 SWH 4194.631 Hz
 FIDRES 4.096319 Hz
 AQ 0.1221108 sec
 RG 6502
 SW 119.200 usec
 DE 6.00 usec
 TK 298.2 K
 CNST2 145.0000000
 d0 0.0000300 usec
 d1 1.8952004 usec
 d2 0.00344828 usec
 d12 0.00002000 usec
 d13 0.00004000 usec
 d16 0.00020000 usec
 DELTA1 0.0022428 usec
 INU 0.00003000 usec

CHANNEL F1
 NUC1 1H
 P1 10.00 usec
 P2 20.00 usec
 PL1 -1.50 dB
 SFO1 400.1313417 MHz

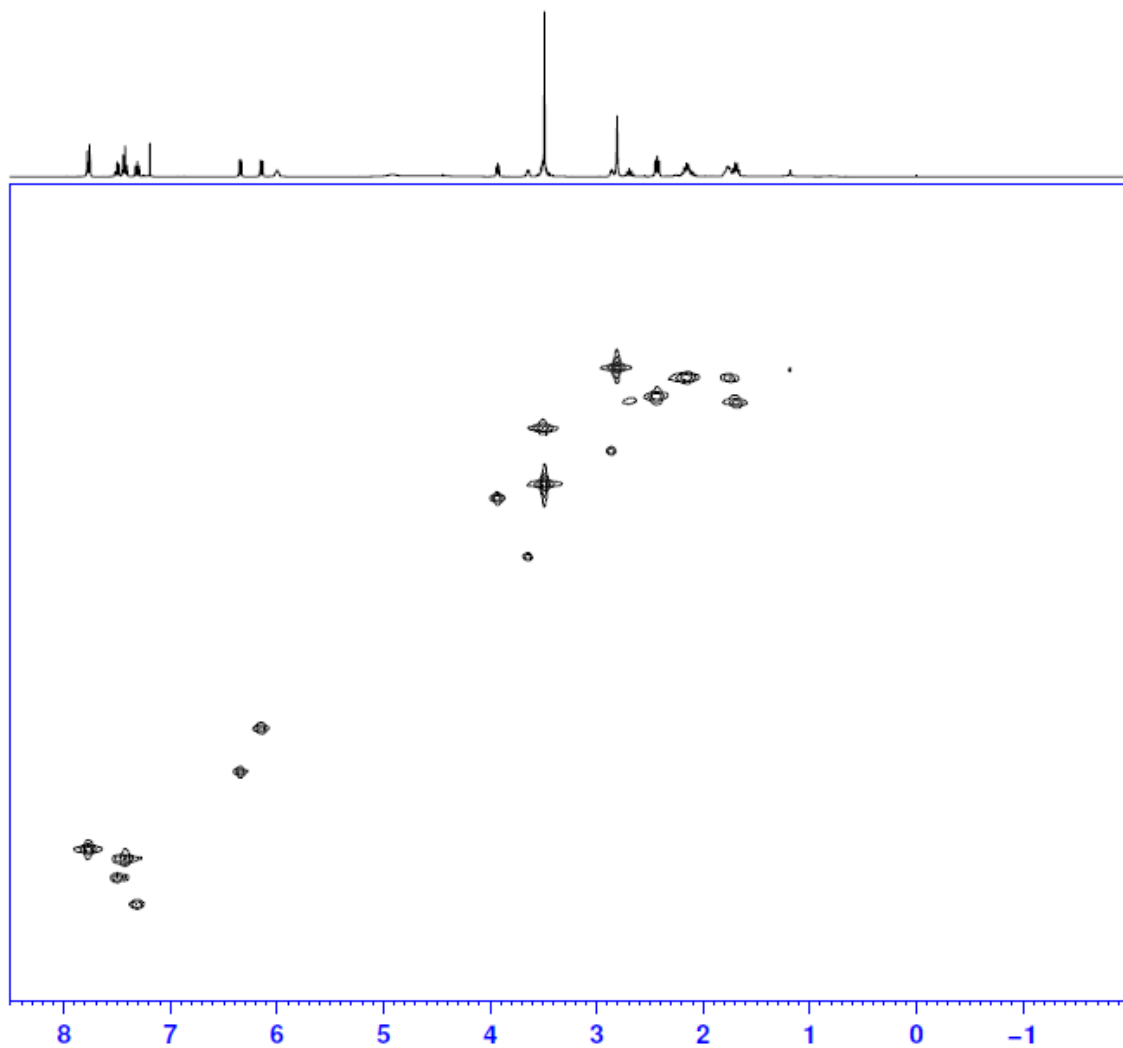
CHANNEL F2
 CPDPRG2 gpgp
 NUC2 13C
 P3 8.00 usec
 PCPD2 74.00 usec
 PL2 -3.00 dB
 PL3 18.00 dB
 SFO2 100.6203140 MHz

GRADIENT CHANNEL
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPNAM3 SINE.100
 GFS1 50.00 %
 GFS2 30.00 %
 GFS3 40.10 %
 F16 1000.00 usec

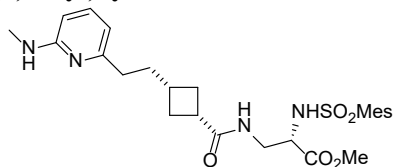
F1 - Acquisition parameters
 NDO 2
 TD 128
 SFO1 100.6203 MHz
 FIDRES 130.208328 Hz
 SW 163.639 ppm
 PRMODE QF

F2 - Processing parameters
 SI 1024
 SF 400.1300347 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

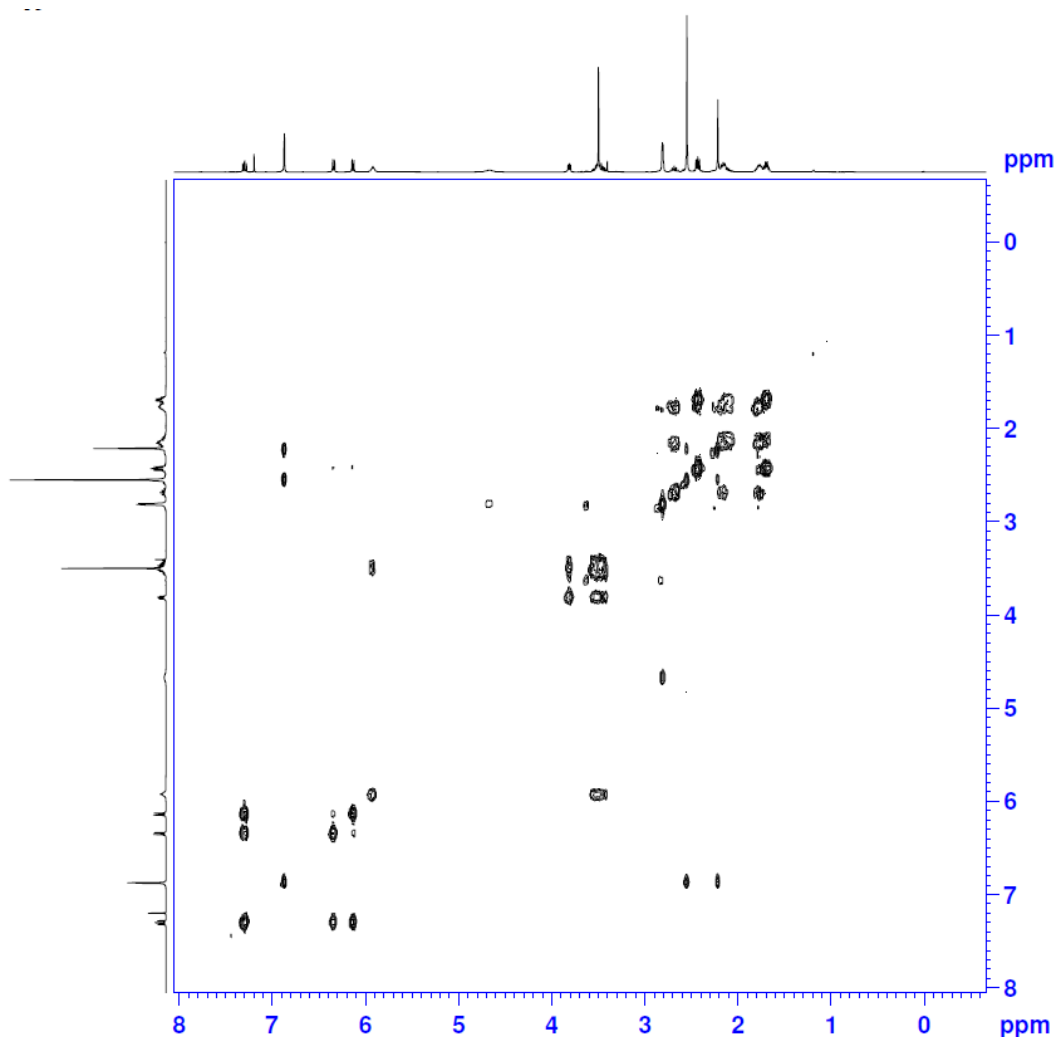
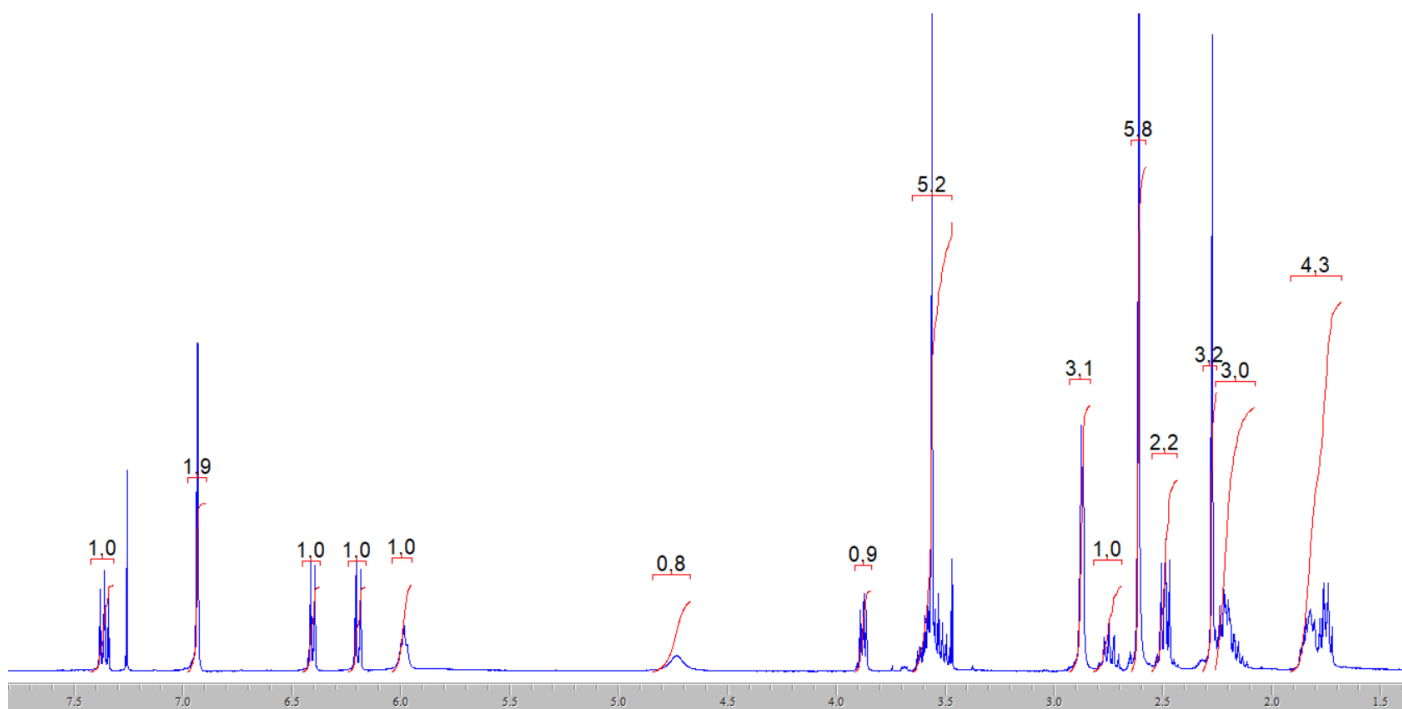
F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 100.617690 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0



Methyl (S)-3-((1r*,3R*)-3-(2-(6-(methylamino)pyridin-2-yl)ethyl)cyclobutane-1-carboxamido)-2-(2,4,6-



trimethylphenylsulfonamido)propanoate [Compound 54]



Current Data Parameters
NAME set7-49
EXPNO 13
PROCNO 1

F2 - Acquisition Parameter:
Date_ 20120106
Time 0.39
INSIRUM DFX400
PROBHD 5 mm QNP 1H/13
PULPROG cosygpmfzf
TD 2048
SOLVENT CDCl3
NS 4
DS 8
SWH 3491.620 Hz
FIDRES 1.704893 Hz
AQ 0.2933236 sec
RG 7298.2
DW 143.200 usec
DE 6.00 usec
TE 298.2 K
DO 0.00000300 sec
D1 1.8988299 sec
d13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00028640 sec

----- CHANNEL f1 -----
NUC1 1H
P1 10.00 usec
PL1 -1.50 dB
SFO1 400.1315125 MHz

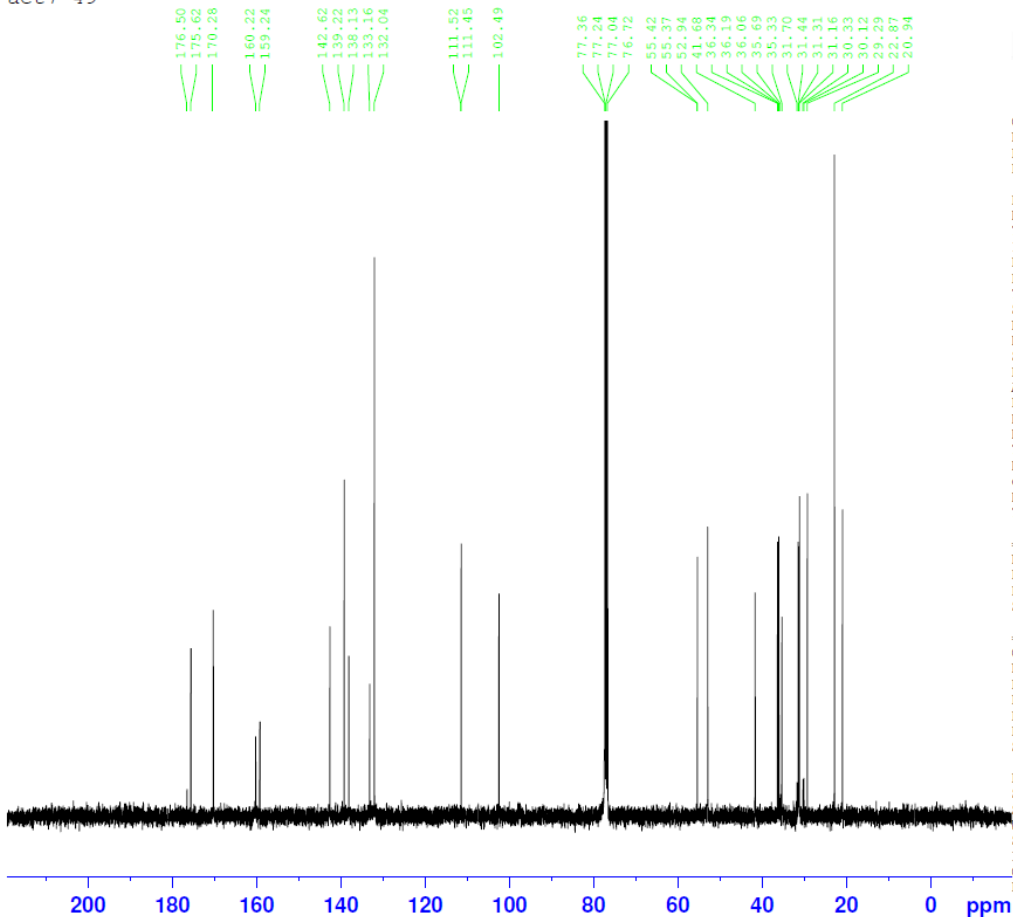
----- GRADIENT CHANNEL -----
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 16.00 %
GPZ2 12.00 %
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameter:
ND0 1
TD 128
SFO1 400.1315 MHz
FIDRES 27.278282 Hz
SW 8.726 ppm
FhMODE QF

F2 - Processing parameters
SI 1024
SF 400.1300346 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.1300346 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

aet7-49



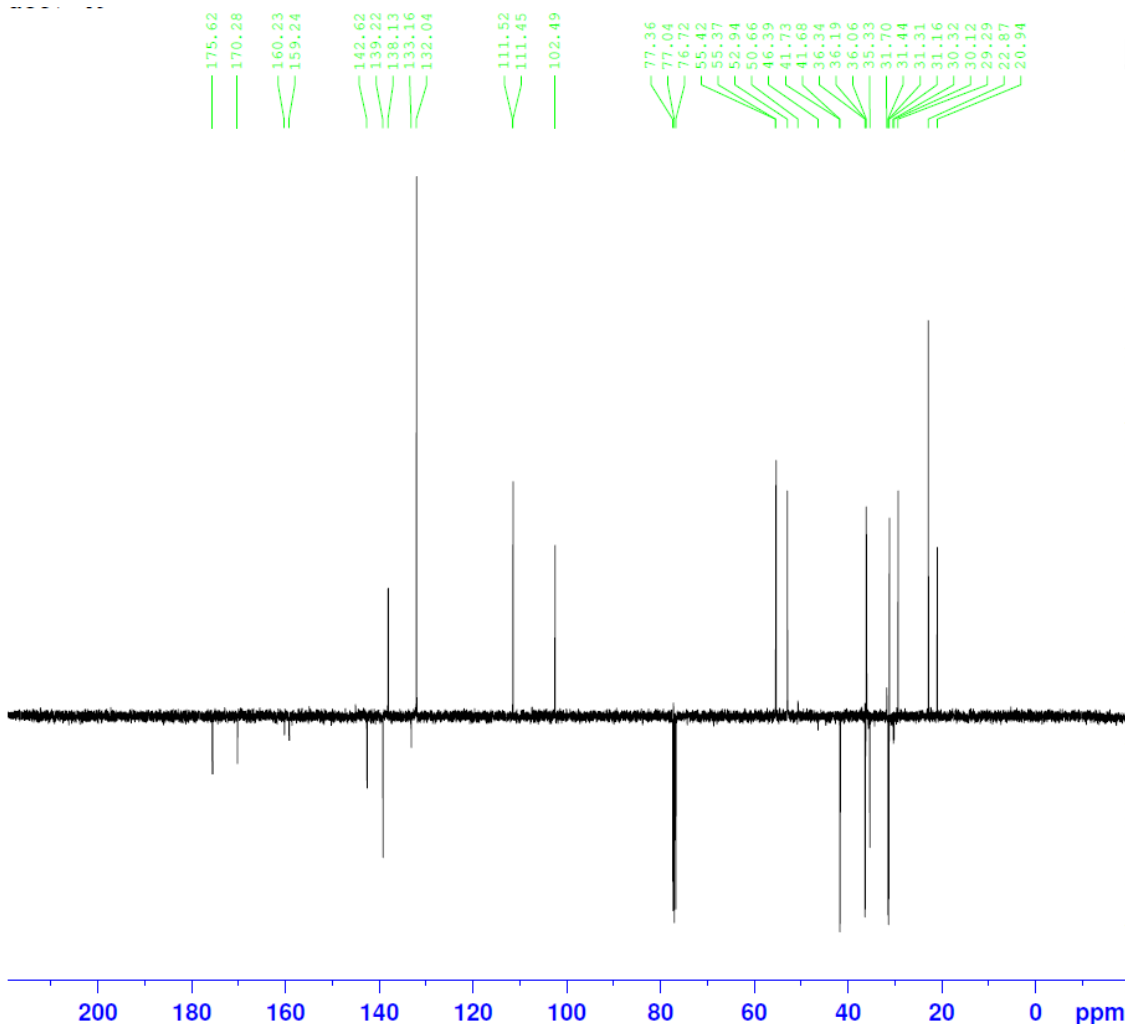
Current Data Parameters
 NAME aet7-49
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120106
 Time 0.08
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 1824.6
 DW 20.850 usec
 DE 6.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.00 usec
 PL1 -2.60 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 PL13 17.50 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
 NAME aet7-49
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120106
 Time 0.38
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG deptq_135
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 11585.2
 DW 20.850 usec
 DE 6.00 usec
 TE 298.2 K
 CNST2 145.0000000
 D1 2.00000000 sec
 d2 0.00344828 sec
 D11 0.03000000 sec
 DELTA 0.00001019 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.00 usec
 P2 16.00 usec
 PL1 -2.60 dB
 SFO1 100.6228300 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 SFO2 400.1316000 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Current Data Parameters
 NAME act7-49
 EXPNO 14
 PRGNO 1

F2 - Acquisition Parameters
 Date_ 20120106
 Time 0.59

INSTRUM Dpx400
 PROBRD 5 mm QNP 1H/13
 PULPROG hmqcpgpgf
 TD 1024
 SOLVENT cdcl3
 NS 4
 DS 4
 SWH 3491.620 Hz
 FIDRES 3.409785 Hz
 AQ 0.1466868 sec
 RG 26008
 DE 143.200 usec
 QE 6.00 usec
 TK 298.2 K
 CNST2 145.0000000
 d0 0.00000300 sec
 d1 1.48054397 sec
 d2 0.00344828 sec
 d12 0.00002000 sec
 d13 0.00000400 sec
 d14 0.00020000 sec
 DELTA1 0.0022428 sec
 INO 0.00003000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 p2 20.00 usec
 PL1 -1.50 dB
 SFO1 400.1315125 MHz

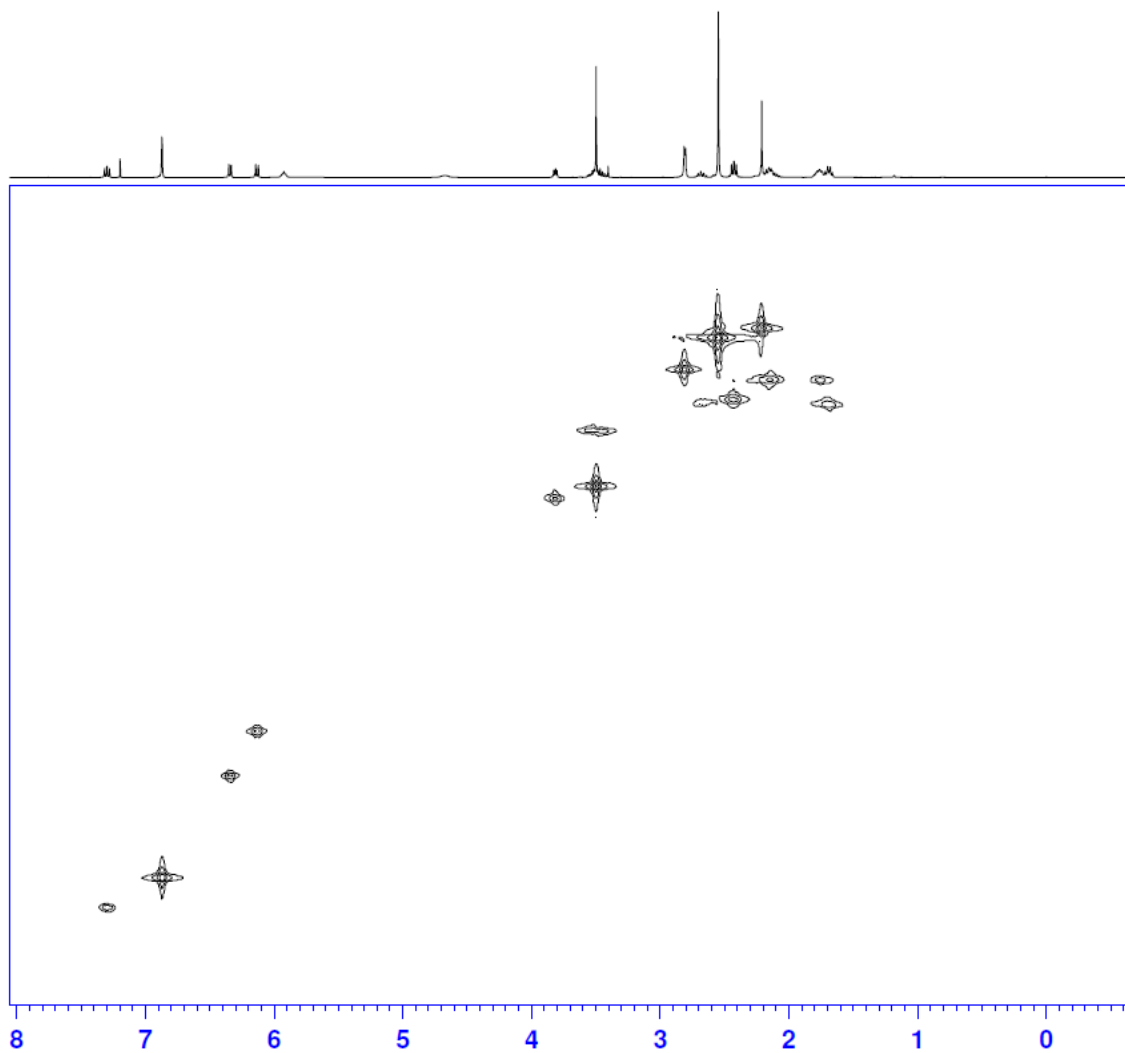
==== CHANNEL f2 =====
 CPDPRG2 garp
 NUC2 13C
 P3 8.00 usec
 PCD2 74.00 usec
 PL2 -3.00 dB
 PL12 18.00 dB
 SFO2 100.6203140 MHz

==== GRADIENT CHANNEL =====
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPNAM3 SINE.100
 GP21 50.00 %
 GP22 30.00 %
 GP23 40.10 %
 P16 1000.00 usec

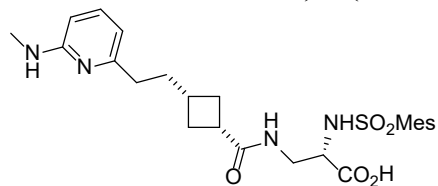
F1 - Acquisition parameters
 ND0 2
 TD 128
 SFO1 100.6203 MHz
 FIDRES 130.208328 Hz
 SW 165.639 ppm
 FRMODE QF

F2 - Processing parameters
 SI 1024
 SF 400.1300346 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

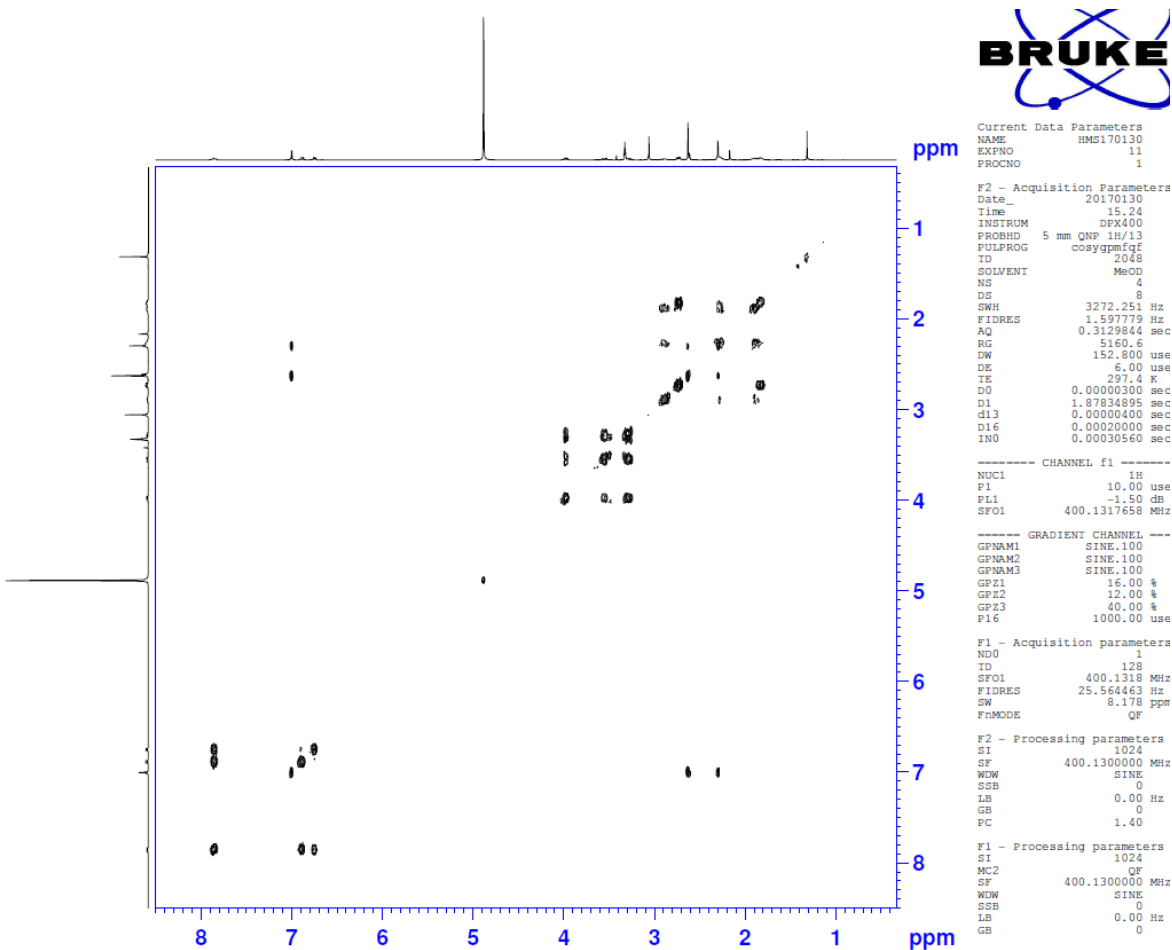
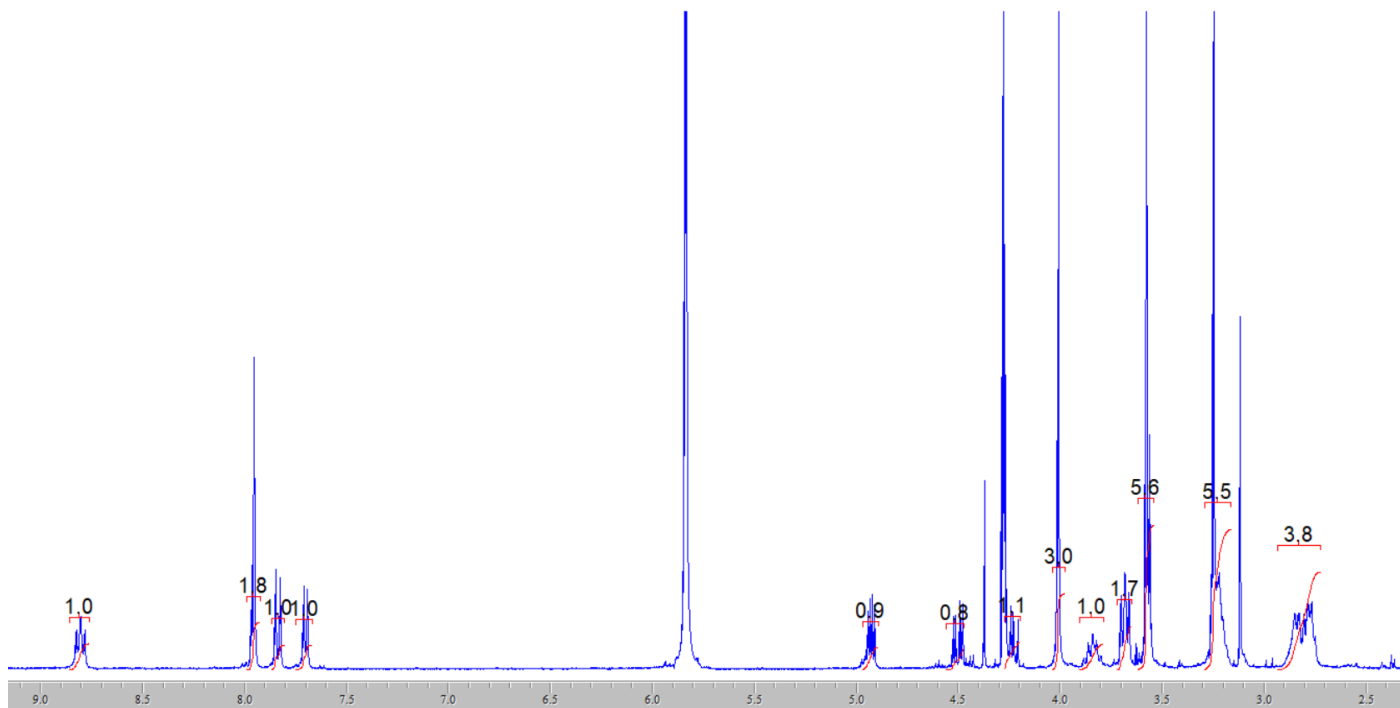
F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 100.6127690 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0



(S)-3-((1*r,3*R**)-3-(2-(6-(methylamino)pyridin-2-yl)ethyl)cyclobutane-1-carboxamido)-2-(2,4,6-**



trimethylphenylsulfonamido)propanoic acid [Compound 55]



BRUKER

Current Data Parameters
NAME HMS170130
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170130
Time 15.24
INSTRUM DFX400
PROBHD 5 mm QNP 1H/13
PULPROG cosygmrgf
ID 2048
SOLVENT MeOD
NS 4
DS 8
SWH 3272.251 Hz
FIDRES 1.597779 Hz
AQ 0.3129844 sec
RG 5160.6
DW 152.800 use
DE 6.00 use
TE 297.4 K
D0 0.00000300 sec
D1 1.87834895 sec
d13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00030560 sec

----- CHANNEL f1 -----
NUC1 1H
P1 10.00 use
PL1 -1.50 dB
SFO1 400.1317658 MHz

----- GRADIENT CHANNEL -----
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 15.00 %
GPZ2 12.00 %
GPZ3 40.00 %
P16 1000.00 use

F1 - Acquisition parameters
ND0 1
ID 128
SFO1 400.1318 MHz
FIDRES 25.564463 Hz
SW 8.178 ppm
FhMODE QF

F2 - Processing parameters
SI 1024
SF 400.1300000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.1300000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0



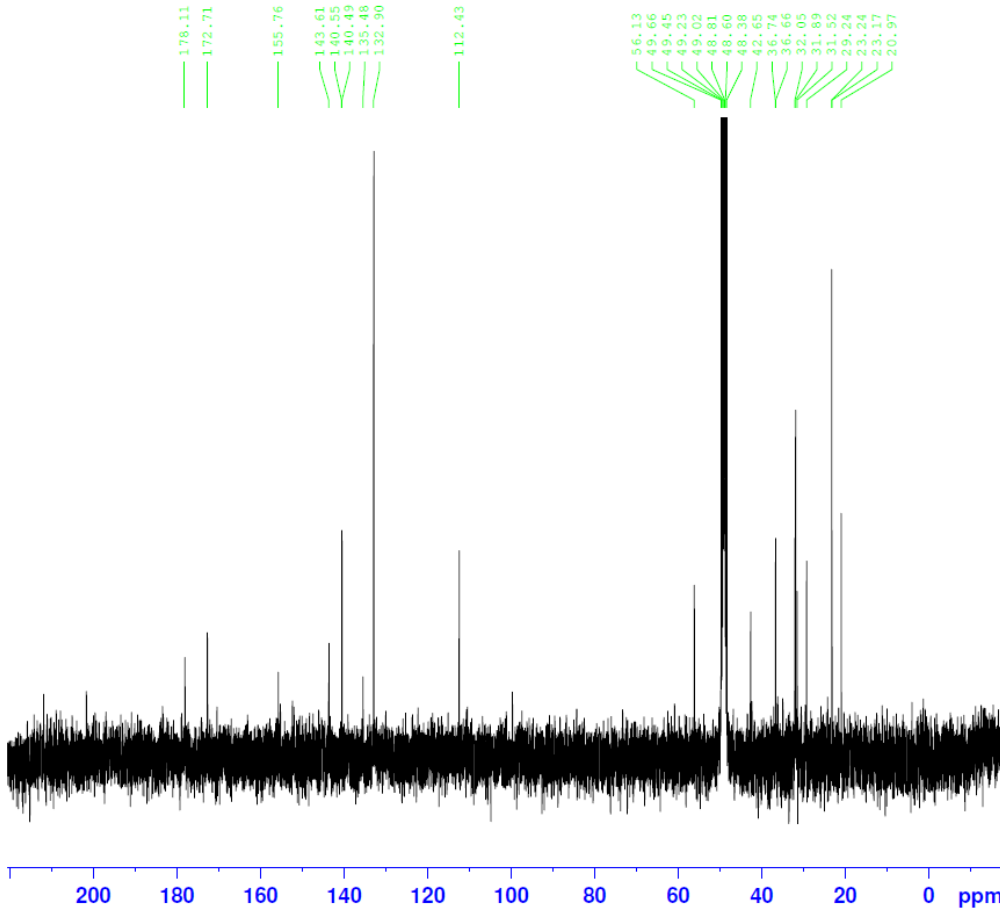
Current Data Parameters
 NAME HMS170130
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170131
 Time 6.23
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT MeOD
 NS 1024
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 18390.4
 DW 20.850 usec
 DE 6.00 usec
 TE 297.4 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.00 usec
 PL1 -2.60 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 PL13 17.50 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6126261 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



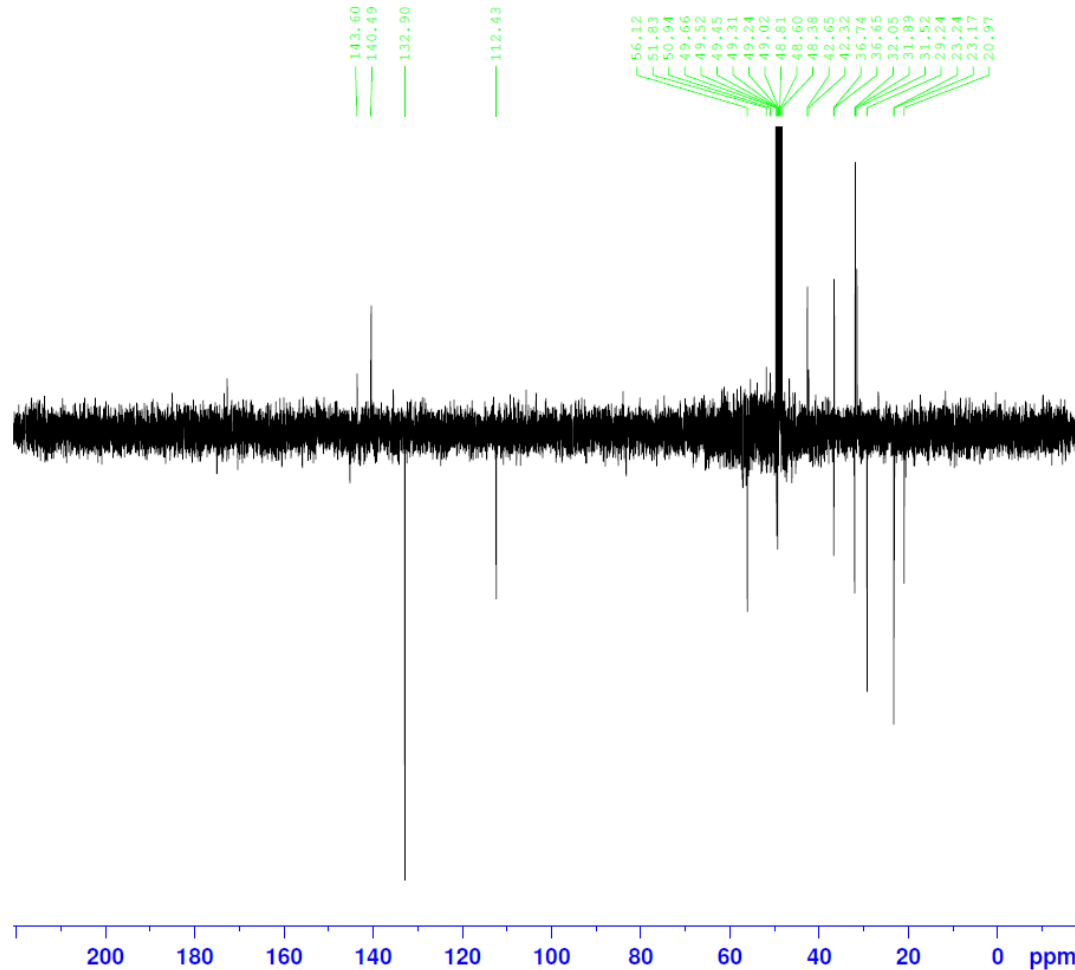
Current Data Parameters
 NAME HMS170130
 EXPNO 13
 PROCNO 1

F2 - Acquisition Parameter:
 Date_ 20170131
 Time 6.53
 INSTRUM DPX400
 PROBHD 5 mm QNP 1H/13
 PULPROG deptg_135
 TD 65536
 SOLVENT MeOD
 NS 512
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 11585.2
 DW 20.850 usec
 DE 6.00 usec
 TE 297.4 K
 CNST2 145.0000000
 D1 2.00000000 sec
 d2 0.00344828 sec
 D11 0.03000000 sec
 DELTA 0.00001146 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.00 usec
 P2 18.00 usec
 PL1 -2.60 dB
 SFO1 100.6228300 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PL2 -1.50 dB
 PL12 17.50 dB
 SFO2 400.1316000 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6126261 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



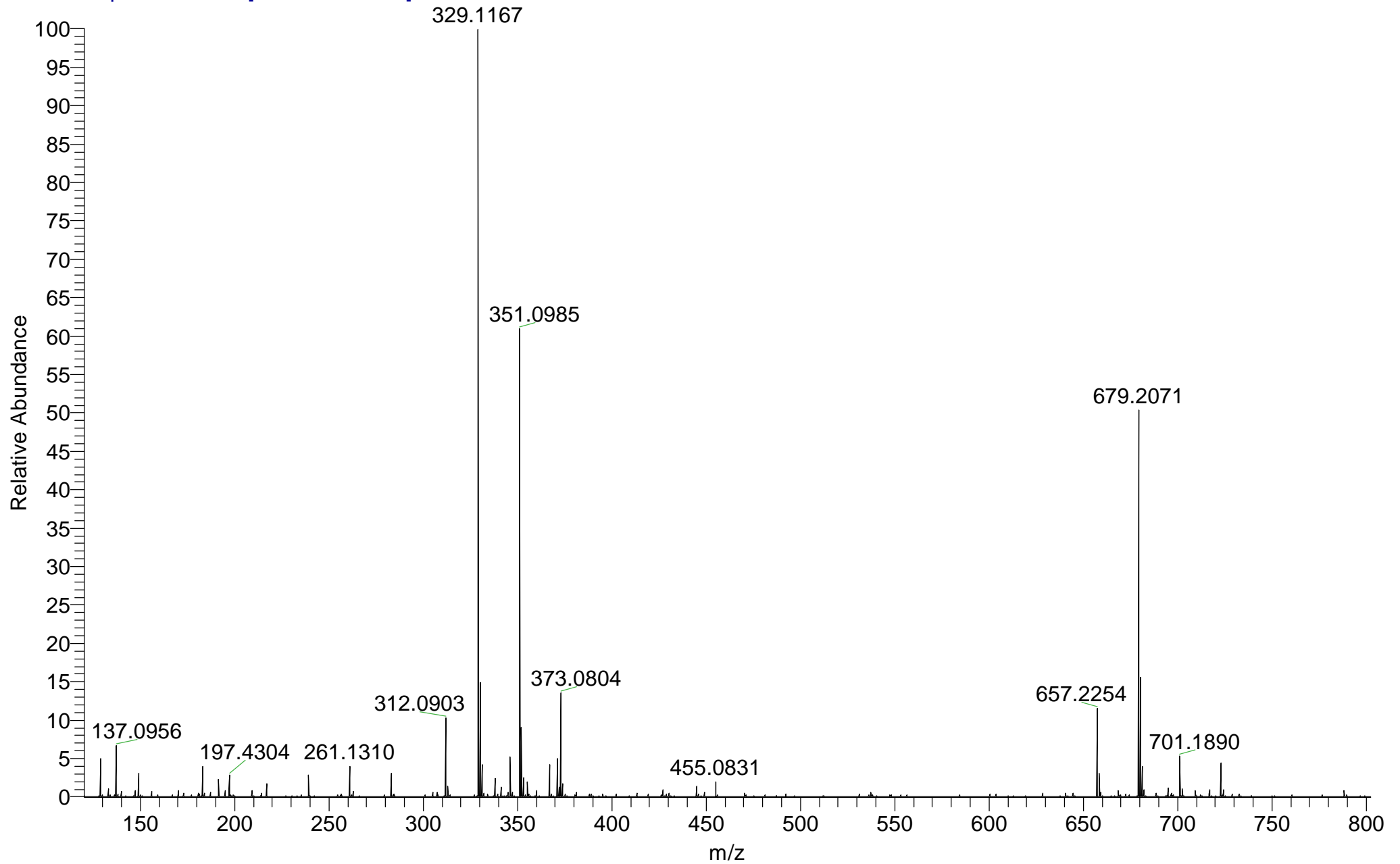
Compound 4

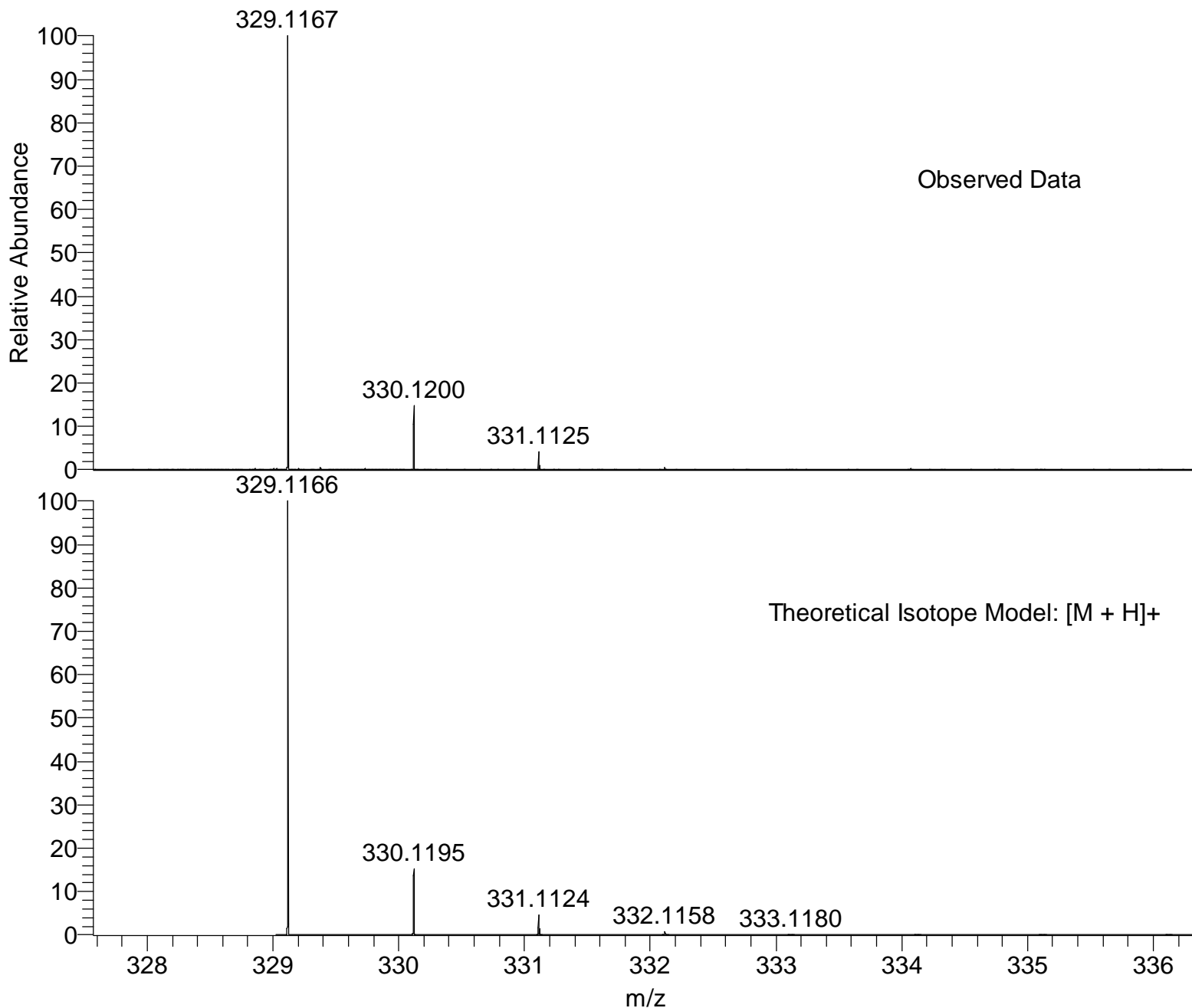
aet9-11 MW=328?
(DCM)/MeOH + NH₄OAc

EPSRC National Centre Swansea
LTQ Orbitrap XL

adam throup
30/11/2012 15:29:41

BRASHE239-OV-HNESP #28-50 RT: 0.71-1.28 AV: 22 SM: 7G NL: 9.24E6
T: FTMS + p NSI Full ms [120.00-2000.00]





NL:
9.24E6
BRASHE239-OV-HNESP#28-
50 RT: 0.71-1.28 AV: 22 T:
FTMS + p NSI Full ms
[120.00-2000.00]

NL:
1.87E4
C₁₄H₂₀N₂O₅SH:
C₁₄H₂₁N₂O₅S₁
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

Isotope: Min. .. Max.
 14 N 0....12
 16 O 0....15
 12 C 0....50
 1 H 0....65
 23 Na 0....0
 32 S 0....4

Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3.. 100 N-Rule: Do not use
 Fits: 100 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
329.1167	329.1166	0.4	5.5	C ₁₄ H ₂₁ O ₅ N ₂ S ₁
	329.1166	0.4	11.0	C ₁₃ H ₁₅ N ₉ S ₁
	329.1164	0.9	-3.0	C ₇ H ₂₃ O ₁₃ N ₁
	329.1164	1.0	2.5	C ₆ H ₁₇ O ₈ N ₈
	329.1172	-1.6	14.5	C ₂₂ H ₁₇ O ₃
	329.1173	-1.7	1.5	C ₇ H ₂₁ O ₃ N ₈ S ₂
	329.1174	-2.2	4.5	C ₁₅ H ₂₅ N ₂ S ₃
	329.1159	2.4	2.0	C ₅ H ₁₉ O ₂ N ₁₁ S ₂
	329.1159	2.5	15.0	C ₂₀ H ₁₅ O ₂ N ₃
	329.1177	-3.1	7.5	C ₇ H ₁₃ O ₄ N ₁₂
	329.1177	-3.1	2.0	C ₈ H ₁₉ O ₉ N ₅
	329.1179	-3.7	10.5	C ₁₅ H ₁₇ O ₁ N ₆ S ₁
	329.1152	4.5	6.0	C ₁₂ H ₁₉ O ₄ N ₅ S ₁

aet9-9 MW=258?
(H₂O)/MeOH + NH₄OAc

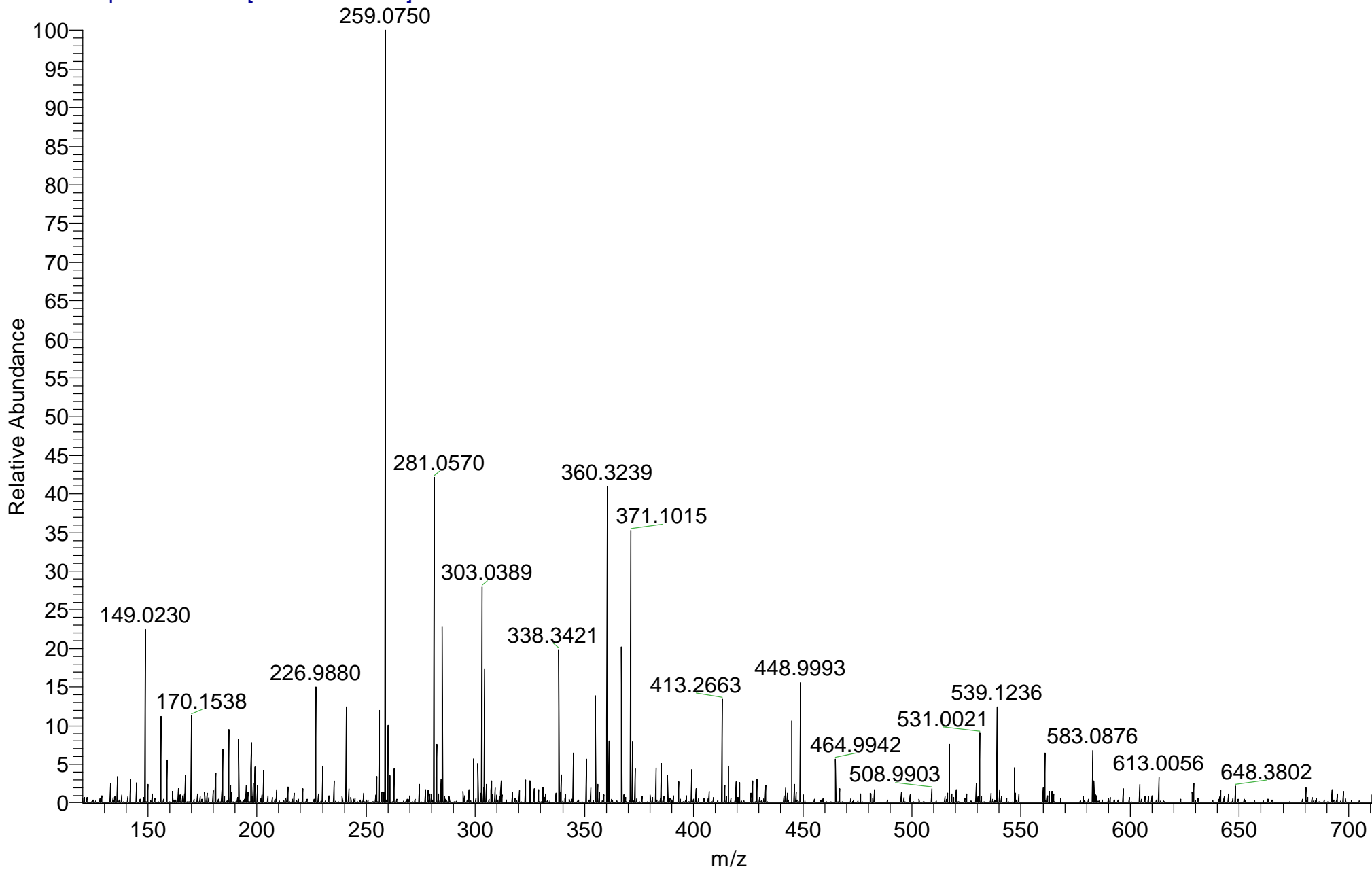
Compound 5

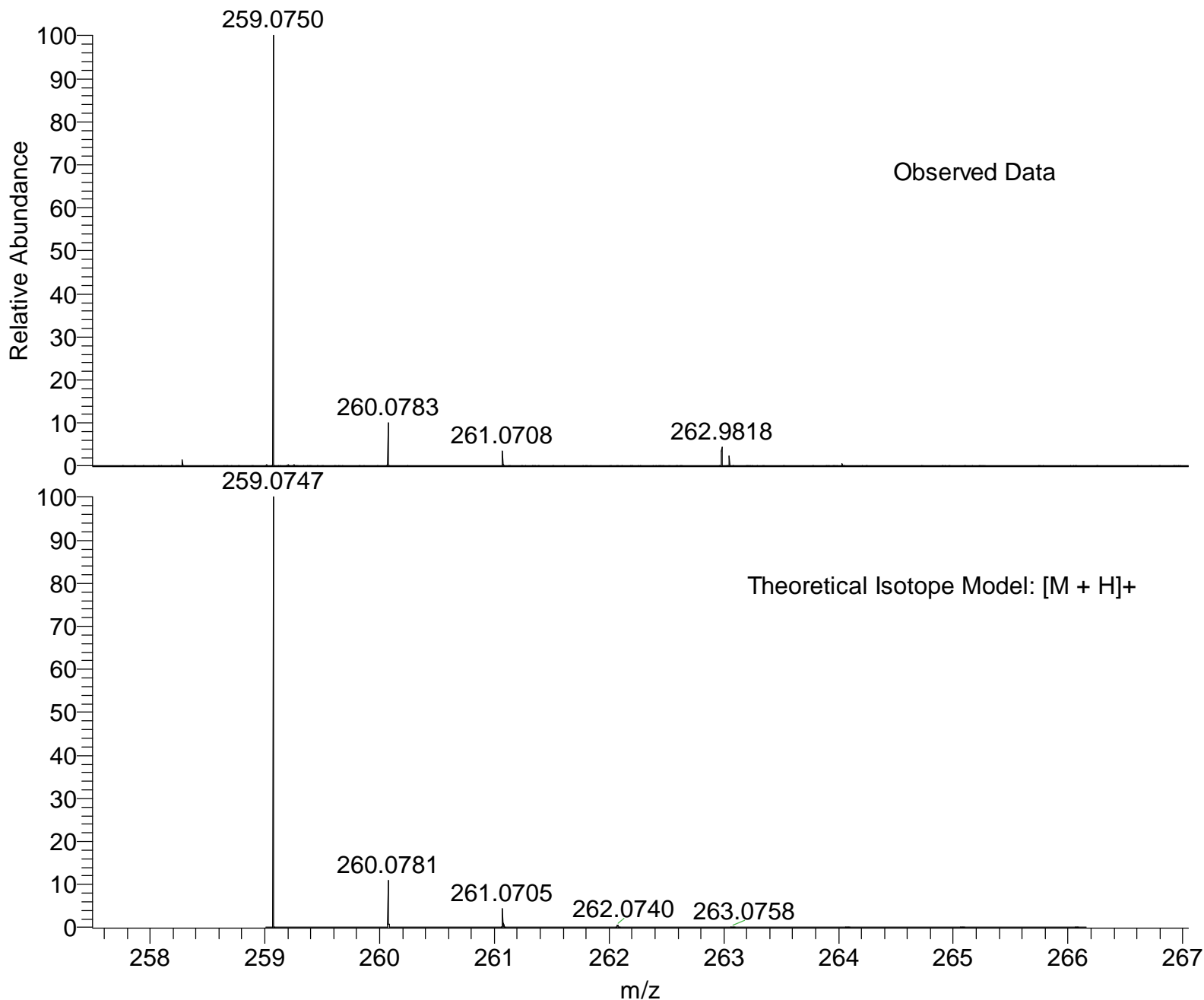
EPSRC National Centre Swansea
LTQ Orbitrap XL

adam throup
30/11/2012 15:22:52

BRASHE237-OV-HNESP #30-50 RT: 0.72-1.28 AV: 21 SM: 7G NL: 1.32E6

T: FTMS + p NSI Full ms [120.00-2000.00]





NL:
1.32E6
BRASHE237-OV-HNESP#30-
50 RT: 0.72-1.28 AV: 21 T:
FTMS + p NSI Full ms
[120.00-2000.00]

NL:
1.96E4
C₁₀ H₁₄ N₂ O₄ SH:
C₁₀ H₁₅ N₂ O₄ S₁
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

Isotope: Min. .. Max.
 14 N 0....12
 16 O 0....14
 12 C 0....50
 1 H 0....65
 23 Na 0....0
 32 S 0....4

Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3.. 100 N-Rule: Do not use
 Fits: 100 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
259.0750	259.0747	1.1	4.5	C ₁₀ H ₁₅ O ₄ N ₂ S ₁
	259.0754	-1.4	13.5	C ₁₈ H ₁₁ O ₂
	259.0754	-1.5	0.5	C ₃ H ₁₅ O ₂ N ₈ S ₂
	259.0745	1.8	1.5	C ₂ H ₁₁ O ₇ N ₈
	259.0759	-3.3	6.5	C ₃ H ₇ O ₃ N ₁₂
	259.0759	-3.3	1.0	C ₄ H ₁₃ O ₈ N ₅
	259.0740	3.7	1.0	C ₁ H ₁₃ O ₁ N ₁₁ S ₂
	259.0740	3.8	14.0	C ₁₆ H ₉ O ₁ N ₃
	259.0760	-4.0	9.5	C ₁₁ H ₁₁ N ₆ S ₁

aet9-13 MW=300?
(H₂O)/MeOH + NH₄OAc

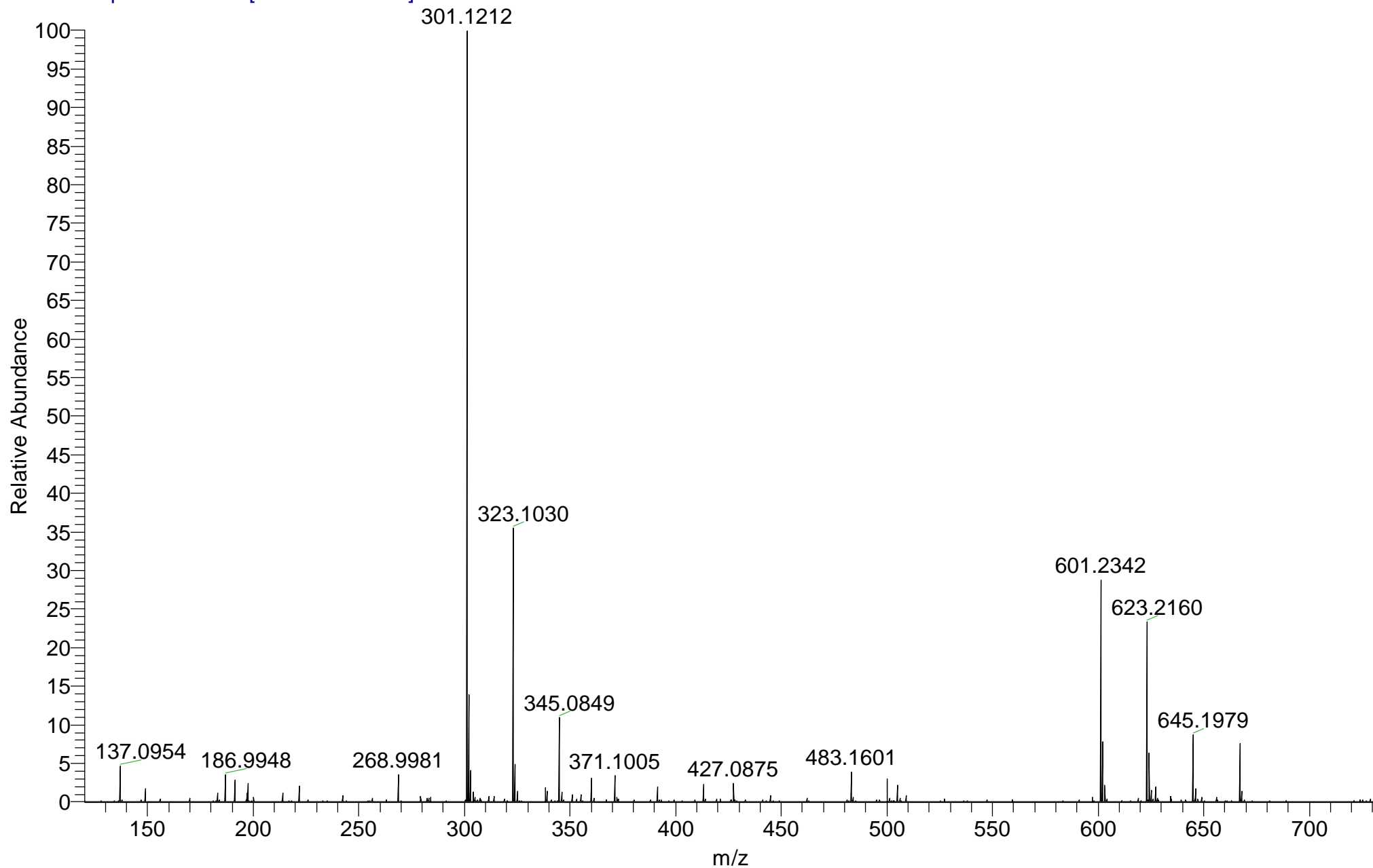
Compound 6

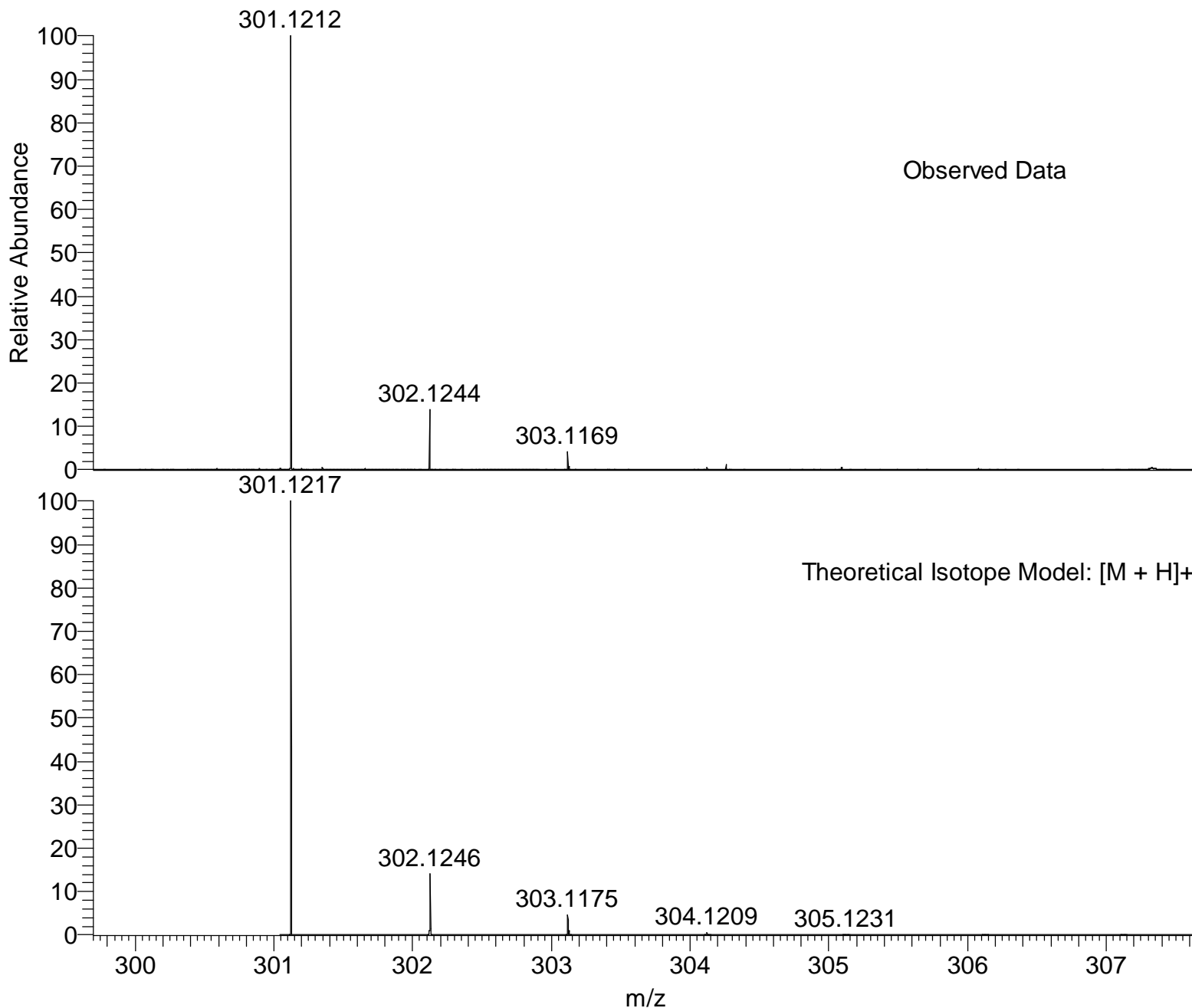
EPSRC National Centre Swansea
LTQ Orbitrap XL

adam throup
30/11/2012 15:26:17

BRASHE238-OV-HNESP #10-24 RT: 0.20-0.58 AV: 14 SM: 7G NL: 1.42E7

T: FTMS + p NSI Full ms [120.00-2000.00]





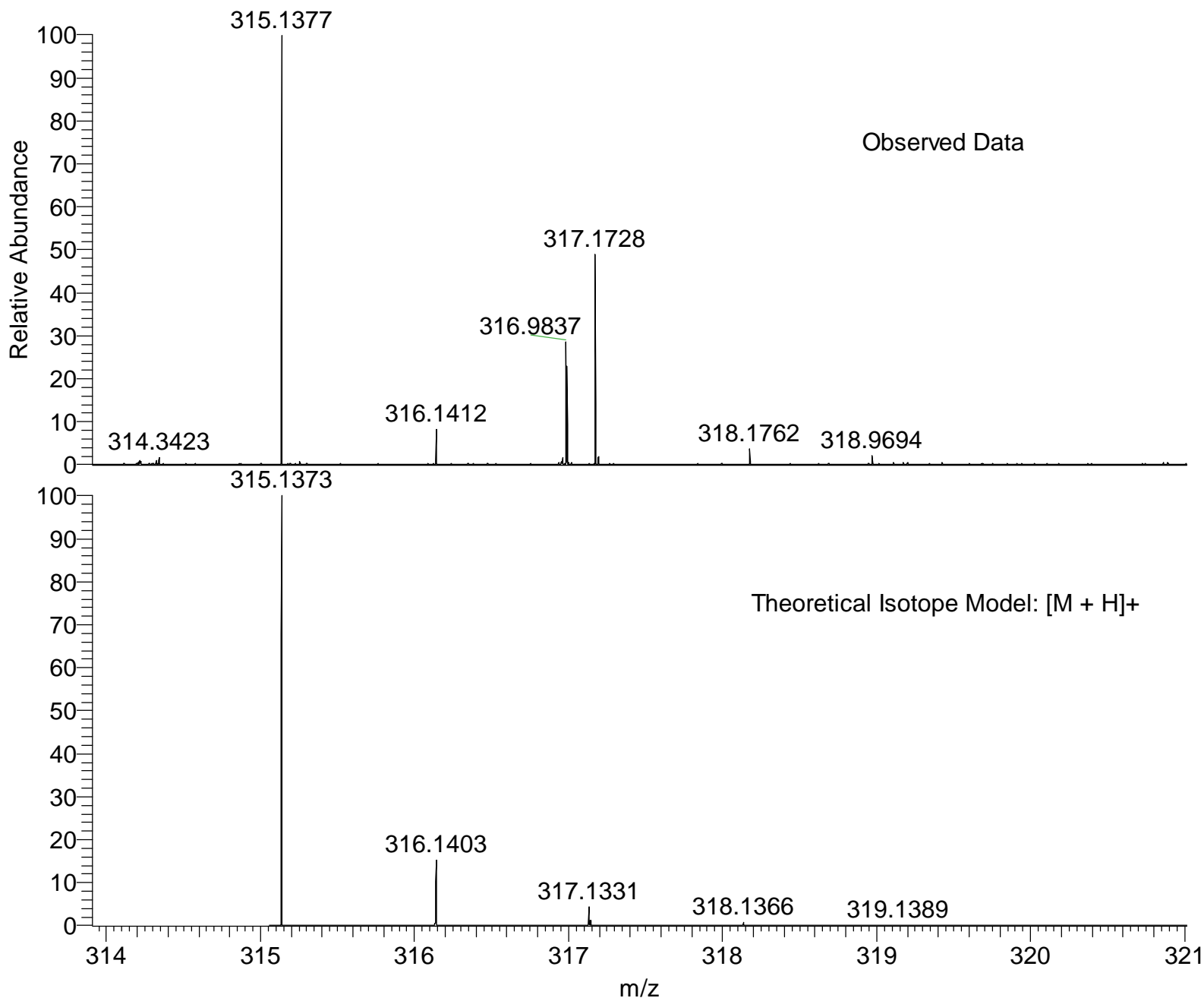
NL:
1.42E7
BRASHE238-OV-HNESP#10-
24 RT: 0.20-0.58 AV: 14 T:
FTMS + p NSI Full ms
[120.00-2000.00]

NL:
1.90E4
C₁₃ H₂₀ N₂ O₄ SH:
C₁₃ H₂₁ N₂ O₄ S₁
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

Isotope: Min. .. Max.
 14 N 0....12
 16 O 0....14
 12 C 0....50
 1 H 0....65
 23 Na 0....0
 32 S 0....4

Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3.. 100 N-Rule: Do not use
 Fits: 100 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
301.1212	301.1210	0.7	1.0	C ₄ H ₁₉ O ₁ N ₁₁ S ₂
	301.1210	0.8	14.0	C ₁₉ H ₁₅ O ₁ N ₃
	301.1215	-0.9	1.5	C ₅ H ₁₇ O ₇ N ₈
	301.1217	-1.5	4.5	C ₁₃ H ₂₁ O ₄ N ₂ S ₁
	301.1203	3.0	5.0	C ₁₁ H ₁₉ O ₃ N ₅ S ₁
	301.1201	3.6	2.0	C ₃ H ₁₅ O ₆ N ₁₁
	301.1223	-3.7	13.5	C ₂₁ H ₁₇ O ₂
	301.1223	-3.8	0.5	C ₆ H ₂₁ O ₂ N ₈ S ₂
	301.1198	4.5	-1.0	C ₁₁ H ₂₇ O ₂ N ₁ S ₃



NL:
5.64E4
BRASHE236-OV-HNESP#33-
51 RT: 0.78-1.29 AV: 19 T:
FTMS + p NSI Full ms
[120.00-2000.00]

NL:
1.88E4
C₁₄H₂₂N₂O₄SH:
C₁₄H₂₃N₂O₄S₁
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

Isotope: Min. .. Max.
 14 N 0....12
 16 O 0....14
 12 C 0....50
 1 H 0....65
 23 Na 0....0
 32 S 0....4

Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3.. 100 N-Rule: Do not use
 Fits: 100 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
315.1377	315.1380	-0.8	13.5	C ₂₂ H ₁₉ O ₂
	315.1380	-0.9	0.5	C ₇ H ₂₃ O ₂ N ₈ S ₂
	315.1373	1.3	4.5	C ₁₄ H ₂₃ O ₄ N ₂ S ₁
	315.1371	1.8	1.5	C ₆ H ₁₉ O ₇ N ₈
	315.1385	-2.4	6.5	C ₇ H ₁₅ O ₃ N ₁₂
	315.1385	-2.4	1.0	C ₈ H ₂₁ O ₈ N ₅
	315.1386	-3.0	9.5	C ₁₅ H ₁₉ N ₆ S ₁
	315.1366	3.3	1.0	C ₅ H ₂₁ O ₁ N ₁₁ S ₂
	315.1366	3.4	14.0	C ₂₀ H ₁₇ O ₁ N ₃
	315.1391	-4.6	-3.0	C ₁ H ₂₁ O ₆ N ₁₁ S ₁

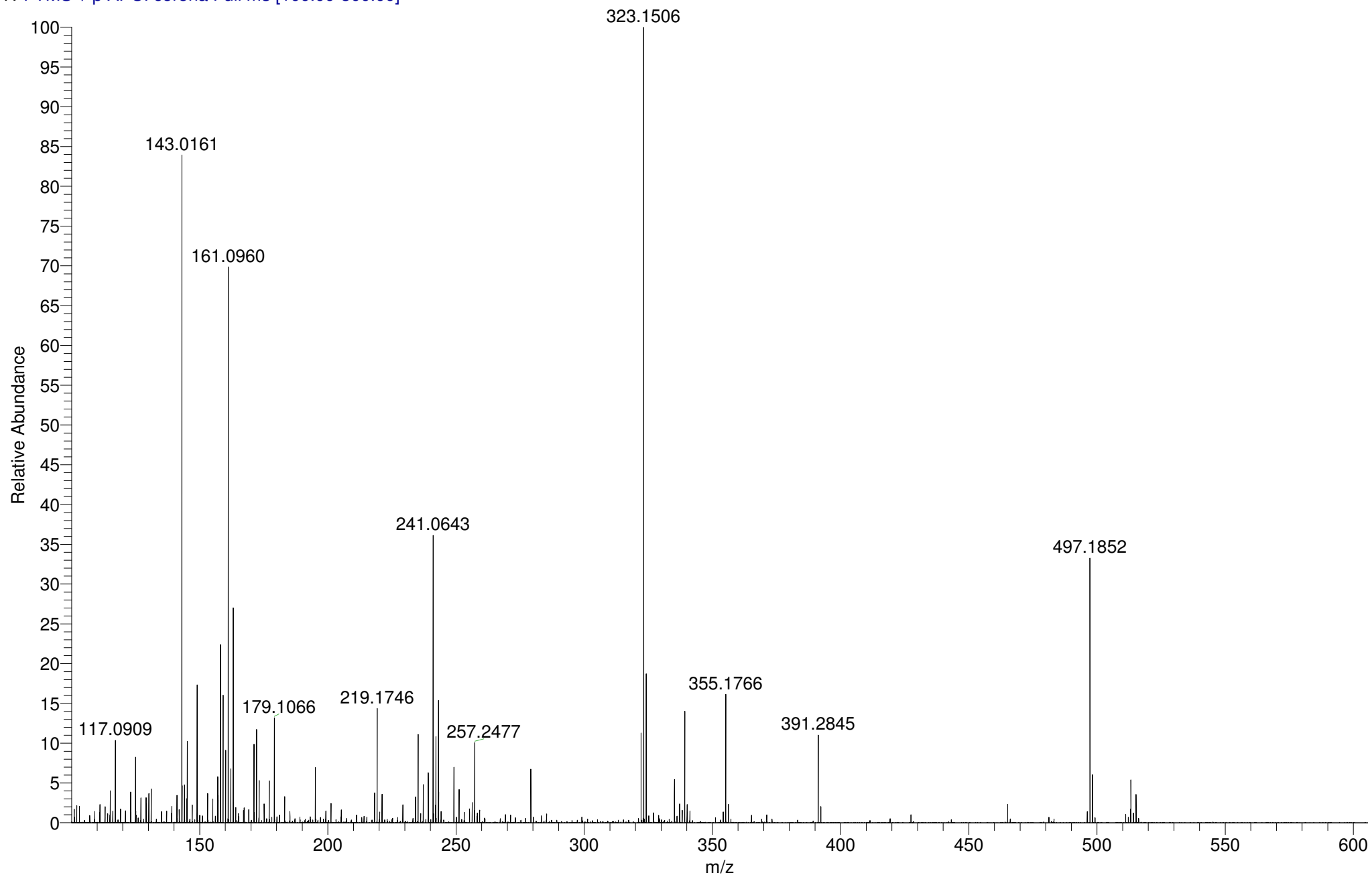
PA1-49 MW=496?
ASAP(SOLID)

Compound 17

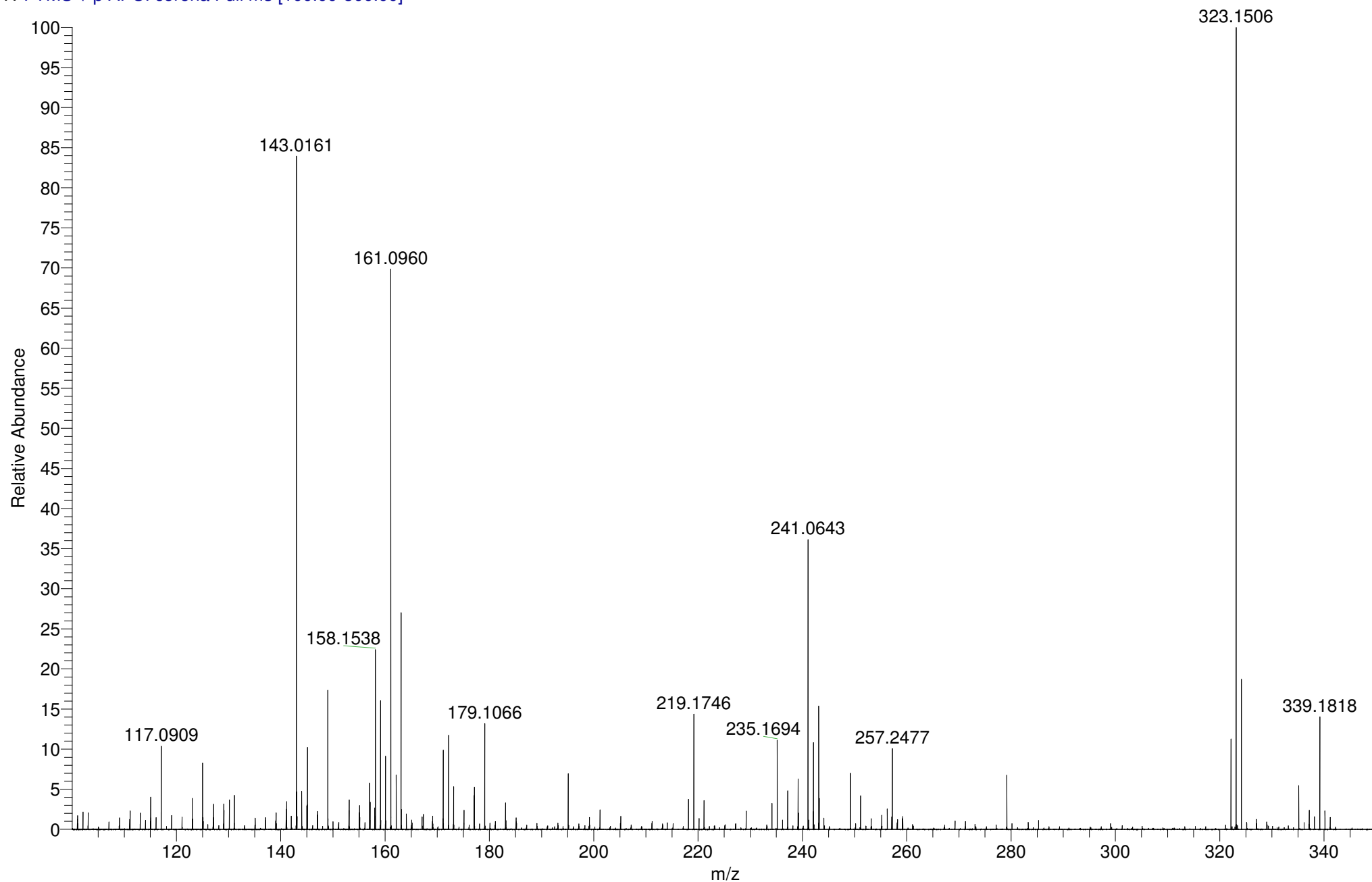
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LTQ Orbitrap XL

Thrup
06/11/2012 11:32:08

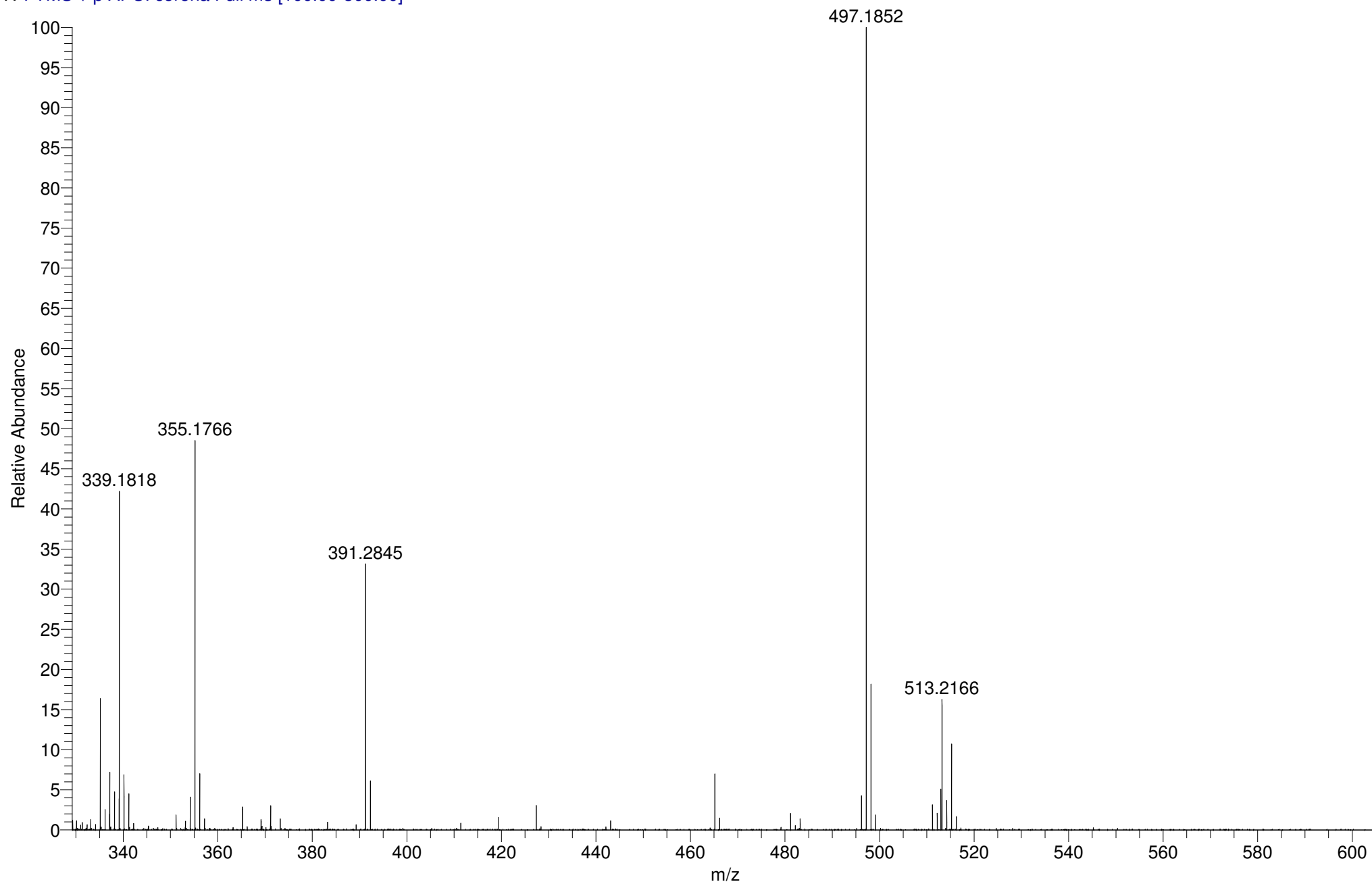
BRASHE228-PG-HASP #127-133 RT: 3.64-3.81 AV: 7 SM: 7G NL: 3.80E6
T: FTMS + p APCI corona Full ms [100.00-800.00]



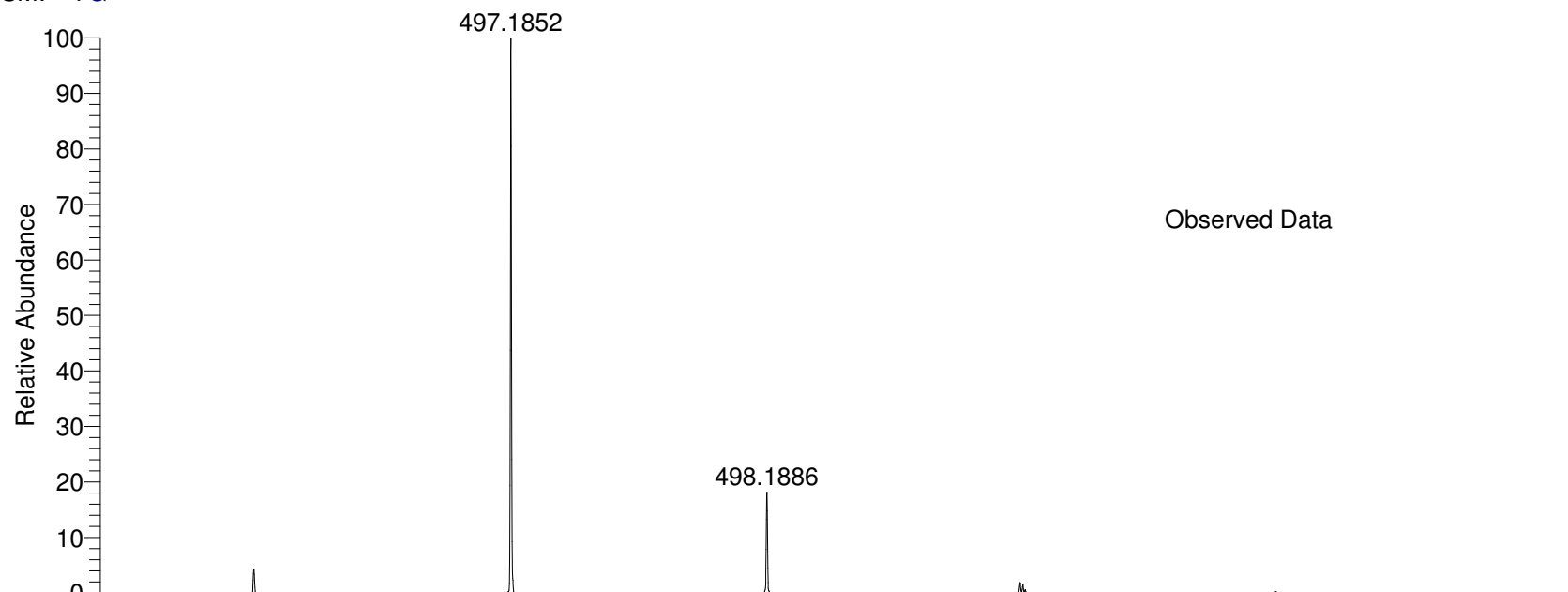
BRASHE228-PG-HASP #127-133 RT: 3.64-3.81 AV: 7 SM: 7G NL: 3.80E6
T: FTMS + p APCI corona Full ms [100.00-800.00]



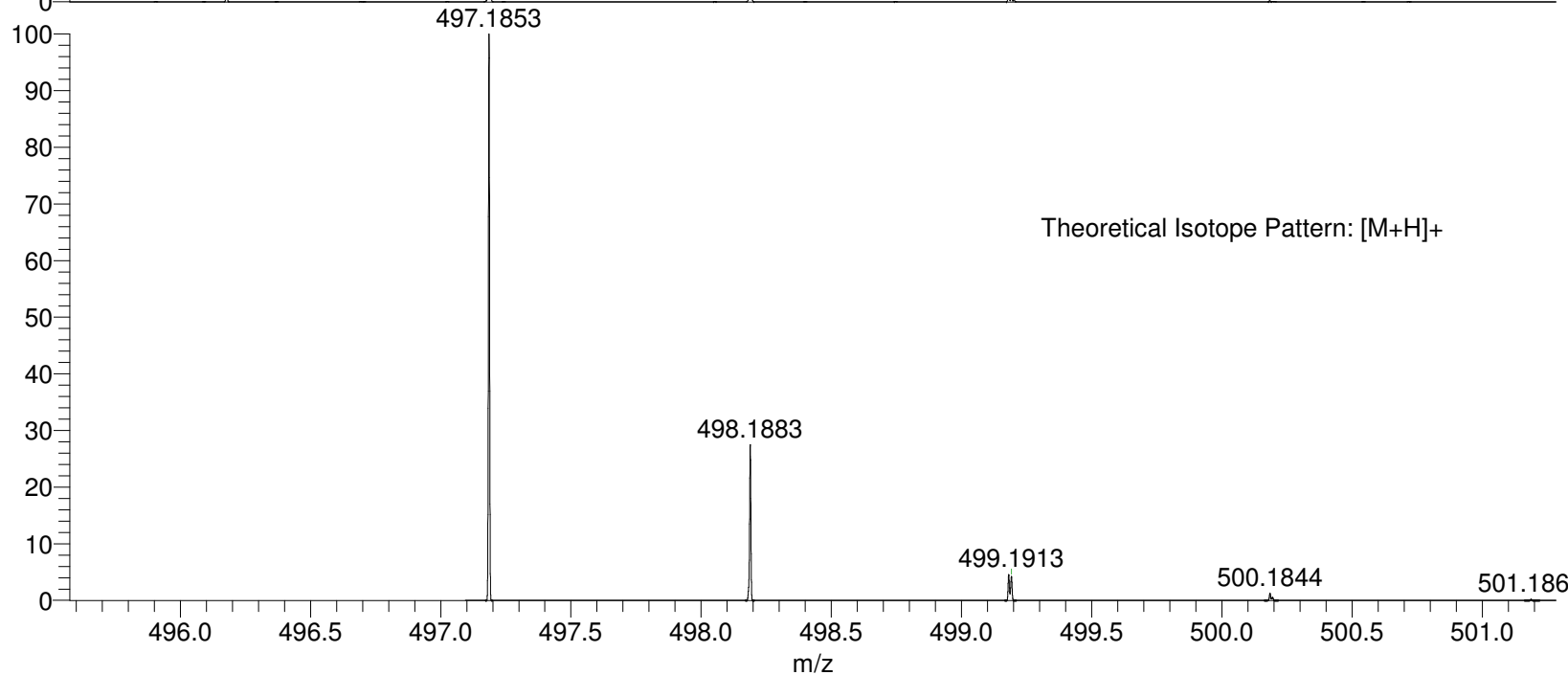
BRASHE228-PG-HASP #127-133 RT: 3.64-3.81 AV: 7 SM: 7G NL: 1.26E6
T: FTMS + p APCI corona Full ms [100.00-800.00]



SM: 7G



NL:
1.26E6
BRASHE228-PG-HASP#127-
133 RT: 3.64-3.81 AV: 7 T:
FTMS + p APCI corona Full ms
[100.00-800.00]



NL:
1.65E4
C25H28N4O5SH:
C25H29N4O5S1
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

Isotope: Min. .. Max.
 14 N 0....16
 16 O 0....15
 12 C 0....80
 1 H 0....100
 23 Na 0....0
 32 S 0....3
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3.. 100
 Fits: 100

N-Rule: Do not use
 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
497.1852	497.1851	0.1	5.0	C ₁₈ H ₃₁ O ₁₃ N ₃
	497.1851	0.1	10.5	C ₁₇ H ₂₅ O ₈ N ₁₀
	497.1853	-0.2	19.0	C ₂₄ H ₂₃ N ₁₁ S ₁
	497.1853	-0.2	13.5	C ₂₅ H ₂₉ O ₅ N ₄ S ₁
	497.1854	-0.3	0.5	C ₁₀ H ₃₃ O ₅ N ₁₂ S ₃
	497.1848	0.7	7.5	C ₂₅ H ₃₇ O ₄ S ₃
	497.1856	-0.9	-2.0	C ₃ H ₂₇ O ₁₄ N ₁₅
	497.1847	1.1	4.5	C ₁₇ H ₃₃ O ₇ N ₆ S ₂
	497.1847	1.1	10.0	C ₁₆ H ₂₇ O ₂ N ₁₃ S ₂
	497.1846	1.2	23.0	C ₃₁ H ₂₃ O ₂ N ₅
	497.1858	-1.2	6.5	C ₁₀ H ₂₅ O ₆ N ₁₆ S ₁
	497.1858	-1.3	1.0	C ₁₁ H ₃₁ O ₁₁ N ₉ S ₁
	497.1845	1.4	1.5	C ₉ H ₂₉ O ₁₀ N ₁₂ S ₁
	497.1860	-1.5	22.5	C ₃₃ H ₂₅ O ₃ N ₂
	497.1860	-1.6	9.5	C ₁₈ H ₂₉ O ₃ N ₁₀ S ₂
	497.1860	-1.6	4.0	C ₁₉ H ₃₅ O ₈ N ₃ S ₂
	497.1862	-2.0	12.5	C ₂₆ H ₃₃ N ₄ S ₃
	497.1842	2.1	17.0	C ₃₁ H ₃₁ O ₁ N ₁ S ₂
	497.1840	2.4	1.0	C ₈ H ₃₁ O ₄ N ₁₅ S ₃
	497.1840	2.5	8.5	C ₂₄ H ₃₃ O ₉ S ₁
	497.1840	2.5	14.0	C ₂₃ H ₂₇ O ₄ N ₇ S ₁
	497.1865	-2.6	15.5	C ₁₈ H ₂₁ O ₄ N ₁₄
	497.1865	-2.6	10.0	C ₁₉ H ₂₇ O ₉ N ₇
	497.1865	-2.6	4.5	C ₂₀ H ₃₃ O ₁₄
	497.1865	-2.6	-3.0	C ₄ H ₃₁ O ₉ N ₁₅ S ₂
	497.1838	2.8	5.5	C ₁₆ H ₂₉ O ₁₂ N ₆
	497.1838	2.8	11.0	C ₁₅ H ₂₃ O ₇ N ₁₃
	497.1867	-2.9	18.5	C ₂₆ H ₂₅ O ₁ N ₈ S ₁
	497.1867	-2.9	13.0	C ₂₇ H ₃₁ O ₆ N ₁ S ₁
	497.1867	-3.0	5.5	C ₁₁ H ₂₉ O ₁ N ₁₆ S ₃
	497.1867	-3.0	0.0	C ₁₂ H ₃₅ O ₆ N ₉ S ₃

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
497.1835	497.1835	3.4	8.0	C ₂₃ H ₃₅ O ₃ N ₃ S ₃
497.1870	497.1870	-3.6	-2.5	C ₅ H ₂₉ O ₁₅ N ₁₂
497.1833	497.1833	3.8	-0.5	C ₁₆ H ₃₇ O ₁₁ N ₂ S ₂
497.1833	497.1833	3.8	5.0	C ₁₅ H ₃₁ O ₆ N ₉ S ₂
497.1833	497.1833	3.8	10.5	C ₁₄ H ₂₅ O ₁ N ₁₆ S ₂
497.1833	497.1833	3.8	18.0	C ₃₀ H ₂₇ O ₆ N ₁
497.1833	497.1833	3.9	23.5	C ₂₉ H ₂₁ O ₁ N ₈
497.1872	497.1872	-3.9	6.0	C ₁₂ H ₂₇ O ₇ N ₁₃ S ₁
497.1872	497.1872	-4.0	0.5	C ₁₃ H ₃₃ O ₁₂ N ₆ S ₁
497.1831	497.1831	4.1	2.0	C ₇ H ₂₇ O ₉ N ₁₅ S ₁
497.1873	497.1873	-4.3	9.0	C ₂₀ H ₃₁ O ₄ N ₇ S ₂
497.1874	497.1874	-4.3	3.5	C ₂₁ H ₃₇ O ₉ S ₂
497.1875	497.1875	-4.7	12.0	C ₂₈ H ₃₅ O ₁ N ₁ S ₃
497.1828	497.1828	4.8	17.5	C ₂₉ H ₂₉ N ₄ S ₂

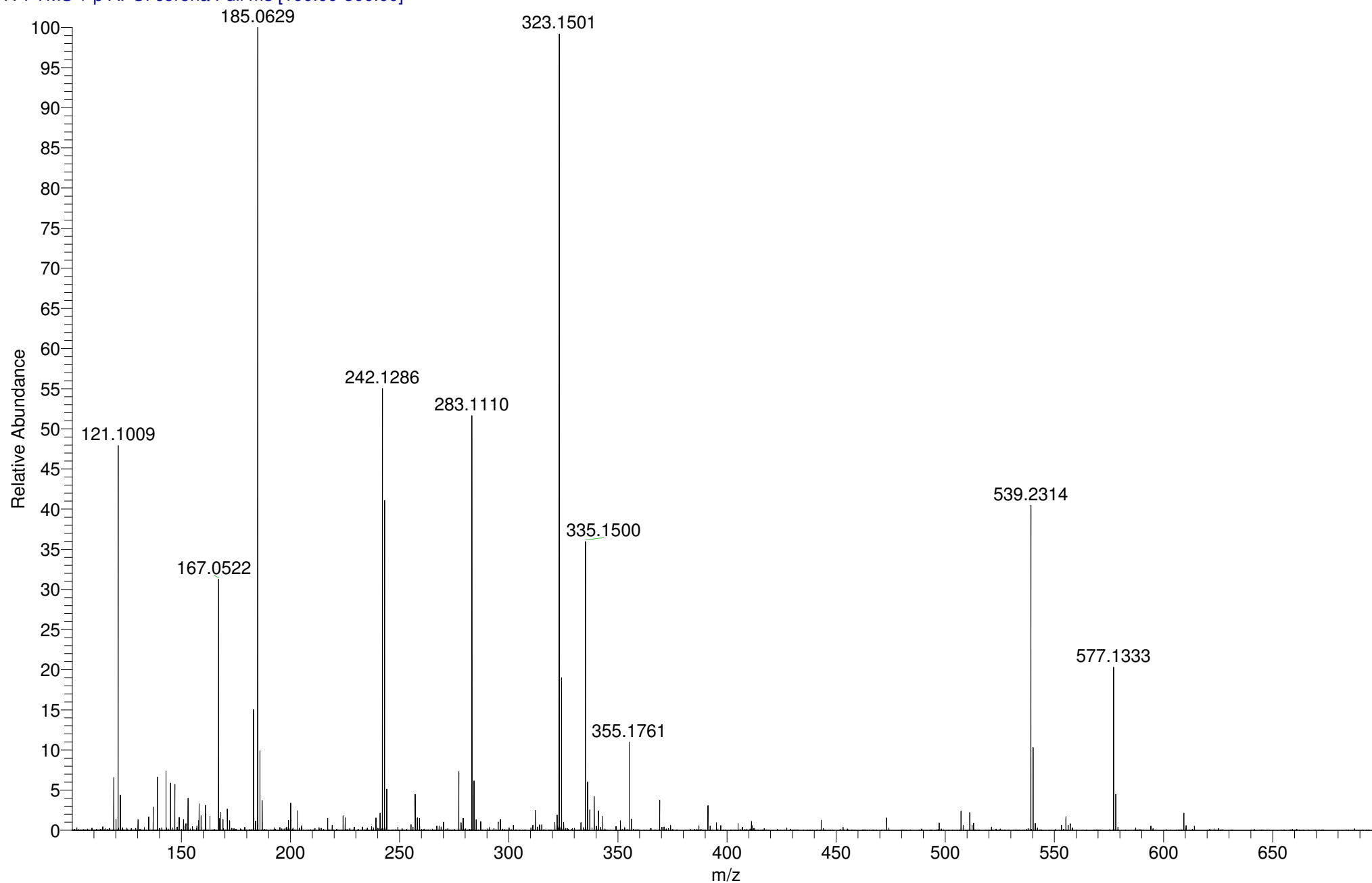
PA1-47 MW=538?
ASAP(DCM)

Compound 18

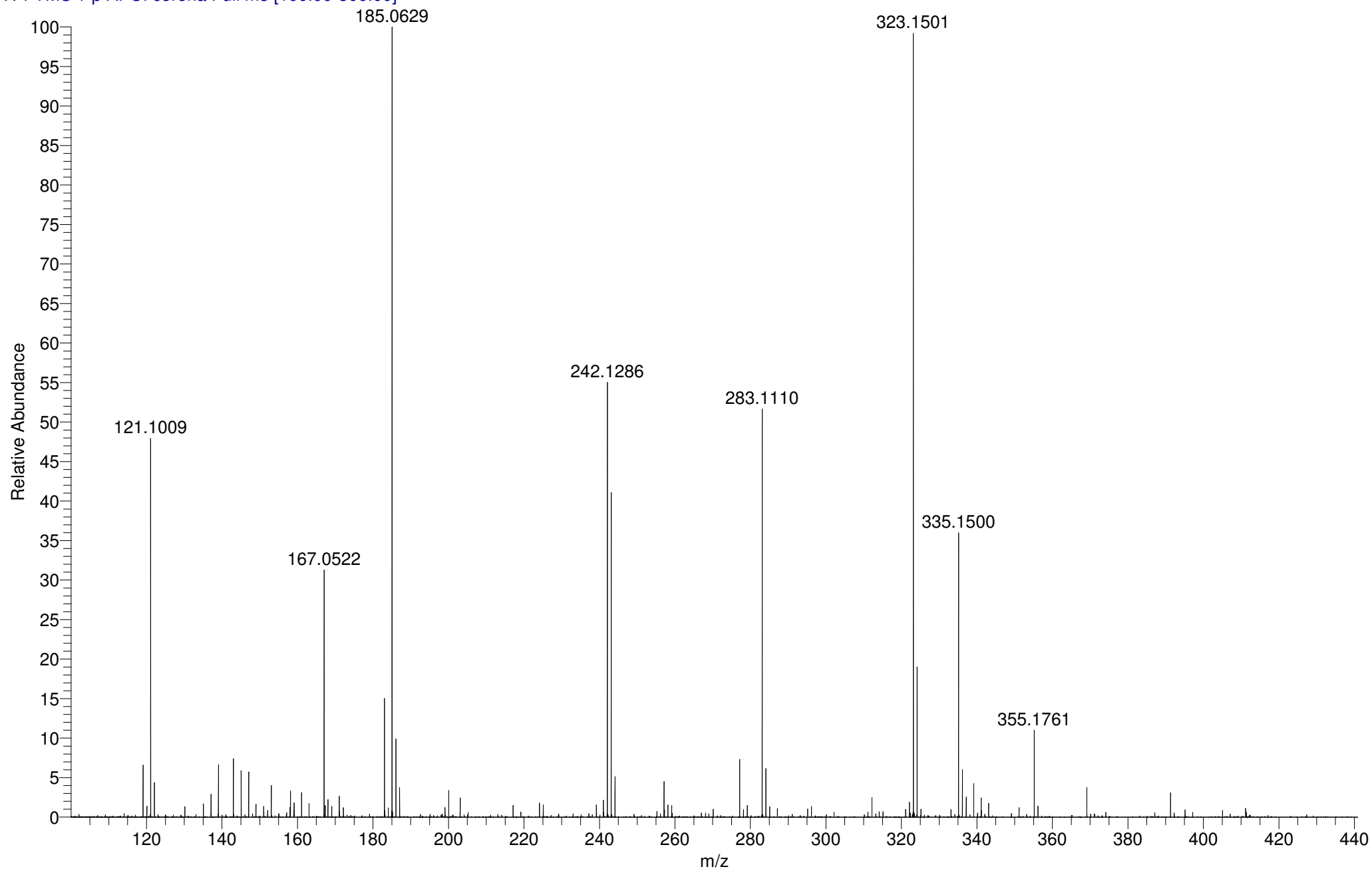
EPSRC National Centre Swansea
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Thrup
06/11/2012 11:41:24

BRASHE229-PG-HASP #34-36 RT: 0.95-1.01 AV: 3 SM: 7G NL: 1.17E7
T: FTMS + p APCI corona Full ms [100.00-800.00]



BRASHE229-PG-HASP #34-36 RT: 0.95-1.01 AV: 3 SM: 7G NL: 1.17E7
T: FTMS + p APCI corona Full ms [100.00-800.00]

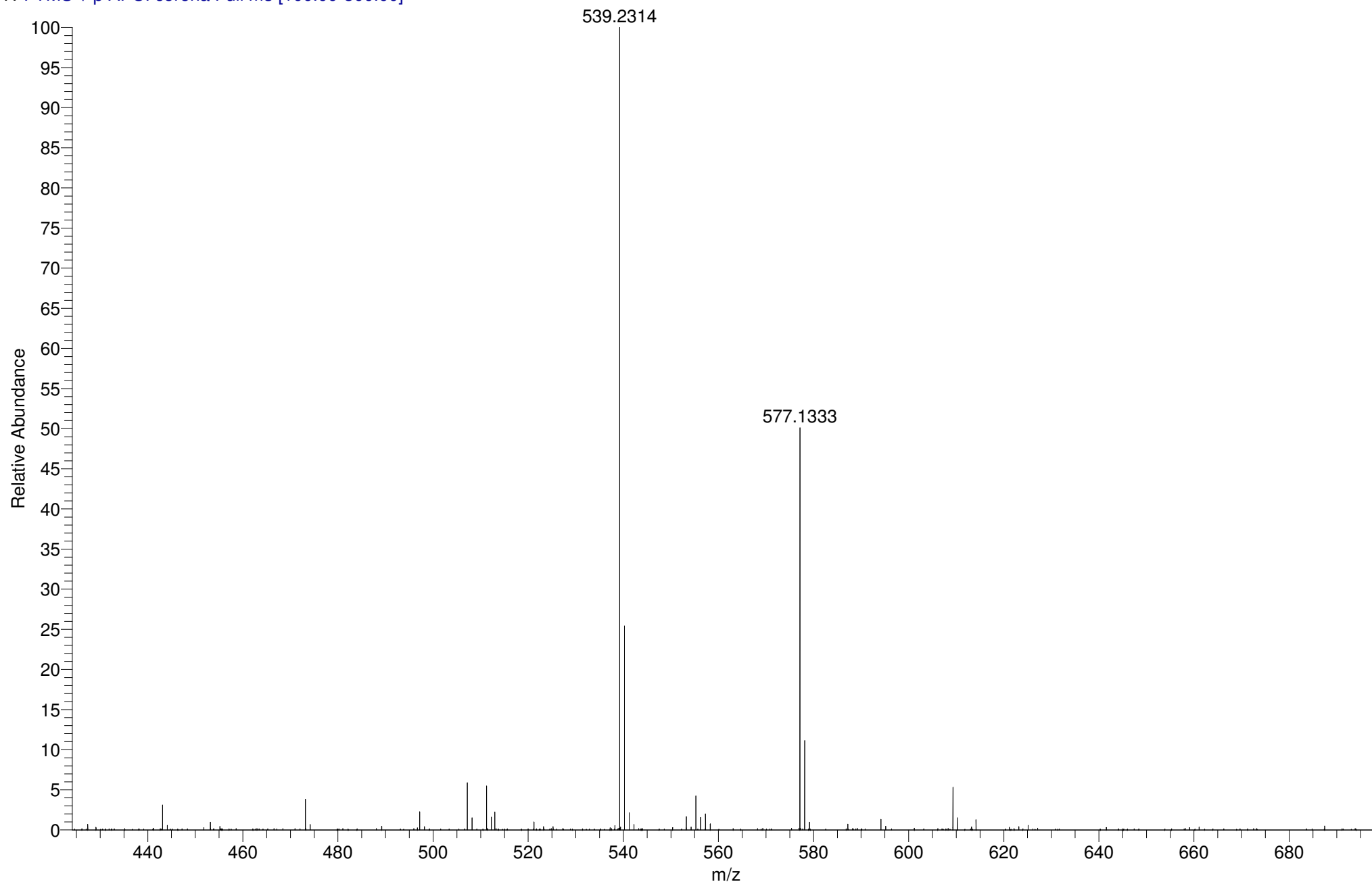


PA1-47 MW=538?
ASAP(DCM)

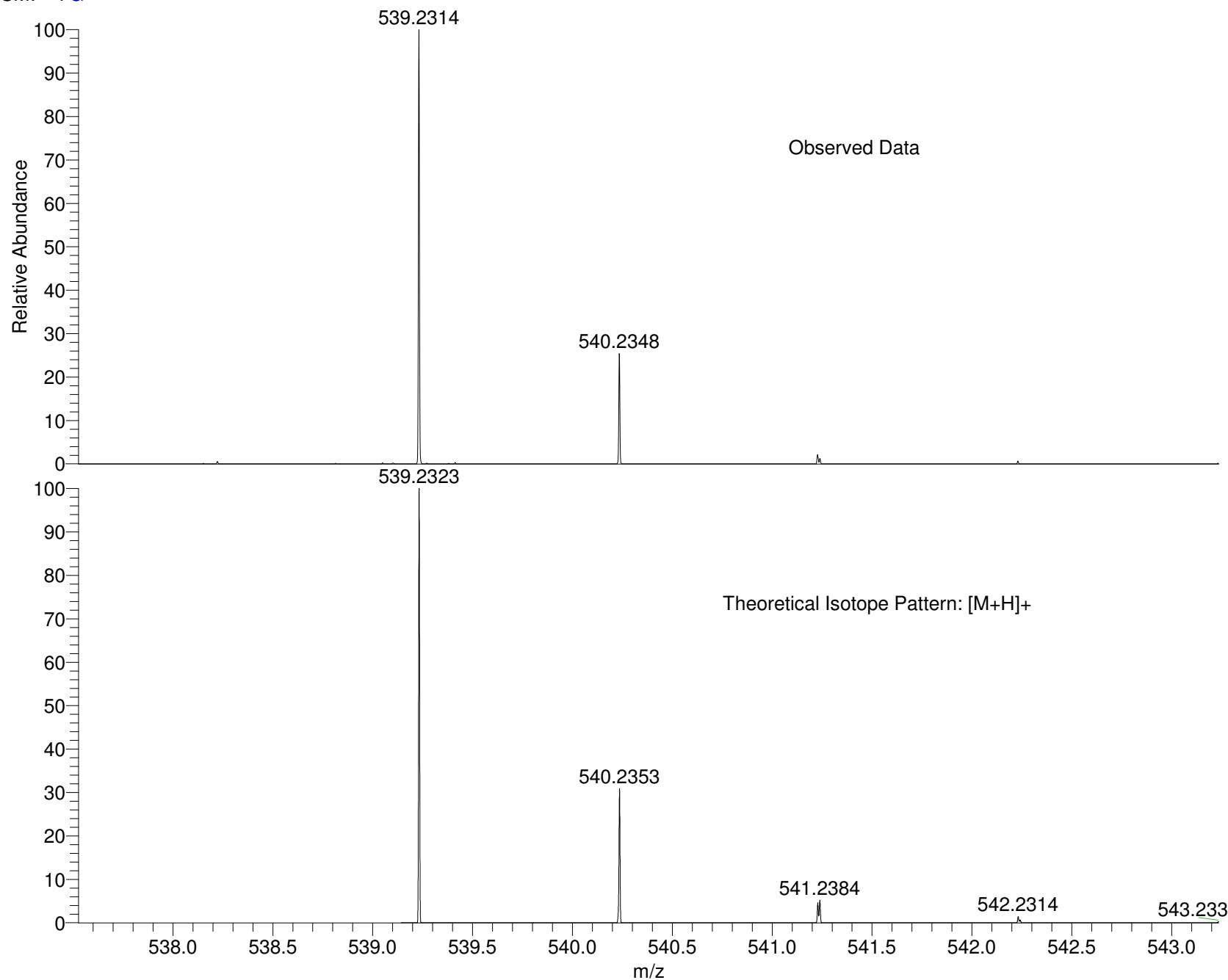
EPSRC National Centre Swansea
LTQ Orbitrap XL

Thrup
06/11/2012 11:41:24

BRASHE229-PG-HASP #34-36 RT: 0.95-1.01 AV: 3 SM: 7G NL: 4.74E6
T: FTMS + p APCI corona Full ms [100.00-800.00]



SM: 7G



NL:
4.74E6
BRASHE229-PG-HASP#34-36
RT: 0.95-1.01 AV: 3 T: FTMS
+ p APCI corona Full ms
[100.00-800.00]

NL:
1.60E4
C₂₈ H₃₄ N₄ O₅ SH:
C₂₈ H₃₅ N₄ O₅ S₁
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

Isotope: Min. . . Max.
 14 N 016
 16 O 015
 12 C 080
 1 H 0100
 23 Na 00
 32 S 03
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3.. 100
 Fits: 100

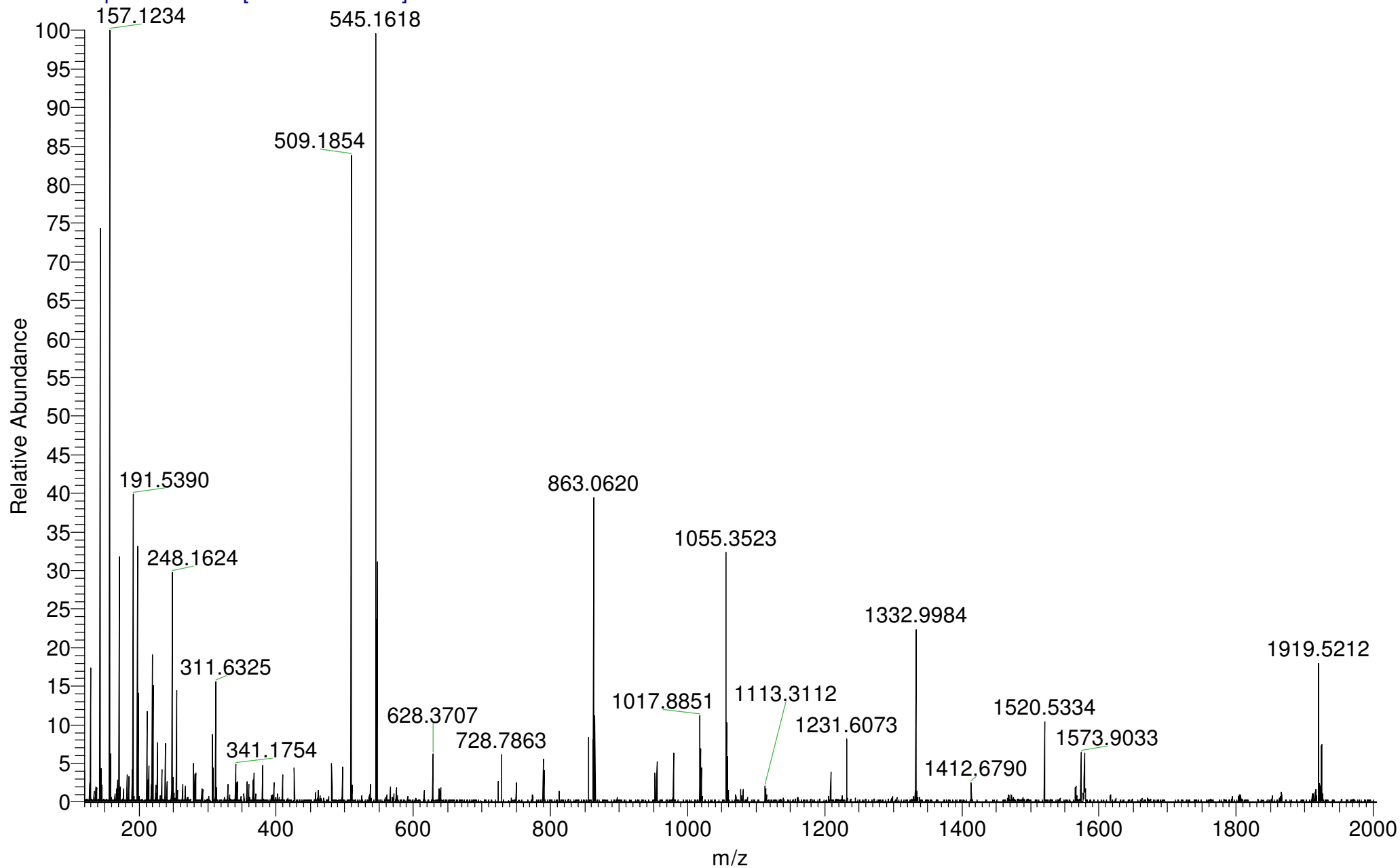
N-Rule: Do not use
 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
539.2314	539.2314	-0.1	1.5	C ₁₂ H ₃₅ O ₁₀ N ₁₂ S ₁
	539.2316	-0.3	23.0	C ₃₄ H ₂₉ O ₂ N ₅
	539.2316	-0.4	10.0	C ₁₉ H ₃₃ O ₂ N ₁₃ S ₂
	539.2316	-0.4	4.5	C ₂₀ H ₃₉ O ₇ N ₆ S ₂
	539.2311	0.5	17.0	C ₃₄ H ₃₇ O ₁ N ₁ S ₂
	539.2318	-0.7	7.5	C ₂₈ H ₄₃ O ₄ S ₃
	539.2310	0.8	1.0	C ₁₁ H ₃₇ O ₄ N ₁₅ S ₃
	539.2309	0.9	8.5	C ₂₇ H ₃₉ O ₉ S ₁
	539.2309	0.9	14.0	C ₂₆ H ₃₃ O ₄ N ₇ S ₁
	539.2307	1.2	5.5	C ₁₉ H ₃₅ O ₁₂ N ₆
	539.2307	1.2	11.0	C ₁₈ H ₂₉ O ₇ N ₁₃
	539.2321	-1.3	10.5	C ₂₀ H ₃₁ O ₈ N ₁₀
	539.2321	-1.3	5.0	C ₂₁ H ₃₇ O ₁₃ N ₃
	539.2323	-1.6	19.0	C ₂₇ H ₂₉ N ₁₁ S ₁
	539.2323	-1.6	13.5	C ₂₈ H ₃₅ O ₅ N ₄ S ₁
	539.2323	-1.7	0.5	C ₁₃ H ₃₉ O ₅ N ₁₂ S ₃
	539.2305	1.8	8.0	C ₂₆ H ₄₁ O ₃ N ₃ S ₃
	539.2303	2.1	-0.5	C ₁₉ H ₄₃ O ₁₁ N ₂ S ₂
	539.2303	2.1	5.0	C ₁₈ H ₃₇ O ₆ N ₉ S ₂
	539.2303	2.1	10.5	C ₁₇ H ₃₁ O ₁ N ₁₆ S ₂
	539.2302	2.2	18.0	C ₃₃ H ₃₃ O ₆ N ₁
	539.2302	2.2	23.5	C ₃₂ H ₂₇ O ₁ N ₈
	539.2326	-2.2	-2.0	C ₆ H ₃₃ O ₁₄ N ₁₅
	539.2301	2.4	2.0	C ₁₀ H ₃₃ O ₉ N ₁₅ S ₁
	539.2328	-2.5	6.5	C ₁₃ H ₃₁ O ₆ N ₁₆ S ₁
	539.2328	-2.5	1.0	C ₁₄ H ₃₇ O ₁₁ N ₉ S ₁
	539.2329	-2.8	22.5	C ₃₆ H ₃₁ O ₃ N ₂
	539.2330	-2.9	9.5	C ₂₁ H ₃₅ O ₃ N ₁₀ S ₂
	539.2330	-2.9	4.0	C ₂₂ H ₄₁ O ₈ N ₃ S ₂
	539.2298	3.0	17.5	C ₃₂ H ₃₅ N ₄ S ₂
	539.2331	-3.2	12.5	C ₂₉ H ₃₉ N ₄ S ₃

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
539.2296	539.2296	3.4	9.0	C ₂₅ H ₃₇ O ₈ N ₃ S ₁
539.2296	539.2296	3.4	14.5	C ₂₄ H ₃₁ O ₃ N ₁₀ S ₁
539.2294	539.2294	3.7	6.0	C ₁₇ H ₃₃ O ₁₁ N ₉
539.2294	539.2294	3.7	11.5	C ₁₆ H ₂₇ O ₆ N ₁₆
539.2334	539.2334	-3.7	15.5	C ₂₁ H ₂₇ O ₄ N ₁₄
539.2334	539.2334	-3.8	10.0	C ₂₂ H ₃₃ O ₉ N ₇
539.2334	539.2334	-3.8	4.5	C ₂₃ H ₃₉ O ₁₄
539.2335	539.2335	-3.8	-3.0	C ₇ H ₃₇ O ₉ N ₁₅ S ₂
539.2336	539.2336	-4.1	18.5	C ₂₉ H ₃₁ O ₁ N ₈ S ₁
539.2336	539.2336	-4.1	13.0	C ₃₀ H ₃₇ O ₆ N ₁ S ₁
539.2336	539.2336	-4.2	5.5	C ₁₄ H ₃₅ O ₁ N ₁₆ S ₃
539.2336	539.2336	-4.2	0.0	C ₁₅ H ₄₁ O ₆ N ₉ S ₃
539.2291	539.2291	4.2	8.5	C ₂₄ H ₃₉ O ₂ N ₆ S ₃
539.2289	539.2289	4.6	0.0	C ₁₇ H ₄₁ O ₁₀ N ₅ S ₂
539.2289	539.2289	4.6	5.5	C ₁₆ H ₃₅ O ₅ N ₁₂ S ₂
539.2289	539.2289	4.6	18.5	C ₃₁ H ₃₁ O ₅ N ₄
539.2289	539.2289	4.7	24.0	C ₃₀ H ₂₅ N ₁₁
539.2339	539.2339	-4.7	-2.5	C ₈ H ₃₅ O ₁₅ N ₁₂
539.2288	539.2288	4.9	-3.0	C ₉ H ₃₇ O ₁₃ N ₁₁ S ₁

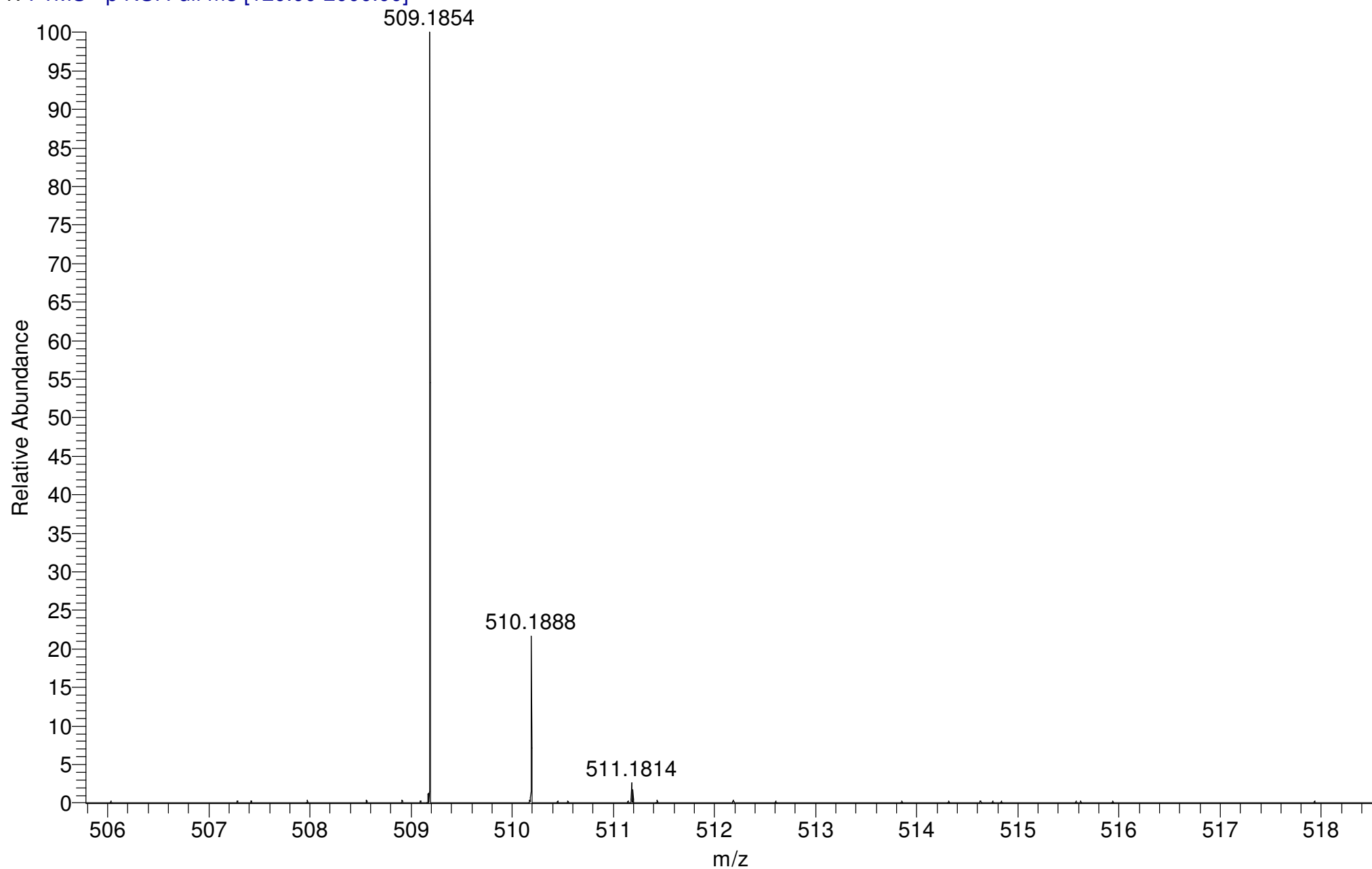
BRASHE253-OV-HNESN #3-7 RT: 0.37-0.74 AV: 5 SM: 7G NL: 2.25E4

T: FTMS - p NSI Full ms [120.00-2000.00]



BRASHE253-OV-HNESN #3-7 RT: 0.37-0.74 AV: 5 SM: 7G NL: 1.89E4

T: FTMS - p NSI Full ms [120.00-2000.00]



Isotope: Min. .. Max.
 12 C 0....60
 1 H 0....70
 14 N 0....15
 16 O 0....15
 23 Na 0....0
 32 S 0....3
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3.. 100
 Fits: 100

N-Rule: Do not use
 Charge: -1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
509.1854	509.1853	0.3	18.0	C ₃₂ H ₃₁ O ₁ N ₁ S ₂
	509.1856	-0.4	2.5	C ₁₀ H ₂₉ O ₁₀ N ₁₂ S ₁
	509.1856	-0.4	-3.0	C ₁₁ H ₃₅ O ₁₅ N ₅ S ₁
	509.1851	0.6	2.0	C ₉ H ₃₁ O ₄ N ₁₅ S ₃
	509.1857	-0.6	24.0	C ₃₂ H ₂₃ O ₂ N ₅
	509.1851	0.6	9.5	C ₂₅ H ₃₃ O ₉ S ₁
	509.1851	0.6	15.0	C ₂₄ H ₂₇ O ₄ N ₇ S ₁
	509.1858	-0.7	11.0	C ₁₇ H ₂₇ O ₂ N ₁₃ S ₂
	509.1858	-0.7	5.5	C ₁₈ H ₃₃ O ₇ N ₆ S ₂
	509.1849	1.0	6.5	C ₁₇ H ₂₉ O ₁₂ N ₆
	509.1849	1.0	12.0	C ₁₆ H ₂₃ O ₇ N ₁₃
	509.1859	-1.1	8.5	C ₂₆ H ₃₇ O ₄ S ₃
	509.1846	1.6	9.0	C ₂₄ H ₃₅ O ₃ N ₃ S ₃
	509.1862	-1.6	11.5	C ₁₈ H ₂₅ O ₈ N ₁₀
	509.1862	-1.6	6.0	C ₁₉ H ₃₁ O ₁₃ N ₃
	509.1844	1.9	0.5	C ₁₇ H ₃₇ O ₁₁ N ₂ S ₂
	509.1844	1.9	6.0	C ₁₆ H ₃₁ O ₆ N ₉ S ₂
	509.1864	-2.0	20.0	C ₂₅ H ₂₃ N ₁₁ S ₁
	509.1864	-2.0	14.5	C ₂₆ H ₂₉ O ₅ N ₄ S ₁
	509.1844	2.0	19.0	C ₃₁ H ₂₇ O ₆ N ₁
	509.1844	2.0	24.5	C ₃₀ H ₂₁ O ₁ N ₈
	509.1864	-2.1	1.5	C ₁₁ H ₃₃ O ₅ N ₁₂ S ₃
	509.1842	2.3	-2.5	C ₉ H ₃₃ O ₁₄ N ₈ S ₁
	509.1842	2.3	3.0	C ₈ H ₂₇ O ₉ N ₁₅ S ₁
	509.1867	-2.6	-1.0	C ₄ H ₂₇ O ₁₄ N ₁₅
	509.1839	2.9	18.5	C ₃₀ H ₂₉ N ₄ S ₂
	509.1869	-3.0	2.0	C ₁₂ H ₃₁ O ₁₁ N ₉ S ₁
	509.1838	3.2	-3.0	C ₈ H ₃₅ O ₈ N ₁₁ S ₃
	509.1871	-3.3	23.5	C ₃₄ H ₂₅ O ₃ N ₂
	509.1837	3.3	10.0	C ₂₃ H ₃₁ O ₈ N ₃ S ₁
	509.1837	3.3	15.5	C ₂₂ H ₂₅ O ₃ N ₁₀ S ₁

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
509.1871	509.1871	-3.3	10.5	C ₁₉ H ₂₉ O ₃ N ₁₀ S ₂
509.1871	509.1871	-3.3	5.0	C ₂₀ H ₃₅ O ₈ N ₃ S ₂
509.1836	509.1836	3.6	7.0	C ₁₅ H ₂₇ O ₁₁ N ₉
509.1873	509.1873	-3.7	13.5	C ₂₇ H ₃₃ N ₄ S ₃
509.1833	509.1833	4.2	9.5	C ₂₂ H ₃₃ O ₂ N ₆ S ₃
509.1876	509.1876	-4.3	16.5	C ₁₉ H ₂₁ O ₄ N ₁₄
509.1876	509.1876	-4.3	11.0	C ₂₀ H ₂₇ O ₉ N ₇
509.1876	509.1876	-4.3	5.5	C ₂₁ H ₃₃ O ₁₄
509.1876	509.1876	-4.3	-2.0	C ₅ H ₃₁ O ₉ N ₁₅ S ₂
509.1831	509.1831	4.6	1.0	C ₁₅ H ₃₅ O ₁₀ N ₅ S ₂
509.1831	509.1831	4.6	6.5	C ₁₄ H ₂₉ O ₅ N ₁₂ S ₂
509.1878	509.1878	-4.6	19.5	C ₂₇ H ₂₅ O ₁ N ₈ S ₁
509.1878	509.1878	-4.6	14.0	C ₂₈ H ₃₁ O ₆ N ₁ S ₁
509.1830	509.1830	4.6	19.5	C ₂₉ H ₂₅ O ₅ N ₄
509.1830	509.1830	4.6	25.0	C ₂₈ H ₁₉ N ₁₁
509.1878	509.1878	-4.7	1.0	C ₁₃ H ₃₅ O ₆ N ₉ S ₃
509.1829	509.1829	4.9	-2.0	C ₇ H ₃₁ O ₁₃ N ₁₁ S ₁

aet9-19 MW=552?
(DCM)/MeOH + NH4OAc

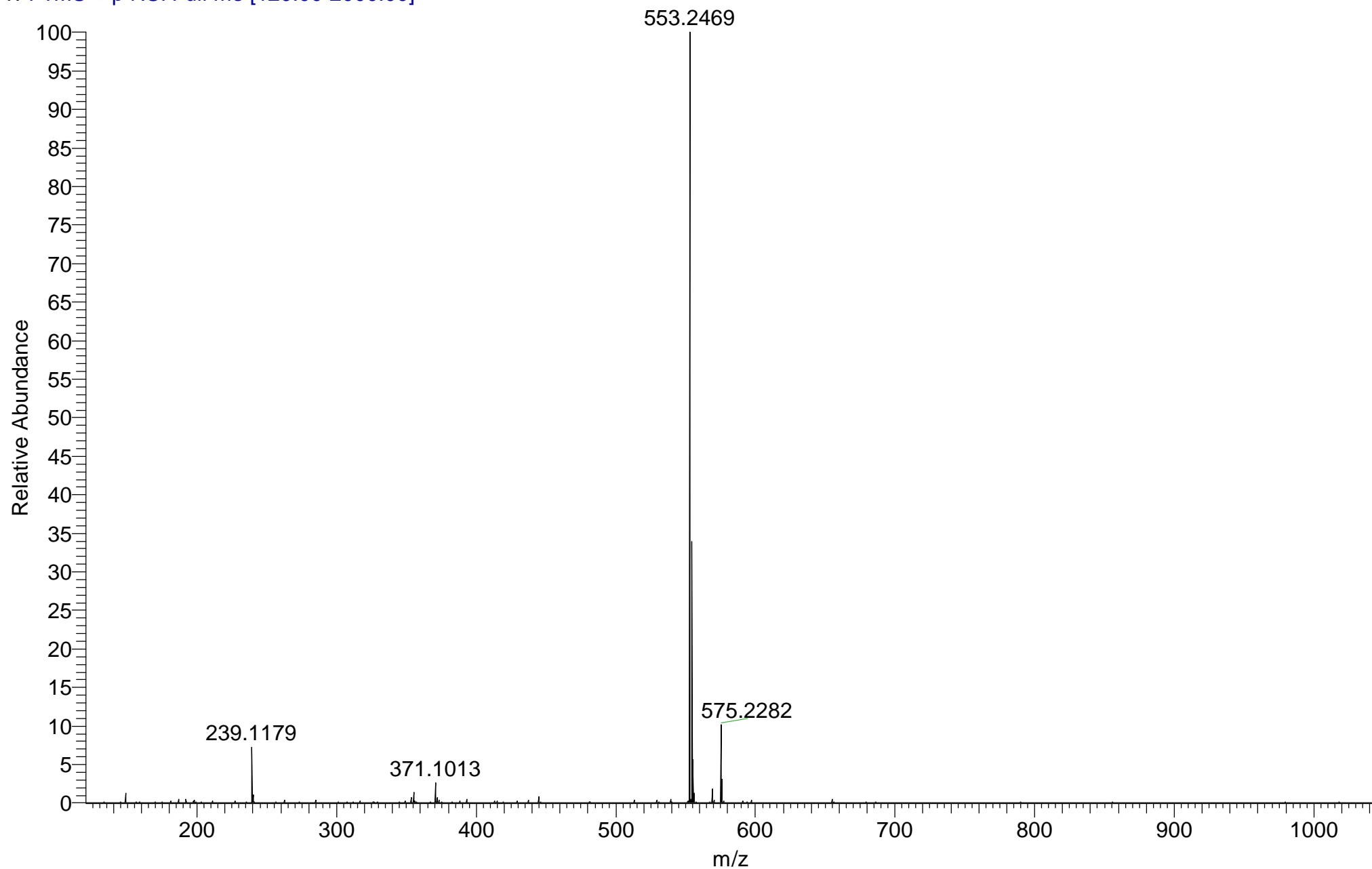
Compound 20

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adam throup
14/01/2013 16:40:17

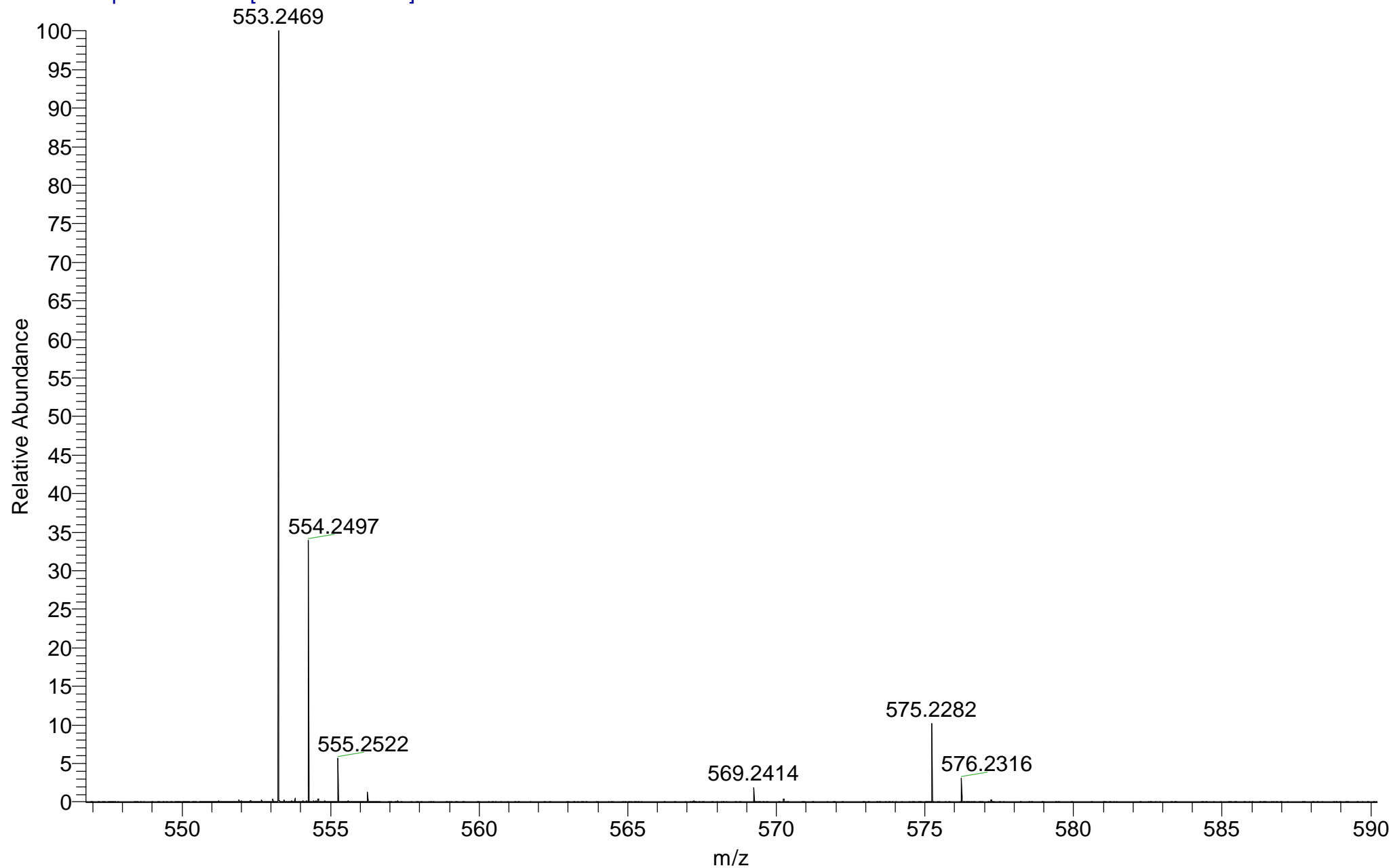
BRASHE246-OJ-HNESP #37-50 RT: 0.95-1.29 AV: 13 SM: 7G NL: 2.62E7

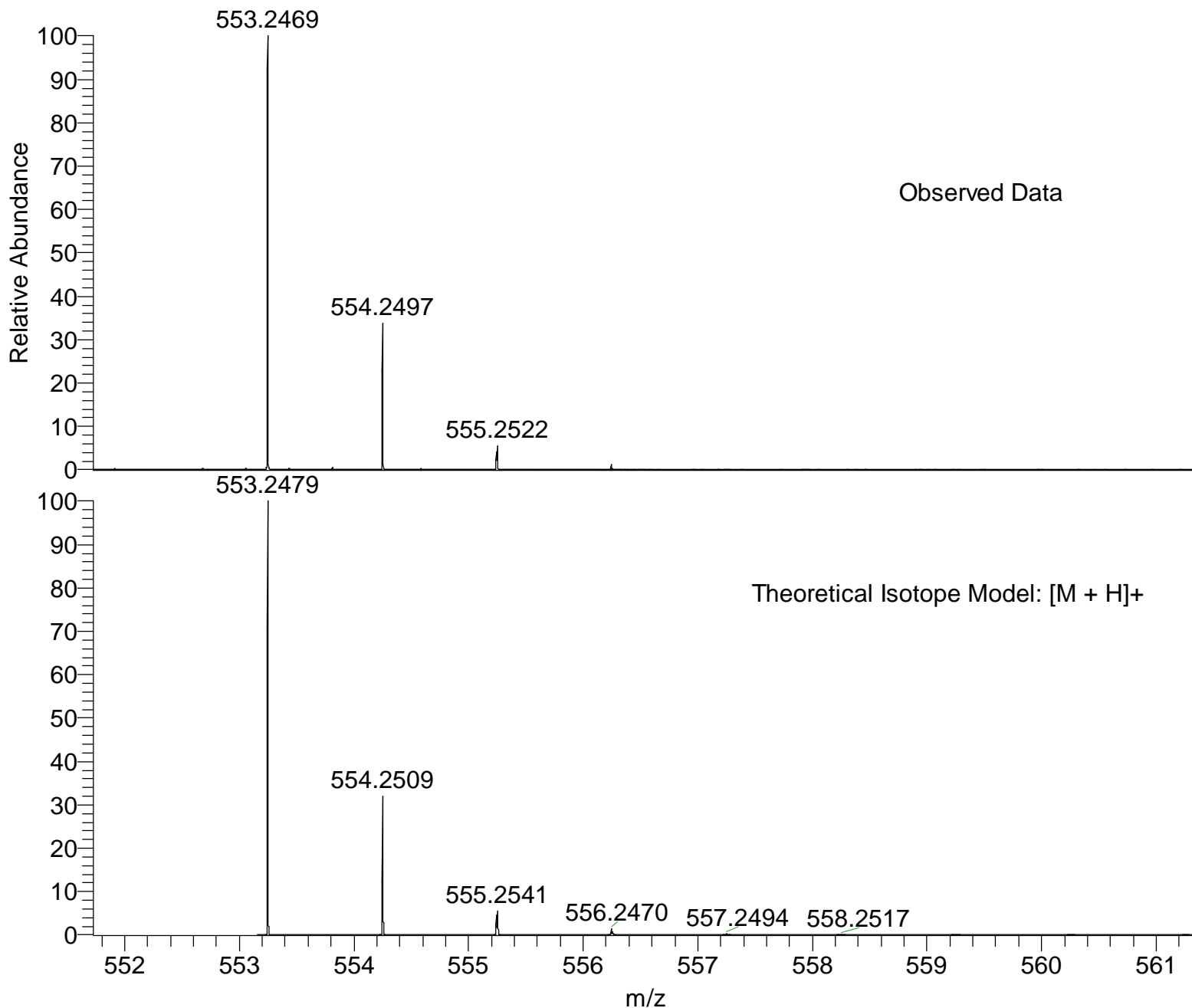
T: FTMS + p NSI Full ms [120.00-2000.00]



BRASHE246-OJ-HNESP #37-50 RT: 0.95-1.29 AV: 13 SM: 7G NL: 2.62E7

T: FTMS + p NSI Full ms [120.00-2000.00]





NL:
2.62E7
BRASHE246-OJ-HNESP#37-
50 RT: 0.95-1.29 AV: 13 T:
FTMS + p NSI Full ms
[120.00-2000.00]

NL:
1.58E4
C₂₉ H₃₆ N₄ O₅ SH:
C₂₉ H₃₇ N₄ O₅ S₁
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

Isotope: Min. .. Max.
 14 N 0....14
 16 O 0....15
 12 C 0....60
 1 H 0....80
 23 Na 0....0
 32 S 0....5

Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3.. 100 N-Rule: Do not use
 Fits: 200 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
553.2469	553.2468	0.2	-1.5	C ₂₁ H ₄₉ O ₆ N ₂ S ₄
	553.2468	0.2	4.0	C ₂₀ H ₄₃ O ₁ N ₉ S ₄
	553.2468	0.3	17.0	C ₃₅ H ₃₉ O ₁ N ₁ S ₂
	553.2471	-0.3	1.5	C ₁₃ H ₃₇ O ₁₀ N ₁₂ S ₁
	553.2466	0.6	8.5	C ₂₈ H ₄₁ O ₉ S ₁
	553.2466	0.6	14.0	C ₂₇ H ₃₅ O ₄ N ₇ S ₁
	553.2472	-0.6	23.0	C ₃₅ H ₃₁ O ₂ N ₅
	553.2473	-0.7	10.0	C ₂₀ H ₃₅ O ₂ N ₁₃ S ₂
	553.2473	-0.7	4.5	C ₂₁ H ₄₁ O ₇ N ₆ S ₂
	553.2464	0.9	5.5	C ₂₀ H ₃₇ O ₁₂ N ₆
	553.2464	0.9	11.0	C ₁₉ H ₃₁ O ₇ N ₁₃
	553.2474	-1.0	7.5	C ₂₉ H ₄₅ O ₄ S ₃
	553.2461	1.4	8.0	C ₂₇ H ₄₃ O ₃ N ₃ S ₃
	553.2477	-1.5	10.5	C ₂₁ H ₃₃ O ₈ N ₁₀
	553.2477	-1.5	5.0	C ₂₂ H ₃₉ O ₁₃ N ₃
	553.2459	1.8	-0.5	C ₂₀ H ₄₅ O ₁₁ N ₂ S ₂
	553.2459	1.8	5.0	C ₁₉ H ₃₉ O ₆ N ₉ S ₂
	553.2459	1.8	18.0	C ₃₄ H ₃₅ O ₆ N ₁
	553.2479	-1.8	19.0	C ₂₈ H ₃₁ N ₁₁ S ₁
	553.2459	1.8	23.5	C ₃₃ H ₂₉ O ₁ N ₈
	553.2479	-1.8	13.5	C ₂₉ H ₃₇ O ₅ N ₄ S ₁
	553.2480	-1.9	0.5	C ₁₄ H ₄₁ O ₅ N ₁₂ S ₃
	553.2481	-2.2	3.5	C ₂₂ H ₄₅ O ₂ N ₆ S ₄
	553.2455	2.6	-1.0	C ₁₉ H ₄₇ O ₅ N ₅ S ₄
	553.2454	2.6	4.5	C ₁₈ H ₄₁ N ₁₂ S ₄
	553.2454	2.7	17.5	C ₃₃ H ₃₇ N ₄ S ₂
	553.2484	-2.8	1.0	C ₁₅ H ₃₉ O ₁₁ N ₉ S ₁
	553.2452	3.0	9.0	C ₂₆ H ₃₉ O ₈ N ₃ S ₁
	553.2452	3.0	14.5	C ₂₅ H ₃₃ O ₃ N ₁₀ S ₁
	553.2486	-3.0	22.5	C ₃₇ H ₃₃ O ₃ N ₂
	553.2486	-3.1	9.5	C ₂₂ H ₃₇ O ₃ N ₁₀ S ₂

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
553.2486	553.2486	-3.1	4.0	C ₂₃ H ₄₃ O ₈ N ₃ S ₂
553.2451	553.2451	3.3	6.0	C ₁₈ H ₃₅ O ₁₁ N ₉
553.2488	553.2488	-3.4	12.5	C ₃₀ H ₄₁ N ₄ S ₃
553.2488	553.2488	-3.5	-0.5	C ₁₅ H ₄₅ N ₁₂ S ₅
553.2448	553.2448	3.9	8.5	C ₂₅ H ₄₁ O ₂ N ₆ S ₃
553.2491	553.2491	-3.9	15.5	C ₂₂ H ₂₉ O ₄ N ₁₄
553.2491	553.2491	-3.9	10.0	C ₂₃ H ₃₅ O ₉ N ₇
553.2491	553.2491	-3.9	4.5	C ₂₄ H ₄₁ O ₁₄
553.2446	553.2446	4.2	0.0	C ₁₈ H ₄₃ O ₁₀ N ₅ S ₂
553.2446	553.2446	4.2	5.5	C ₁₇ H ₃₇ O ₅ N ₁₂ S ₂
553.2445	553.2445	4.3	18.5	C ₃₂ H ₃₃ O ₅ N ₄
553.2493	553.2493	-4.3	18.5	C ₃₀ H ₃₃ O ₁ N ₈ S ₁
553.2445	553.2445	4.3	24.0	C ₃₁ H ₂₇ N ₁₁
553.2493	553.2493	-4.3	13.0	C ₃₁ H ₃₉ O ₆ N ₁ S ₁
553.2493	553.2493	-4.3	0.0	C ₁₆ H ₄₃ O ₆ N ₉ S ₃
553.2444	553.2444	4.5	-3.0	C ₁₀ H ₃₉ O ₁₃ N ₁₁ S ₁
553.2495	553.2495	-4.7	3.0	C ₂₄ H ₄₇ O ₃ N ₃ S ₄
553.2443	553.2443	4.7	2.5	C ₂₅ H ₄₉ O ₁ N ₂ S ₅
553.2496	553.2496	-4.9	-2.5	C ₉ H ₃₇ O ₁₅ N ₁₂

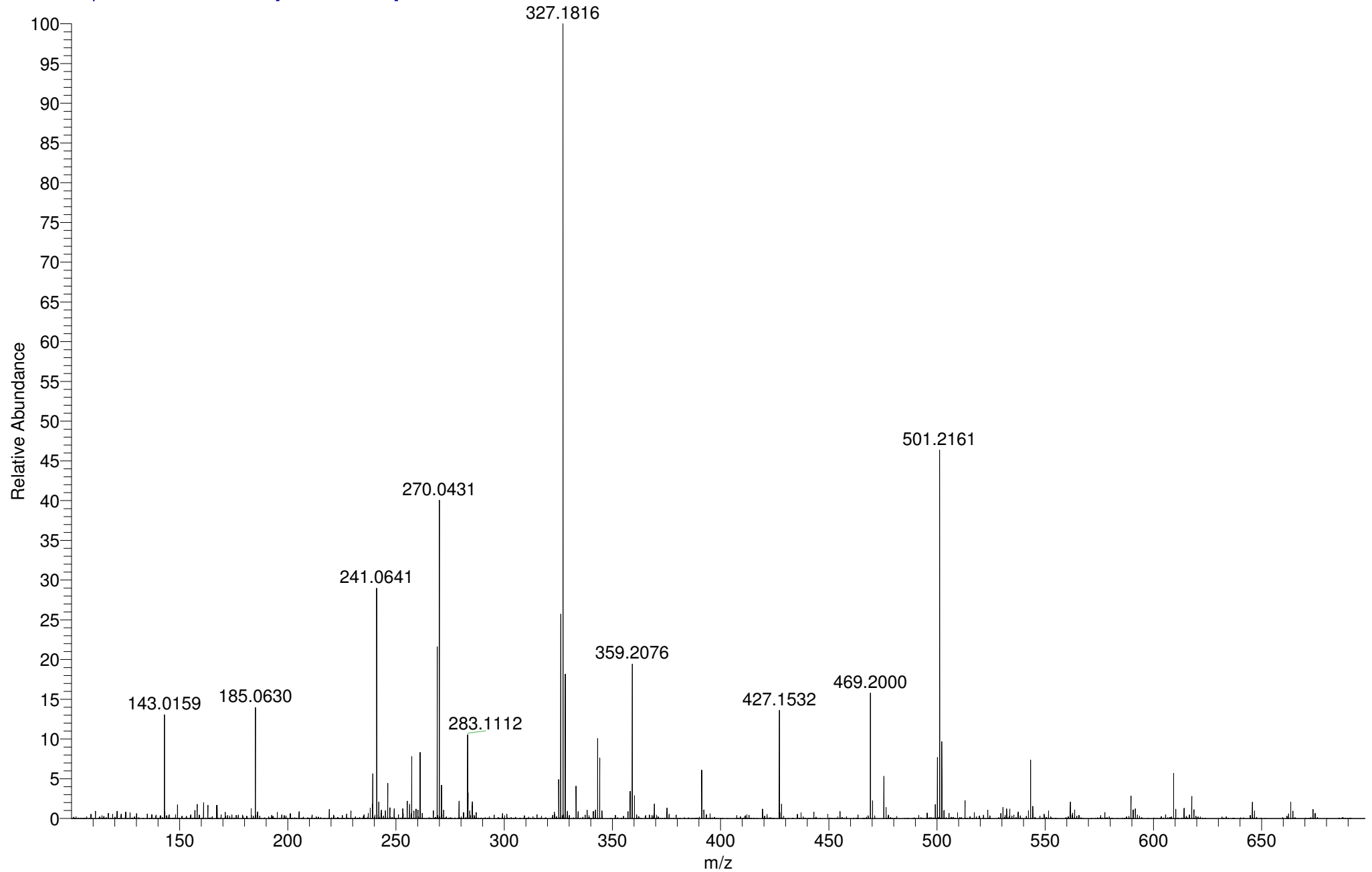
Compound 21

AET9-3 MW=500?
ASAP(SOLID)

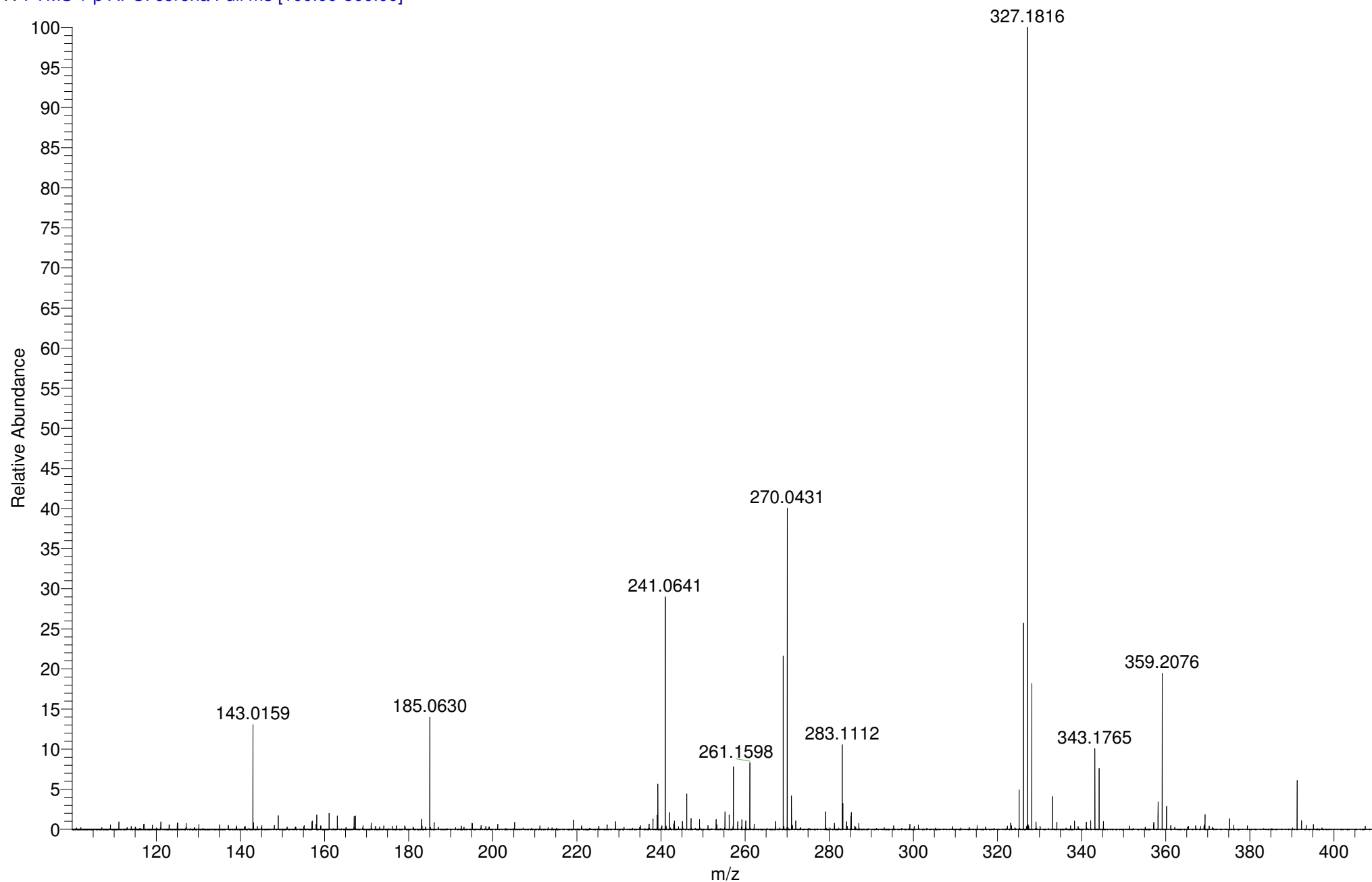
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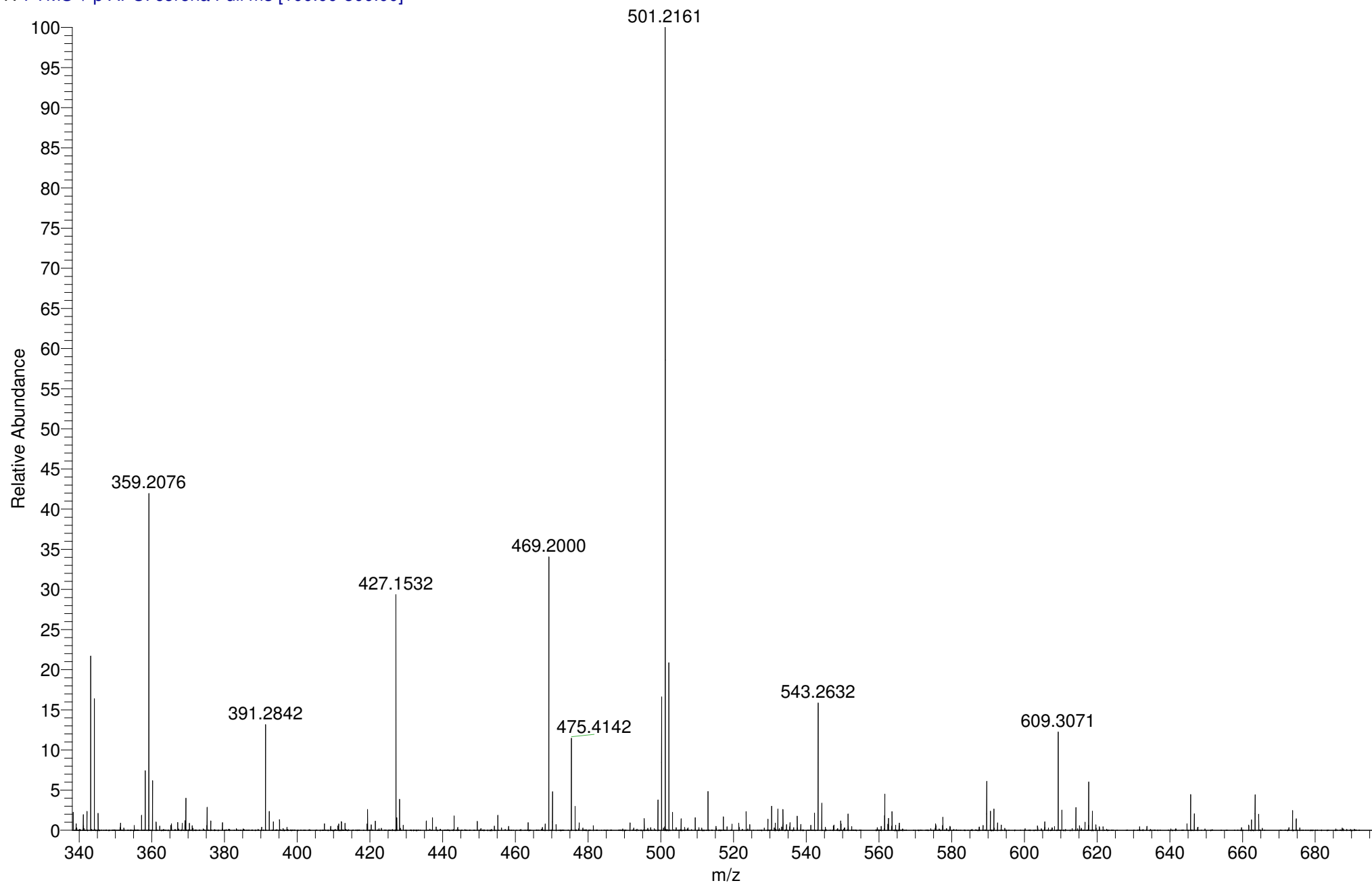
BRASHE235-PG-HASP #33-40 RT: 0.92-1.12 AV: 8 SM: 7G NL: 5.61E6
T: FTMS + p APCI corona Full ms [100.00-800.00]

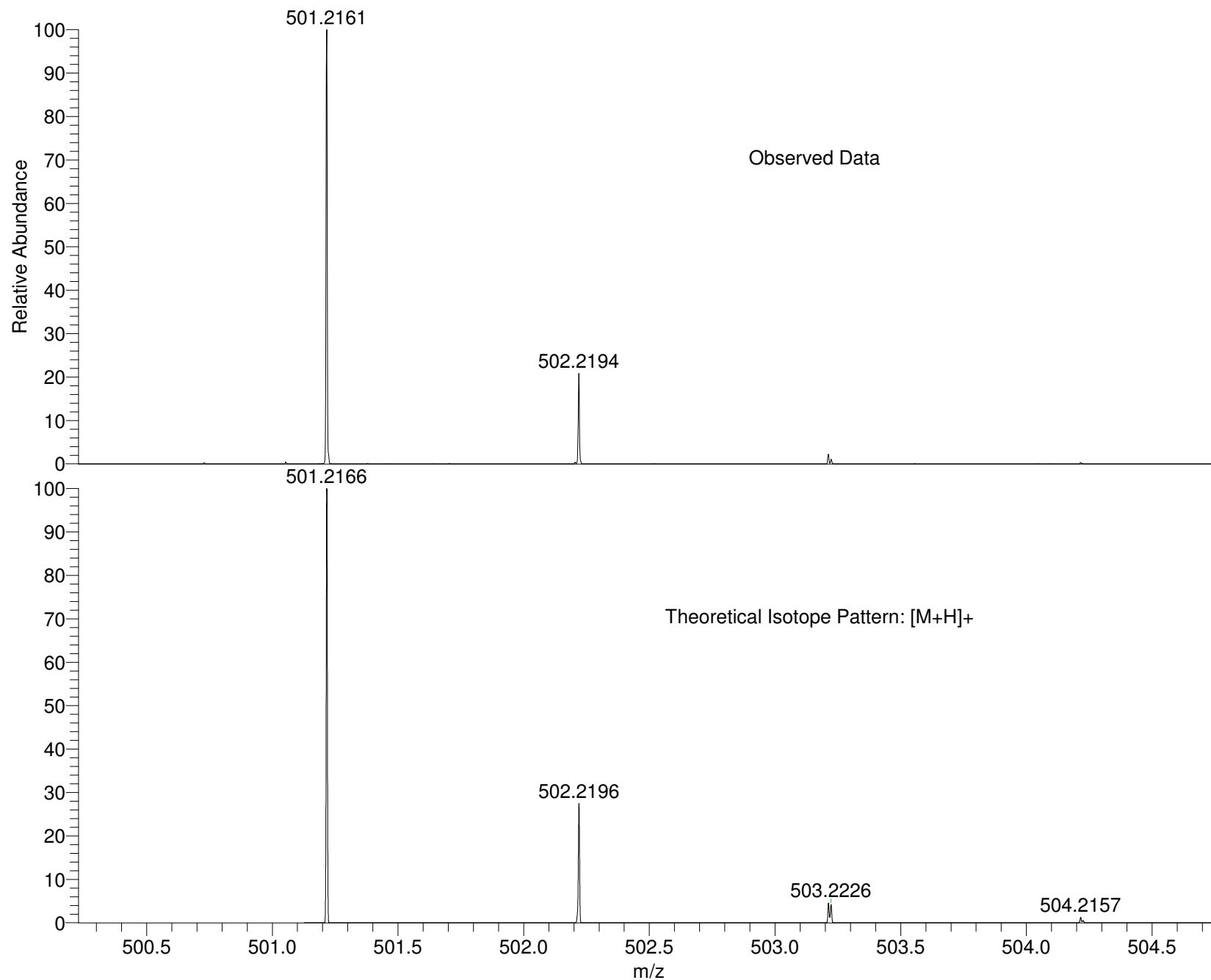


BRASHE235-PG-HASP #33-40 RT: 0.92-1.12 AV: 8 SM: 7G NL: 5.61E6
T: FTMS + p APCI corona Full ms [100.00-800.00]



BRASHE235-PG-HASP #33-40 RT: 0.92-1.12 AV: 8 SM: 7G NL: 2.60E6
T: FTMS + p APCI corona Full ms [100.00-800.00]





NL:
2.60E6
BRASHE235-PG-HASP#33-40
RT: 0.92-1.12 AV: 8 T: FTMS
+ p APCI corona Full ms
[100.00-800.00]

NL:
1.65E4
C₂₅H₃₂N₄O₅SH:
C₂₅H₃₃N₄O₅S₁
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

Isotope: Min. .. Max.
 14 N 0....16
 16 O 0....15
 12 C 0....80
 1 H 0....100
 23 Na 0....0
 32 S 0....3
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3.. 100
 Fits: 100

N-Rule: Do not use
 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
501.2161	501.2161	-0.1	5.5	C ₂₅ H ₄₁ O ₄ S ₃
	501.2160	0.3	2.5	C ₁₇ H ₃₇ O ₇ N ₆ S ₂
	501.2160	0.3	8.0	C ₁₆ H ₃₁ O ₂ N ₁₃ S ₂
	501.2159	0.3	21.0	C ₃₁ H ₂₇ O ₂ N ₅ S ₁
	501.2158	0.6	-0.5	C ₉ H ₃₃ O ₁₀ N ₁₂ S ₁
	501.2164	-0.7	8.5	C ₁₇ H ₂₉ O ₈ N ₁₀
	501.2164	-0.7	3.0	C ₁₈ H ₃₅ O ₁₃ N ₃
	501.2166	-1.0	17.0	C ₂₄ H ₂₇ N ₁₁ S ₁
	501.2166	-1.0	11.5	C ₂₅ H ₃₃ O ₅ N ₄ S ₁
	501.2167	-1.1	-1.5	C ₁₀ H ₃₇ O ₅ N ₁₂ S ₃
	501.2155	1.3	15.0	C ₃₁ H ₃₅ O ₁ N ₁ S ₂
	501.2153	1.6	-1.0	C ₈ H ₃₅ O ₄ N ₁₅ S ₃
	501.2153	1.6	6.5	C ₂₄ H ₃₇ O ₉ S ₁
	501.2153	1.6	12.0	C ₂₃ H ₃₁ O ₄ N ₇ S ₁
	501.2151	2.0	3.5	C ₁₆ H ₃₃ O ₁₂ N ₆
	501.2151	2.0	9.0	C ₁₅ H ₂₇ O ₇ N ₁₃
	501.2171	-2.0	4.5	C ₁₀ H ₂₉ O ₆ N ₁₆ S ₁
	501.2171	-2.0	-1.0	C ₁₁ H ₃₅ O ₁₁ N ₉ S ₁
	501.2173	-2.3	20.5	C ₃₃ H ₂₉ O ₃ N ₂
	501.2173	-2.4	7.5	C ₁₈ H ₃₃ O ₃ N ₁₀ S ₂
	501.2173	-2.4	2.0	C ₁₉ H ₃₉ O ₈ N ₃ S ₂
	501.2148	2.6	6.0	C ₂₃ H ₃₉ O ₃ N ₃ S ₃
	501.2175	-2.8	10.5	C ₂₆ H ₃₇ N ₄ S ₃
	501.2146	2.9	-2.5	C ₁₆ H ₄₁ O ₁₁ N ₂ S ₂
	501.2146	2.9	3.0	C ₁₅ H ₃₅ O ₆ N ₉ S ₂
	501.2146	3.0	8.5	C ₁₄ H ₂₉ O ₁ N ₁₆ S ₂
	501.2146	3.0	16.0	C ₃₀ H ₃₁ O ₆ N ₁
	501.2146	3.0	21.5	C ₂₉ H ₂₅ O ₁ N ₈
	501.2144	3.3	0.0	C ₇ H ₃₁ O ₉ N ₁₅ S ₁
	501.2178	-3.3	13.5	C ₁₈ H ₂₅ O ₄ N ₁₄
	501.2178	-3.3	8.0	C ₁₉ H ₃₁ O ₉ N ₇

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
501.2178	501.2178	-3.4	2.5	C ₂₀ H ₃₇ O ₁₄
501.2180	501.2180	-3.7	16.5	C ₂₆ H ₂₉ O ₁ N ₈ S ₁
501.2180	501.2180	-3.7	11.0	C ₂₇ H ₃₅ O ₆ N ₁ S ₁
501.2180	501.2180	-3.8	3.5	C ₁₁ H ₃₃ O ₁ N ₁₆ S ₃
501.2180	501.2180	-3.8	-2.0	C ₁₂ H ₃₉ O ₆ N ₉ S ₃
501.2141	501.2141	4.0	15.5	C ₂₉ H ₃₃ N ₄ S ₂
501.2139	501.2139	4.3	7.0	C ₂₂ H ₃₅ O ₈ N ₃ S ₁
501.2139	501.2139	4.3	12.5	C ₂₁ H ₂₉ O ₃ N ₁₀ S ₁
501.2138	501.2138	4.7	4.0	C ₁₄ H ₃₁ O ₁₁ N ₉
501.2137	501.2137	4.7	9.5	C ₁₃ H ₂₅ O ₆ N ₁₆
501.2185	501.2185	-4.7	4.0	C ₁₂ H ₃₁ O ₇ N ₁₃ S ₁
501.2185	501.2185	-4.7	-1.5	C ₁₃ H ₃₇ O ₁₂ N ₆ S ₁

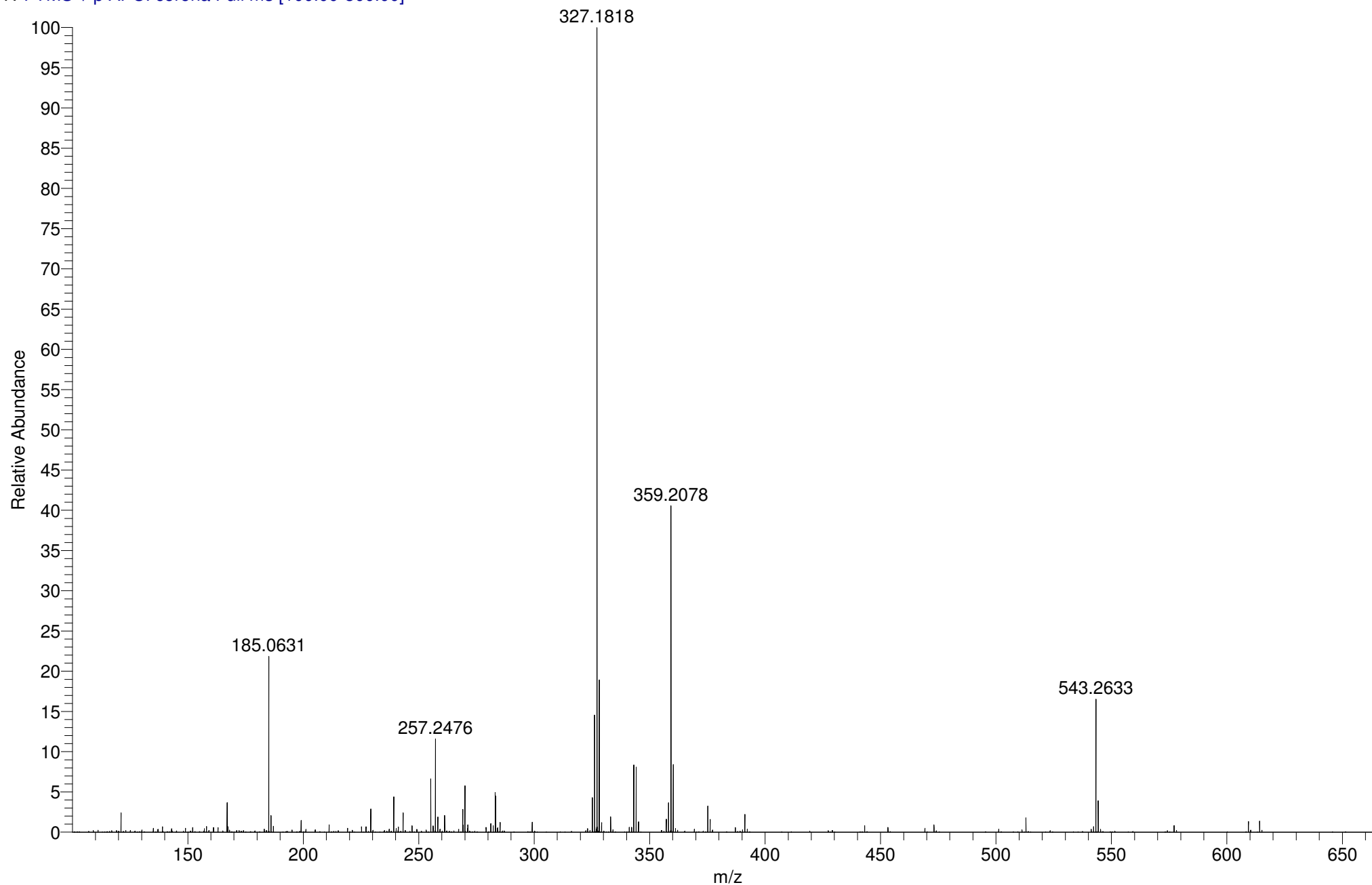
AET9-4 MW=542?
ASAP(SOLID)

Compound 22

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06/11/2012 12:17:45

BRASHE234-PG-HASP #45-50 RT: 1.26-1.41 AV: 6 SM: 7G NL: 1.58E7
T: FTMS + p APCI corona Full ms [100.00-800.00]

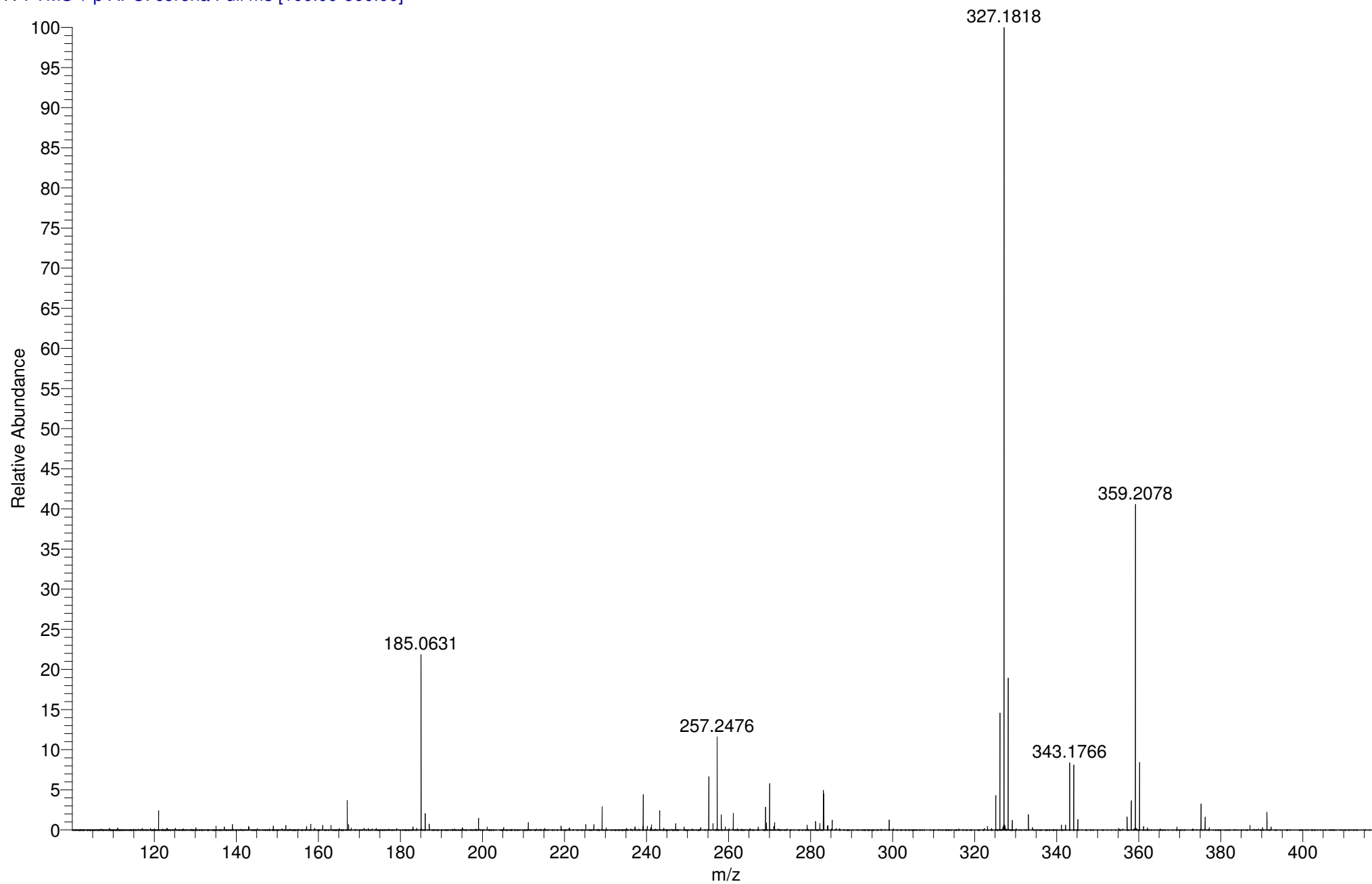


AET9-4 MW=542?
ASAP(SOLID)

EPSRC National Centre Swansea
LTQ Orbitrap XL

Throup
06/11/2012 12:17:45

BRASHE234-PG-HASP #45-50 RT: 1.26-1.41 AV: 6 SM: 7G NL: 1.58E7
T: FTMS + p APCI corona Full ms [100.00-800.00]

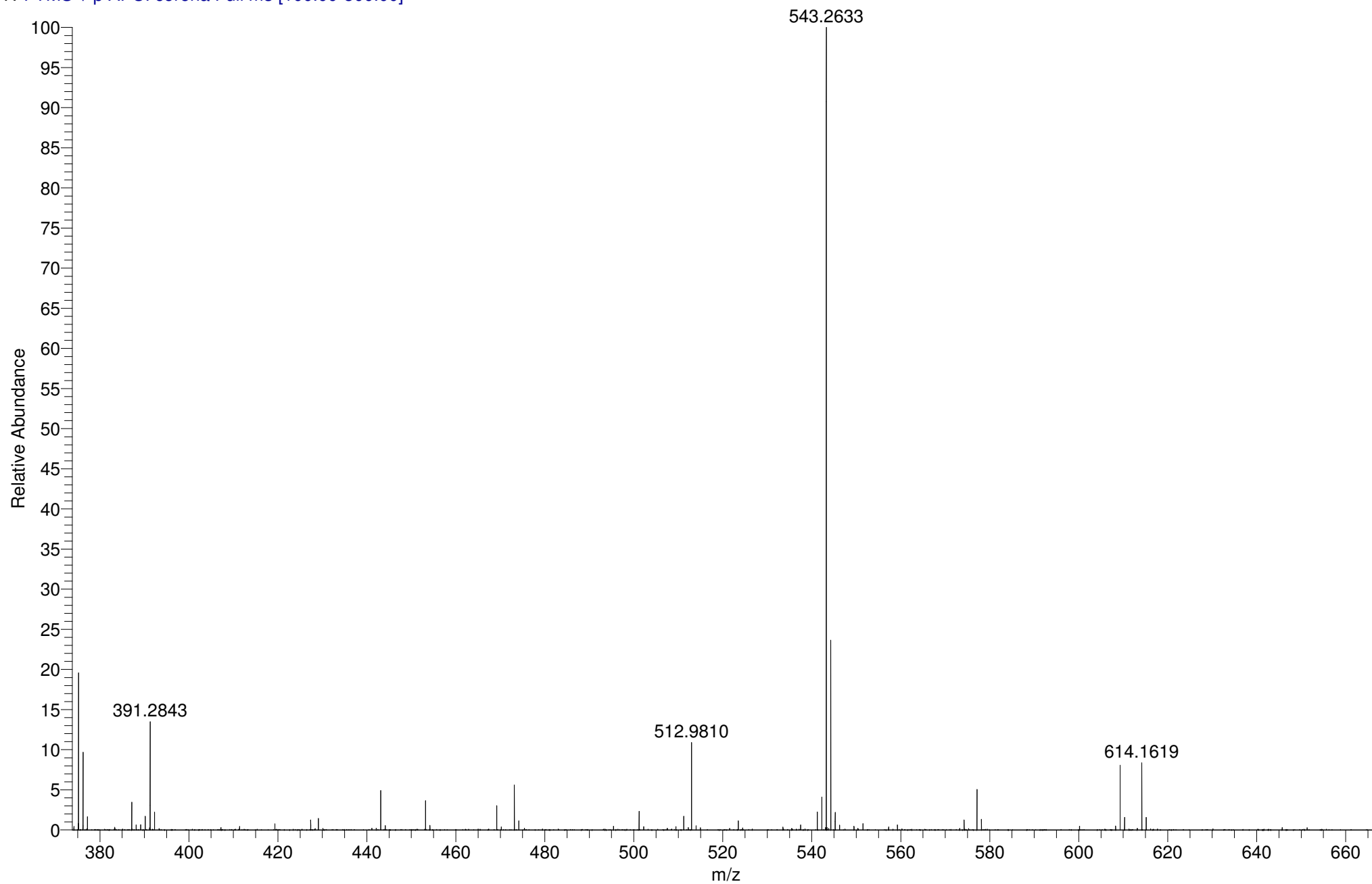


AET9-4 MW=542?
ASAP(SOLID)

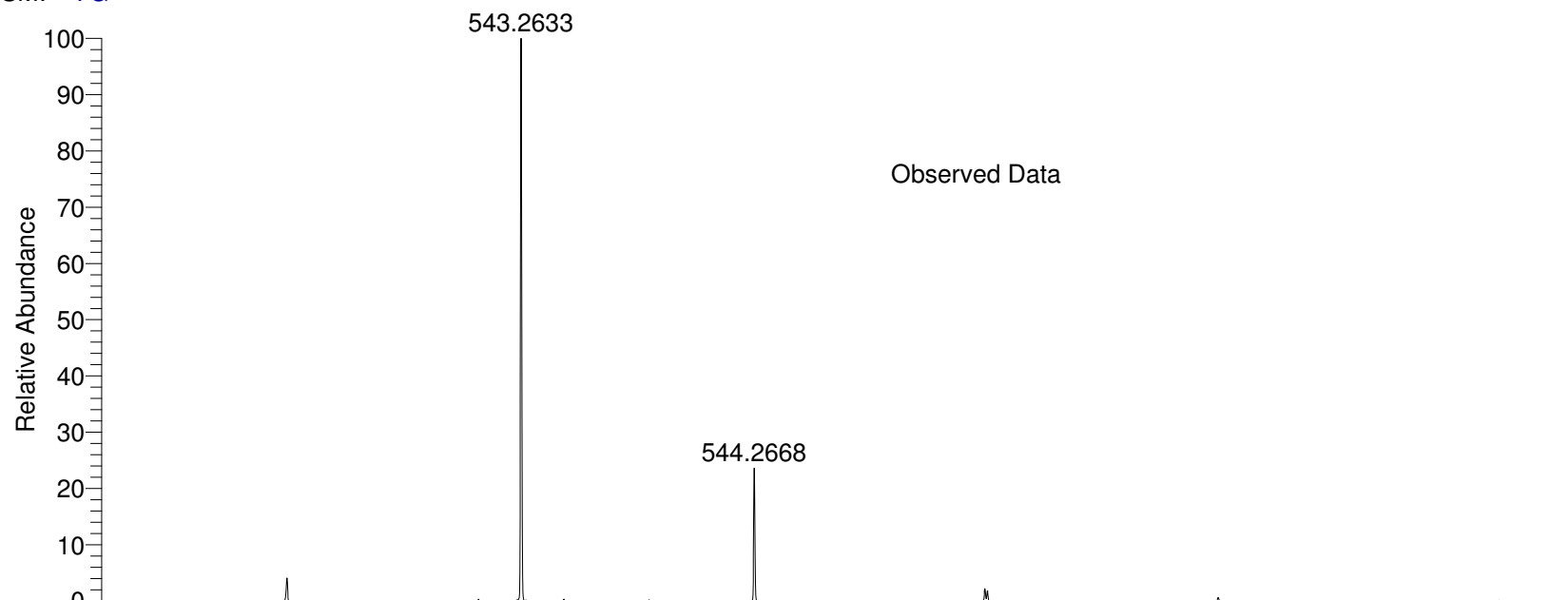
EPSRC National Centre Swansea
LTQ Orbitrap XL

Thrup
06/11/2012 12:17:45

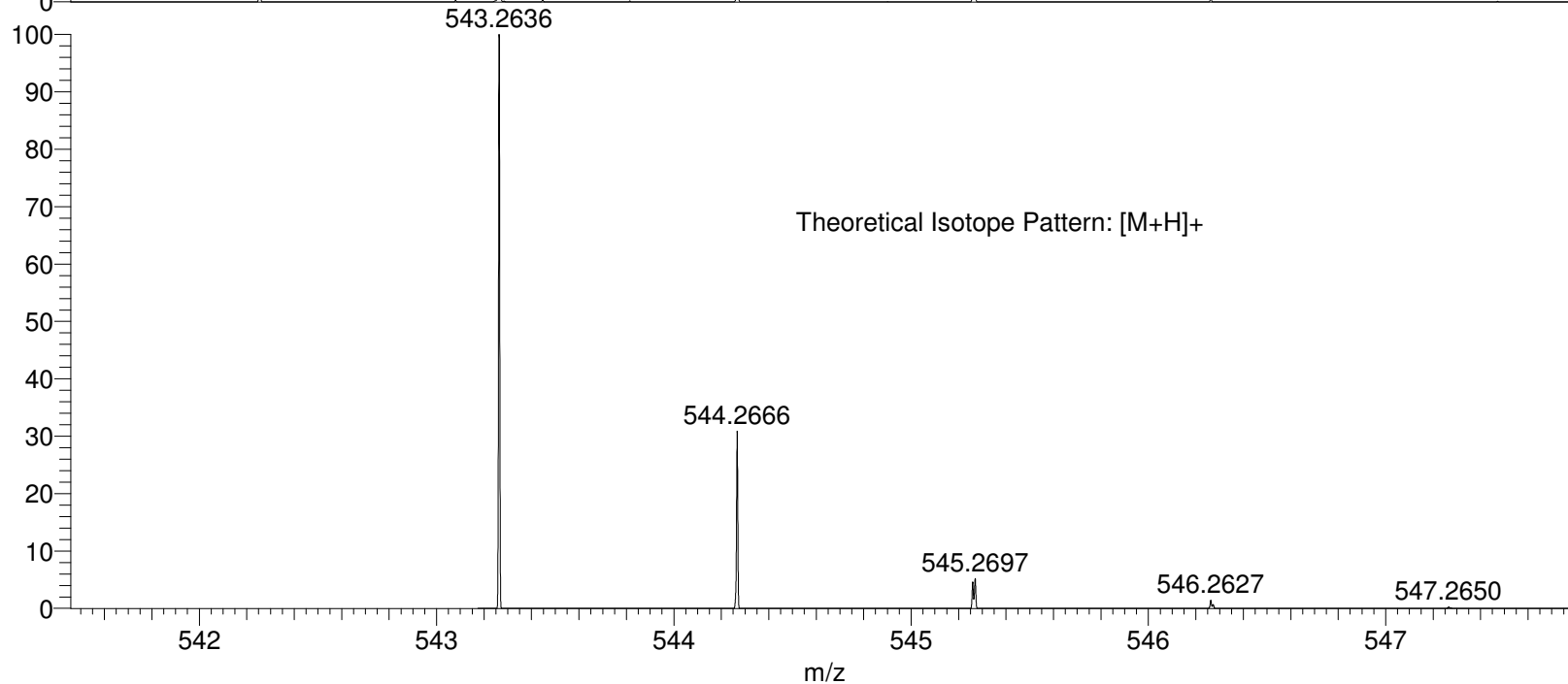
BRASHE234-PG-HASP #45-50 RT: 1.26-1.41 AV: 6 SM: 7G NL: 2.61E6
T: FTMS + p APCI corona Full ms [100.00-800.00]



SM: 7G



NL:
2.61E6
BRASHE234-PG-HASP#45-50
RT: 1.26-1.41 AV: 6 T: FTMS
+ p APCI corona Full ms
[100.00-800.00]



NL:
1.60E4
C₂₈H₃₈N₄O₅SH:
C₂₈H₃₉N₄O₅S₁
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

Isotope: Min. .. Max.
 14 N 0....16
 16 O 0....15
 12 C 0....80
 1 H 0....100
 23 Na 0....0
 32 S 0....3
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3.. 100
 Fits: 100

N-Rule: Do not use
 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
543.2633	543.2634	-0.2	8.5	C ₂₀ H ₃₅ O ₈ N ₁₀
	543.2634	-0.2	3.0	C ₂₁ H ₄₁ O ₁₃ N ₃
	543.2631	0.4	5.5	C ₂₈ H ₄₇ O ₄ S ₃
	543.2636	-0.5	17.0	C ₂₇ H ₃₃ N ₁₁ S ₁
	543.2636	-0.5	11.5	C ₂₈ H ₃₉ O ₅ N ₄ S ₁
	543.2636	-0.6	-1.5	C ₁₃ H ₄₃ O ₅ N ₁₂ S ₃
	543.2629	0.7	2.5	C ₂₀ H ₄₃ O ₇ N ₆ S ₂
	543.2629	0.7	8.0	C ₁₉ H ₃₇ O ₂ N ₁₃ S ₂
	543.2629	0.8	21.0	C ₃₄ H ₃₃ O ₂ N ₅
	543.2627	1.0	-0.5	C ₁₂ H ₃₉ O ₁₀ N ₁₂ S ₁
	543.2641	-1.4	4.5	C ₁₃ H ₃₅ O ₆ N ₁₆ S ₁
	543.2641	-1.4	-1.0	C ₁₄ H ₄₁ O ₁₁ N ₉ S ₁
	543.2624	1.6	15.0	C ₃₄ H ₄₁ O ₁ N ₁ S ₂
	543.2642	-1.7	20.5	C ₃₆ H ₃₅ O ₃ N ₂
	543.2643	-1.8	7.5	C ₂₁ H ₃₉ O ₃ N ₁₀ S ₂
	543.2643	-1.8	2.0	C ₂₂ H ₄₅ O ₈ N ₃ S ₂
	543.2623	1.9	-1.0	C ₁₁ H ₄₁ O ₄ N ₁₅ S ₃
	543.2622	2.0	6.5	C ₂₇ H ₄₃ O ₉ S ₁
	543.2622	2.0	12.0	C ₂₆ H ₃₇ O ₄ N ₇ S ₁
	543.2644	-2.1	10.5	C ₂₉ H ₄₃ N ₄ S ₃
	543.2620	2.3	3.5	C ₁₉ H ₃₉ O ₁₂ N ₆
	543.2620	2.3	9.0	C ₁₈ H ₃₃ O ₇ N ₁₃
	543.2647	-2.6	13.5	C ₂₁ H ₃₁ O ₄ N ₁₄
	543.2647	-2.6	8.0	C ₂₂ H ₃₇ O ₉ N ₇
	543.2647	-2.6	2.5	C ₂₃ H ₄₃ O ₁₄
	543.2618	2.8	6.0	C ₂₆ H ₄₅ O ₃ N ₃ S ₃
	543.2649	-3.0	16.5	C ₂₉ H ₃₅ O ₁ N ₈ S ₁
	543.2649	-3.0	11.0	C ₃₀ H ₄₁ O ₆ N ₁ S ₁
	543.2649	-3.0	3.5	C ₁₄ H ₃₉ O ₁ N ₁₆ S ₃
	543.2649	-3.0	-2.0	C ₁₅ H ₄₅ O ₆ N ₉ S ₃
	543.2616	3.2	-2.5	C ₁₉ H ₄₇ O ₁₁ N ₂ S ₂

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
543.2616	543.2616	3.2	3.0	C ₁₈ H ₄₁ O ₆ N ₉ S ₂
543.2616	543.2616	3.2	8.5	C ₁₇ H ₃₅ O ₁ N ₁₆ S ₂
543.2615	543.2615	3.2	16.0	C ₃₃ H ₃₇ O ₆ N ₁
543.2615	543.2615	3.3	21.5	C ₃₂ H ₃₁ O ₁ N ₈
543.2614	543.2614	3.5	0.0	C ₁₀ H ₃₇ O ₉ N ₁₅ S ₁
543.2654	543.2654	-3.9	4.0	C ₁₅ H ₃₇ O ₇ N ₁₃ S ₁
543.2654	543.2654	-3.9	-1.5	C ₁₆ H ₄₃ O ₁₂ N ₆ S ₁
543.2611	543.2611	4.1	15.5	C ₃₂ H ₃₉ N ₄ S ₂
543.2656	543.2656	-4.2	7.0	C ₂₃ H ₄₁ O ₄ N ₇ S ₂
543.2656	543.2656	-4.2	1.5	C ₂₄ H ₄₇ O ₉ S ₂
543.2609	543.2609	4.4	7.0	C ₂₅ H ₄₁ O ₈ N ₃ S ₁
543.2609	543.2609	4.5	12.5	C ₂₄ H ₃₅ O ₃ N ₁₀ S ₁
543.2658	543.2658	-4.6	10.0	C ₃₁ H ₄₅ O ₁ N ₁ S ₃
543.2607	543.2607	4.8	4.0	C ₁₇ H ₃₇ O ₁₁ N ₉
543.2607	543.2607	4.8	9.5	C ₁₆ H ₃₁ O ₆ N ₁₆

aet9-20-1 MW=556?
(DCM)/MeOH + NH4OAc

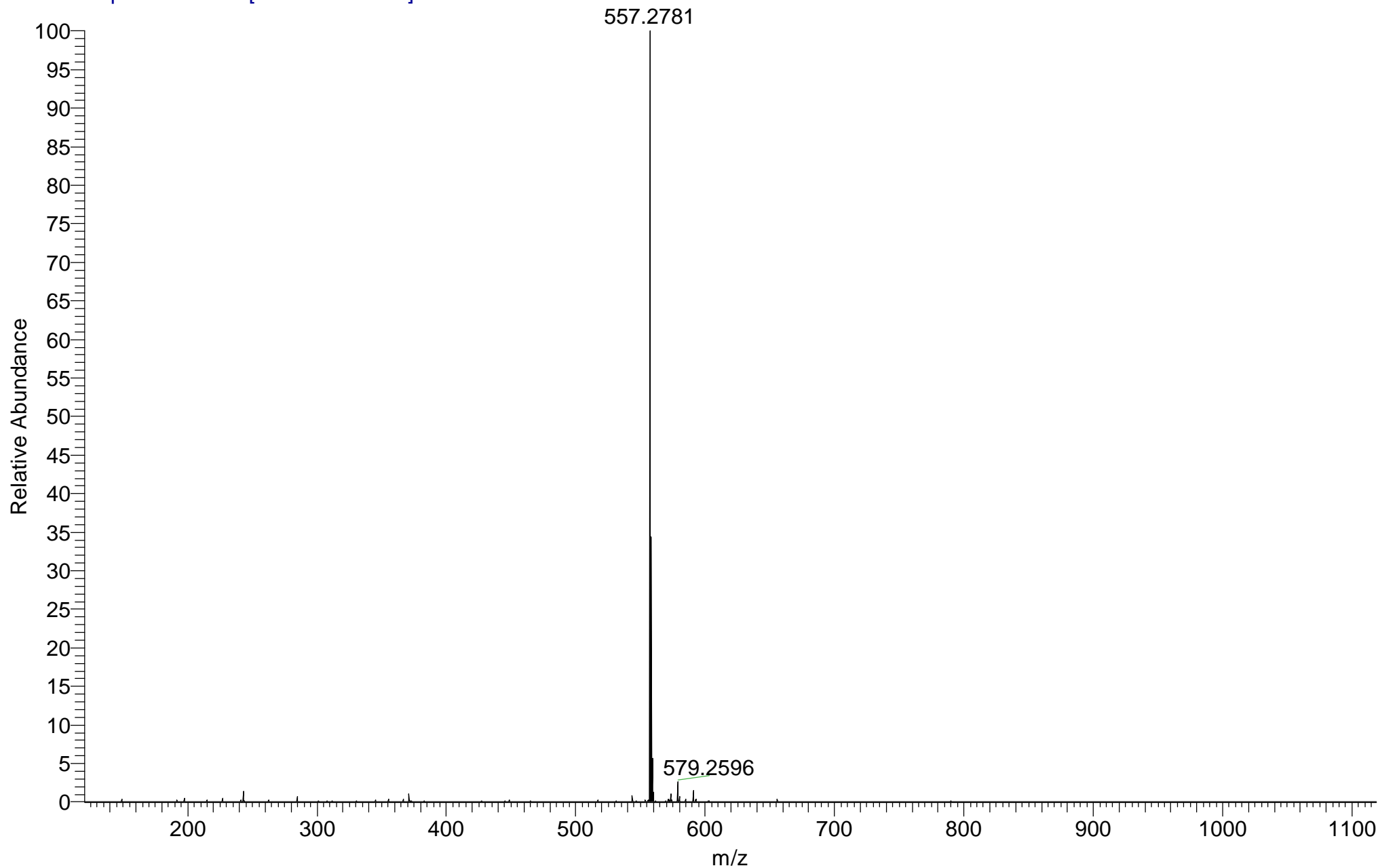
Compound 24

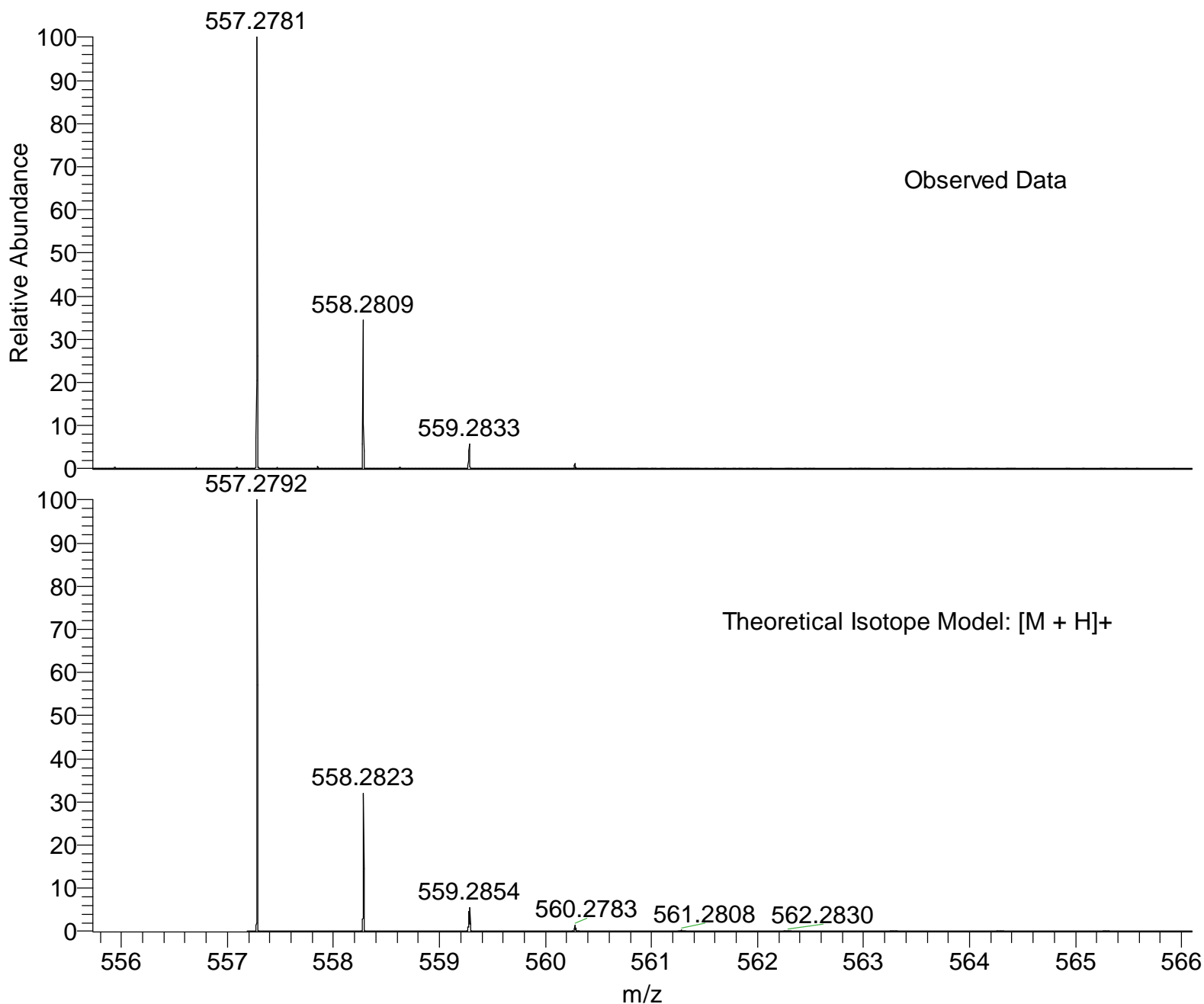
EPSRC National Centre Swansea
LTQ Orbitrap XL

adam throup
14/01/2013 16:43:46

BRASHE247-OJ-HNESP #27-50 RT: 0.72-1.28 AV: 22 SM: 7G NL: 7.74E7

T: FTMS + p NSI Full ms [120.00-2000.00]





NL:
7.74E7
BRASHE247-OJ-HNESP#27-
50 RT: 0.72-1.28 AV: 22 T:
FTMS + p NSI Full ms
[120.00-2000.00]

NL:
1.58E4
C₂₉H₄₀N₄O₅SH:
C₂₉H₄₁N₄O₅S₁
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

Isotope: Min. .. Max.
 14 N 0....14
 16 O 0....15
 12 C 0....60
 1 H 0....80
 23 Na 0....0
 32 S 0....5

Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3.. 100 N-Rule: Do not use
 Fits: 200 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
557.2781	557.2781	0.0	2.0	C ₂₀ H ₄₇ O ₁ N ₉ S ₄
	557.2781	0.1	15.0	C ₃₅ H ₄₃ O ₁ N ₁ S ₂
	557.2779	0.4	6.5	C ₂₈ H ₄₅ O ₉ S ₁
	557.2779	0.4	12.0	C ₂₇ H ₃₉ O ₄ N ₇ S ₁
	557.2784	-0.5	-0.5	C ₁₃ H ₄₁ O ₁₀ N ₁₂ S ₁
	557.2777	0.7	3.5	C ₂₀ H ₄₁ O ₁₂ N ₆
	557.2777	0.7	9.0	C ₁₉ H ₃₅ O ₇ N ₁₃
	557.2785	-0.8	21.0	C ₃₅ H ₃₅ O ₂ N ₅
	557.2786	-0.8	8.0	C ₂₀ H ₃₉ O ₂ N ₁₃ S ₂
	557.2786	-0.8	2.5	C ₂₁ H ₄₅ O ₇ N ₆ S ₂
	557.2787	-1.2	5.5	C ₂₉ H ₄₉ O ₄ S ₃
	557.2774	1.2	6.0	C ₂₇ H ₄₇ O ₃ N ₃ S ₃
	557.2772	1.6	-2.5	C ₂₀ H ₄₉ O ₁₁ N ₂ S ₂
	557.2772	1.6	3.0	C ₁₉ H ₄₃ O ₆ N ₉ S ₂
	557.2772	1.6	16.0	C ₃₄ H ₃₉ O ₆ N ₁
	557.2772	1.6	21.5	C ₃₃ H ₃₃ O ₁ N ₈
	557.2790	-1.7	8.5	C ₂₁ H ₃₇ O ₈ N ₁₀
	557.2790	-1.7	3.0	C ₂₂ H ₄₃ O ₁₃ N ₃
	557.2792	-2.0	17.0	C ₂₈ H ₃₅ N ₁₁ S ₁
	557.2792	-2.0	11.5	C ₂₉ H ₄₁ O ₅ N ₄ S ₁
	557.2793	-2.1	-1.5	C ₁₄ H ₄₅ O ₅ N ₁₂ S ₃
	557.2794	-2.4	1.5	C ₂₂ H ₄₉ O ₂ N ₆ S ₄
	557.2768	2.4	-3.0	C ₁₉ H ₅₁ O ₅ N ₅ S ₄
	557.2767	2.4	2.5	C ₁₈ H ₄₅ N ₁₂ S ₄
	557.2767	2.5	15.5	C ₃₃ H ₄₁ N ₄ S ₂
	557.2765	2.8	7.0	C ₂₆ H ₄₃ O ₈ N ₃ S ₁
	557.2765	2.8	12.5	C ₂₅ H ₃₇ O ₃ N ₁₀ S ₁
	557.2797	-2.9	-1.0	C ₁₅ H ₄₃ O ₁₁ N ₉ S ₁
	557.2764	3.1	4.0	C ₁₈ H ₃₉ O ₁₁ N ₉
	557.2799	-3.2	20.5	C ₃₇ H ₃₇ O ₃ N ₂
	557.2799	-3.2	7.5	C ₂₂ H ₄₁ O ₃ N ₁₀ S ₂

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
557.2799	557.2799	-3.2	2.0	C ₂₃ H ₄₇ O ₈ N ₃ S ₂
557.2801	557.2801	-3.6	10.5	C ₃₀ H ₄₅ N ₄ S ₃
557.2801	557.2801	-3.6	-2.5	C ₁₅ H ₄₉ N ₁₂ S ₅
557.2761	557.2761	3.7	6.5	C ₂₅ H ₄₅ O ₂ N ₆ S ₃
557.2759	557.2759	4.0	-2.0	C ₁₈ H ₄₇ O ₁₀ N ₅ S ₂
557.2759	557.2759	4.0	3.5	C ₁₇ H ₄₁ O ₅ N ₁₂ S ₂
557.2758	557.2758	4.0	16.5	C ₃₂ H ₃₇ O ₅ N ₄
557.2758	557.2758	4.1	22.0	C ₃₁ H ₃₁ N ₁₁
557.2804	557.2804	-4.1	13.5	C ₂₂ H ₃₃ O ₄ N ₁₄
557.2804	557.2804	-4.1	8.0	C ₂₃ H ₃₉ O ₉ N ₇
557.2804	557.2804	-4.1	2.5	C ₂₄ H ₄₅ O ₁₄
557.2806	557.2806	-4.4	16.5	C ₃₀ H ₃₇ O ₁ N ₈ S ₁
557.2806	557.2806	-4.4	11.0	C ₃₁ H ₄₃ O ₆ N ₁ S ₁
557.2806	557.2806	-4.5	-2.0	C ₁₆ H ₄₇ O ₆ N ₉ S ₃
557.2756	557.2756	4.5	0.5	C ₂₅ H ₅₃ O ₁ N ₂ S ₅
557.2808	557.2808	-4.8	1.0	C ₂₄ H ₅₁ O ₃ N ₃ S ₄
557.2754	557.2754	4.8	-2.5	C ₁₇ H ₄₉ O ₄ N ₈ S ₄
557.2754	557.2754	4.9	10.5	C ₃₂ H ₄₅ O ₄ S ₂

aet7-16 MW=227?
(DCM)/MeOH + NH4OAc

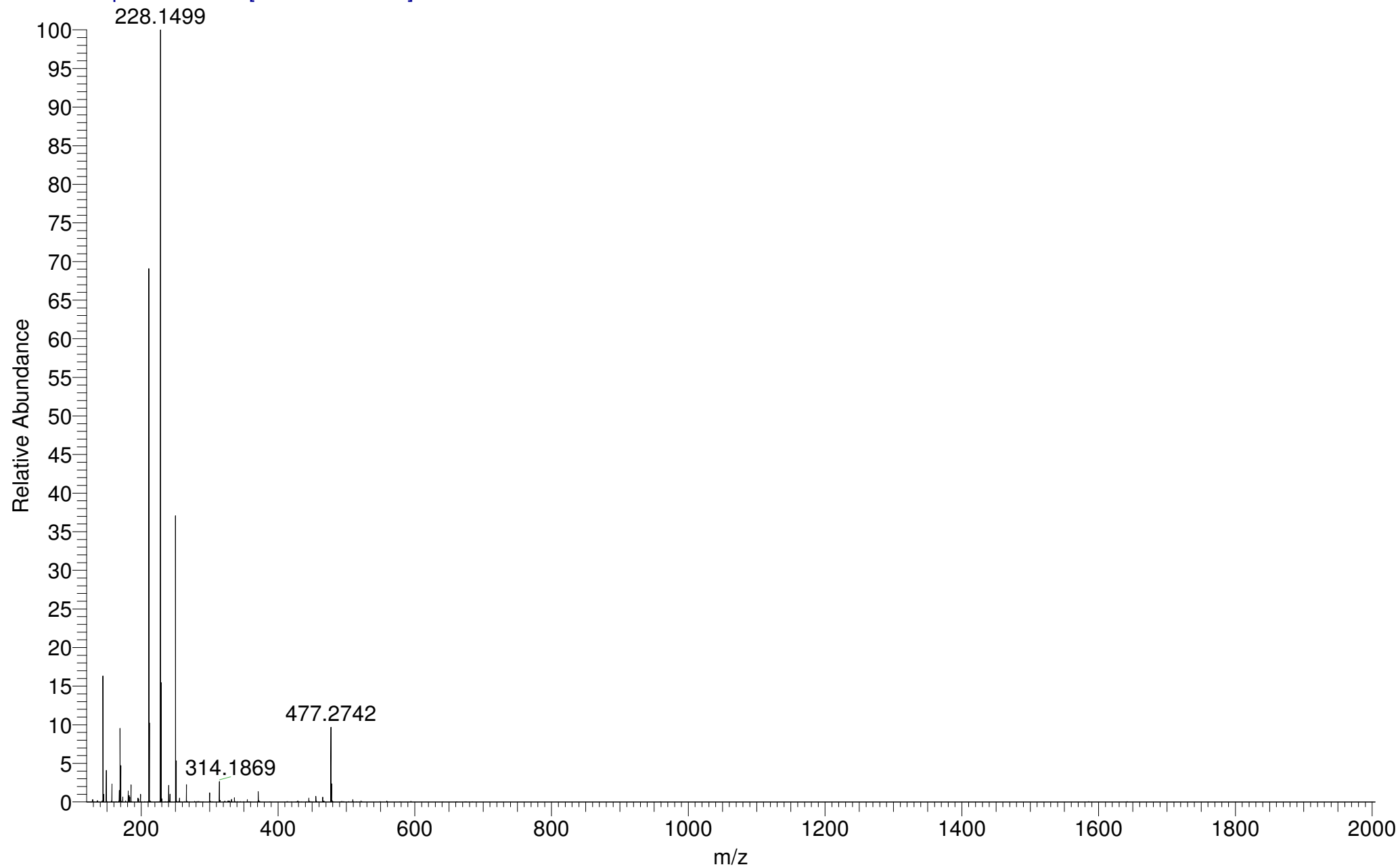
Compound 25

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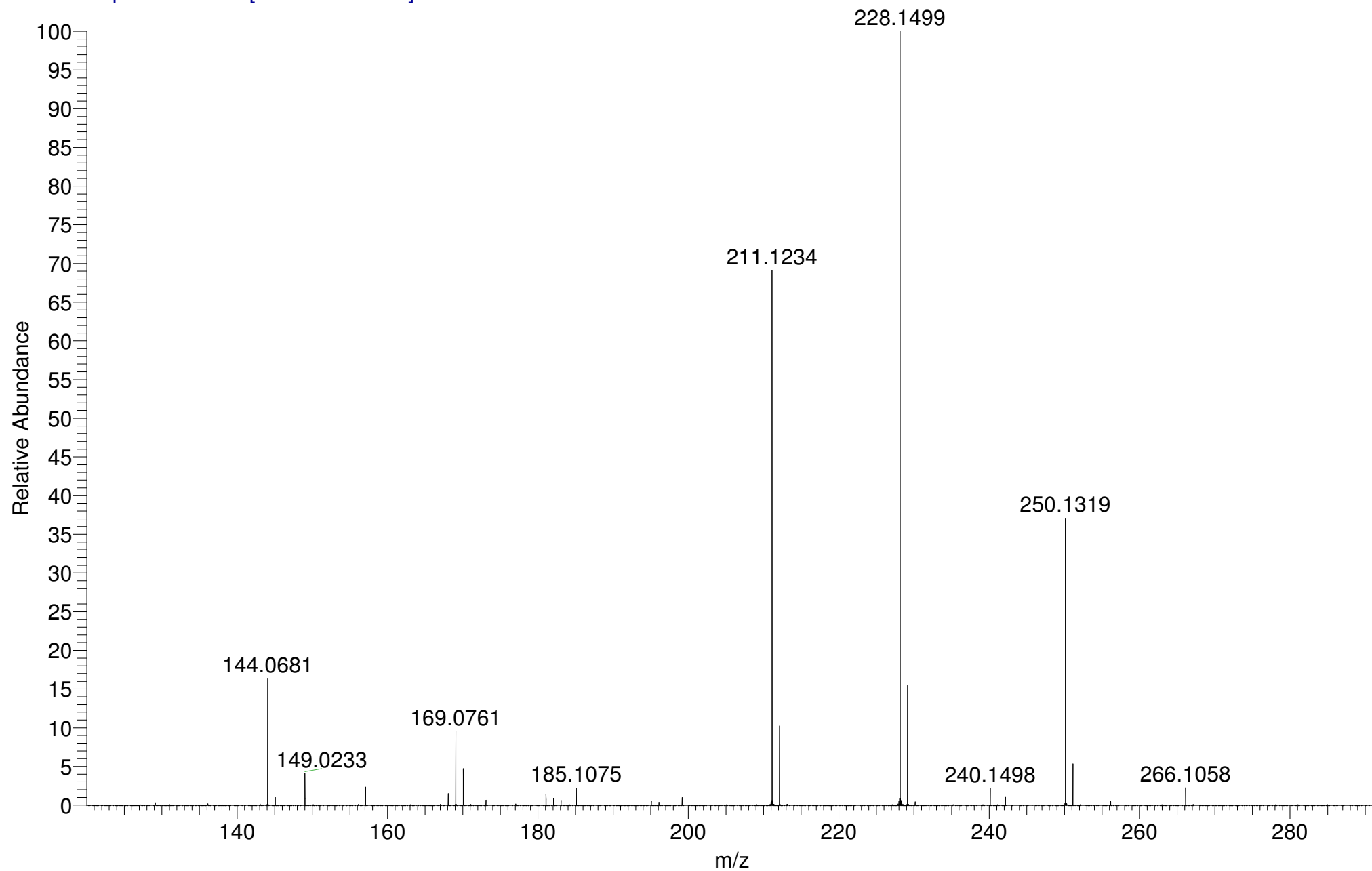
adam throup
05/12/2011 13:10:59

BRASHE162-PV-HNESP #21-32 RT: 0.86-1.18 AV: 12 SM: 7G NL: 1.50E7

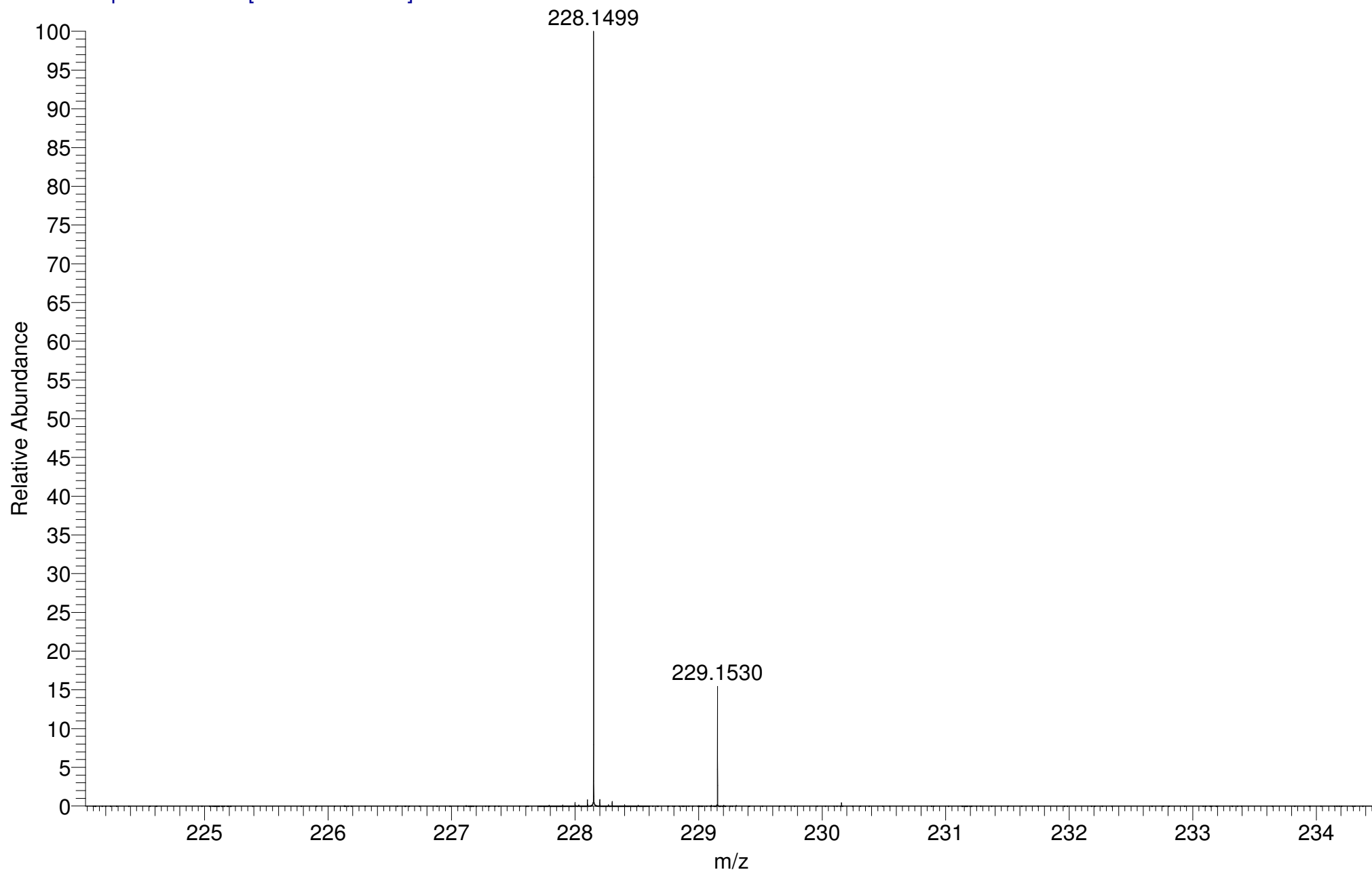
T: FTMS + p NSI Full ms [120.00-2000.00]



BRASHE162-PV-HNESP #21-32 RT: 0.86-1.18 AV: 12 SM: 7G NL: 1.50E7
T: FTMS + p NSI Full ms [120.00-2000.00]



BRASHE162-PV-HNESP #21-32 RT: 0.86-1.18 AV: 12 SM: 7G NL: 1.50E7
T: FTMS + p NSI Full ms [120.00-2000.00]



Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
228.1499	228.1495	1.6	7.5	C ₁₄ H ₁₈ N ₃
	228.1509	-4.2	7.0	C ₁₆ H ₂₀ O ₁

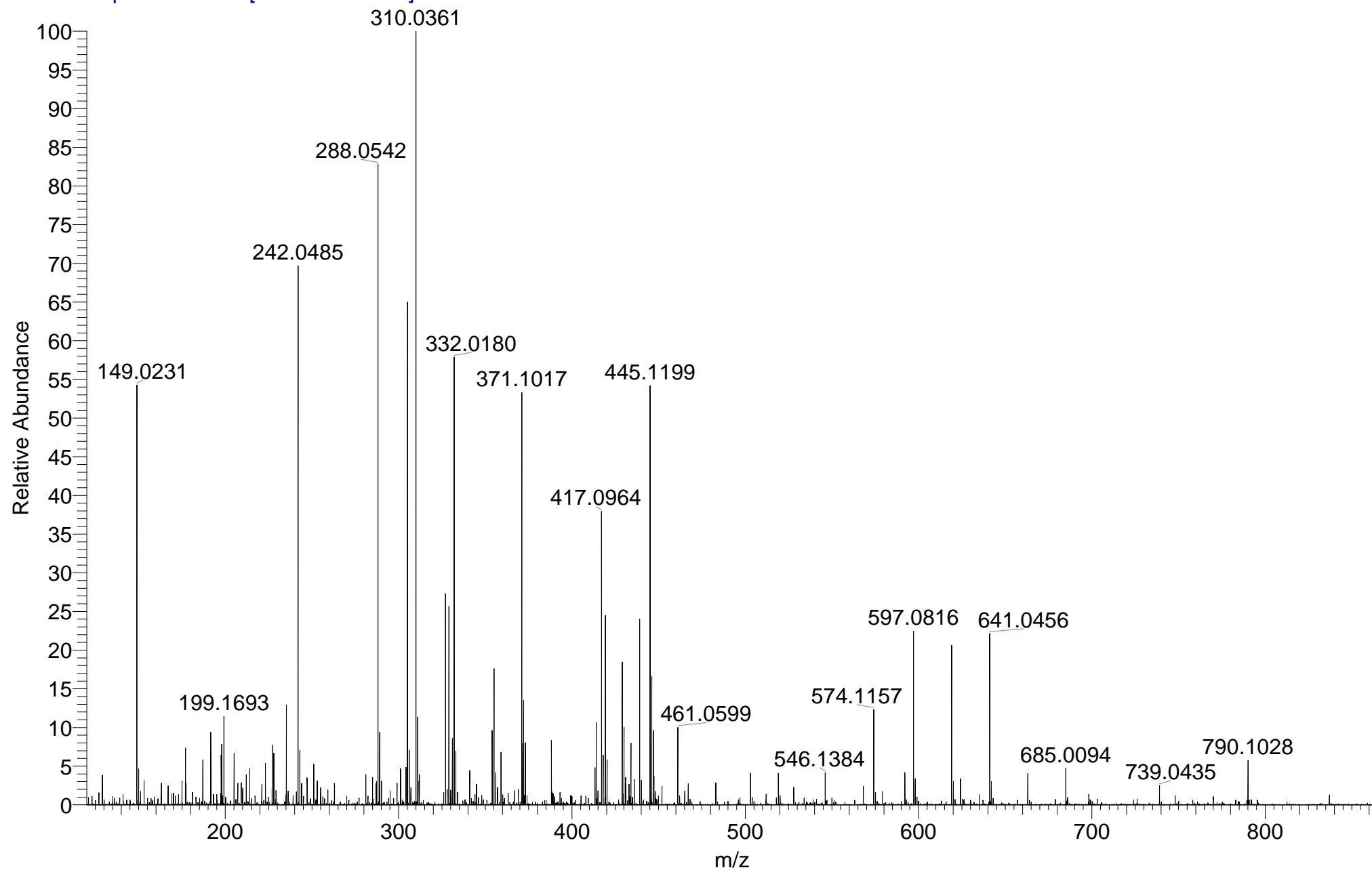
AET7-76 MW=287?
(DCM)/MeOH + NH4OAc

Compound 26

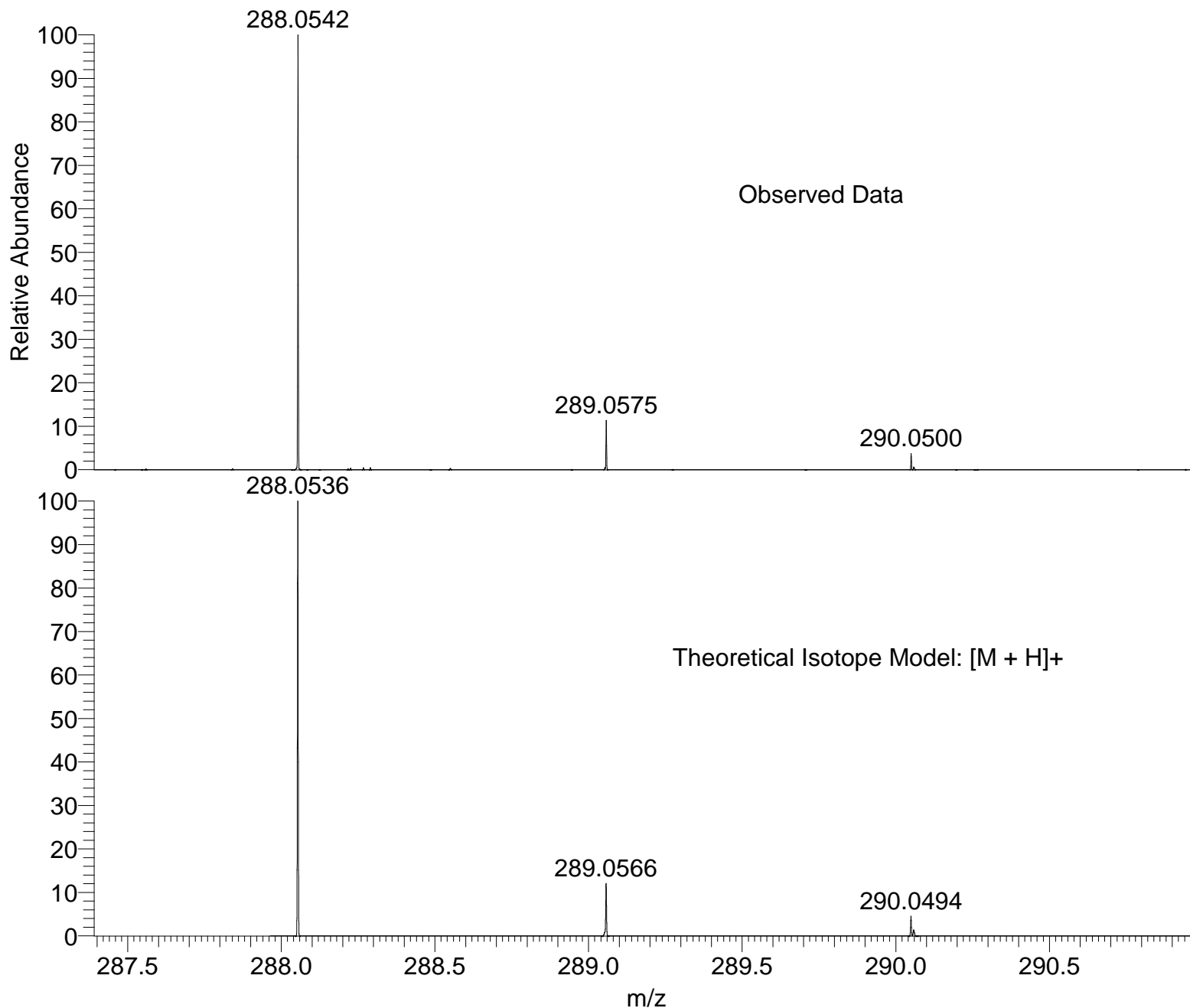
EPSRC National Centre Swansea
LTQ Orbitrap XL

adam throup
11/04/2012 12:20:42

BRASHE191-OJ-HNESP #28-32 RT: 0.75-0.88 AV: 5 SM: 7G NL: 2.03E5
T: FTMS + p NSI Full ms [120.00-2000.00]



SM: 7G



NL:
1.68E5
BRASHE191-OJ-HNESP#28-
32 RT: 0.75-0.88 AV: 5 T:
FTMS + p NSI Full ms
[120.00-2000.00]

NL:
1.94E4
C₁₁H₁₃NO₆SH:
C₁₁H₁₄N₁O₆S₁
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

Isotope: Min. .. Max.
 14 N 0....10
 16 O 0....15
 12 C 0....65
 1 H 0....75
 23 Na 0....0
 32 S 0....2
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3.. 100
 Fits: 500

N-Rule: Do not use
 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
288.0542	288.0543	-0.4	1.5	C ₄ H ₁₄ O ₄ N ₇ S ₂
	288.0536	2.0	5.5	C ₁₁ H ₁₄ O ₆ N ₁ S ₁
	288.0536	2.0	11.0	C ₁₀ H ₈ O ₁ N ₈ S ₁
	288.0548	-2.1	2.0	C ₅ H ₁₂ O ₁₀ N ₄
	288.0535	2.6	-3.0	C ₄ H ₁₆ O ₁₄
	288.0535	2.6	2.5	C ₃ H ₁₀ O ₉ N ₇
	288.0550	-2.7	10.5	C ₁₂ H ₁₀ O ₂ N ₅ S ₁
	288.0530	4.2	2.0	C ₂ H ₁₂ O ₃ N ₁₀ S ₂
	288.0529	4.4	15.0	C ₁₇ H ₈ O ₃ N ₂
	288.0556	-4.9	19.5	C ₂₀ H ₆ N ₃

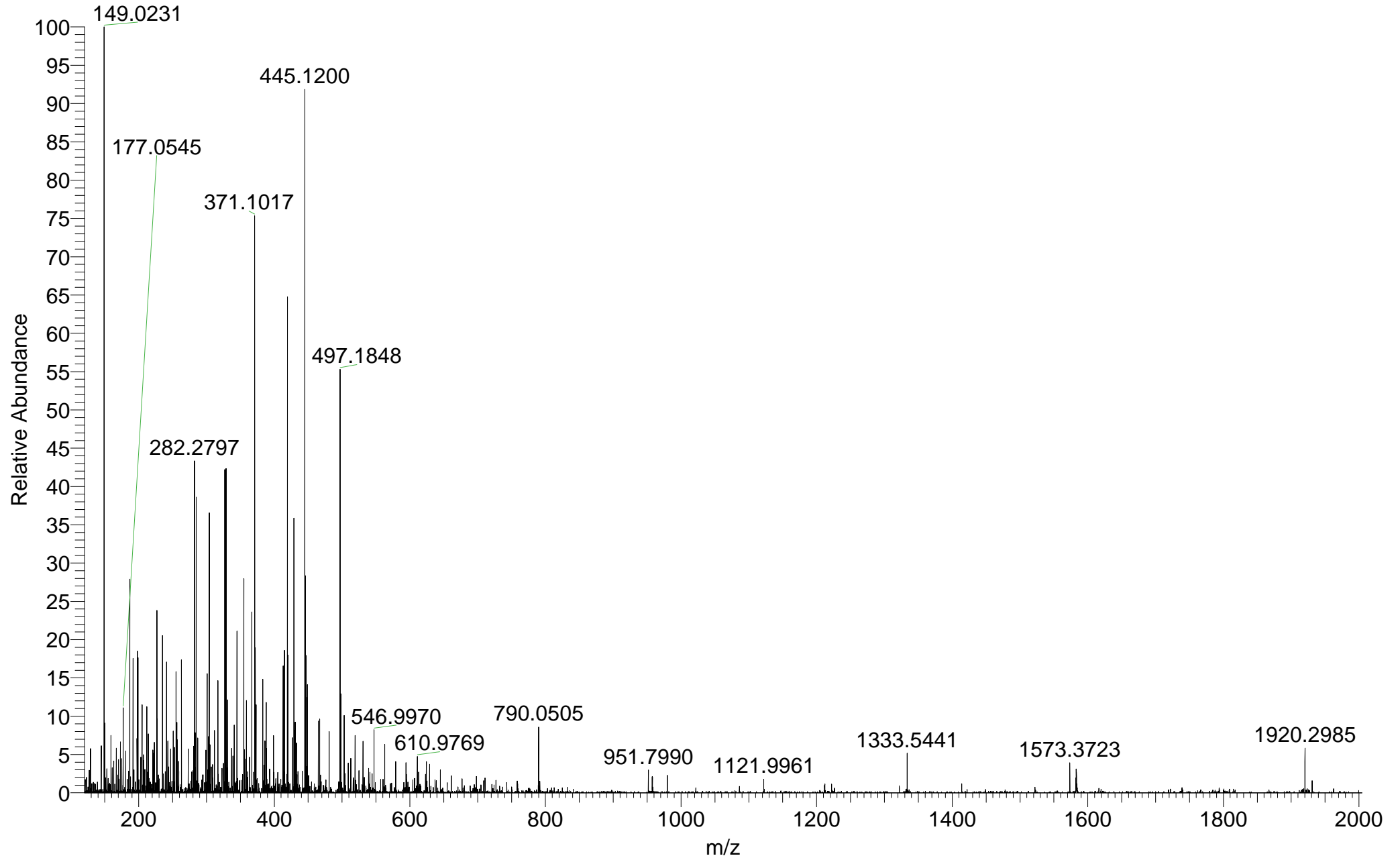
Compound 28

AET7-77-2 MW=497?
(DCM)/MeOH + NH₄OAc

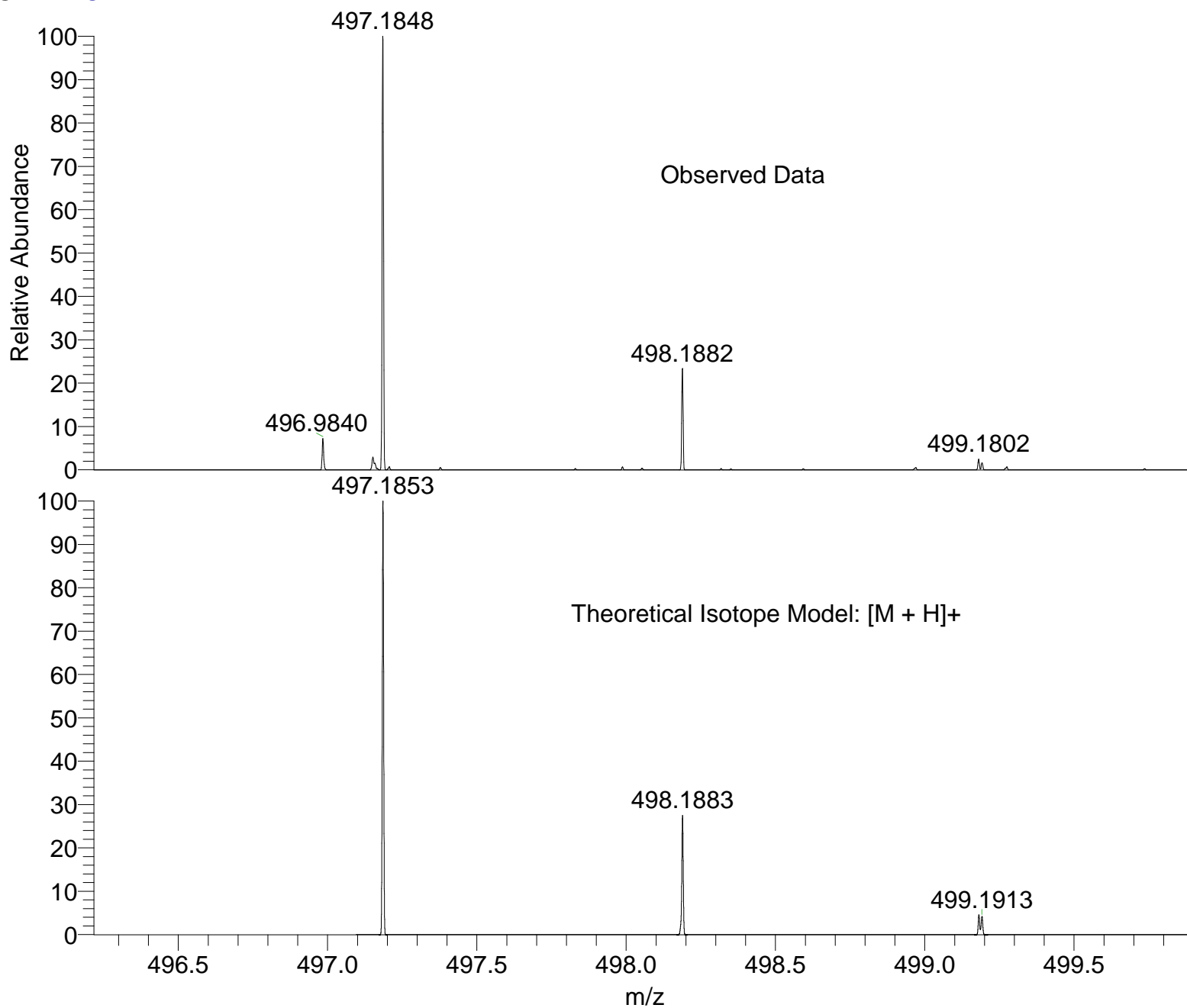
EPSRC National Centre Swansea
LTQ Orbitrap XL

adam throup
11/04/2012 12:31:00

BRASHE194-OJ-HNESP #32-34 RT: 0.83-0.89 AV: 3 SM: 7G NL: 1.61E5
T: FTMS + p NSI Full ms [120.00-2000.00]



SM: 7G



NL:
8.92E4
BRASHE194-OJ-HNESP#32-
34 RT: 0.83-0.89 AV: 3 T:
FTMS + p NSI Full ms
[120.00-2000.00]

NL:
1.65E4
C₂₅ H₂₈ N₄ O₅ SH:
C₂₅ H₂₉ N₄ O₅ S₁
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

Isotope: Min. .. Max.
 14 N 0....10
 16 O 0....15
 12 C 0....65
 1 H 0....75
 23 Na 0....0
 32 S 0....2
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3.. 100
 Fits: 500

N-Rule: Do not use
 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
497.1848	497.1847	0.3	4.5	C ₁₇ H ₃₃ O ₇ N ₆ S ₂
	497.1846	0.3	23.0	C ₃₁ H ₂₃ O ₂ N ₅
	497.1851	-0.7	10.5	C ₁₇ H ₂₅ O ₈ N ₁₀
	497.1851	-0.7	5.0	C ₁₈ H ₃₁ O ₁₃ N ₃
	497.1853	-1.0	13.5	C ₂₅ H ₂₉ O ₅ N ₄ S ₁
	497.1842	1.3	17.0	C ₃₁ H ₃₁ O ₁ N ₁ S ₂
	497.1840	1.6	8.5	C ₂₄ H ₃₃ O ₉ S ₁
	497.1840	1.7	14.0	C ₂₃ H ₂₇ O ₄ N ₇ S ₁
	497.1838	2.0	5.5	C ₁₆ H ₂₉ O ₁₂ N ₆
	497.1858	-2.1	1.0	C ₁₁ H ₃₁ O ₁₁ N ₉ S ₁
	497.1860	-2.4	22.5	C ₃₃ H ₂₅ O ₃ N ₂
	497.1860	-2.4	9.5	C ₁₈ H ₂₉ O ₃ N ₁₀ S ₂
	497.1860	-2.4	4.0	C ₁₉ H ₃₅ O ₈ N ₃ S ₂
	497.1833	3.0	-0.5	C ₁₆ H ₃₇ O ₁₁ N ₂ S ₂
	497.1833	3.0	5.0	C ₁₅ H ₃₁ O ₆ N ₉ S ₂
	497.1833	3.0	18.0	C ₃₀ H ₂₇ O ₆ N ₁
	497.1833	3.0	23.5	C ₂₉ H ₂₁ O ₁ N ₈
	497.1865	-3.4	10.0	C ₁₉ H ₂₇ O ₉ N ₇
	497.1865	-3.4	4.5	C ₂₀ H ₃₃ O ₁₄
	497.1867	-3.7	18.5	C ₂₆ H ₂₅ O ₁ N ₈ S ₁
	497.1867	-3.7	13.0	C ₂₇ H ₃₁ O ₆ N ₁ S ₁
	497.1828	4.0	17.5	C ₂₉ H ₂₉ N ₄ S ₂
	497.1826	4.4	9.0	C ₂₂ H ₃₁ O ₈ N ₃ S ₁
	497.1826	4.4	14.5	C ₂₁ H ₂₅ O ₃ N ₁₀ S ₁
	497.1825	4.7	6.0	C ₁₄ H ₂₇ O ₁₁ N ₉
	497.1872	-4.8	0.5	C ₁₃ H ₃₃ O ₁₂ N ₆ S ₁

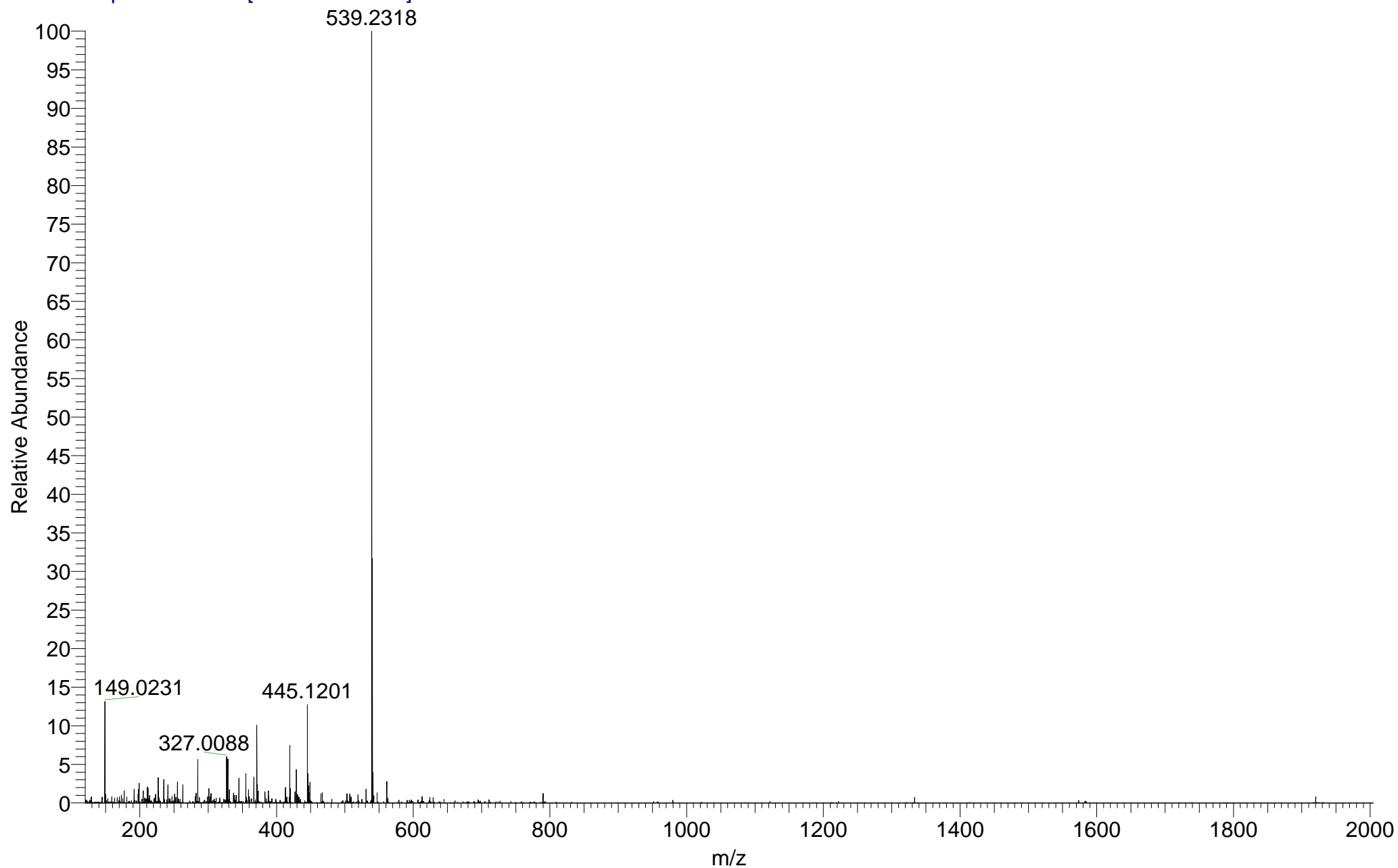
Compound 29

AET7-78-2 MW=538?
(DCM)/MeOH + NH₄OAc

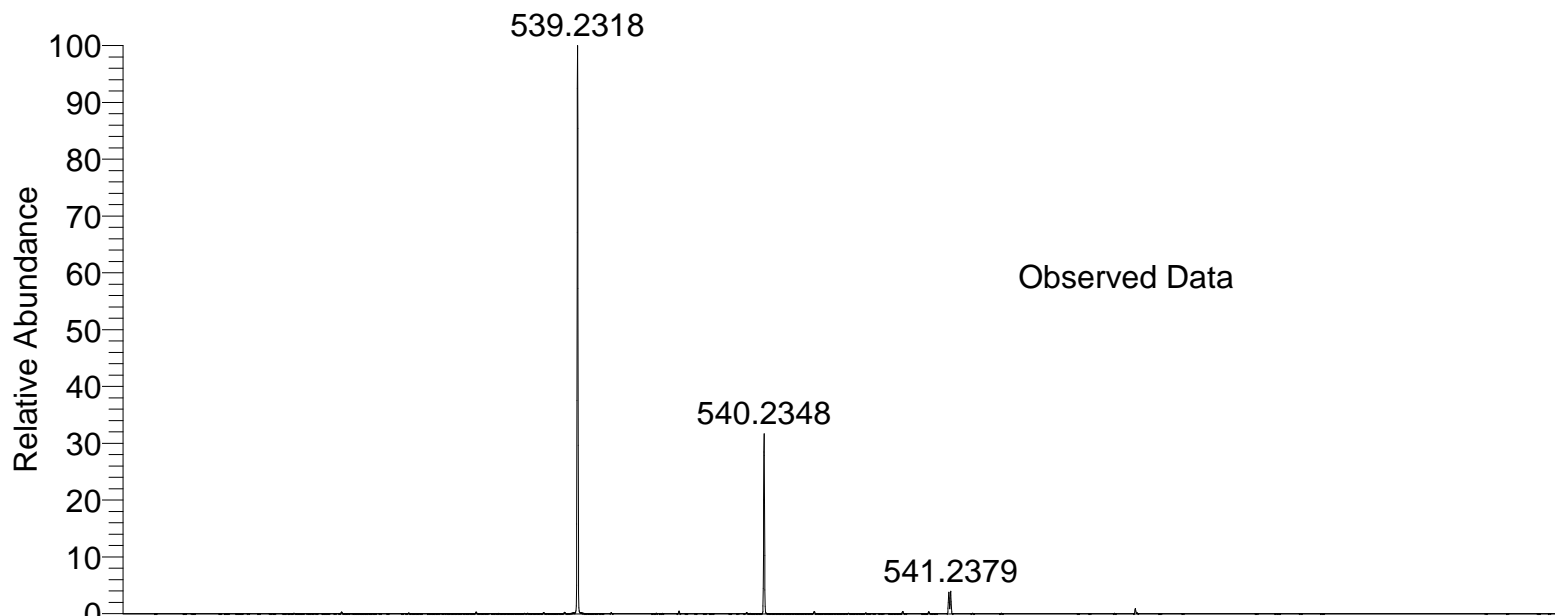
EPSRC National Centre Swansea
LTQ Orbitrap XL

adam throup
11/04/2012 12:27:35

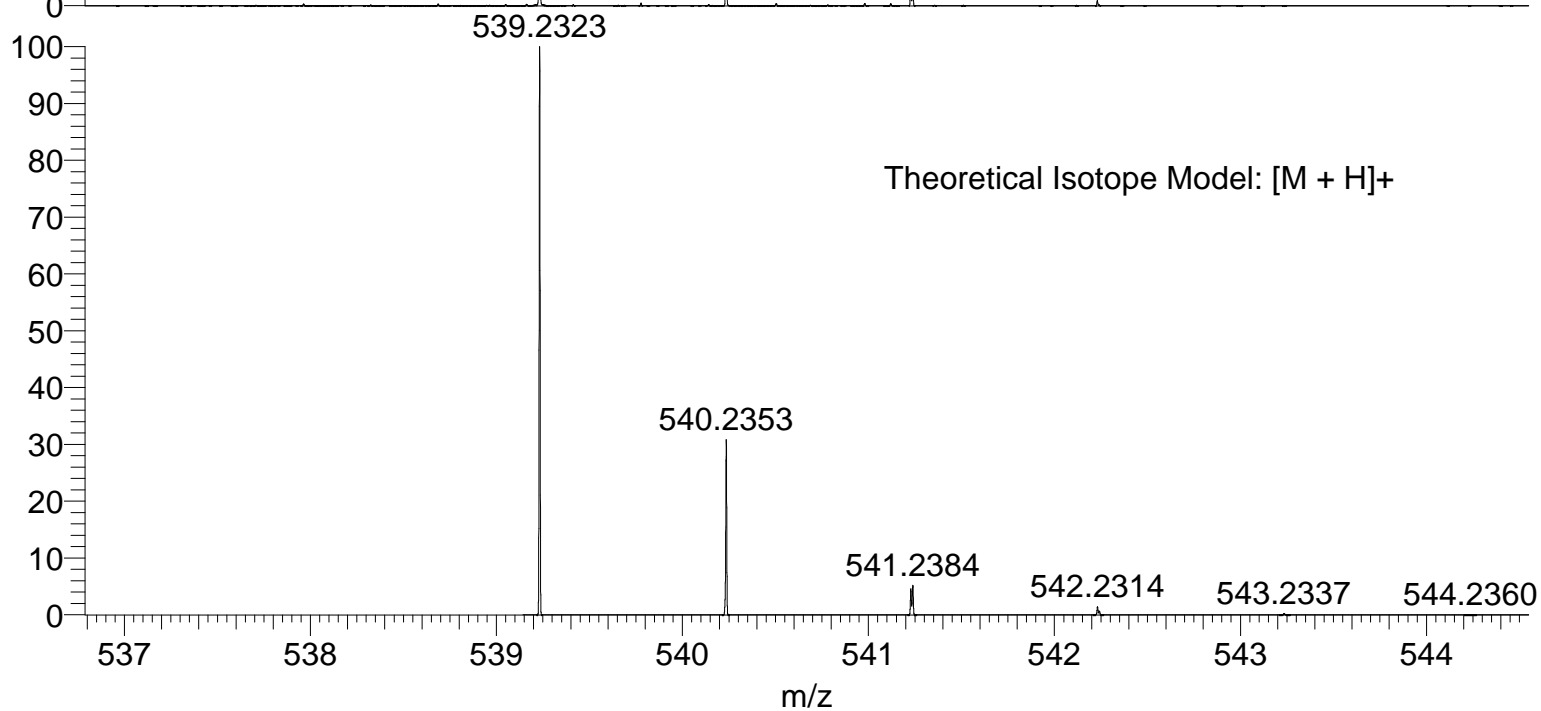
BRASHE193-OJ-HNESP #31-38 RT: 0.81-1.02 AV: 8 SM: 7G NL: 1.33E6
T: FTMS + p NSI Full ms [120.00-2000.00]



SM: 7G



NL:
1.33E6
BRASHE193-OJ-HNESP#31-
38 RT: 0.81-1.02 AV: 8 T:
FTMS + p NSI Full ms
[120.00-2000.00]



NL:
1.60E4
C₂₈ H₃₄ N₄ O₅ SH:
C₂₈ H₃₅ N₄ O₅ S₁
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

Isotope: Min. .. Max.
 14 N 0....10
 16 O 0....15
 12 C 0....65
 1 H 0....75
 23 Na 0....0
 32 S 0....2
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3.. 100
 Fits: 500

N-Rule: Do not use
 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
539.2318	539.2316	0.3	4.5	C ₂₀ H ₃₉ O ₇ N ₆ S ₂
	539.2316	0.4	23.0	C ₃₄ H ₂₉ O ₂ N ₅
	539.2321	-0.5	10.5	C ₂₀ H ₃₁ O ₈ N ₁₀
	539.2321	-0.5	5.0	C ₂₁ H ₃₇ O ₁₃ N ₃
	539.2323	-0.9	13.5	C ₂₈ H ₃₅ O ₅ N ₄ S ₁
	539.2311	1.3	17.0	C ₃₄ H ₃₇ O ₁ N ₁ S ₂
	539.2309	1.6	8.5	C ₂₇ H ₃₉ O ₉ S ₁
	539.2309	1.6	14.0	C ₂₆ H ₃₃ O ₄ N ₇ S ₁
	539.2328	-1.8	1.0	C ₁₄ H ₃₇ O ₁₁ N ₉ S ₁
	539.2307	2.0	5.5	C ₁₉ H ₃₅ O ₁₂ N ₆
	539.2329	-2.1	22.5	C ₃₆ H ₃₁ O ₃ N ₂
	539.2330	-2.1	9.5	C ₂₁ H ₃₅ O ₃ N ₁₀ S ₂
	539.2330	-2.1	4.0	C ₂₂ H ₄₁ O ₈ N ₃ S ₂
	539.2303	2.8	-0.5	C ₁₉ H ₄₃ O ₁₁ N ₂ S ₂
	539.2303	2.8	5.0	C ₁₈ H ₃₇ O ₆ N ₉ S ₂
	539.2302	2.9	18.0	C ₃₃ H ₃₃ O ₆ N ₁
	539.2302	2.9	23.5	C ₃₂ H ₂₇ O ₁ N ₈
	539.2334	-3.0	10.0	C ₂₂ H ₃₃ O ₉ N ₇
	539.2334	-3.0	4.5	C ₂₃ H ₃₉ O ₁₄
	539.2336	-3.3	18.5	C ₂₉ H ₃₁ O ₁ N ₈ S ₁
	539.2336	-3.4	13.0	C ₃₀ H ₃₇ O ₆ N ₁ S ₁
	539.2298	3.8	17.5	C ₃₂ H ₃₅ N ₄ S ₂
	539.2296	4.1	9.0	C ₂₅ H ₃₇ O ₈ N ₃ S ₁
	539.2296	4.1	14.5	C ₂₄ H ₃₁ O ₃ N ₁₀ S ₁
	539.2341	-4.3	0.5	C ₁₆ H ₃₉ O ₁₂ N ₆ S ₁
	539.2294	4.4	6.0	C ₁₇ H ₃₃ O ₁₁ N ₉
	539.2343	-4.6	9.0	C ₂₃ H ₃₇ O ₄ N ₇ S ₂
	539.2343	-4.6	3.5	C ₂₄ H ₄₃ O ₉ S ₂

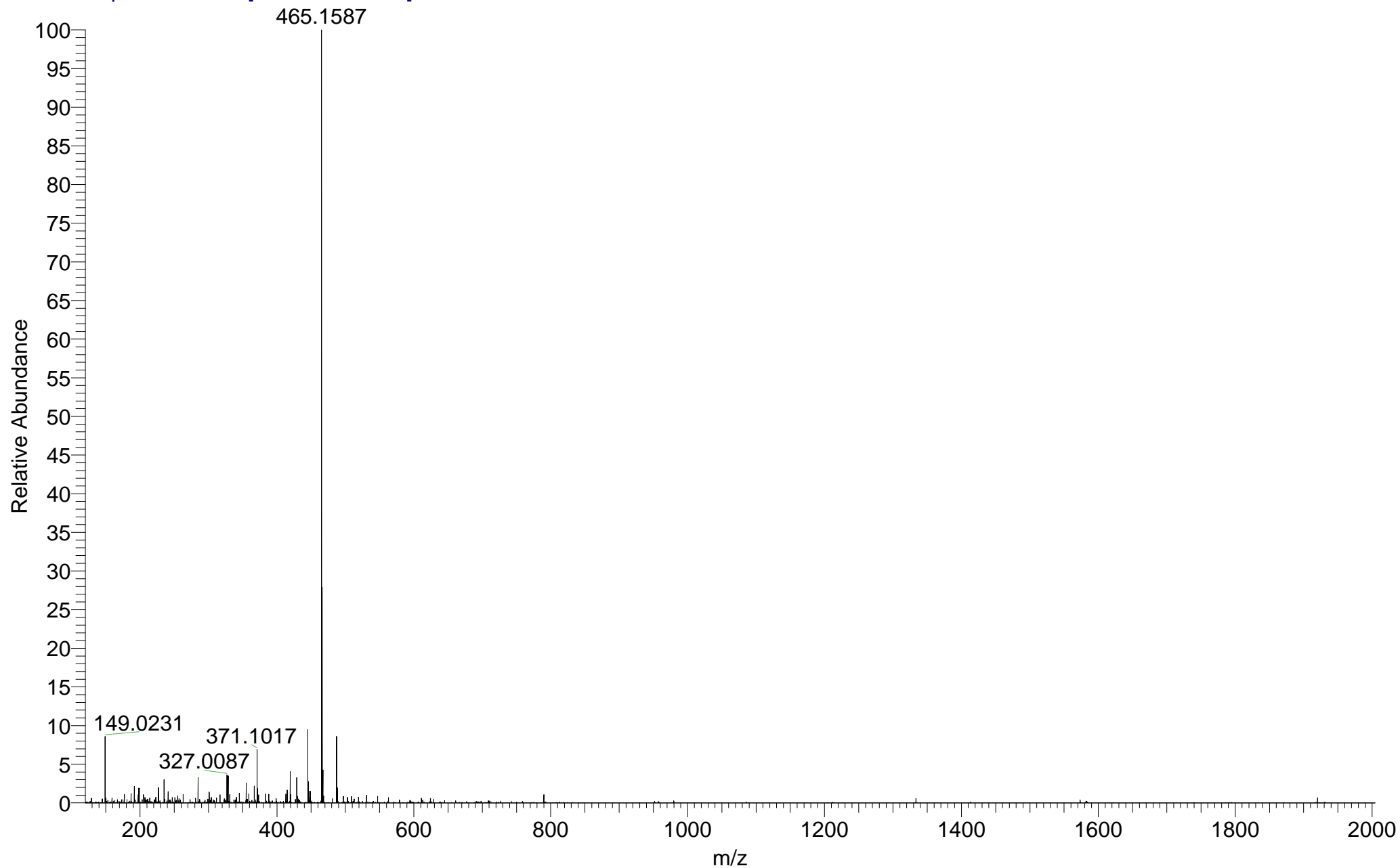
AET7-77-1 MW=464?
(DCM)/MeOH + NH4OAc

Compound 30

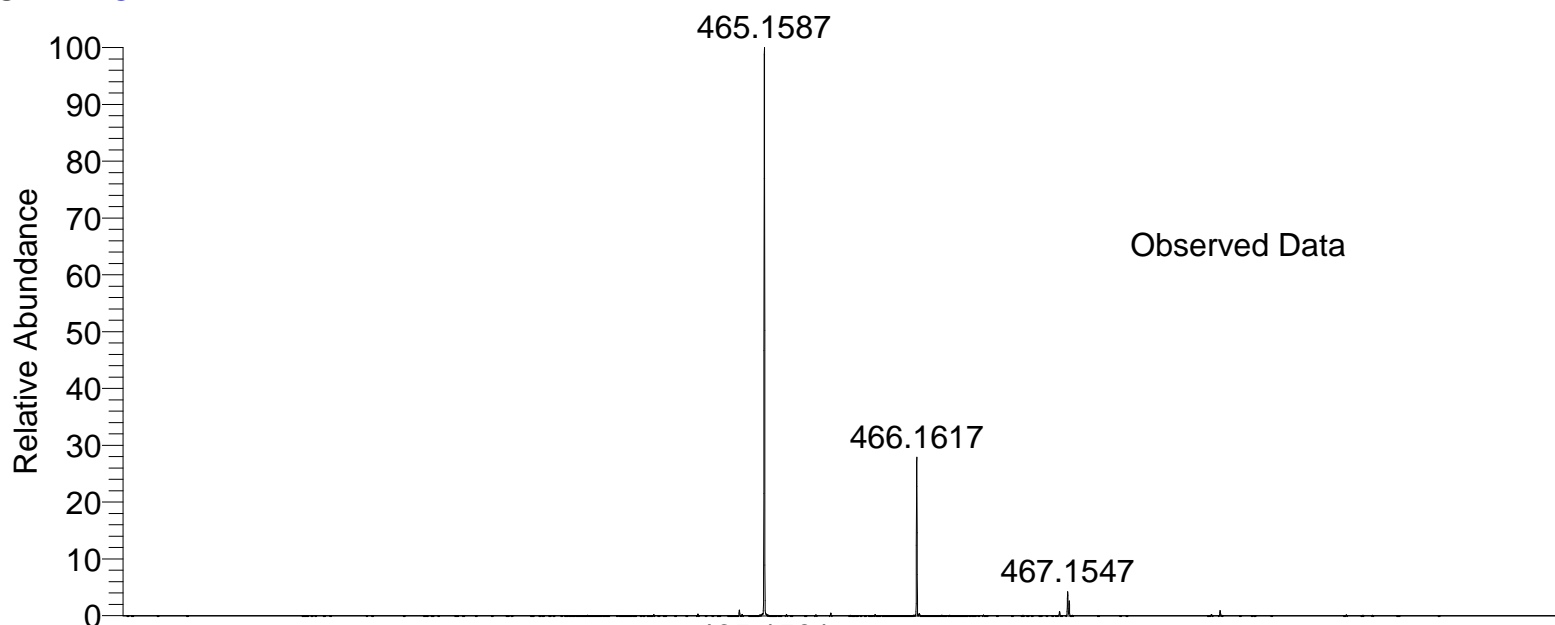
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adam throup
11/04/2012 12:24:09

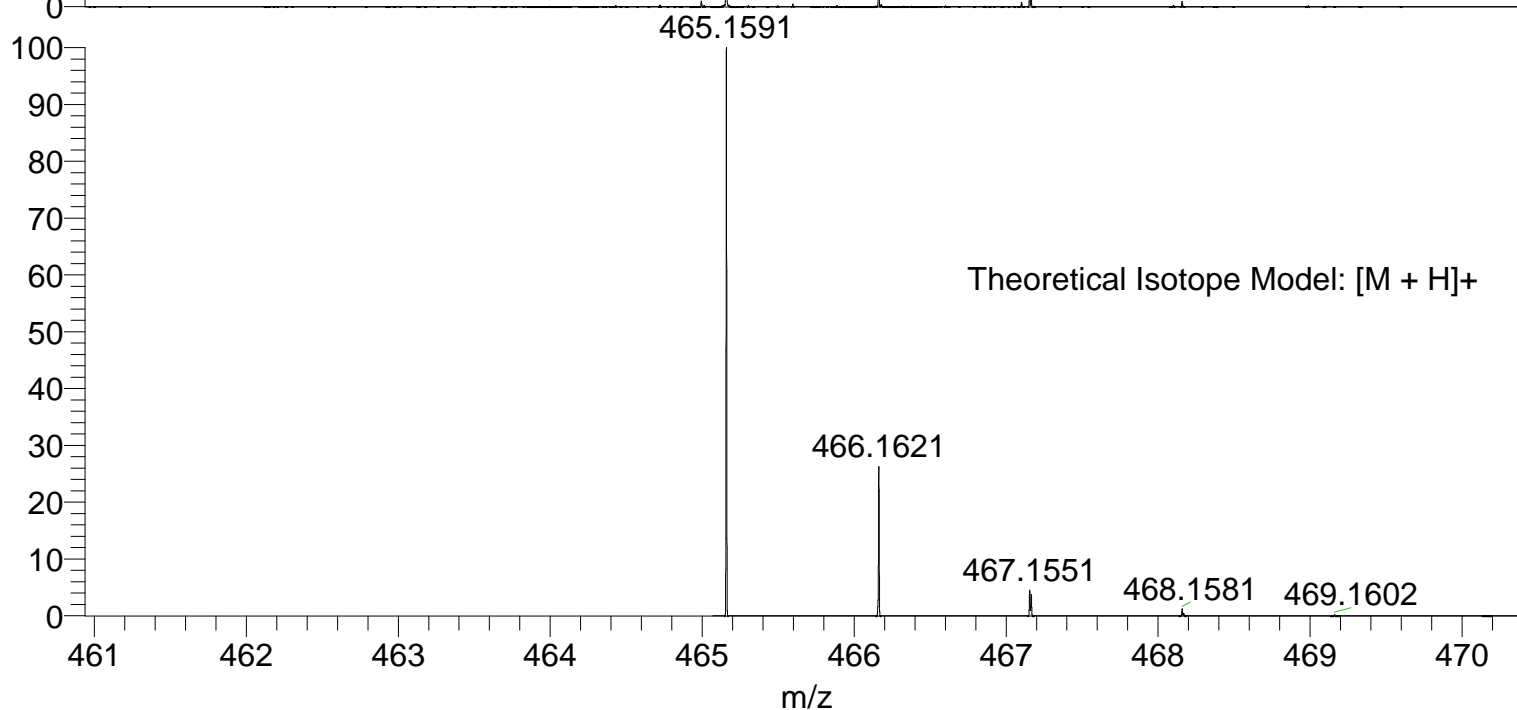
BRASHE192-OJ-HNESP #32-36 RT: 0.84-0.96 AV: 5 SM: 7G NL: 1.90E6
T: FTMS + p NSI Full ms [120.00-2000.00]



SM: 7G



NL:
1.90E6
BRASHE192-OJ-HNESP#32-
36 RT: 0.84-0.96 AV: 5 T:
FTMS + p NSI Full ms
[120.00-2000.00]



NL:
1.67E4
C₂₄ H₂₄ N₄ O₄ SH:
C₂₄ H₂₅ N₄ O₄ S₁
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

Isotope: Min. .. Max.
 14 N 0....10
 16 O 0....15
 12 C 0....65
 1 H 0....75
 23 Na 0....0
 32 S 0....2
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3.. 100
 Fits: 500

N-Rule: Do not use
 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
465.1587	465.1589	-0.5	11.5	C ₁₆ H ₂₁ O ₇ N ₁₀
	465.1589	-0.5	6.0	C ₁₇ H ₂₇ O ₁₂ N ₃
	465.1585	0.5	5.5	C ₁₆ H ₂₉ O ₆ N ₆ S ₂
	465.1584	0.6	24.0	C ₃₀ H ₁₉ O ₁ N ₅
	465.1591	-0.9	14.5	C ₂₄ H ₂₅ O ₄ N ₄ S ₁
	465.1583	0.9	-3.0	C ₉ H ₃₁ O ₁₄ N ₅ S ₁
	465.1579	1.6	18.0	C ₃₀ H ₂₇ N ₁ S ₂
	465.1596	-2.0	2.0	C ₁₀ H ₂₇ O ₁₀ N ₉ S ₁
	465.1578	2.0	9.5	C ₂₃ H ₂₉ O ₈ S ₁
	465.1578	2.0	15.0	C ₂₂ H ₂₃ O ₃ N ₇ S ₁
	465.1598	-2.3	23.5	C ₃₂ H ₂₁ O ₂ N ₂
	465.1598	-2.3	10.5	C ₁₇ H ₂₅ O ₂ N ₁₀ S ₂
	465.1598	-2.4	5.0	C ₁₈ H ₃₁ O ₇ N ₃ S ₂
	465.1576	2.4	6.5	C ₁₅ H ₂₅ O ₁₁ N ₆
	465.1603	-3.4	11.0	C ₁₈ H ₂₃ O ₈ N ₇
	465.1603	-3.4	5.5	C ₁₉ H ₂₉ O ₁₃
	465.1571	3.4	0.5	C ₁₅ H ₃₃ O ₁₀ N ₂ S ₂
	465.1571	3.4	6.0	C ₁₄ H ₂₇ O ₅ N ₉ S ₂
	465.1571	3.5	19.0	C ₂₉ H ₂₃ O ₅ N ₁
	465.1571	3.5	24.5	C ₂₈ H ₁₇ N ₈
	465.1604	-3.7	19.5	C ₂₅ H ₂₁ N ₈ S ₁
	465.1604	-3.8	14.0	C ₂₆ H ₂₇ O ₅ N ₁ S ₁
	465.1569	3.8	-2.5	C ₇ H ₂₉ O ₁₃ N ₈ S ₁
	465.1610	-4.8	1.5	C ₁₂ H ₂₉ O ₁₁ N ₆ S ₁
	465.1564	4.9	10.0	C ₂₁ H ₂₇ O ₇ N ₃ S ₁
	465.1564	4.9	15.5	C ₂₀ H ₂₁ O ₂ N ₁₀ S ₁

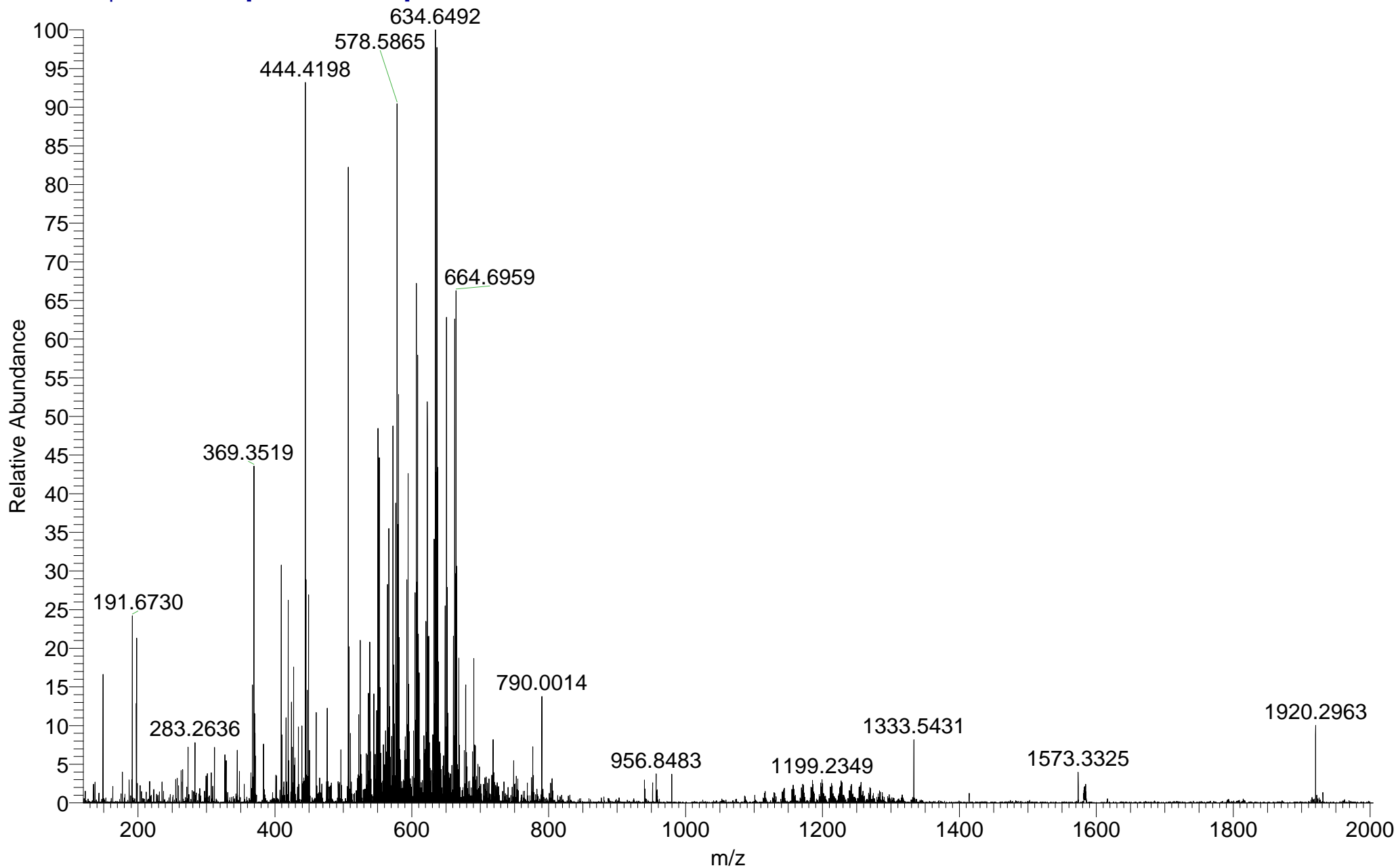
AET7-78-1 MW=507?
(DCM)/MeOH + NH4OAc

Compound 31

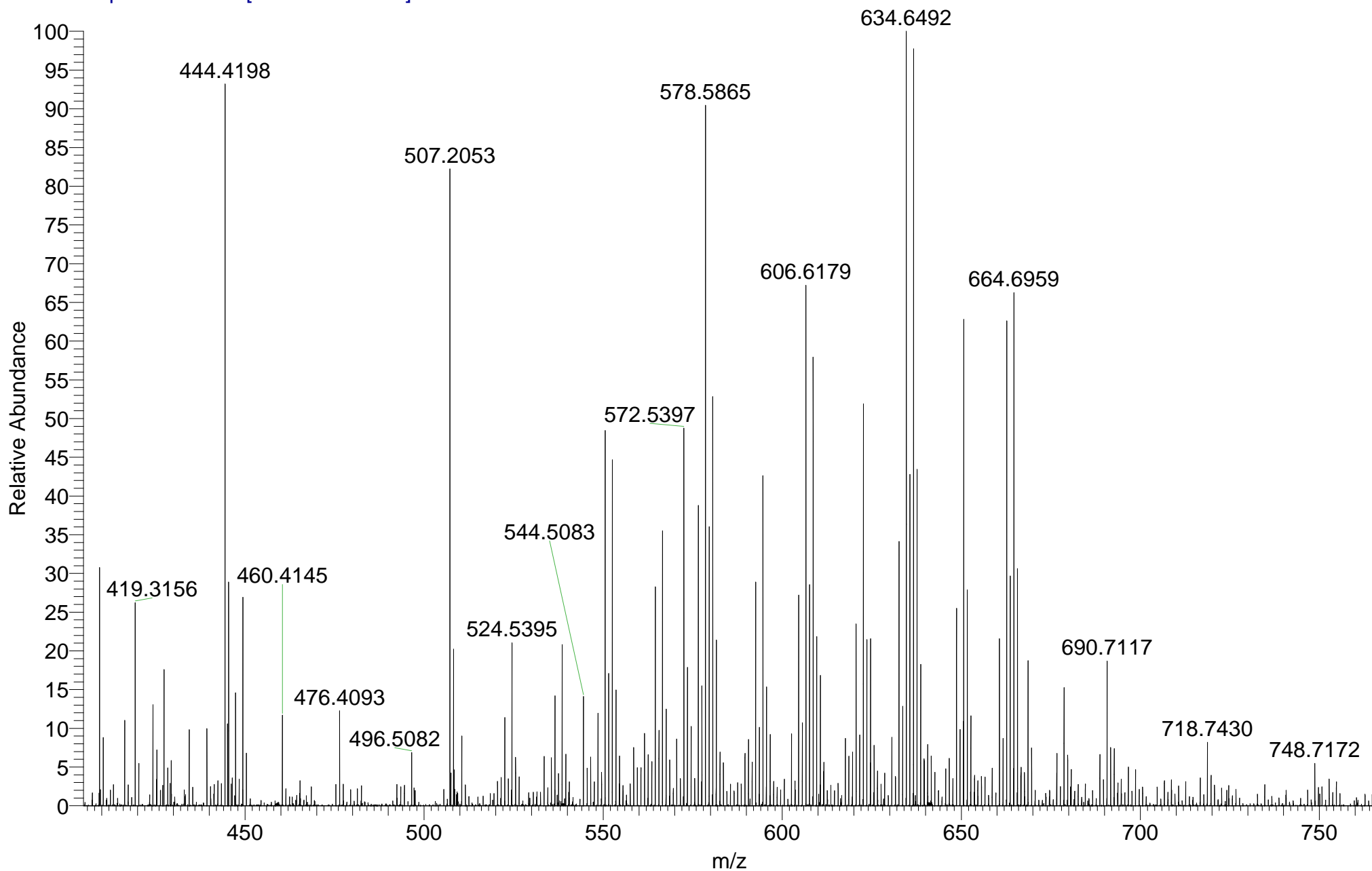
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adam throup
11/04/2012 12:34:26

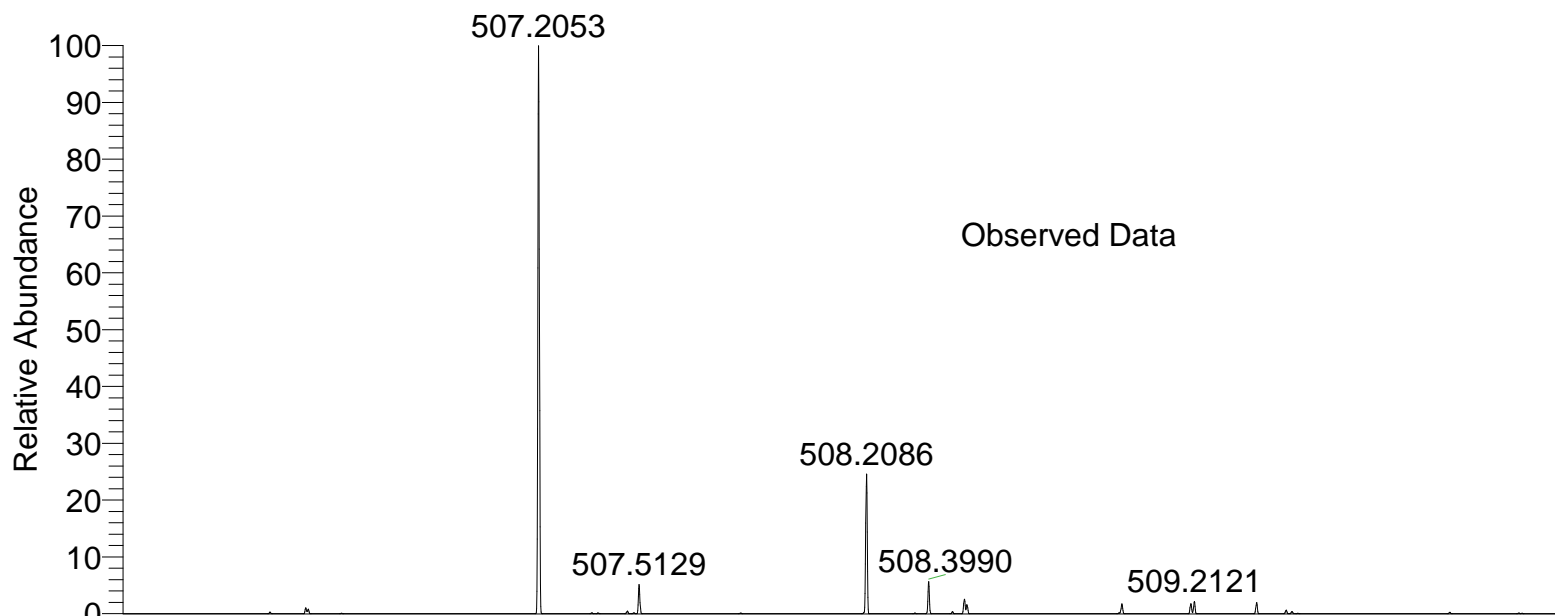
BRASHE195-OJ-HNESP #28-34 RT: 0.72-0.86 AV: 7 SM: 7G NL: 9.10E5
T: FTMS + p NSI Full ms [120.00-2000.00]



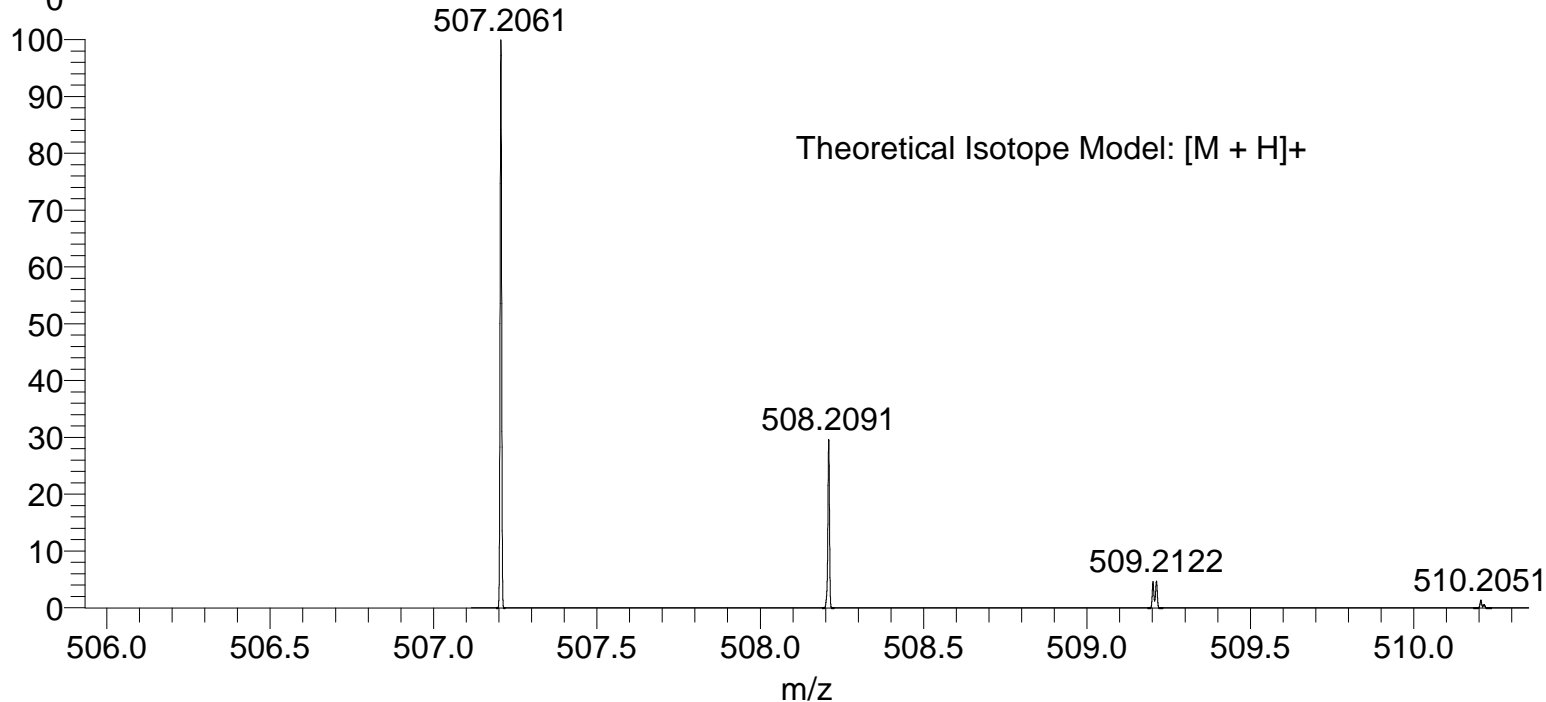
BRASHE195-OJ-HNESP #28-34 RT: 0.72-0.86 AV: 7 SM: 7G NL: 9.10E5
T: FTMS + p NSI Full ms [120.00-2000.00]



SM: 7G



NL:
7.48E5
BRASHE195-OJ-HNESP#28-
34 RT: 0.72-0.86 AV: 7 T:
FTMS + p NSI Full ms
[120.00-2000.00]



NL:
1.62E4
C₂₇ H₃₀ N₄ O₄ SH:
C₂₇ H₃₁ N₄ O₄ S₁
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

Isotope: Min. .. Max.
 14 N 0....10
 16 O 0....15
 12 C 0....65
 1 H 0....75
 23 Na 0....0
 32 S 0....2
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3.. 100
 Fits: 500

N-Rule: Do not use
 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
507.2053	507.2054	-0.1	24.0	C ₃₃ H ₂₅ O ₁ N ₅
	507.2052	0.2	-3.0	C ₁₂ H ₃₇ O ₁₄ N ₅ S ₁
	507.2054	-0.2	5.5	C ₁₉ H ₃₅ O ₆ N ₆ S ₂
	507.2049	0.8	18.0	C ₃₃ H ₃₃ N ₁ S ₂
	507.2059	-1.1	11.5	C ₁₉ H ₂₇ O ₇ N ₁₀
	507.2059	-1.1	6.0	C ₂₀ H ₃₃ O ₁₂ N ₃
	507.2047	1.2	9.5	C ₂₆ H ₃₅ O ₈ S ₁
	507.2047	1.2	15.0	C ₂₅ H ₂₉ O ₃ N ₇ S ₁
	507.2061	-1.5	14.5	C ₂₇ H ₃₁ O ₄ N ₄ S ₁
	507.2045	1.5	6.5	C ₁₈ H ₃₁ O ₁₁ N ₆
	507.2041	2.4	0.5	C ₁₈ H ₃₉ O ₁₀ N ₂ S ₂
	507.2041	2.4	6.0	C ₁₇ H ₃₃ O ₅ N ₉ S ₂
	507.2066	-2.5	2.0	C ₁₃ H ₃₃ O ₁₀ N ₉ S ₁
	507.2040	2.5	19.0	C ₃₂ H ₂₉ O ₅ N ₁
	507.2040	2.5	24.5	C ₃₁ H ₂₃ N ₈
	507.2067	-2.8	23.5	C ₃₅ H ₂₇ O ₂ N ₂
	507.2039	2.8	-2.5	C ₁₀ H ₃₅ O ₁₃ N ₈ S ₁
	507.2067	-2.8	10.5	C ₂₀ H ₃₁ O ₂ N ₁₀ S ₂
	507.2067	-2.8	5.0	C ₂₁ H ₃₇ O ₇ N ₃ S ₂
	507.2072	-3.8	11.0	C ₂₁ H ₂₉ O ₈ N ₇
	507.2072	-3.8	5.5	C ₂₂ H ₃₅ O ₁₃
	507.2034	3.8	10.0	C ₂₄ H ₃₃ O ₇ N ₃ S ₁
	507.2034	3.8	15.5	C ₂₃ H ₂₇ O ₂ N ₁₀ S ₁
	507.2074	-4.1	19.5	C ₂₈ H ₂₇ N ₈ S ₁
	507.2074	-4.1	14.0	C ₂₉ H ₃₃ O ₅ N ₁ S ₁
	507.2032	4.2	1.5	C ₁₇ H ₃₅ O ₁₅ N ₂
	507.2032	4.2	7.0	C ₁₆ H ₂₉ O ₁₀ N ₉

aet7-93-2 MW=500?
(DCM)/MeOH + NH4OAc

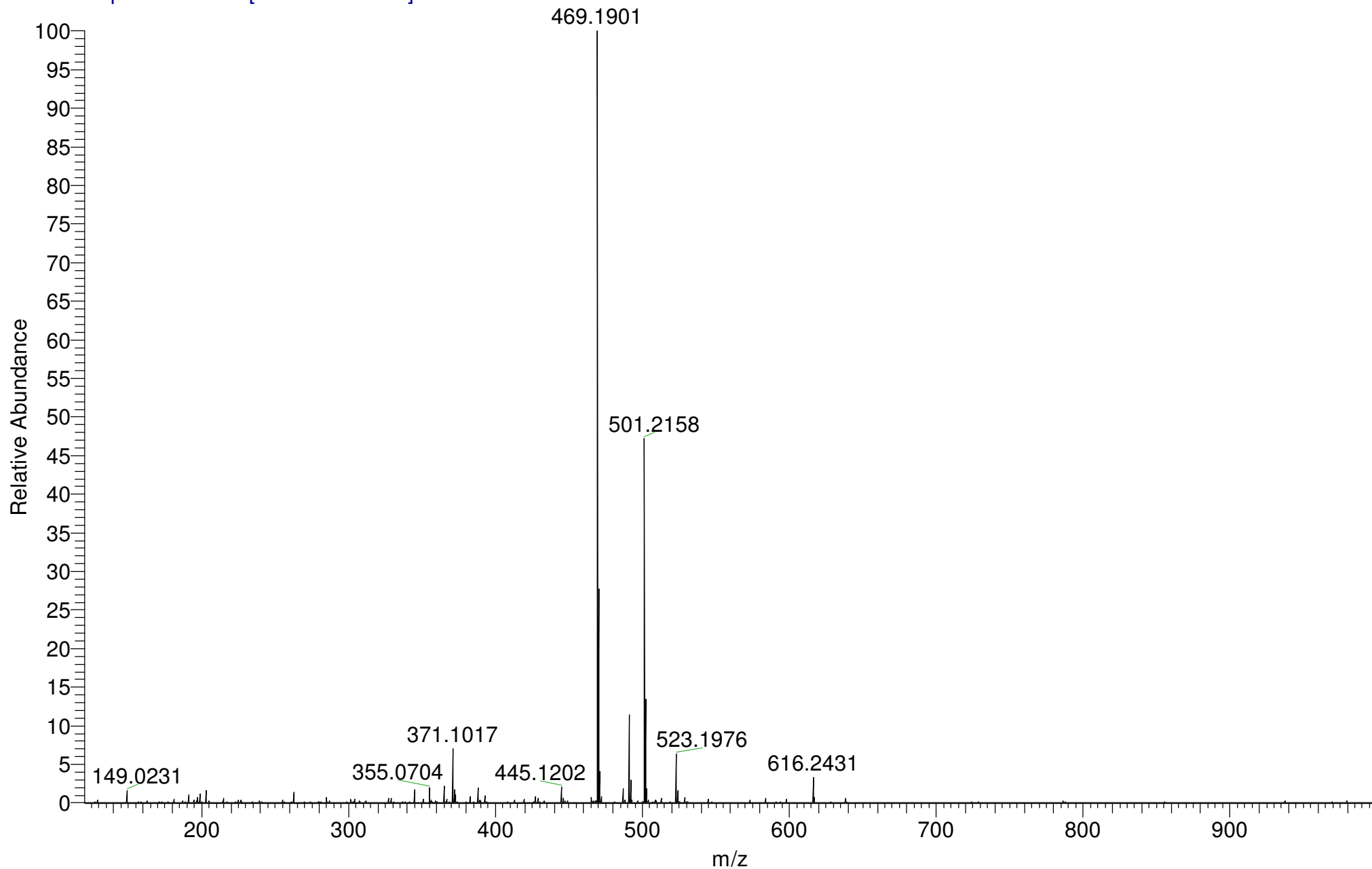
Compound 32

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adam throup
21/06/2012 11:37:09

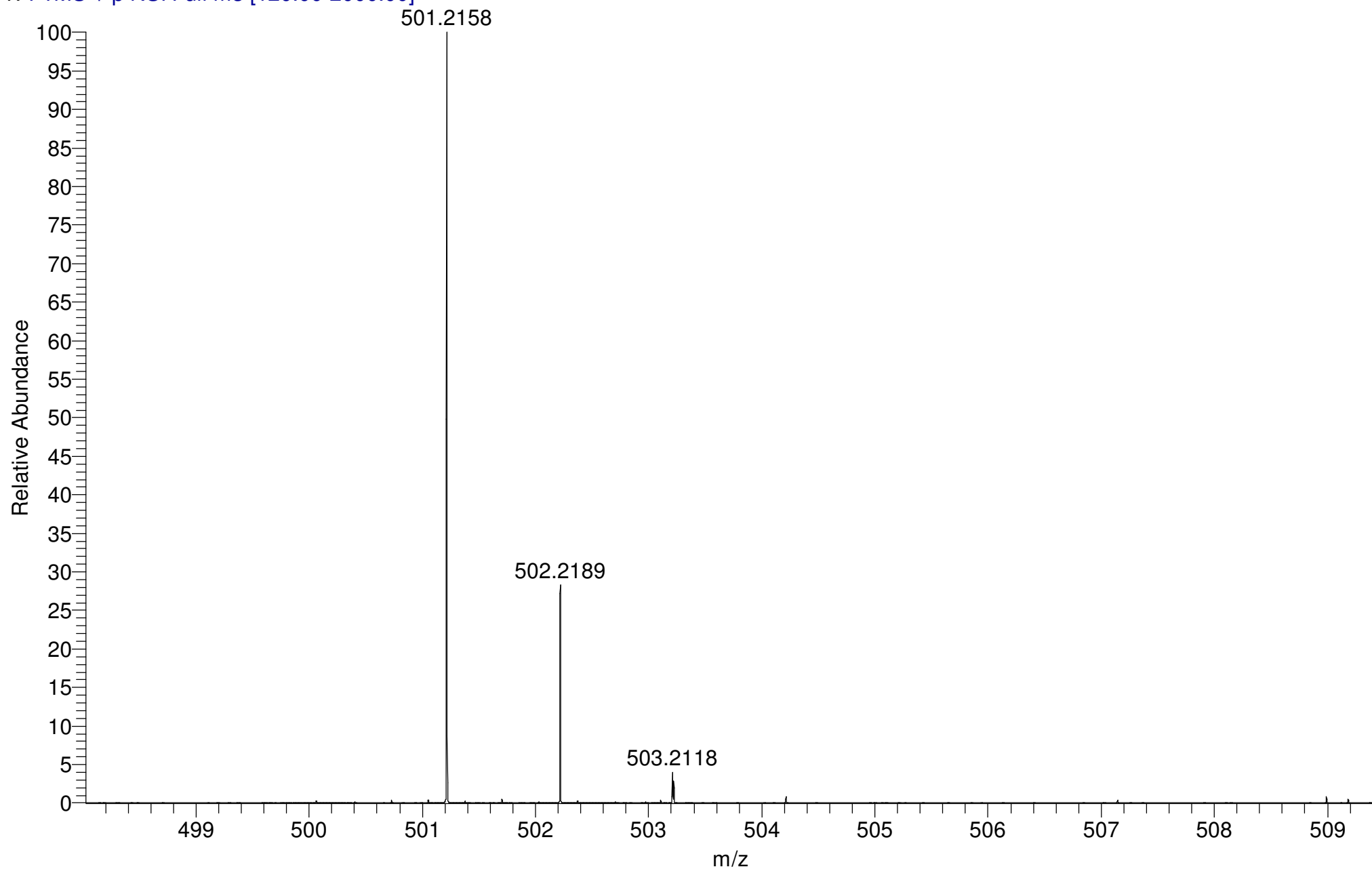
BRASHE219-OJ-HNESP #31-49 RT: 0.77-1.29 AV: 19 SM: 7G NL: 5.19E6

T: FTMS + p NSI Full ms [120.00-2000.00]



BRASHE219-OJ-HNESP #31-49 RT: 0.77-1.29 AV: 19 SM: 7G NL: 2.45E6

T: FTMS + p NSI Full ms [120.00-2000.00]



Isotope: Min. .. Max.
 12 C 0....60
 1 H 0....70
 14 N 0....15
 16 O 0....15
 23 Na 0....0
 32 S 0....3
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3.. 100
 Fits: 100

N-Rule: Do not use
 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
501.2158	501.2158	0.0	-0.5	C ₉ H ₃₃ O ₁₀ N ₁₂ S ₁
	501.2159	-0.3	21.0	C ₃₁ H ₂₇ O ₂ N ₅
	501.2160	-0.3	8.0	C ₁₆ H ₃₁ O ₂ N ₁₃ S ₂
	501.2160	-0.3	2.5	C ₁₇ H ₃₇ O ₇ N ₆ S ₂
	501.2155	0.7	15.0	C ₃₁ H ₃₅ O ₁ N ₁ S ₂
	501.2161	-0.7	5.5	C ₂₅ H ₄₁ O ₄ S ₃
	501.2153	1.0	-1.0	C ₈ H ₃₅ O ₄ N ₁₅ S ₃
	501.2153	1.0	6.5	C ₂₄ H ₃₇ O ₉ S ₁
	501.2153	1.0	12.0	C ₂₃ H ₃₁ O ₄ N ₇ S ₁
	501.2164	-1.3	8.5	C ₁₇ H ₂₉ O ₈ N ₁₀
	501.2164	-1.3	3.0	C ₁₈ H ₃₅ O ₁₃ N ₃
	501.2151	1.4	3.5	C ₁₆ H ₃₃ O ₁₂ N ₆
	501.2151	1.4	9.0	C ₁₅ H ₂₇ O ₇ N ₁₃
	501.2166	-1.6	17.0	C ₂₄ H ₂₇ N ₁₁ S ₁
	501.2166	-1.6	11.5	C ₂₅ H ₃₃ O ₅ N ₄ S ₁
	501.2167	-1.7	-1.5	C ₁₀ H ₃₇ O ₅ N ₁₂ S ₃
	501.2148	2.0	6.0	C ₂₃ H ₃₉ O ₃ N ₃ S ₃
	501.2146	2.3	-2.5	C ₁₆ H ₄₁ O ₁₁ N ₂ S ₂
	501.2146	2.3	3.0	C ₁₅ H ₃₅ O ₆ N ₉ S ₂
	501.2146	2.4	16.0	C ₃₀ H ₃₁ O ₆ N ₁
	501.2146	2.4	21.5	C ₂₉ H ₂₅ O ₁ N ₈
	501.2171	-2.6	-1.0	C ₁₁ H ₃₅ O ₁₁ N ₉ S ₁
	501.2144	2.7	0.0	C ₇ H ₃₁ O ₉ N ₁₅ S ₁
	501.2173	-2.9	20.5	C ₃₃ H ₂₉ O ₃ N ₂
	501.2173	-3.0	7.5	C ₁₈ H ₃₃ O ₃ N ₁₀ S ₂
	501.2173	-3.0	2.0	C ₁₉ H ₃₉ O ₈ N ₃ S ₂
	501.2141	3.4	15.5	C ₂₉ H ₃₃ N ₄ S ₂
	501.2175	-3.4	10.5	C ₂₆ H ₃₇ N ₄ S ₃
	501.2139	3.7	7.0	C ₂₂ H ₃₅ O ₈ N ₃ S ₁
	501.2139	3.7	12.5	C ₂₁ H ₂₉ O ₃ N ₁₀ S ₁
	501.2178	-3.9	13.5	C ₁₈ H ₂₅ O ₄ N ₁₄

aet7-96 MW=542?
(DCM)/MeOH + NH4OAc

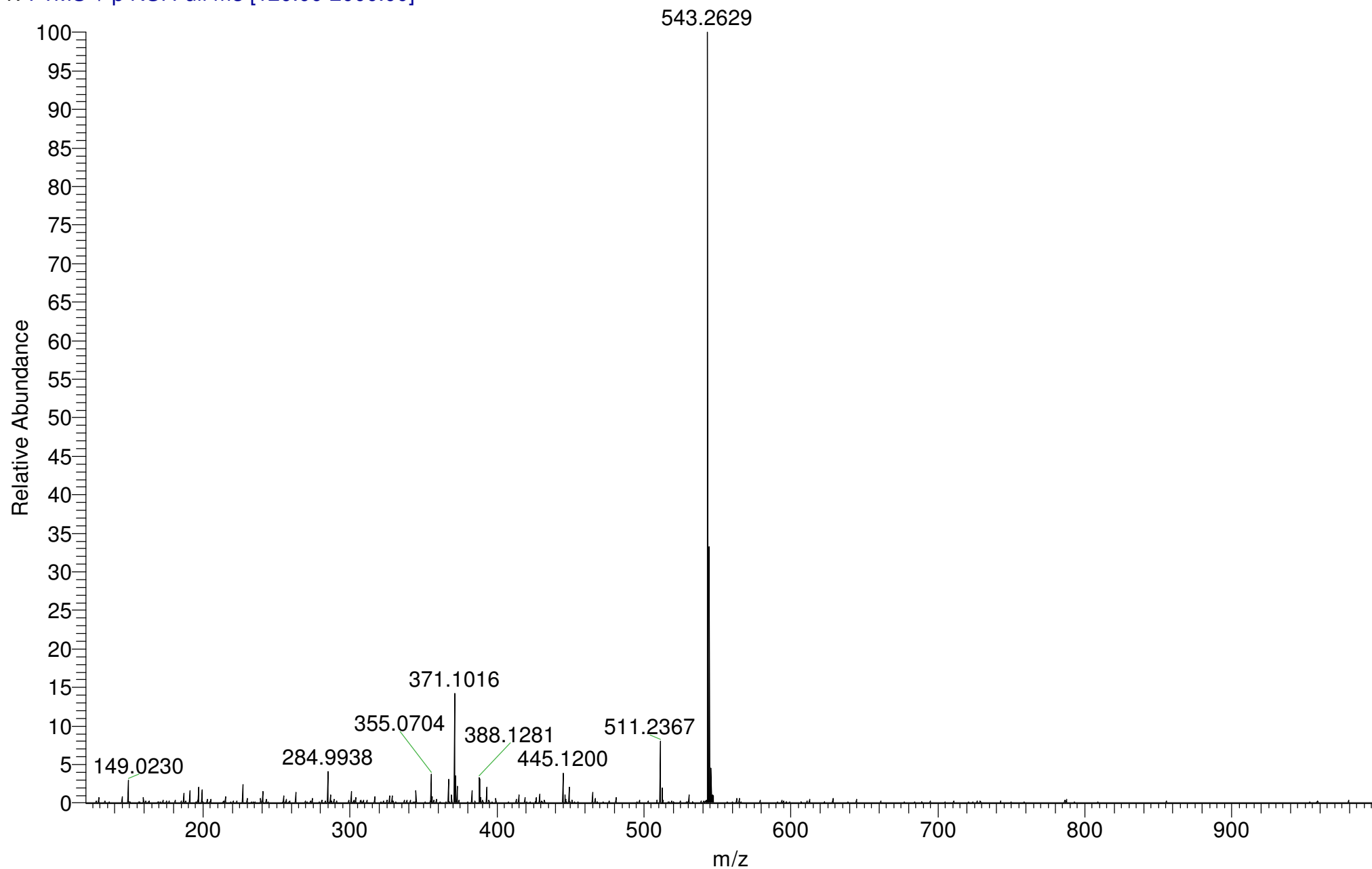
Compound 33

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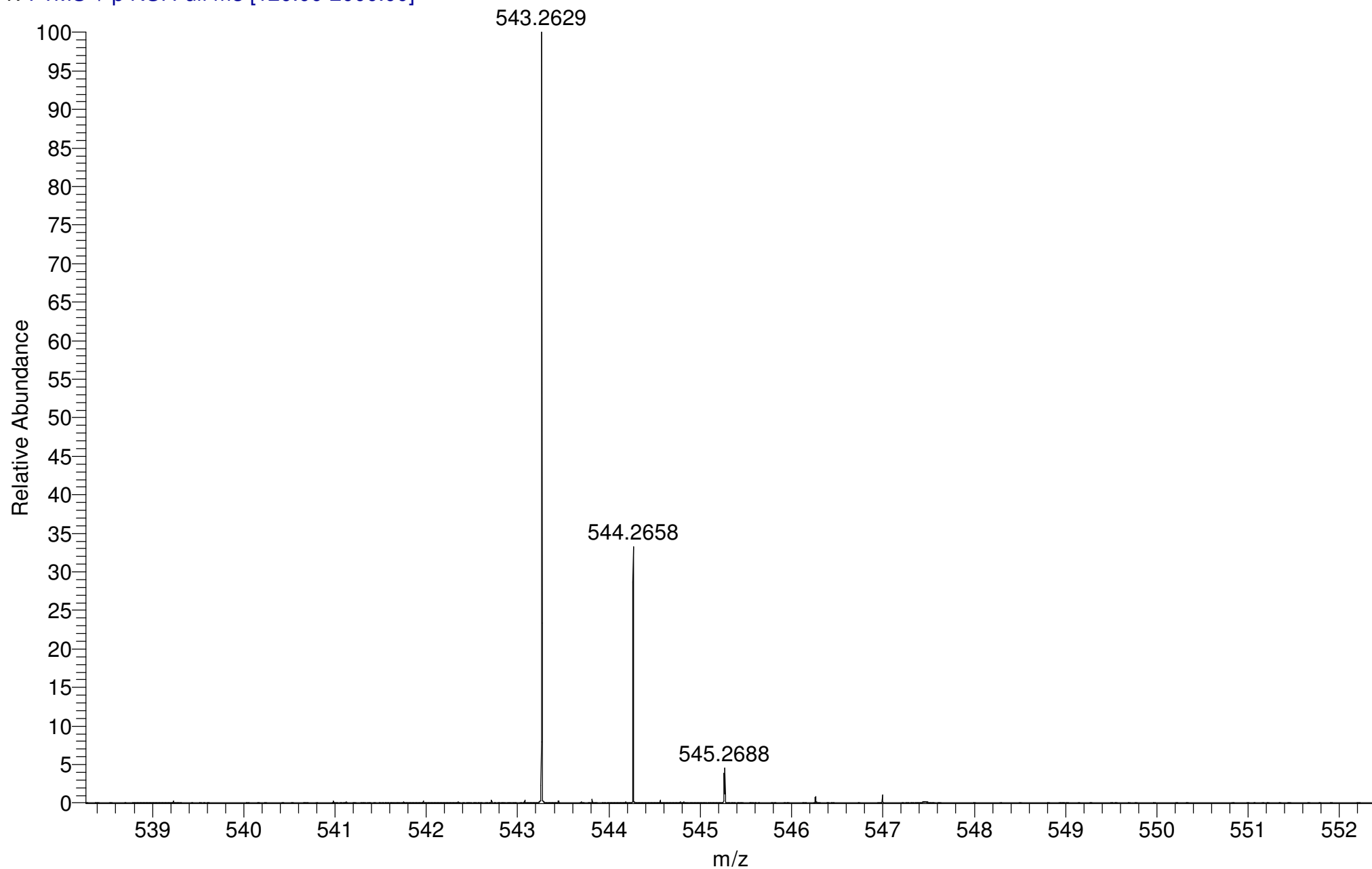
adam throup
21/06/2012 11:33:42

BRASHE218-OJ-HNESP #34-46 RT: 0.86-1.21 AV: 13 SM: 7G NL: 3.26E6

T: FTMS + p NSI Full ms [120.00-2000.00]



BRASHE218-OJ-HNESP #34-46 RT: 0.86-1.21 AV: 13 SM: 7G NL: 3.26E6
T: FTMS + p NSI Full ms [120.00-2000.00]



Isotope: Min. .. Max.
 12 C 0....60
 1 H 0....70
 14 N 0....15
 16 O 0....15
 23 Na 0....0
 32 S 0....3
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3.. 100
 Fits: 100

N-Rule: Do not use
 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
543.2629	543.2629	-0.0	8.0	C ₁₉ H ₃₇ O ₂ N ₁₃ S ₂
	543.2629	-0.0	2.5	C ₂₀ H ₄₃ O ₇ N ₆ S ₂
	543.2629	0.0	21.0	C ₃₄ H ₃₃ O ₂ N ₅
	543.2627	0.3	-0.5	C ₁₂ H ₃₉ O ₁₀ N ₁₂ S ₁
	543.2631	-0.4	5.5	C ₂₈ H ₄₇ O ₄ S ₃
	543.2634	-0.9	8.5	C ₂₀ H ₃₅ O ₈ N ₁₀
	543.2634	-0.9	3.0	C ₂₁ H ₄₁ O ₁₃ N ₃
	543.2624	0.9	15.0	C ₃₄ H ₄₁ O ₁ N ₁ S ₂
	543.2623	1.2	-1.0	C ₁₁ H ₄₁ O ₄ N ₁₅ S ₃
	543.2636	-1.2	17.0	C ₂₇ H ₃₃ N ₁₁ S ₁
	543.2636	-1.2	11.5	C ₂₈ H ₃₉ O ₅ N ₄ S ₁
	543.2622	1.2	6.5	C ₂₇ H ₄₃ O ₉ S ₁
	543.2622	1.2	12.0	C ₂₆ H ₃₇ O ₄ N ₇ S ₁
	543.2636	-1.3	-1.5	C ₁₃ H ₄₃ O ₅ N ₁₂ S ₃
	543.2620	1.6	3.5	C ₁₉ H ₃₉ O ₁₂ N ₆
	543.2620	1.6	9.0	C ₁₈ H ₃₃ O ₇ N ₁₃
	543.2618	2.1	6.0	C ₂₆ H ₄₅ O ₃ N ₃ S ₃
	543.2641	-2.2	-1.0	C ₁₄ H ₄₁ O ₁₁ N ₉ S ₁
	543.2642	-2.4	20.5	C ₃₆ H ₃₅ O ₃ N ₂
	543.2616	2.4	-2.5	C ₁₉ H ₄₇ O ₁₁ N ₂ S ₂
	543.2616	2.4	3.0	C ₁₈ H ₄₁ O ₆ N ₉ S ₂
	543.2643	-2.5	7.5	C ₂₁ H ₃₉ O ₃ N ₁₀ S ₂
	543.2643	-2.5	2.0	C ₂₂ H ₄₅ O ₈ N ₃ S ₂
	543.2615	2.5	16.0	C ₃₃ H ₃₇ O ₆ N ₁
	543.2615	2.5	21.5	C ₃₂ H ₃₁ O ₁ N ₈
	543.2614	2.8	0.0	C ₁₀ H ₃₇ O ₉ N ₁₅ S ₁
	543.2644	-2.8	10.5	C ₂₉ H ₄₃ N ₄ S ₃
	543.2647	-3.4	13.5	C ₂₁ H ₃₁ O ₄ N ₁₄
	543.2647	-3.4	8.0	C ₂₂ H ₃₇ O ₉ N ₇
	543.2647	-3.4	2.5	C ₂₃ H ₄₃ O ₁₄
	543.2611	3.4	15.5	C ₃₂ H ₃₉ N ₄ S ₂

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
543.2649	543.2649	-3.7	16.5	C ₂₉ H ₃₅ O ₁ N ₈ S ₁
543.2649	543.2649	-3.7	11.0	C ₃₀ H ₄₁ O ₆ N ₁ S ₁
543.2609	543.2609	3.7	7.0	C ₂₅ H ₄₁ O ₈ N ₃ S ₁
543.2609	543.2609	3.7	12.5	C ₂₄ H ₃₅ O ₃ N ₁₀ S ₁
543.2649	543.2649	-3.8	-2.0	C ₁₅ H ₄₅ O ₆ N ₉ S ₃
543.2607	543.2607	4.0	4.0	C ₁₇ H ₃₇ O ₁₁ N ₉
543.2604	543.2604	4.6	6.5	C ₂₄ H ₄₃ O ₂ N ₆ S ₃
543.2654	543.2654	-4.6	4.0	C ₁₅ H ₃₇ O ₇ N ₁₃ S ₁
543.2654	543.2654	-4.6	-1.5	C ₁₆ H ₄₃ O ₁₂ N ₆ S ₁
543.2602	543.2602	4.9	-2.0	C ₁₇ H ₄₅ O ₁₀ N ₅ S ₂
543.2602	543.2602	4.9	3.5	C ₁₆ H ₃₉ O ₅ N ₁₂ S ₂
543.2656	543.2656	-5.0	7.0	C ₂₃ H ₄₁ O ₄ N ₇ S ₂
543.2656	543.2656	-5.0	1.5	C ₂₄ H ₄₇ O ₉ S ₂
543.2602	543.2602	5.0	16.5	C ₃₁ H ₃₅ O ₅ N ₄
543.2602	543.2602	5.0	22.0	C ₃₀ H ₂₉ N ₁₁

aet9-1-2 MW=468?
(DCM)/MeOH + NH4OAc

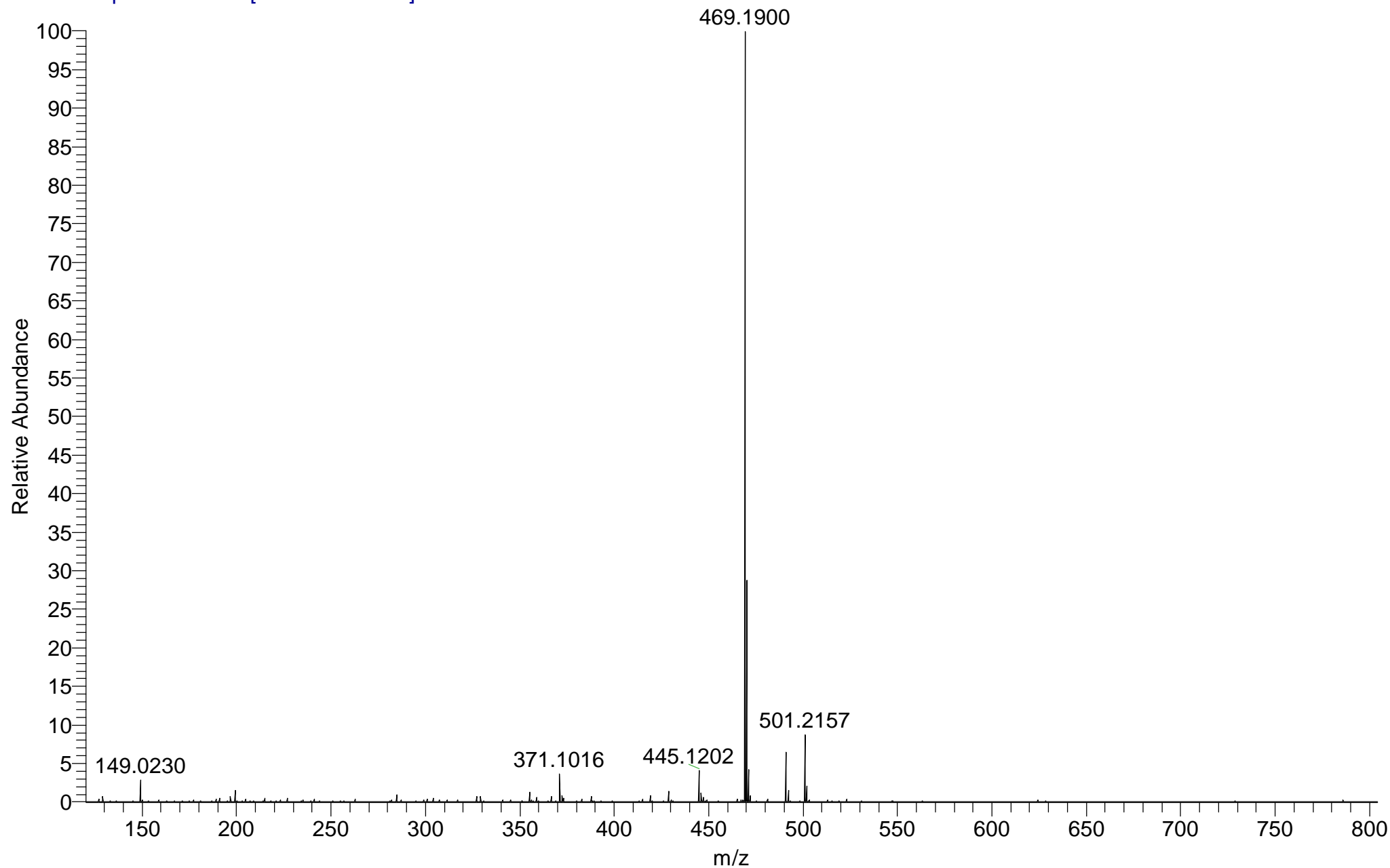
Compound 34

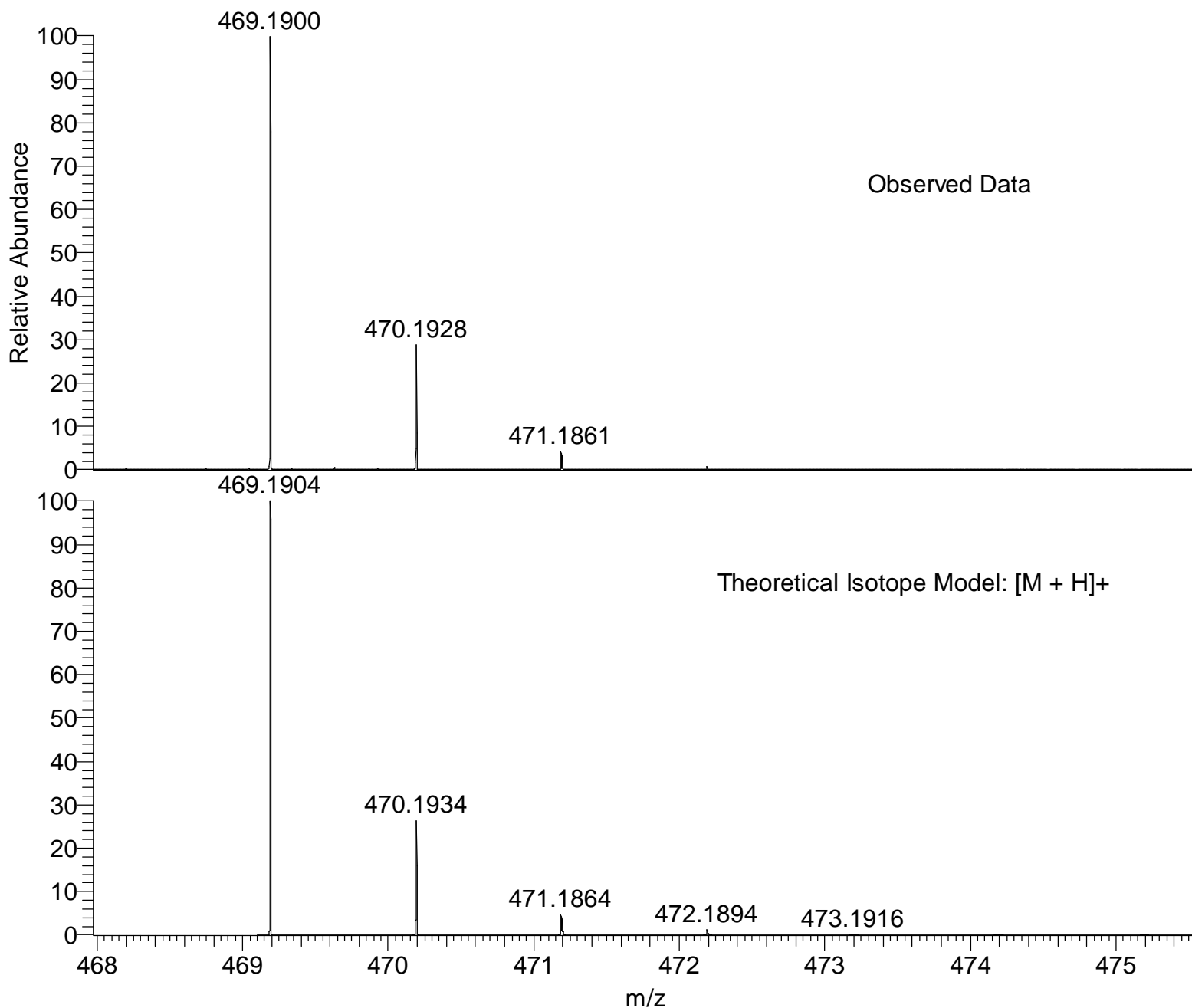
EPSRC National Centre Swansea
LTQ Orbitrap XL

adam throup
01/08/2012 10:21:47

BRASHE223-OJ-HNESP #31-49 RT: 0.75-1.28 AV: 19 SM: 7G NL: 3.30E6

T: FTMS + p NSI Full ms [120.00-2000.00]





NL:
3.30E6
BRASHE223-OJ-HNESP#31-
49 RT: 0.75-1.28 AV: 19 T:
FTMS + p NSI Full ms
[120.00-2000.00]

NL:
1.67E4
C₂₄ H₂₈ N₄ O₄ SH:
C₂₄ H₂₉ N₄ O₄ S₁
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

Isotope: Min. .. Max.
 14 N 0....14
 16 O 0....14
 12 C 0....60
 1 H 0....70
 23 Na 0....0
 32 S 0....4

Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3.. 100 N-Rule: Do not use
 Fits: 100 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
469.1900	469.1899	0.1	6.5	C ₂₄ H ₃₇ O ₃ S ₃
	469.1902	-0.5	9.5	C ₁₆ H ₂₅ O ₇ N ₁₀
	469.1902	-0.5	4.0	C ₁₇ H ₃₁ O ₁₂ N ₃
	469.1898	0.5	3.5	C ₁₆ H ₃₃ O ₆ N ₆ S ₂
	469.1897	0.5	9.0	C ₁₅ H ₂₇ O ₁ N ₁₃ S ₂
	469.1897	0.6	22.0	C ₃₀ H ₂₃ O ₁ N ₅ S ₂
	469.1904	-0.9	12.5	C ₂₄ H ₂₉ O ₄ N ₄ S ₁
	469.1896	0.9	0.5	C ₈ H ₂₉ O ₉ N ₁₂ S ₁
	469.1904	-0.9	-0.5	C ₉ H ₃₃ O ₄ N ₁₂ S ₃
	469.1906	-1.3	2.5	C ₁₇ H ₃₇ O ₁ N ₆ S ₄
	469.1893	1.5	-2.5	C ₁₆ H ₄₁ O ₅ N ₂ S ₄
	469.1893	1.5	3.0	C ₁₅ H ₃₅ N ₉ S ₄
	469.1892	1.6	16.0	C ₃₀ H ₃₁ N ₁ S ₂
	469.1909	-1.9	0.0	C ₁₀ H ₃₁ O ₁₀ N ₉ S ₁
	469.1891	2.0	7.5	C ₂₃ H ₃₃ O ₈ S ₁
	469.1891	2.0	13.0	C ₂₂ H ₂₇ O ₃ N ₇ S ₁
	469.1911	-2.2	21.5	C ₃₂ H ₂₅ O ₂ N ₂ S ₂
	469.1911	-2.3	8.5	C ₁₇ H ₂₉ O ₂ N ₁₀ S ₂
	469.1911	-2.3	3.0	C ₁₈ H ₃₅ O ₇ N ₃ S ₂
	469.1889	2.4	4.5	C ₁₅ H ₂₉ O ₁₁ N ₆
	469.1889	2.4	10.0	C ₁₄ H ₂₃ O ₆ N ₁₃
	469.1886	3.0	7.0	C ₂₂ H ₃₅ O ₂ N ₃ S ₃
	469.1916	-3.3	14.5	C ₁₇ H ₂₁ O ₃ N ₁₄
	469.1916	-3.3	9.0	C ₁₈ H ₂₇ O ₈ N ₇
	469.1916	-3.3	3.5	C ₁₉ H ₃₃ O ₁₃
	469.1884	3.4	-1.5	C ₁₅ H ₃₇ O ₁₀ N ₂ S ₂
	469.1884	3.4	4.0	C ₁₄ H ₃₁ O ₅ N ₉ S ₂
	469.1884	3.5	17.0	C ₂₉ H ₂₇ O ₅ N ₁
	469.1884	3.5	22.5	C ₂₈ H ₂₁ N ₈
	469.1917	-3.7	17.5	C ₂₅ H ₂₅ N ₈ S ₁
	469.1917	-3.7	12.0	C ₂₆ H ₃₁ O ₅ N ₁ S ₁

aet9-2-2 MW=510?
(DCM)/MeOH + NH4OAc

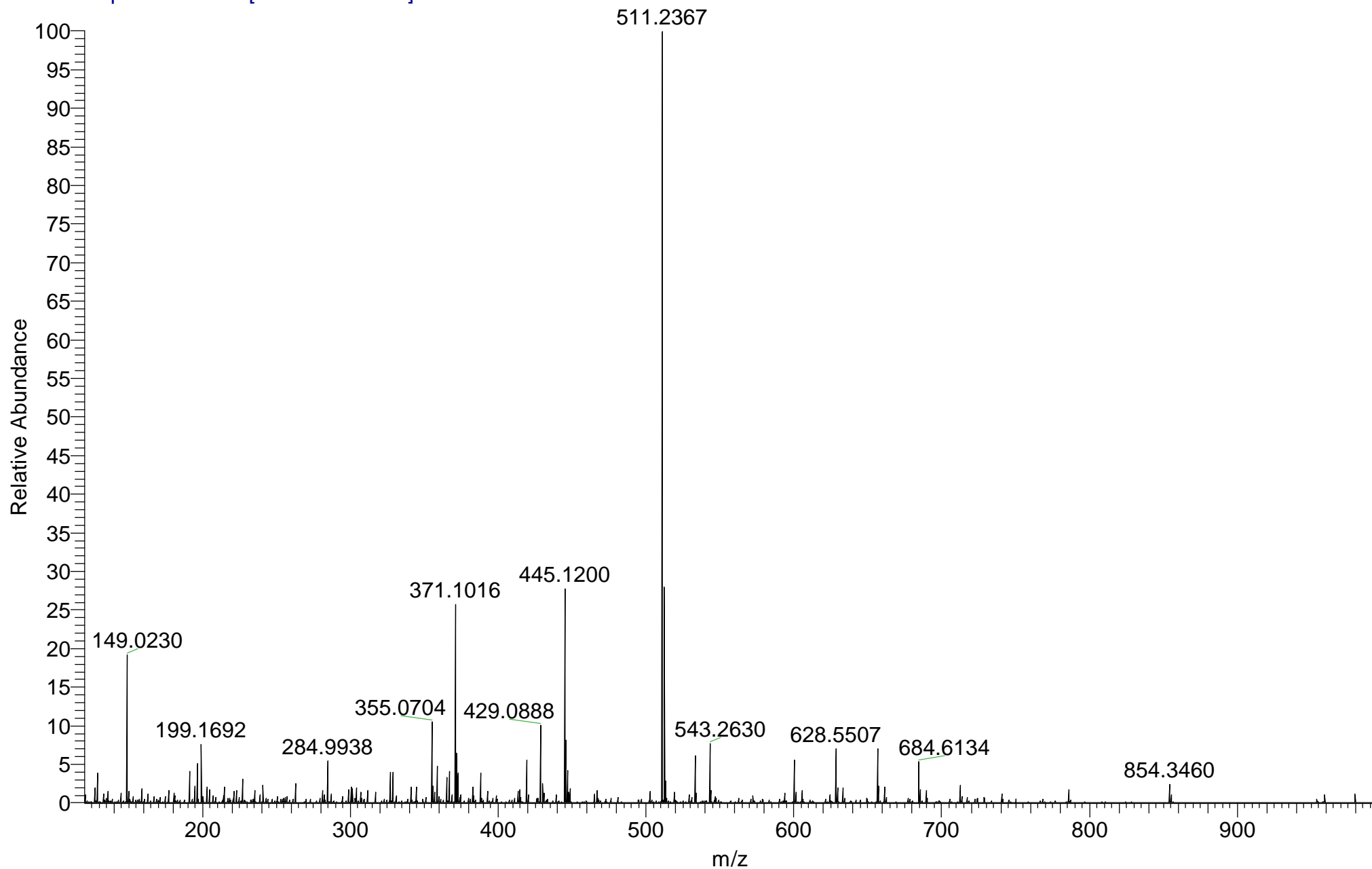
Compound 35

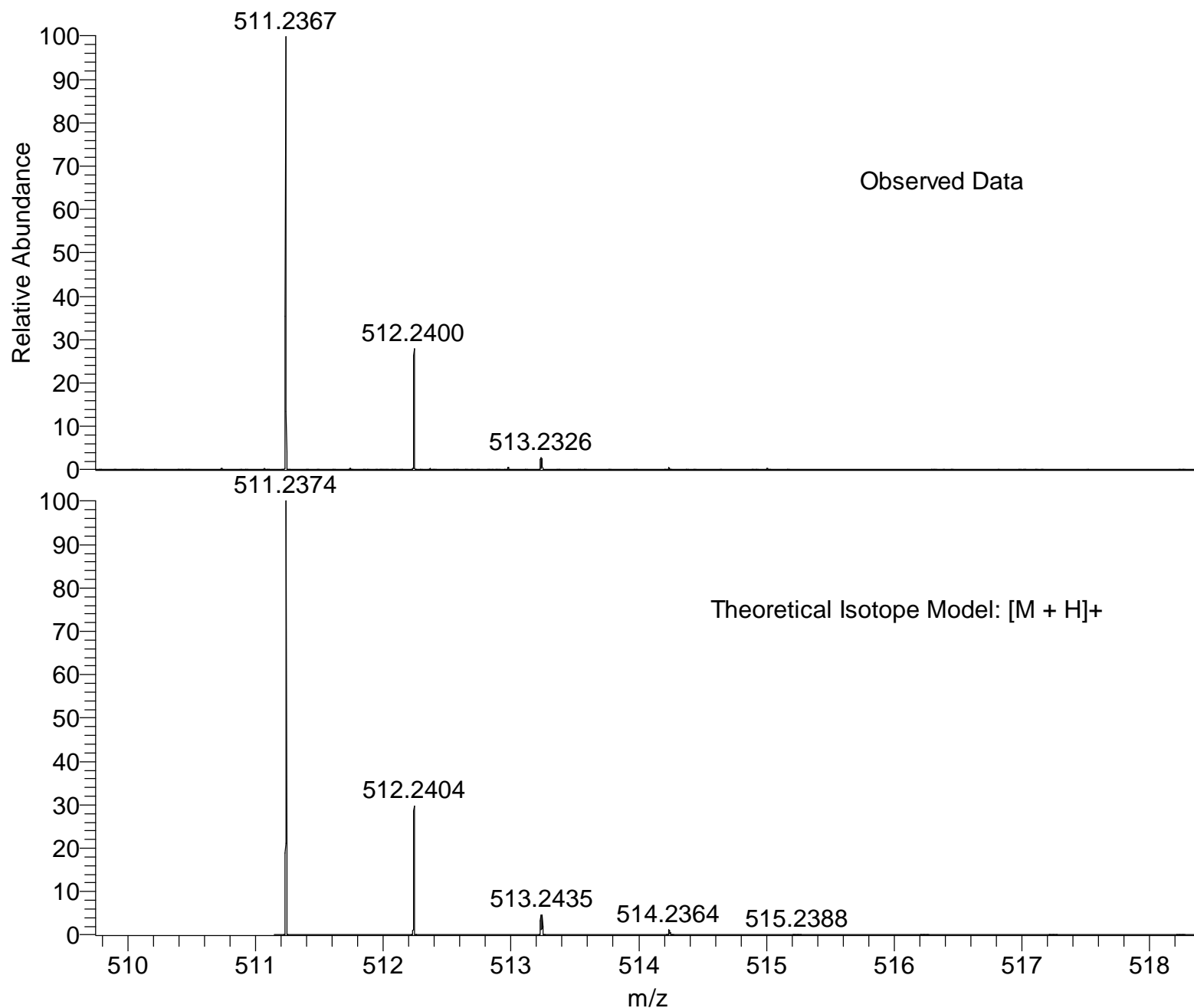
EPSRC National Centre Swansea
LTQ Orbitrap XL

adam throup
01/08/2012 10:25:14

BRASHE224-OJ-HNESP #29-50 RT: 0.71-1.29 AV: 21 SM: 7G NL: 4.81E5

T: FTMS + p NSI Full ms [120.00-2000.00]





NL:
4.81E5
BRASHE224-OJ-HNESP#29-
50 RT: 0.71-1.29 AV: 21 T:
FTMS + p NSI Full ms
[120.00-2000.00]

NL:
1.62E4
C₂₇ H₃₄ N₄ O₄ SH:
C₂₇ H₃₅ N₄ O₄ S₁
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

Isotope: Min. .. Max.
 14 N 0....14
 16 O 0....14
 12 C 0....60
 1 H 0....75
 23 Na 0....0
 32 S 0....4

Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3.. 100 N-Rule: Do not use
 Fits: 100 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
511.2367	511.2367	-0.0	3.5	C ₁₉ H ₃₉ O ₆ N ₆ S ₂
	511.2367	0.0	9.0	C ₁₈ H ₃₃ O ₁ N ₁₃ S ₂
	511.2367	0.1	22.0	C ₃₃ H ₂₉ O ₁ N ₅
	511.2365	0.4	0.5	C ₁₁ H ₃₅ O ₉ N ₁₂ S ₁
	511.2369	-0.4	6.5	C ₂₇ H ₄₃ O ₃ S ₃
	511.2362	0.9	-2.5	C ₁₉ H ₄₇ O ₅ N ₂ S ₄
	511.2372	-0.9	9.5	C ₁₉ H ₃₁ O ₇ N ₁₀
	511.2362	0.9	3.0	C ₁₈ H ₄₁ N ₉ S ₄
	511.2372	-0.9	4.0	C ₂₀ H ₃₇ O ₁₂ N ₃
	511.2362	1.0	16.0	C ₃₃ H ₃₇ N ₁ S ₂
	511.2374	-1.3	12.5	C ₂₇ H ₃₅ O ₄ N ₄ S ₁
	511.2360	1.3	7.5	C ₂₆ H ₃₉ O ₈ S ₁
	511.2374	-1.3	-0.5	C ₁₂ H ₃₉ O ₄ N ₁₂ S ₃
	511.2360	1.3	13.0	C ₂₅ H ₃₃ O ₃ N ₇ S ₁
	511.2358	1.7	4.5	C ₁₈ H ₃₅ O ₁₁ N ₆
	511.2376	-1.7	2.5	C ₂₀ H ₄₃ O ₁ N ₆ S ₄
	511.2358	1.7	10.0	C ₁₇ H ₂₉ O ₆ N ₁₃
	511.2355	2.3	7.0	C ₂₅ H ₄₁ O ₂ N ₃ S ₃
	511.2379	-2.3	0.0	C ₁₃ H ₃₇ O ₁₀ N ₉ S ₁
	511.2380	-2.6	21.5	C ₃₅ H ₃₁ O ₂ N ₂
	511.2354	2.6	-1.5	C ₁₈ H ₄₃ O ₁₀ N ₂ S ₂
	511.2380	-2.6	8.5	C ₂₀ H ₃₅ O ₂ N ₁₀ S ₂
	511.2354	2.6	4.0	C ₁₇ H ₃₇ O ₅ N ₉ S ₂
	511.2380	-2.6	3.0	C ₂₁ H ₄₁ O ₇ N ₃ S ₂
	511.2353	2.7	17.0	C ₃₂ H ₃₃ O ₅ N ₁
	511.2353	2.7	22.5	C ₃₁ H ₂₇ N ₈
	511.2385	-3.5	14.5	C ₂₀ H ₂₇ O ₃ N ₁₄
	511.2349	3.5	-2.0	C ₁₇ H ₄₅ O ₄ N ₅ S ₄
	511.2385	-3.5	9.0	C ₂₁ H ₃₃ O ₈ N ₇
	511.2385	-3.6	3.5	C ₂₂ H ₃₉ O ₁₃
	511.2387	-3.9	17.5	C ₂₈ H ₃₁ N ₈ S ₁

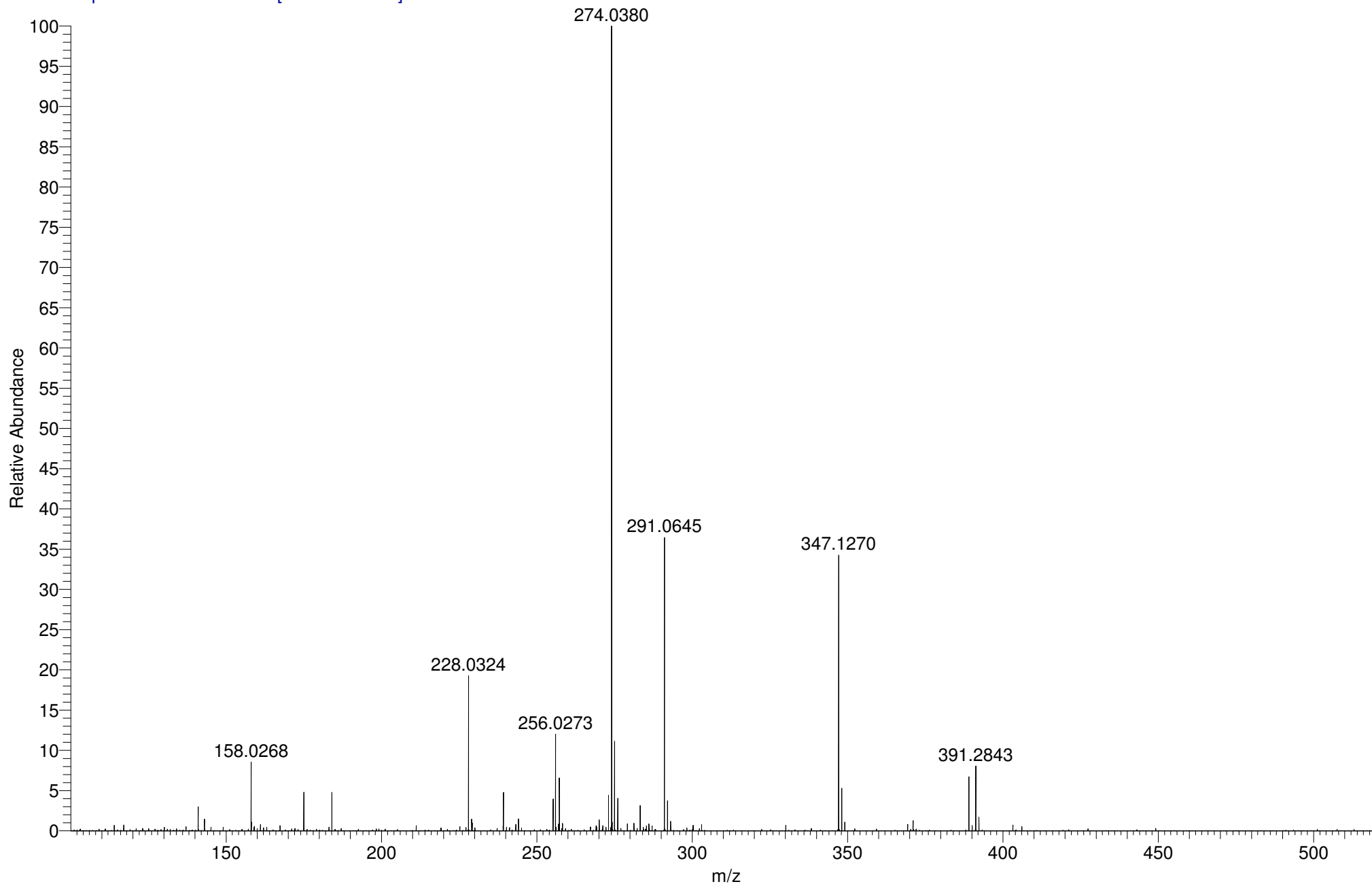
AET9-6 MW=329?
ASAP(SOLID + NH4OAc)

Compound 36

EPSRC National Centre Swansea
LTQ Orbitrap XL

Throup
06/11/2012 12:06:57

BRASHE233-PG-HASP #135-137 RT: 3.87-3.92 AV: 3 SM: 7G NL: 2.04E7
T: FTMS + p APCI corona Full ms [100.00-800.00]

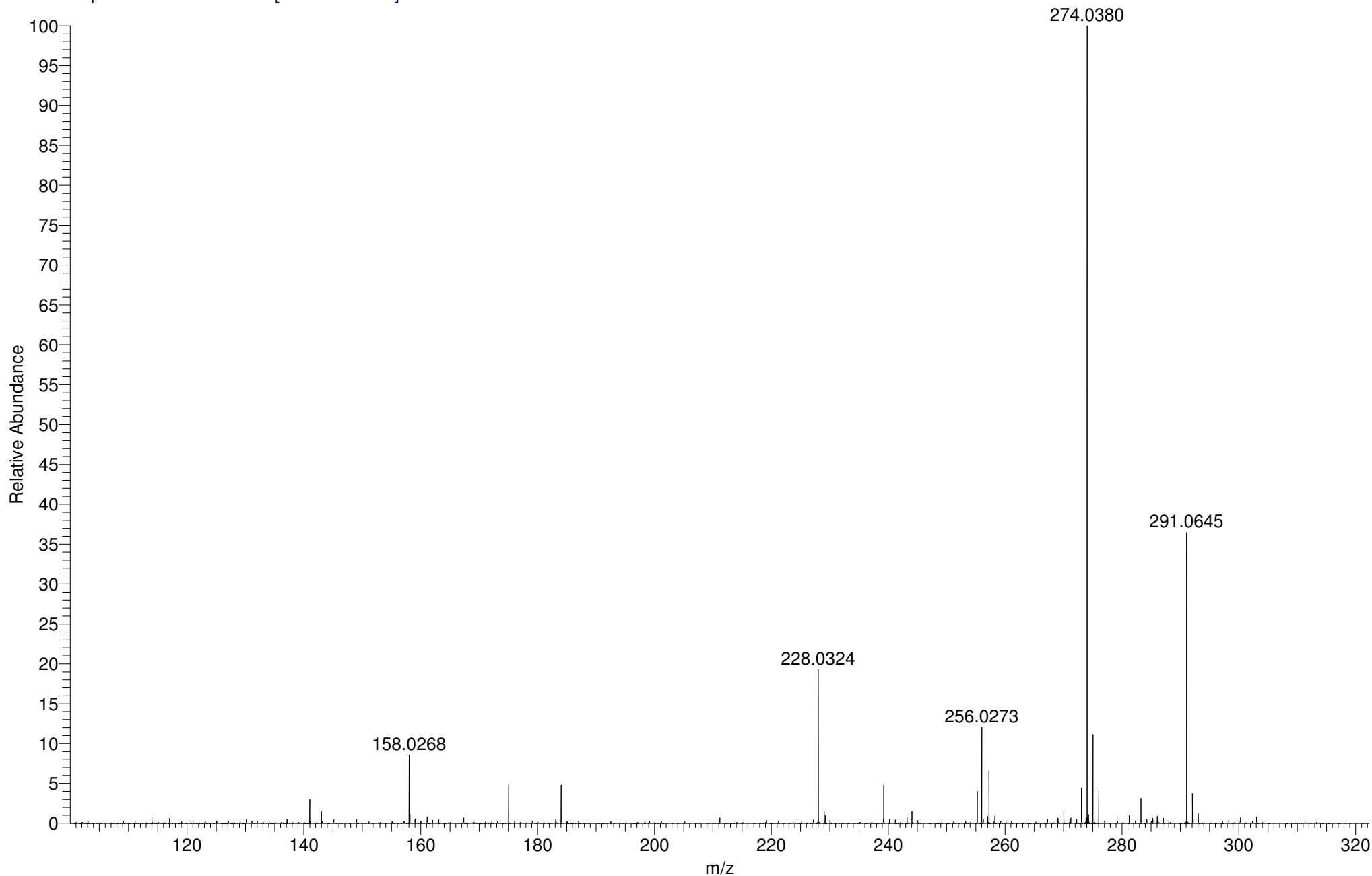


AET9-6 MW=329?
ASAP(SOLID + NH4OAc)

EPSRC National Centre Swansea
LTQ Orbitrap XL

Thrup
06/11/2012 12:06:57

BRASHE233-PG-HASP #135-137 RT: 3.87-3.92 AV: 3 SM: 7G NL: 2.04E7
T: FTMS + p APCI corona Full ms [100.00-800.00]

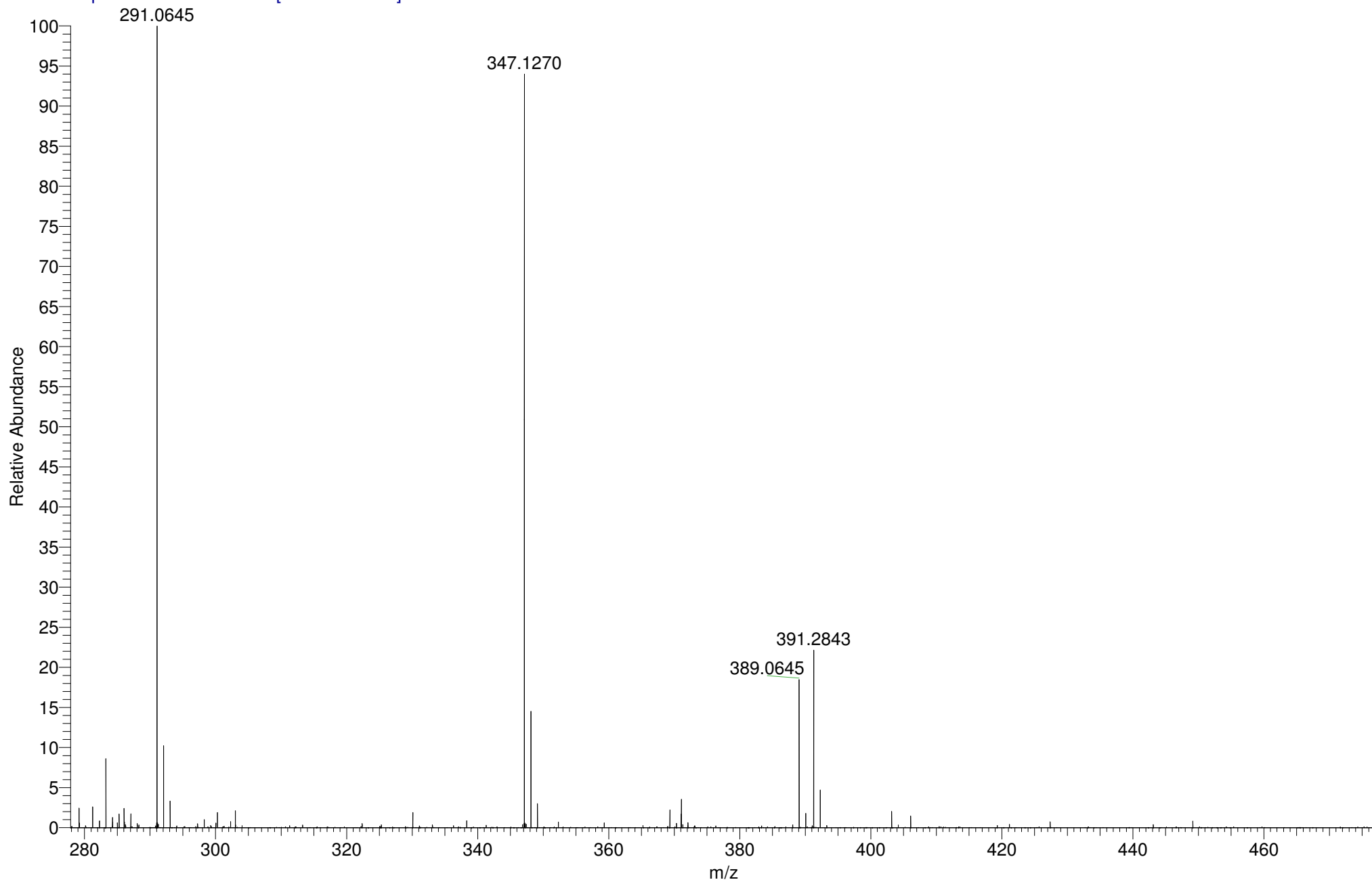


AET9-6 MW=329?
ASAP(SOLID + NH4OAc)

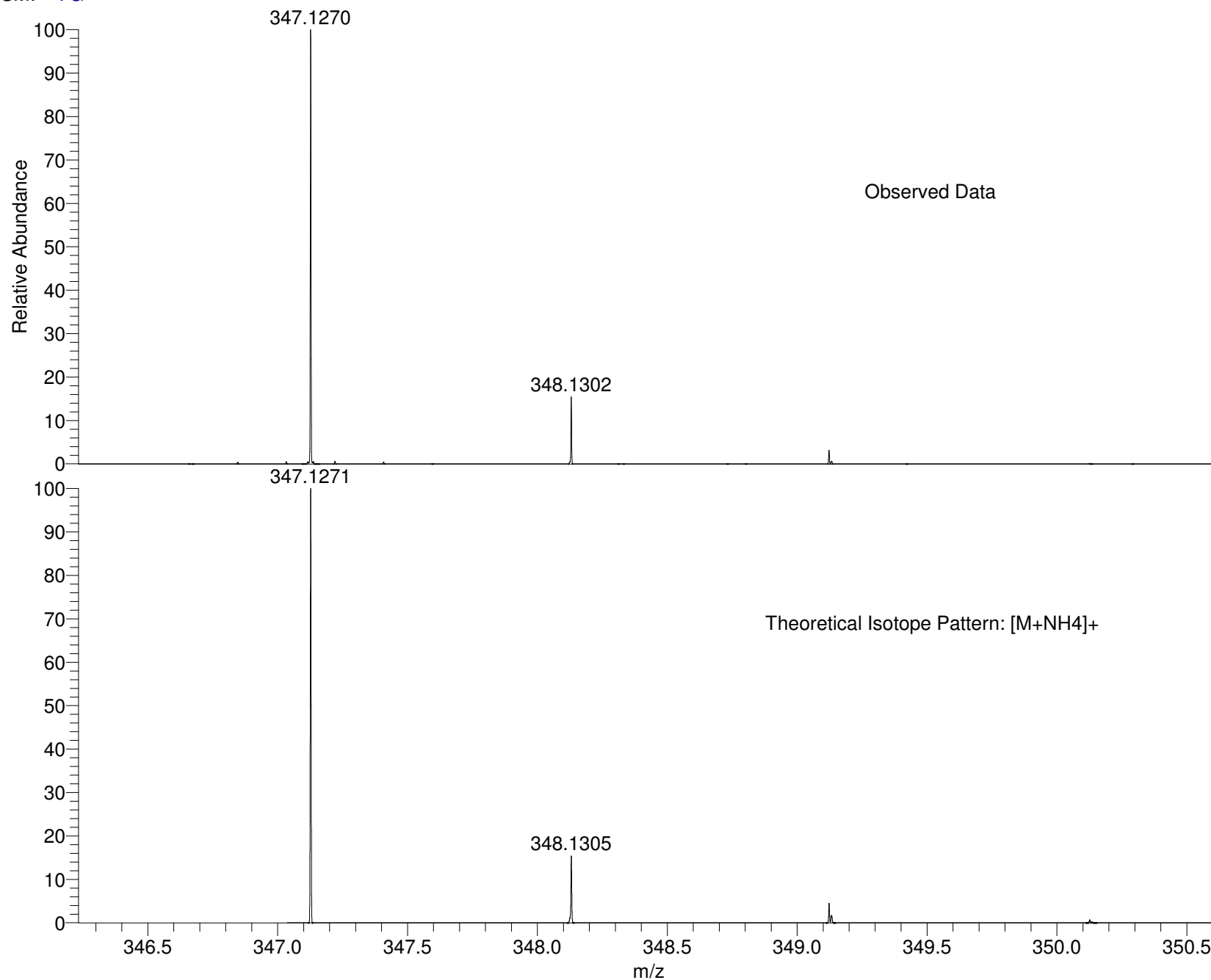
EPSRC National Centre Swansea
LTQ Orbitrap XL

Thrup
06/11/2012 12:06:57

BRASHE233-PG-HASP #135-137 RT: 3.87-3.92 AV: 3 SM: 7G NL: 7.44E6
T: FTMS + p APCI corona Full ms [100.00-800.00]



SM: 7G



NL:
7.00E6
BRASHE233-PG-HASP#135-
137 RT: 3.87-3.92 AV: 3 T:
FTMS + p APCI corona Full ms
[100.00-800.00]

NL:
1.87E4
C₁₄H₁₉NO₆SNH₄:
C₁₄H₂₃N₂O₆S₁
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

Isotope: Min. .. Max.
 14 N 0....16
 16 O 0....15
 12 C 0....80
 1 H 0....100
 23 Na 0....0
 32 S 0....3
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3.. 100
 Fits: 100

N-Rule: Do not use
 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
347.1270	347.1270	0.1	1.5	C ₆ H ₁₉ O ₉ N ₈
	347.1269	0.2	7.0	C ₅ H ₁₃ O ₄ N ₁₅
	347.1271	-0.4	10.0	C ₁₃ H ₁₇ O ₁ N ₉ S ₁
	347.1271	-0.4	4.5	C ₁₄ H ₂₃ O ₆ N ₂ S ₁
	347.1267	1.0	4.0	C ₁₃ H ₂₅ N ₅ S ₃
	347.1265	1.5	1.0	C ₅ H ₂₁ O ₃ N ₁₁ S ₂
	347.1264	1.6	14.0	C ₂₀ H ₁₇ O ₃ N ₃
	347.1278	-2.3	13.5	C ₂₂ H ₁₉ O ₄
	347.1278	-2.4	0.5	C ₇ H ₂₃ O ₄ N ₈ S ₂
	347.1280	-2.9	3.5	C ₁₅ H ₂₇ O ₁ N ₂ S ₃
	347.1258	3.5	5.0	C ₁₂ H ₂₁ O ₅ N ₅ S ₁
	347.1258	3.5	10.5	C ₁₁ H ₁₅ N ₁₂ S ₁
	347.1283	-3.7	6.5	C ₇ H ₁₅ O ₅ N ₁₂
	347.1283	-3.7	1.0	C ₈ H ₂₁ O ₁₀ N ₅
	347.1256	4.0	2.0	C ₄ H ₁₇ O ₈ N ₁₁
	347.1285	-4.2	9.5	C ₁₅ H ₁₉ O ₂ N ₆ S ₁
	347.1253	4.8	-1.0	C ₁₂ H ₂₉ O ₄ N ₁ S ₃

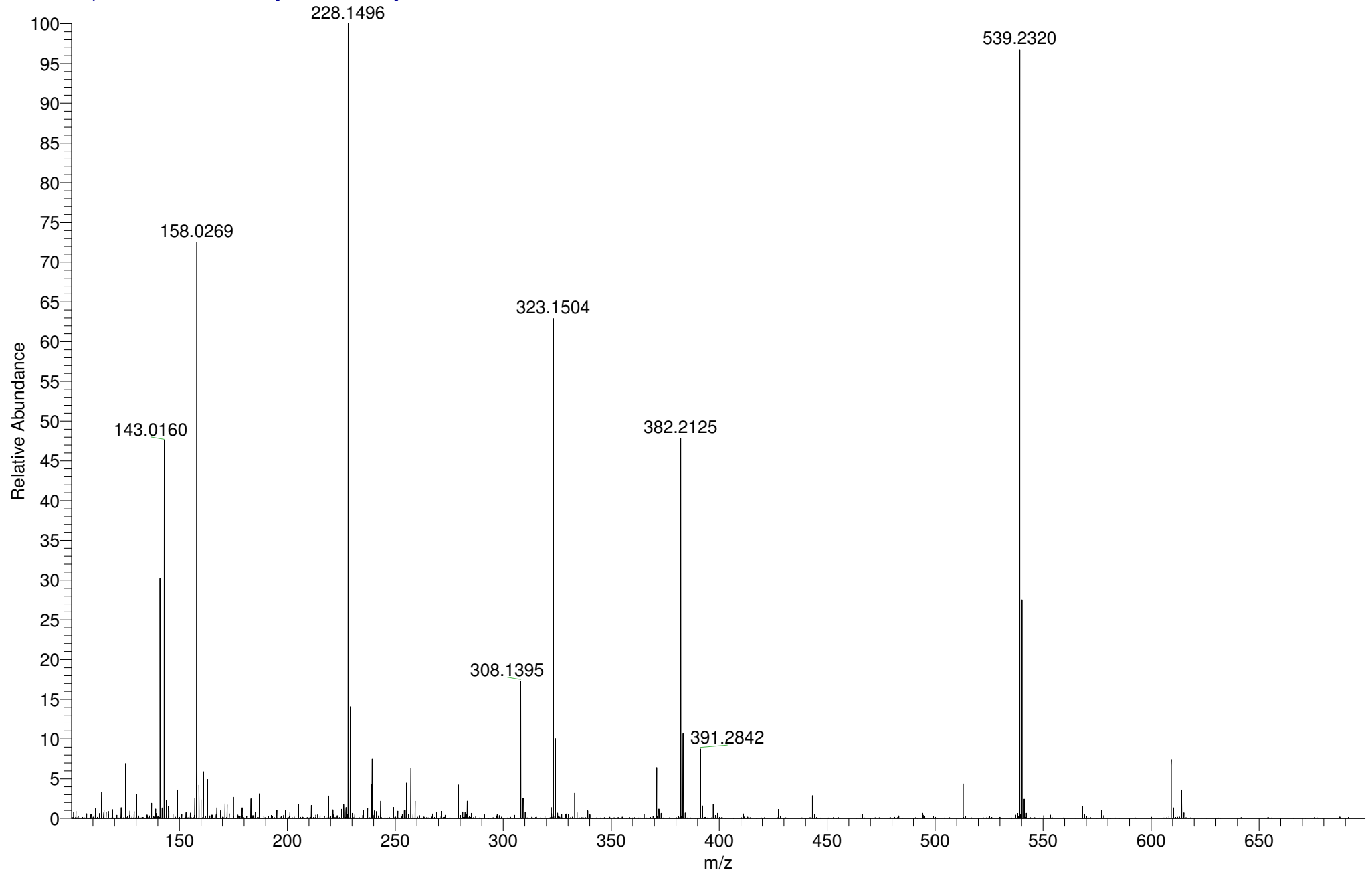
Compound 37

AET9-8 MW=538?
ASAP(SOLID)

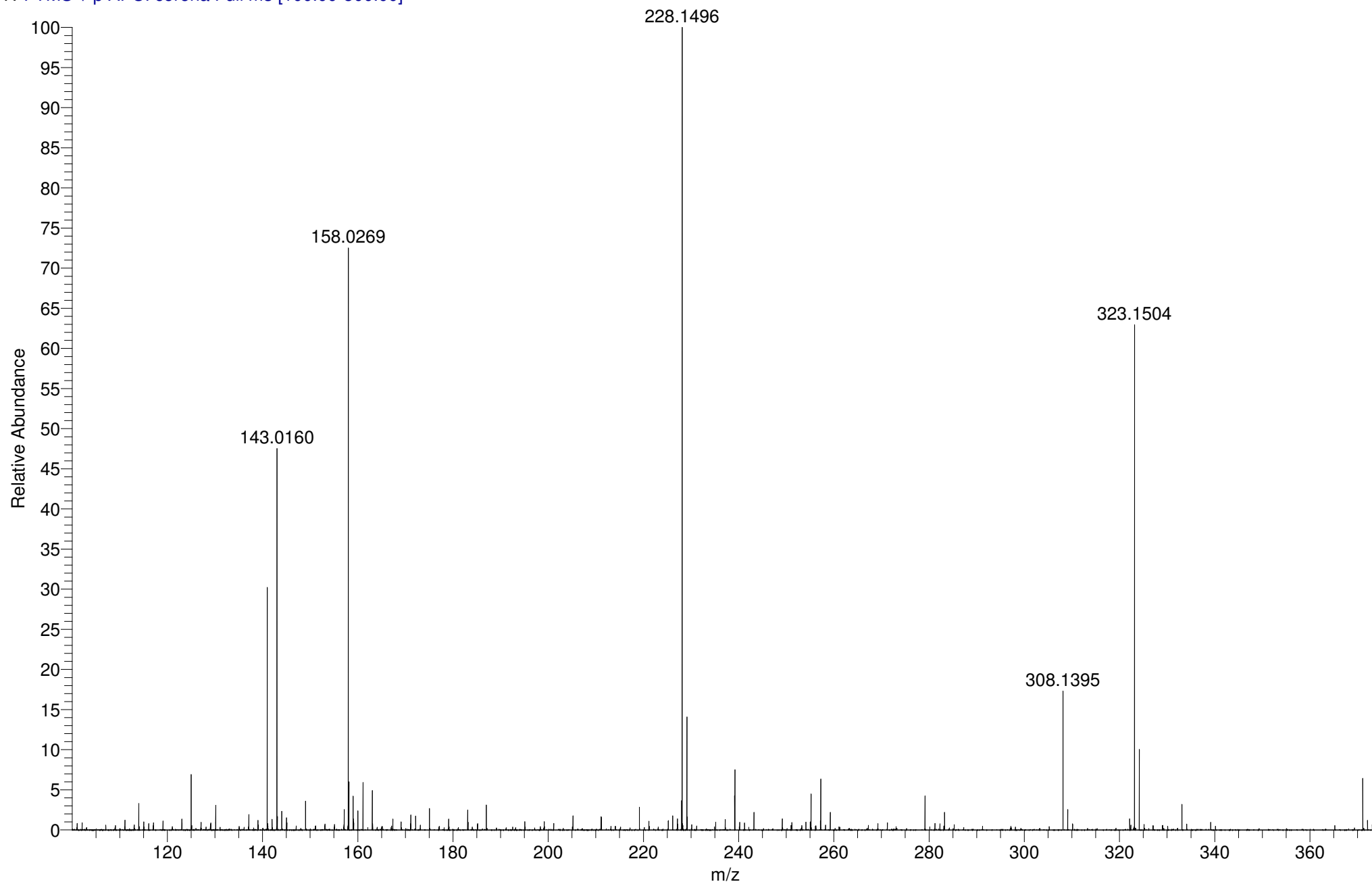
EPSRC National Centre Swansea
LTQ Orbitrap XL

Throup
06/11/2012 11:52:53

BRASHE231-PG-HASP #27-30 RT: 0.75-0.84 AV: 4 SM: 7G NL: 3.59E6
T: FTMS + p APCI corona Full ms [100.00-800.00]



BRASHE231-PG-HASP #27-30 RT: 0.75-0.84 AV: 4 SM: 7G NL: 3.59E6
T: FTMS + p APCI corona Full ms [100.00-800.00]

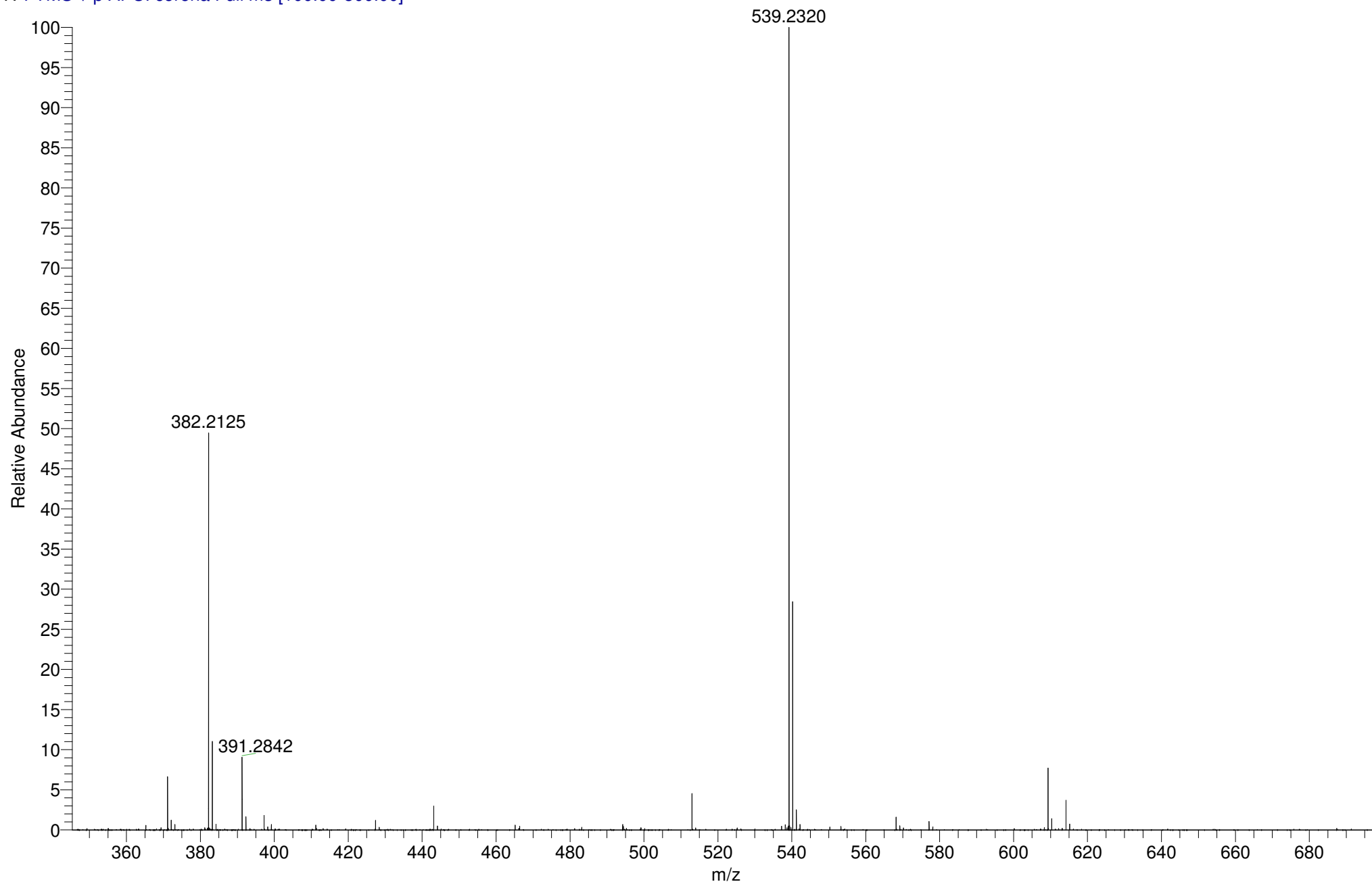


AET9-8 MW=538?
ASAP(SOLID)

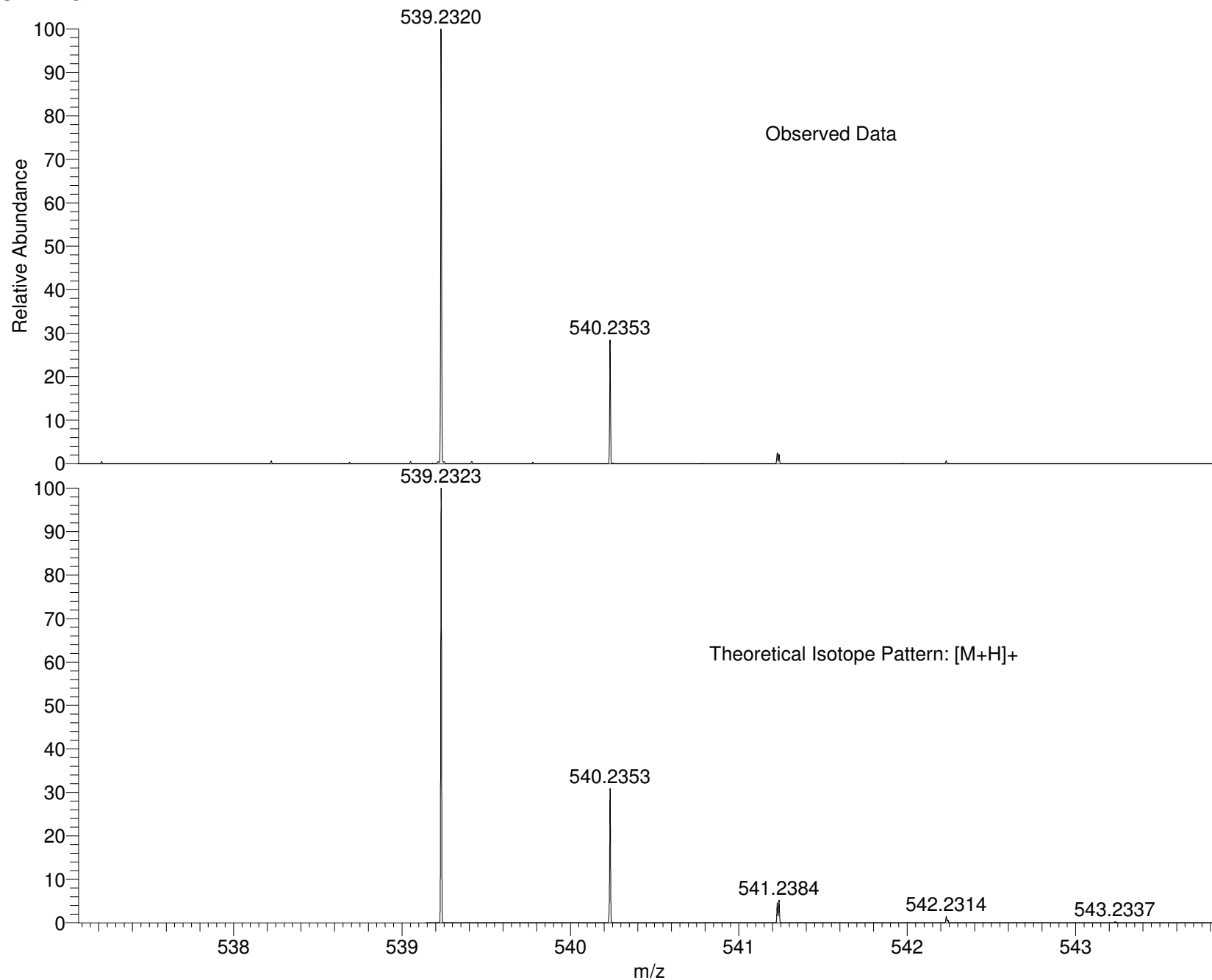
EPSRC National Centre Swansea
LTQ Orbitrap XL

Thrup
06/11/2012 11:52:53

BRASHE231-PG-HASP #27-30 RT: 0.75-0.84 AV: 4 SM: 7G NL: 3.47E6
T: FTMS + p APCI corona Full ms [100.00-800.00]



SM: 7G



NL:
3.47E6
BRASHE231-PG-HASP#27-30
RT: 0.75-0.84 AV: 4 T: FTMS
+ p APCI corona Full ms
[100.00-800.00]

NL:
1.60E4
C₂₈H₃₄N₄O₅SH:
C₂₈H₃₅N₄O₅S₁
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

Isotope: Min. .. Max.
 14 N 0....16
 16 O 0....15
 12 C 0....80
 1 H 0....100
 23 Na 0....0
 32 S 0....3
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3.. 100
 Fits: 100

N-Rule: Do not use
 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
539.2320	539.2321	-0.2	10.5	C ₂₀ H ₃₁ O ₈ N ₁₀
	539.2321	-0.2	5.0	C ₂₁ H ₃₇ O ₁₃ N ₃
	539.2318	0.4	7.5	C ₂₈ H ₄₃ O ₄ S ₃
	539.2323	-0.5	19.0	C ₂₇ H ₂₉ N ₁₁ S ₁
	539.2323	-0.5	13.5	C ₂₈ H ₃₅ O ₅ N ₄ S ₁
	539.2323	-0.6	0.5	C ₁₃ H ₃₉ O ₅ N ₁₂ S ₃
	539.2316	0.7	4.5	C ₂₀ H ₃₉ O ₇ N ₆ S ₂
	539.2316	0.7	10.0	C ₁₉ H ₃₃ O ₂ N ₁₃ S ₂
	539.2316	0.8	23.0	C ₃₄ H ₂₉ O ₂ N ₅
	539.2314	1.1	1.5	C ₁₂ H ₃₅ O ₁₀ N ₁₂ S ₁
	539.2326	-1.1	-2.0	C ₆ H ₃₃ O ₁₄ N ₁₅
	539.2328	-1.4	6.5	C ₁₃ H ₃₁ O ₆ N ₁₆ S ₁
	539.2328	-1.4	1.0	C ₁₄ H ₃₇ O ₁₁ N ₉ S ₁
	539.2311	1.7	17.0	C ₃₄ H ₃₇ O ₁ N ₁ S ₂
	539.2329	-1.7	22.5	C ₃₄ H ₃₁ O ₃ N ₂
	539.2330	-1.8	9.5	C ₂₁ H ₃₅ O ₃ N ₁₀ S ₂
	539.2330	-1.8	4.0	C ₂₂ H ₄₁ O ₈ N ₃ S ₂
	539.2310	1.9	1.0	C ₁₁ H ₃₇ O ₄ N ₁₅ S ₃
	539.2309	2.0	8.5	C ₂₇ H ₃₉ O ₉ S ₁
	539.2309	2.0	14.0	C ₂₆ H ₃₃ O ₄ N ₇ S ₁
	539.2331	-2.1	12.5	C ₂₉ H ₃₉ N ₄ S ₃
	539.2307	2.3	5.5	C ₁₉ H ₃₅ O ₁₂ N ₆
	539.2307	2.3	11.0	C ₁₈ H ₂₉ O ₇ N ₁₃
	539.2334	-2.6	15.5	C ₂₁ H ₂₇ O ₄ N ₁₄
	539.2334	-2.6	10.0	C ₂₂ H ₃₃ O ₉ N ₇
	539.2334	-2.7	4.5	C ₂₃ H ₃₉ O ₁₄
	539.2335	-2.7	-3.0	C ₇ H ₃₇ O ₉ N ₁₅ S ₂
	539.2305	2.9	8.0	C ₂₆ H ₄₁ O ₃ N ₃ S ₃
	539.2336	-3.0	18.5	C ₂₉ H ₃₁ O ₁ N ₈ S ₁
	539.2336	-3.0	13.0	C ₃₀ H ₃₇ O ₆ N ₁ S ₁
	539.2336	-3.0	5.5	C ₁₄ H ₃₅ O ₁ N ₁₆ S ₃

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
539.2336		-3.0	0.0	C ₁₅ H ₄₁ O ₆ N ₉ S ₃
539.2303		3.2	-0.5	C ₁₉ H ₄₃ O ₁₁ N ₂ S ₂
539.2303		3.2	5.0	C ₁₈ H ₃₇ O ₆ N ₉ S ₂
539.2303		3.2	10.5	C ₁₇ H ₃₁ O ₁ N ₁₆ S ₂
539.2302		3.3	18.0	C ₃₃ H ₃₃ O ₆ N ₁
539.2302		3.3	23.5	C ₃₂ H ₂₇ O ₁ N ₈
539.2301		3.5	2.0	C ₁₀ H ₃₃ O ₉ N ₁₅ S ₁
539.2339		-3.6	-2.5	C ₈ H ₃₅ O ₁₅ N ₁₂
539.2341		-3.9	6.0	C ₁₅ H ₃₃ O ₇ N ₁₃ S ₁
539.2341		-3.9	0.5	C ₁₆ H ₃₉ O ₁₂ N ₆ S ₁
539.2298		4.1	17.5	C ₃₂ H ₃₅ N ₄ S ₂
539.2343		-4.3	9.0	C ₂₃ H ₃₇ O ₄ N ₇ S ₂
539.2343		-4.3	3.5	C ₂₄ H ₄₃ O ₉ S ₂
539.2296		4.5	9.0	C ₂₅ H ₃₇ O ₈ N ₃ S ₁
539.2296		4.5	14.5	C ₂₄ H ₃₁ O ₃ N ₁₀ S ₁
539.2345		-4.6	12.0	C ₃₁ H ₄₁ O ₁ N ₁ S ₃
539.2294		4.8	6.0	C ₁₇ H ₃₃ O ₁₁ N ₉
539.2294		4.8	11.5	C ₁₆ H ₂₇ O ₆ N ₁₆

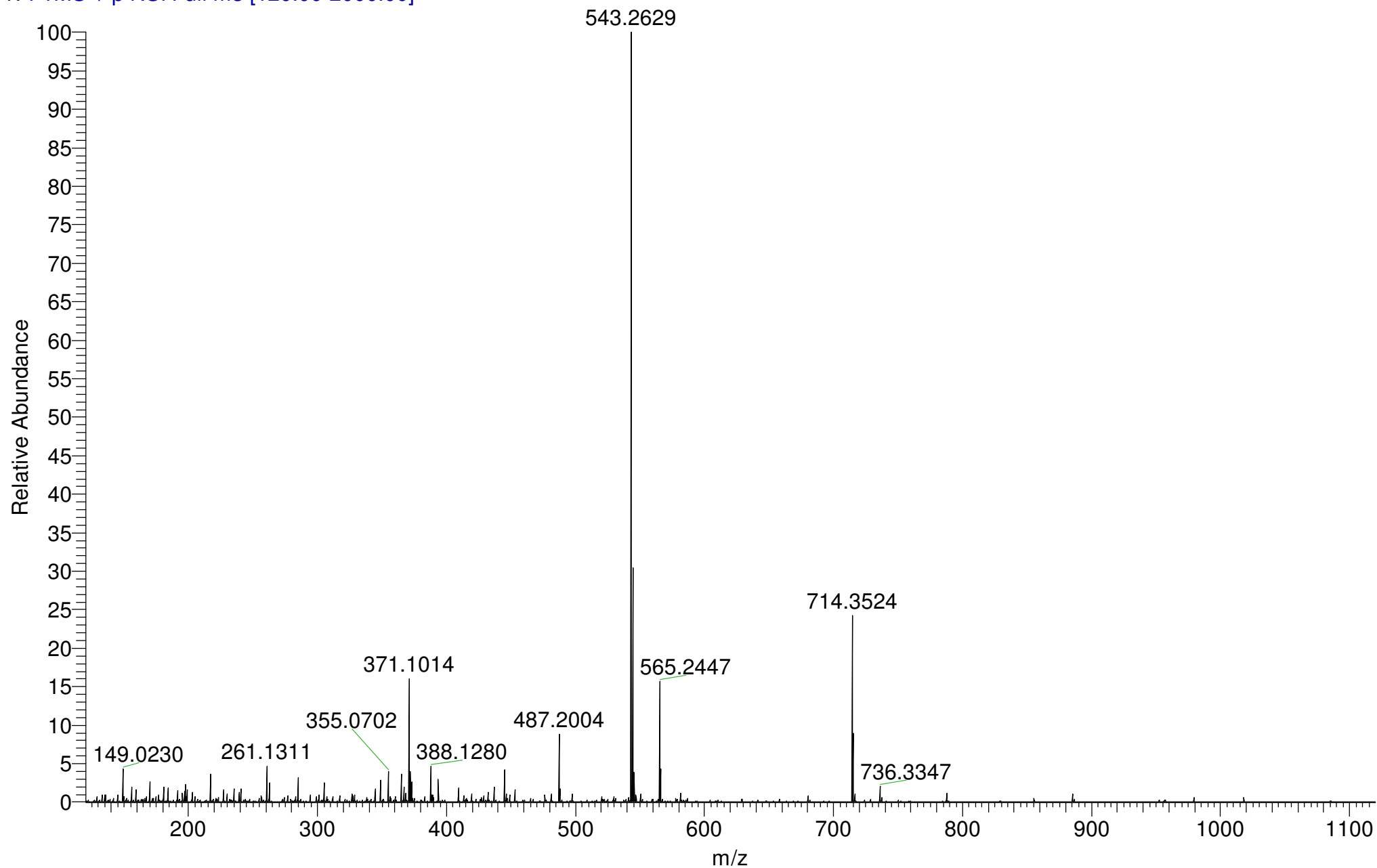
AET9-12 MW=542?
(DCM)/MeOH + NH4OAc

Compound 39

EPSRC National Centre Swansea
LTQ Orbitrap XL

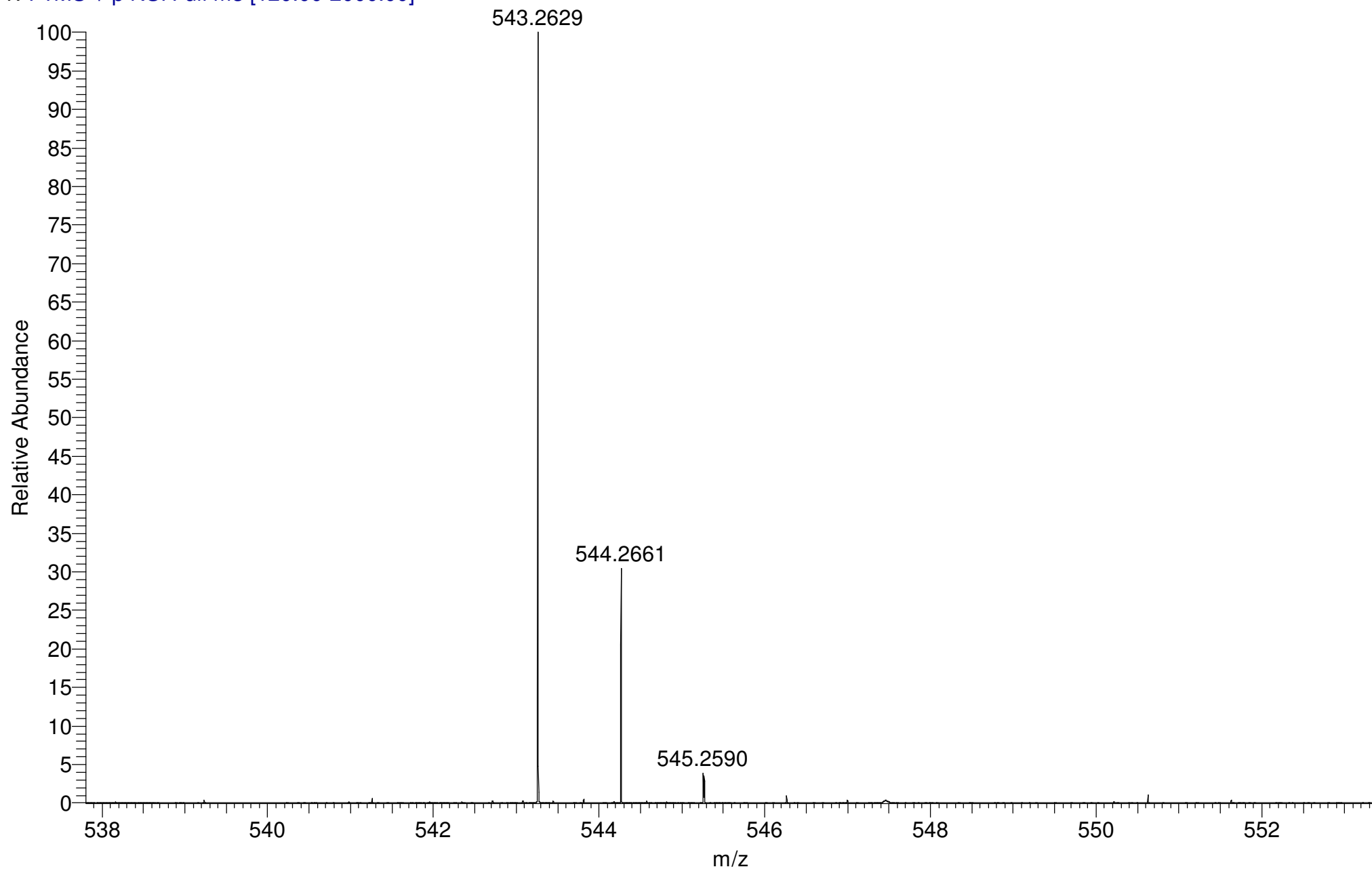
adam throup
06/11/2012 11:01:27

BRASHE230-OJ-HNESP #31-49 RT: 0.77-1.28 AV: 19 SM: 7G NL: 5.17E6
T: FTMS + p NSI Full ms [120.00-2000.00]



BRASHE230-OJ-HNESP #31-49 RT: 0.77-1.28 AV: 19 SM: 7G NL: 5.17E6

T: FTMS + p NSI Full ms [120.00-2000.00]



Isotope: Min. .. Max.
 12 C 0....60
 1 H 0....70
 14 N 0....15
 16 O 0....15
 23 Na 0....0
 32 S 0....3
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3.. 100
 Fits: 100

N-Rule: Do not use
 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
543.2629	543.2629	-0.0	8.0	C ₁₉ H ₃₇ O ₂ N ₁₃ S ₂
	543.2629	-0.0	2.5	C ₂₀ H ₄₃ O ₇ N ₆ S ₂
	543.2629	0.0	21.0	C ₃₄ H ₃₃ O ₂ N ₅
	543.2627	0.3	-0.5	C ₁₂ H ₃₉ O ₁₀ N ₁₂ S ₁
	543.2631	-0.4	5.5	C ₂₈ H ₄₇ O ₄ S ₃
	543.2634	-0.9	8.5	C ₂₀ H ₃₅ O ₈ N ₁₀
	543.2634	-0.9	3.0	C ₂₁ H ₄₁ O ₁₃ N ₃
	543.2624	0.9	15.0	C ₃₄ H ₄₁ O ₁ N ₁ S ₂
	543.2623	1.2	-1.0	C ₁₁ H ₄₁ O ₄ N ₁₅ S ₃
	543.2636	-1.2	17.0	C ₂₇ H ₃₃ N ₁₁ S ₁
	543.2636	-1.2	11.5	C ₂₈ H ₃₉ O ₅ N ₄ S ₁
	543.2622	1.2	6.5	C ₂₇ H ₄₃ O ₉ S ₁
	543.2622	1.2	12.0	C ₂₆ H ₃₇ O ₄ N ₇ S ₁
	543.2636	-1.3	-1.5	C ₁₃ H ₄₃ O ₅ N ₁₂ S ₃
	543.2620	1.6	3.5	C ₁₉ H ₃₉ O ₁₂ N ₆
	543.2620	1.6	9.0	C ₁₈ H ₃₃ O ₇ N ₁₃
	543.2618	2.1	6.0	C ₂₆ H ₄₅ O ₃ N ₃ S ₃
	543.2641	-2.2	-1.0	C ₁₄ H ₄₁ O ₁₁ N ₉ S ₁
	543.2642	-2.4	20.5	C ₃₆ H ₃₅ O ₃ N ₂
	543.2616	2.4	-2.5	C ₁₉ H ₄₇ O ₁₁ N ₂ S ₂
	543.2616	2.4	3.0	C ₁₈ H ₄₁ O ₆ N ₉ S ₂
	543.2643	-2.5	7.5	C ₂₁ H ₃₉ O ₃ N ₁₀ S ₂
	543.2643	-2.5	2.0	C ₂₂ H ₄₅ O ₈ N ₃ S ₂
	543.2615	2.5	16.0	C ₃₃ H ₃₇ O ₆ N ₁
	543.2615	2.5	21.5	C ₃₂ H ₃₁ O ₁ N ₈
	543.2614	2.8	0.0	C ₁₀ H ₃₇ O ₉ N ₁₅ S ₁
	543.2644	-2.8	10.5	C ₂₉ H ₄₃ N ₄ S ₃
	543.2647	-3.4	13.5	C ₂₁ H ₃₁ O ₄ N ₁₄
	543.2647	-3.4	8.0	C ₂₂ H ₃₇ O ₉ N ₇
	543.2647	-3.4	2.5	C ₂₃ H ₄₃ O ₁₄
	543.2611	3.4	15.5	C ₃₂ H ₃₉ N ₄ S ₂

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
543.2649	543.2649	-3.7	16.5	C ₂₉ H ₃₅ O ₁ N ₈ S ₁
543.2649	543.2649	-3.7	11.0	C ₃₀ H ₄₁ O ₆ N ₁ S ₁
543.2609	543.2609	3.7	7.0	C ₂₅ H ₄₁ O ₈ N ₃ S ₁
543.2609	543.2609	3.7	12.5	C ₂₄ H ₃₅ O ₃ N ₁₀ S ₁
543.2649	543.2649	-3.8	-2.0	C ₁₅ H ₄₅ O ₆ N ₉ S ₃
543.2607	543.2607	4.0	4.0	C ₁₇ H ₃₇ O ₁₁ N ₉
543.2604	543.2604	4.6	6.5	C ₂₄ H ₄₃ O ₂ N ₆ S ₃
543.2654	543.2654	-4.6	4.0	C ₁₅ H ₃₇ O ₇ N ₁₃ S ₁
543.2654	543.2654	-4.6	-1.5	C ₁₆ H ₄₃ O ₁₂ N ₆ S ₁
543.2602	543.2602	4.9	-2.0	C ₁₇ H ₄₅ O ₁₀ N ₅ S ₂
543.2602	543.2602	4.9	3.5	C ₁₆ H ₃₉ O ₅ N ₁₂ S ₂
543.2656	543.2656	-5.0	7.0	C ₂₃ H ₄₁ O ₄ N ₇ S ₂
543.2656	543.2656	-5.0	1.5	C ₂₄ H ₄₇ O ₉ S ₂
543.2602	543.2602	5.0	16.5	C ₃₁ H ₃₅ O ₅ N ₄
543.2602	543.2602	5.0	22.0	C ₃₀ H ₂₉ N ₁₁

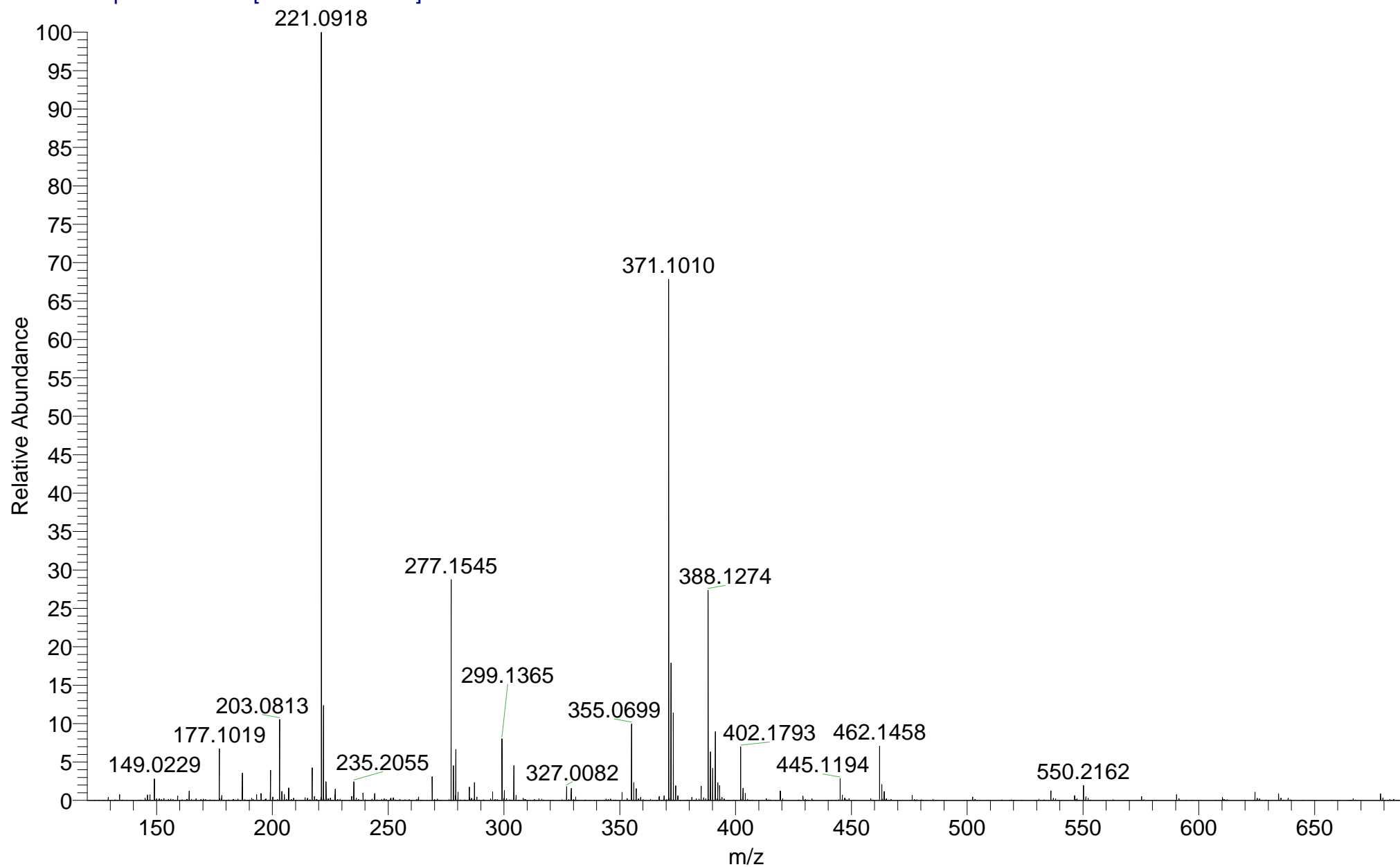
15-177-a
(DCM)/MeOH + NH4OAc
C15H20N2O3

Compound 46

EPSRC National Facility Swansea
LTQ Orbitrap XL

BRASHE
23/01/2017 11:34:10

BRASHE_0U5ZN_#6-12 RT: 0.11-0.37 AV: 6 SM: 7G NL: 3.59E6
T: FTMS + p NSI Full ms [120.00-1935.00]

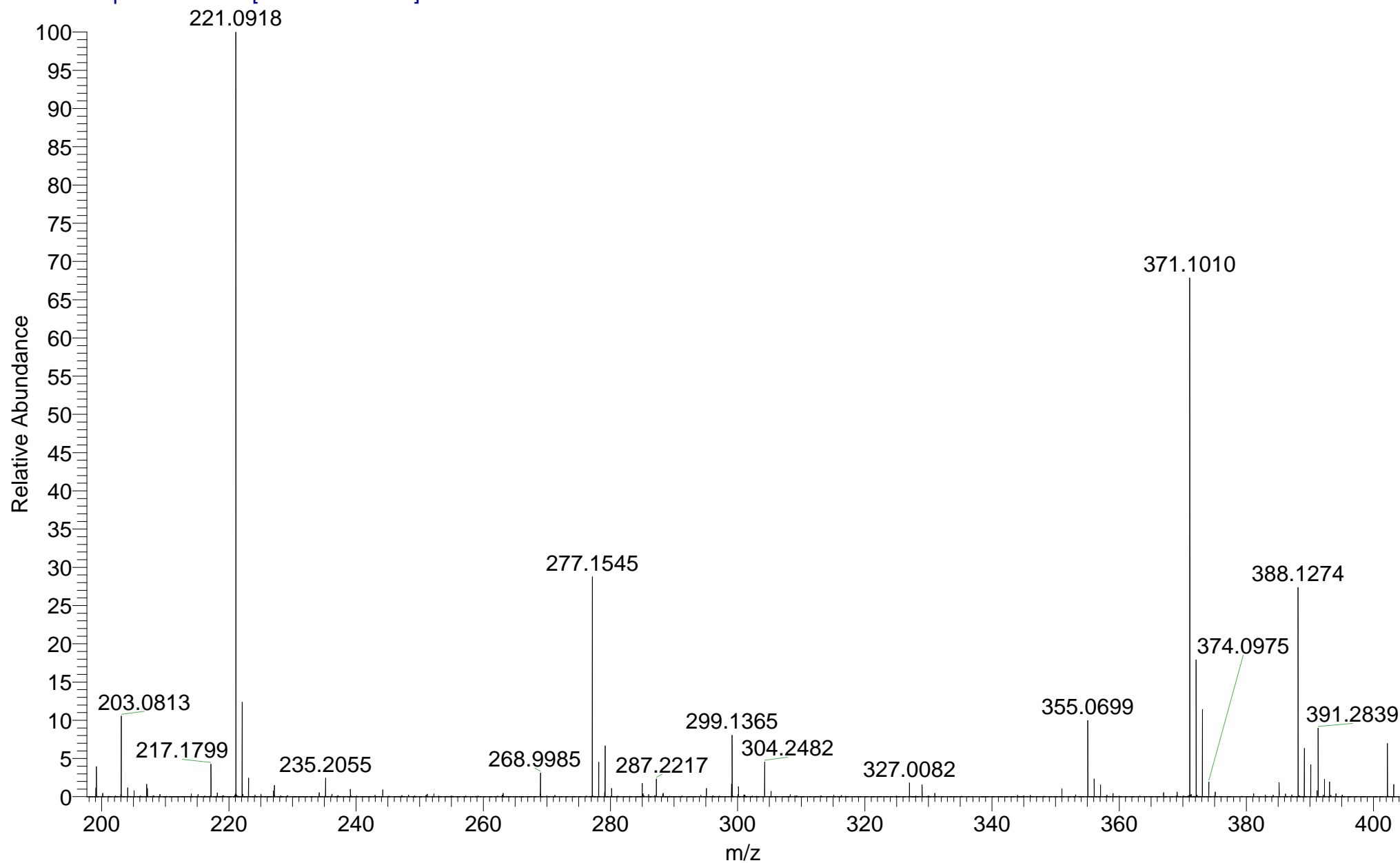


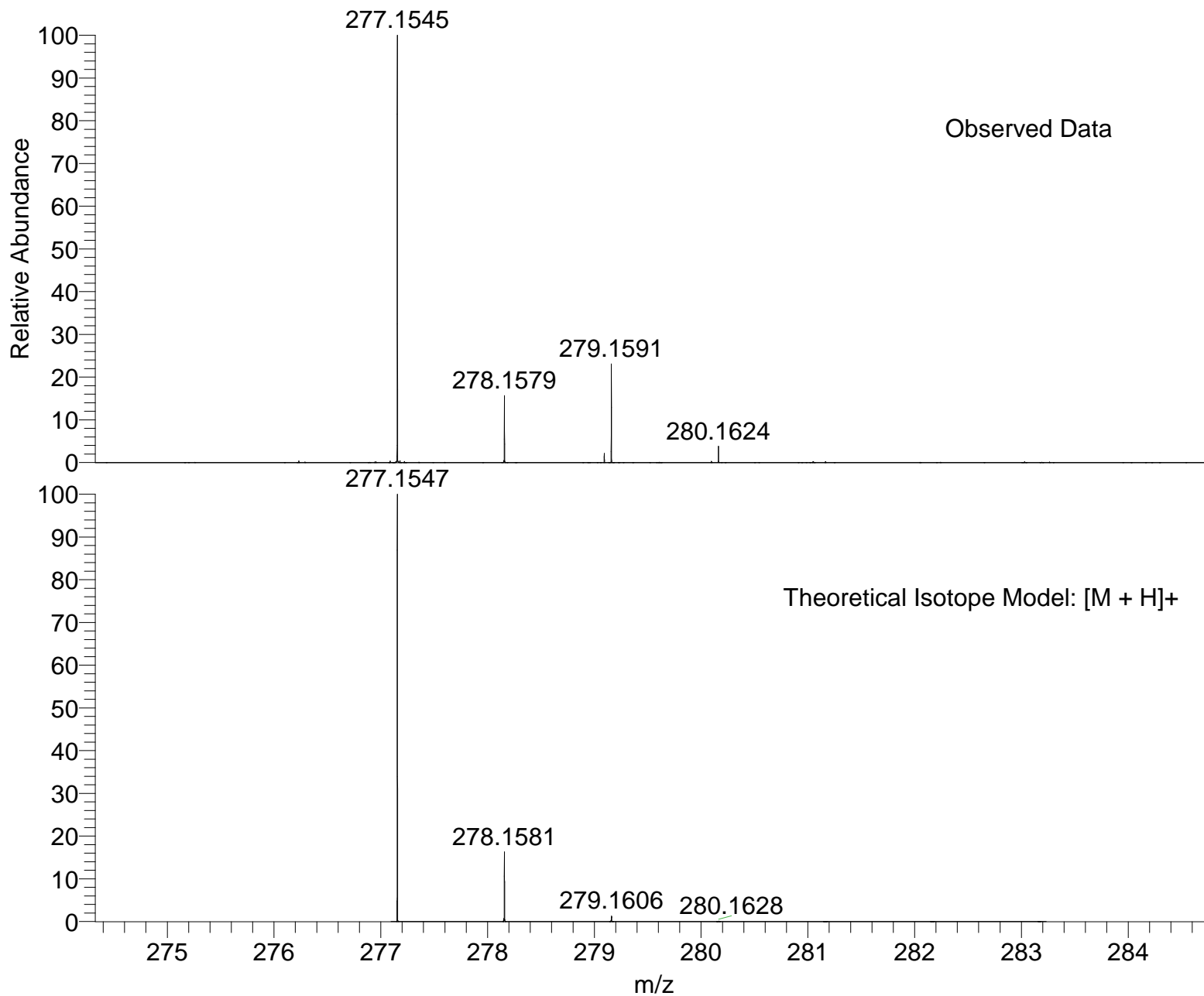
15-177-a
(DCM)/MeOH + NH4OAc
C15H20N2O3

EPSRC National Facility Swansea
LTQ Orbitrap XL

BRASHE
23/01/2017 11:34:10

BRASHE_0U5ZN_#6-12 RT: 0.11-0.37 AV: 6 SM: 7G NL: 3.59E6
T: FTMS + p NSI Full ms [120.00-1935.00]





NL:
1.03E6
BRASHE_OU5ZN_#6-12 RT:
0.11-0.37 AV: 6 T: FTMS + p
NSI Full ms [120.00-1935.00]

NL:
1.96E4
C₁₅H₂₀N₂O₃H:
C₁₅H₂₁N₂O₃
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

Isotope: Min. .. Max.
 14 N 0....15
 16 O 0....15
 12 C 0....60
 1 H 0....70
 23 Na 0....0
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3.. 100
 Fits: 100

N-Rule: Do not use
 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
277.1545	277.1547	-0.6	6.5	C ₁₅ H ₂₁ O ₃ N ₂
	277.1552	-2.4	-0.5	H ₁₇ O ₄ N ₁₄
	277.1533	4.2	7.0	C ₁₃ H ₁₉ O ₂ N ₅

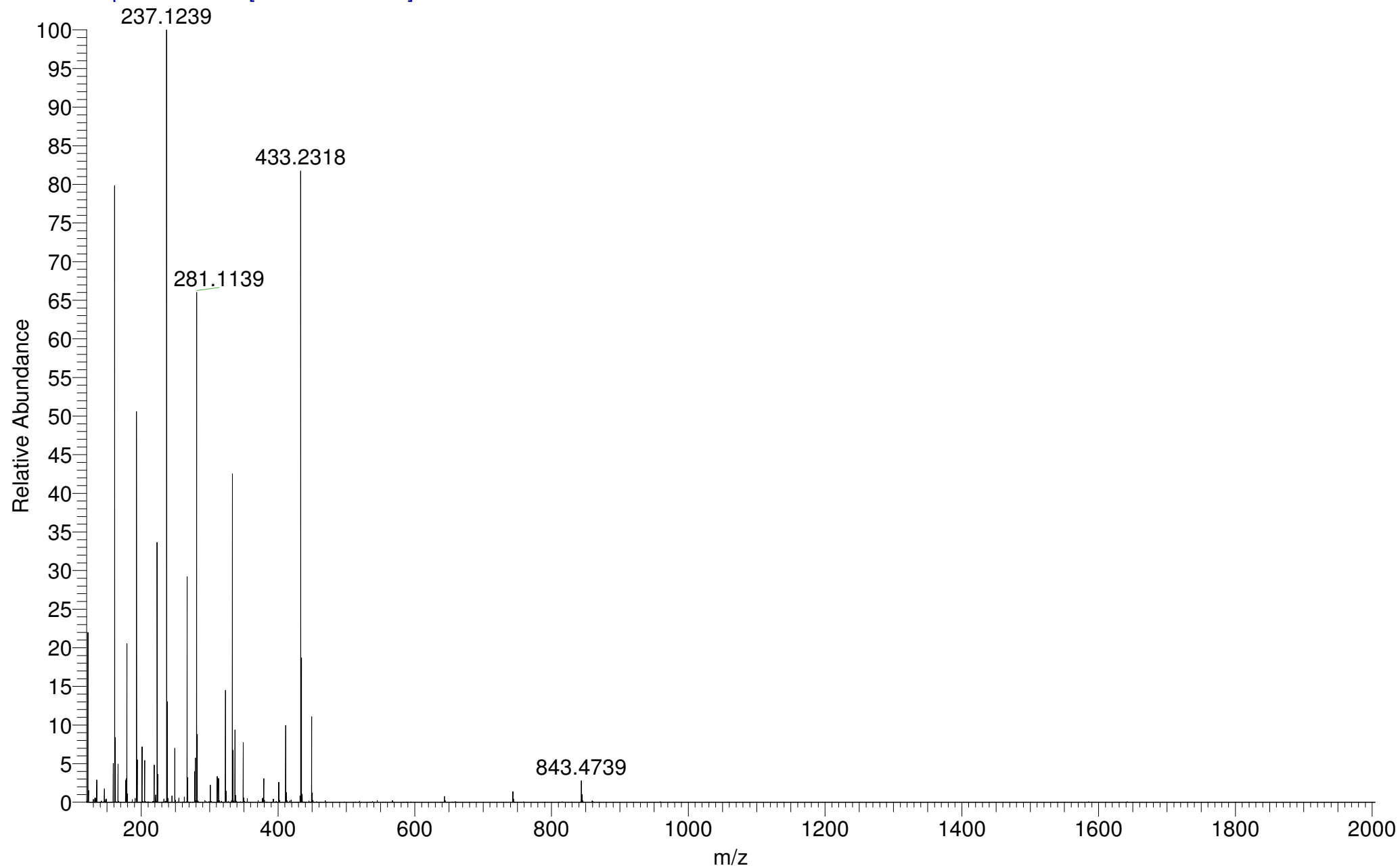
aet7-23 MW=278?
(?)/MeOH + NH4OAc

Compound 43

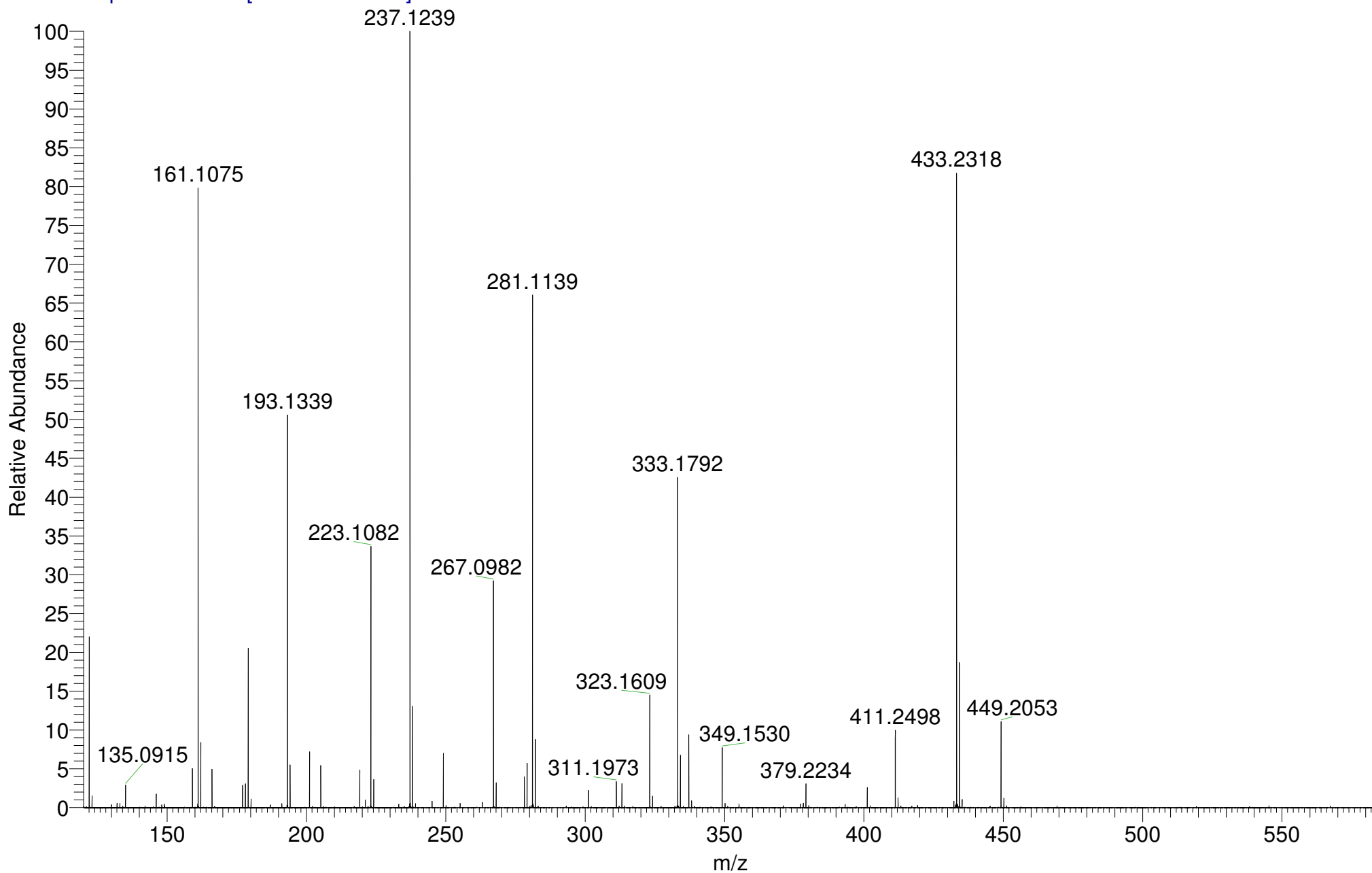
EPSRC National Centre Swansea
LTQ Orbitrap XL

adam throup
05/12/2011 13:14:33

BRASHE163-PV-HNESP #20-35 RT: 0.82-1.25 AV: 16 SM: 7G NL: 2.40E7
T: FTMS + p NSI Full ms [120.00-2000.00]



BRASHE163-PV-HNESP #20-35 RT: 0.82-1.25 AV: 16 SM: 7G NL: 2.40E7
T: FTMS + p NSI Full ms [120.00-2000.00]

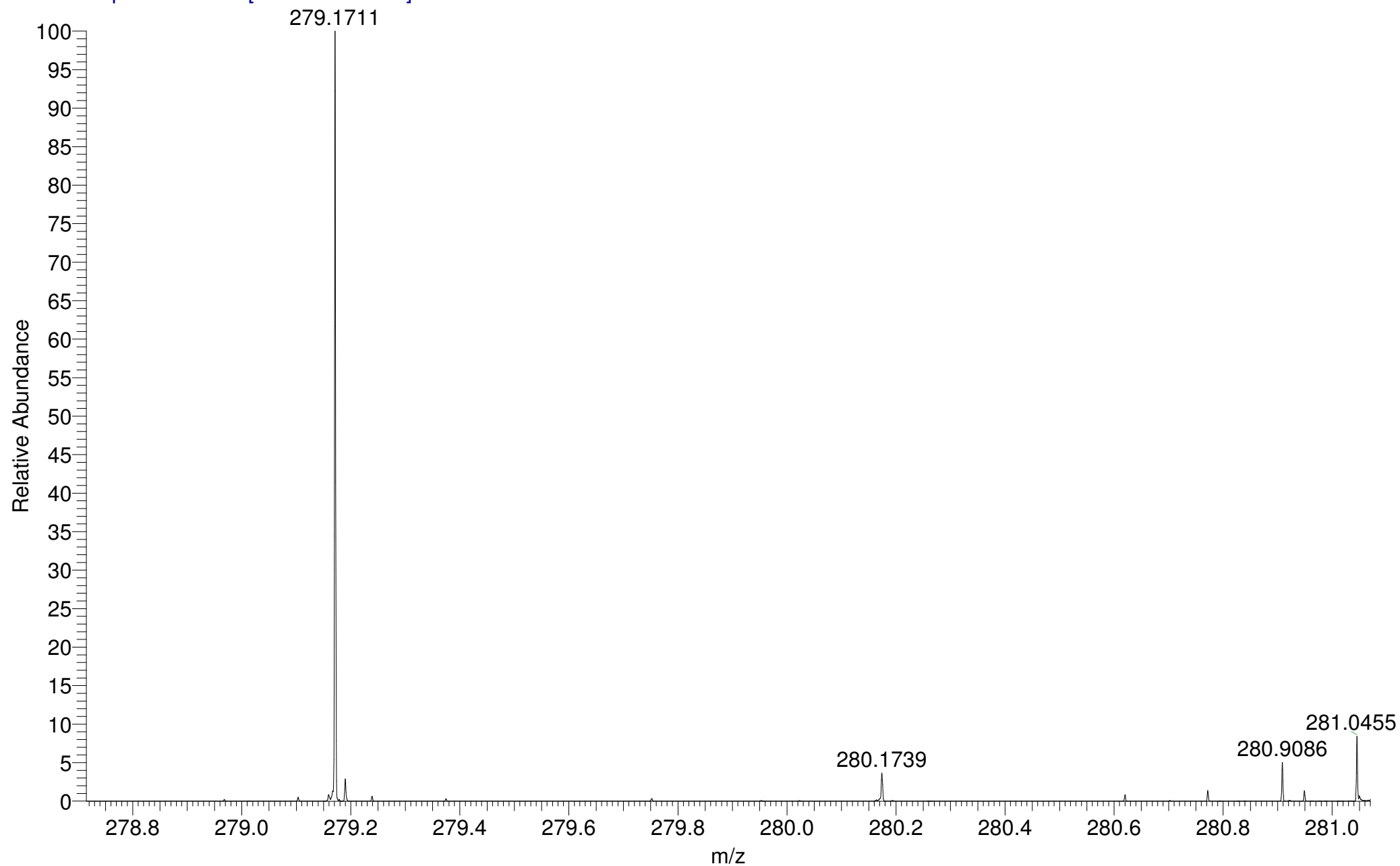


aet7-23 MW=278?
(?)/MeOH + NH4OAc

EPSRC National Centre Swansea
LTQ Orbitrap XL

adam throup
05/12/2011 13:14:33

BRASHE163-PV-HNESP #20-35 RT: 0.82-1.25 AV: 16 SM: 7G NL: 1.38E6
T: FTMS + p NSI Full ms [120.00-2000.00]



Isotope: Min. .. Max.
14 N 0....10
16 O 0....15
12 C 0....60
1 H 0....90
23 Na 0....0
Tolerance Window: +- 5.00 ppm
Db/Ring Equiv: -3.. 100
Fits: 100

N-Rule: Do not use
Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
279.1711	279.1703	2.8	5.5	C ₁₅ H ₂₃ O ₃ N ₂

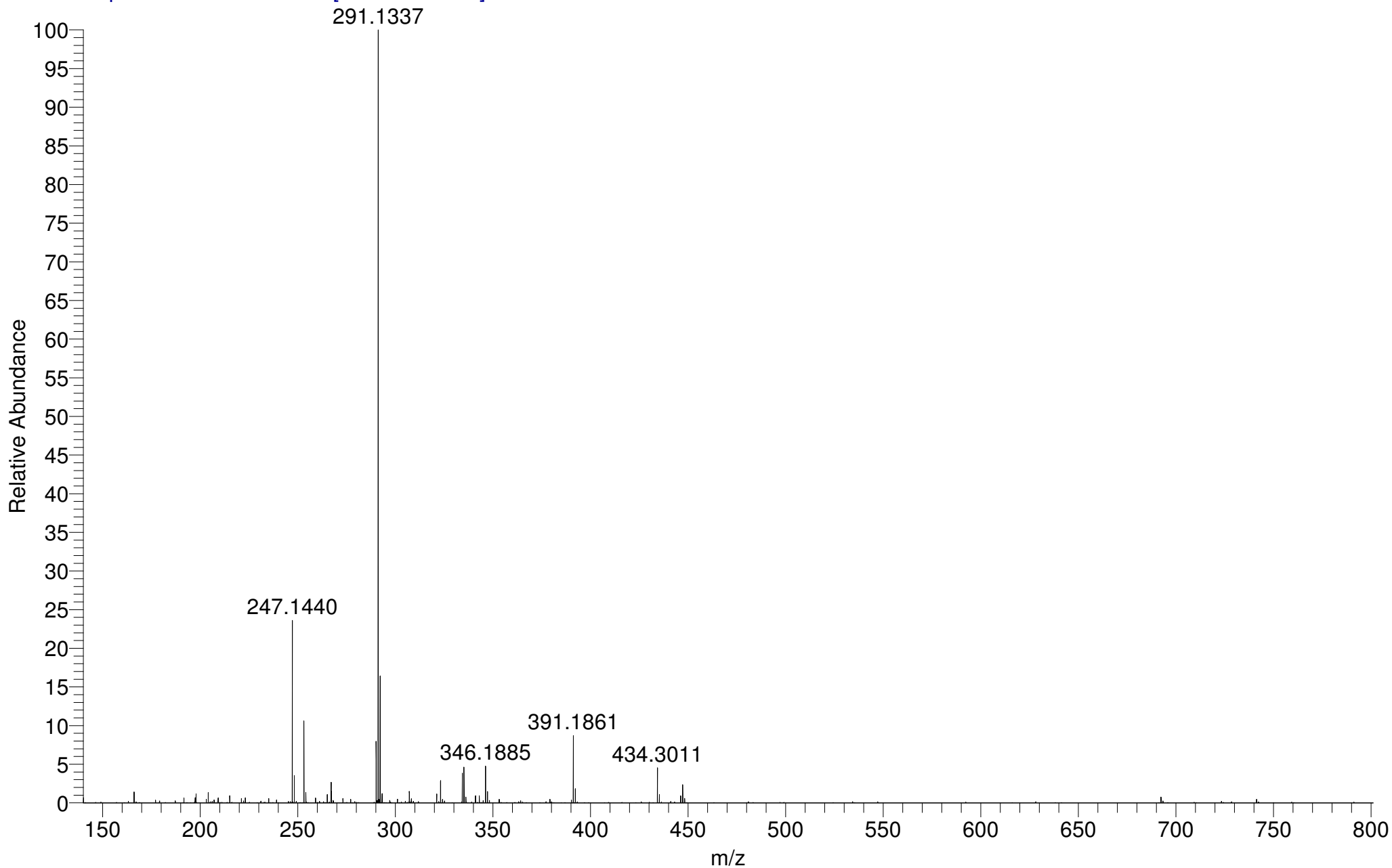
aet7-26 MW=345?
ASAP

Compound 47

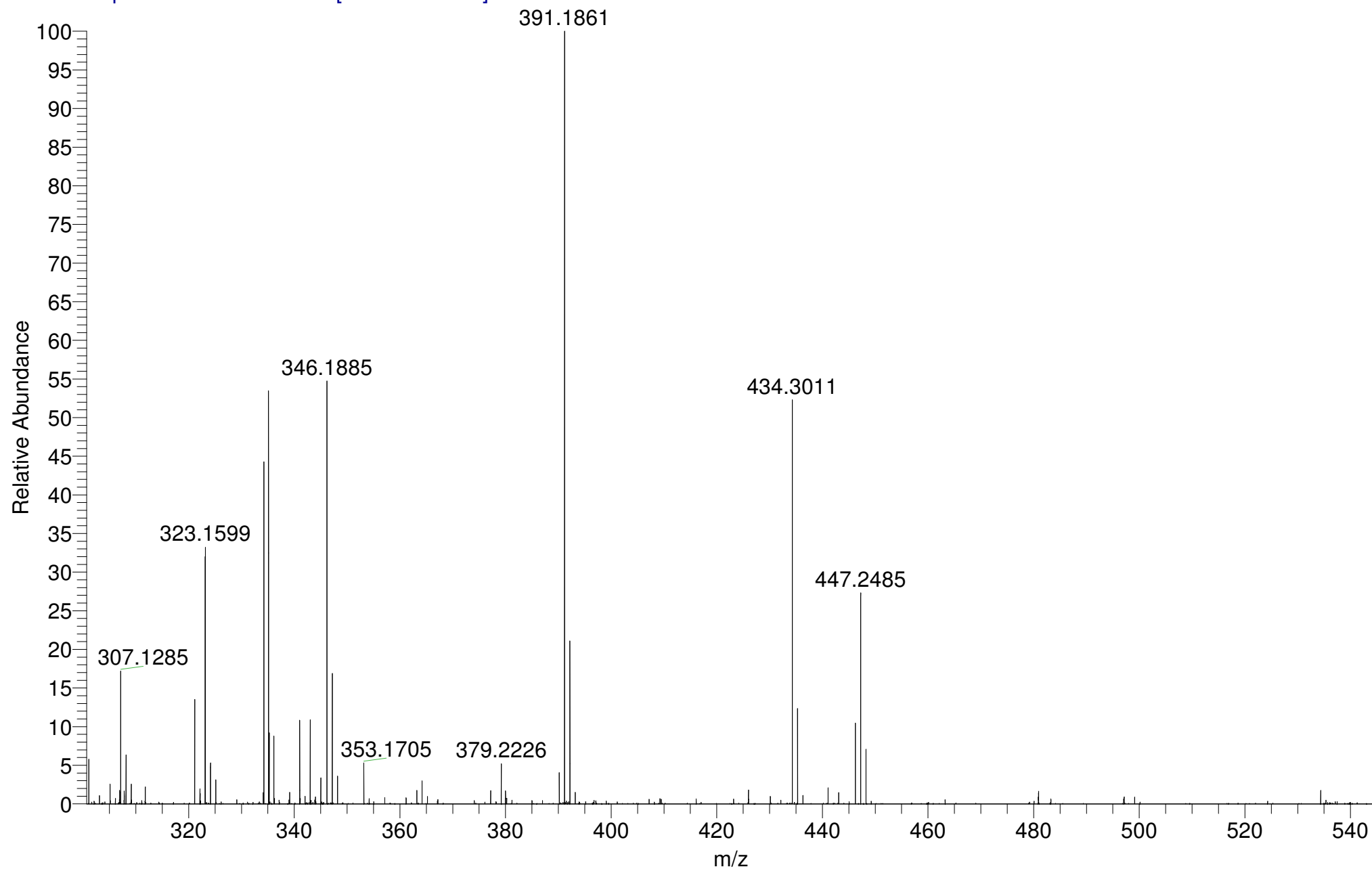
EPSRC National Centre Swansea
LTQ Orbitrap XL

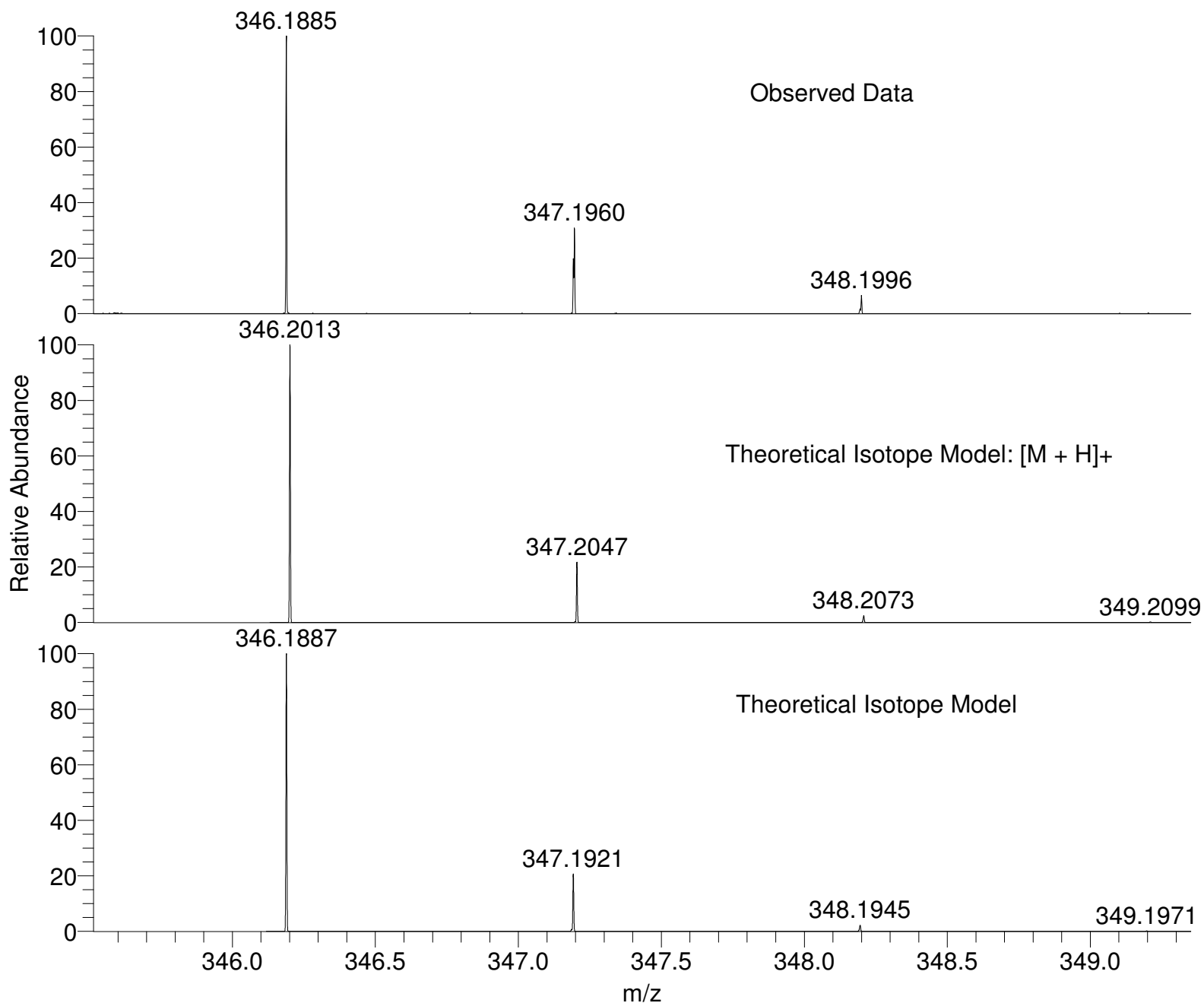
adam throup
13/12/2011 14:03:44

BRASHE168-OC-HASP #32-33 RT: 1.01-1.04 AV: 2 SM: 7G NL: 2.20E8
T: FTMS + p APCI corona Full ms [140.00-800.00]



BRASHE168-OC-HASP #32-33 RT: 1.01-1.04 AV: 2 SM: 7G NL: 1.91E7
T: FTMS + p APCI corona Full ms [140.00-800.00]





NL:
1.05E7
BRASHE168-OC-HASP#32-33
RT: 1.01-1.04 AV: 2 T: FTMS
+ p APCI corona Full ms
[140.00-800.00]

NL:
1.86E4
C₂₀ H₂₇ NO₄ H:
C₂₀ H₂₈ N₁ O₄
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

NL:
1.87E4
C₁₉ H₂₆ N₂ O₄:
C₁₉ H₂₆ N₂ O₄
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

Isotope: Min. .. Max.
 12 C 0....40
 1 H 0....60
 14 N 0....10
 16 O 0....10
 23 Na 0....0
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3.. 100
 Fits: 200

N-Rule: Do not use
 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
346.1885	346.1887	-0.6	8.0	C ₁₉ H ₂₆ O ₄ N ₂
	346.1874	3.3	8.5	C ₁₇ H ₂₄ O ₃ N ₅
	346.1900	-4.5	13.0	C ₂₀ H ₂₂ N ₆

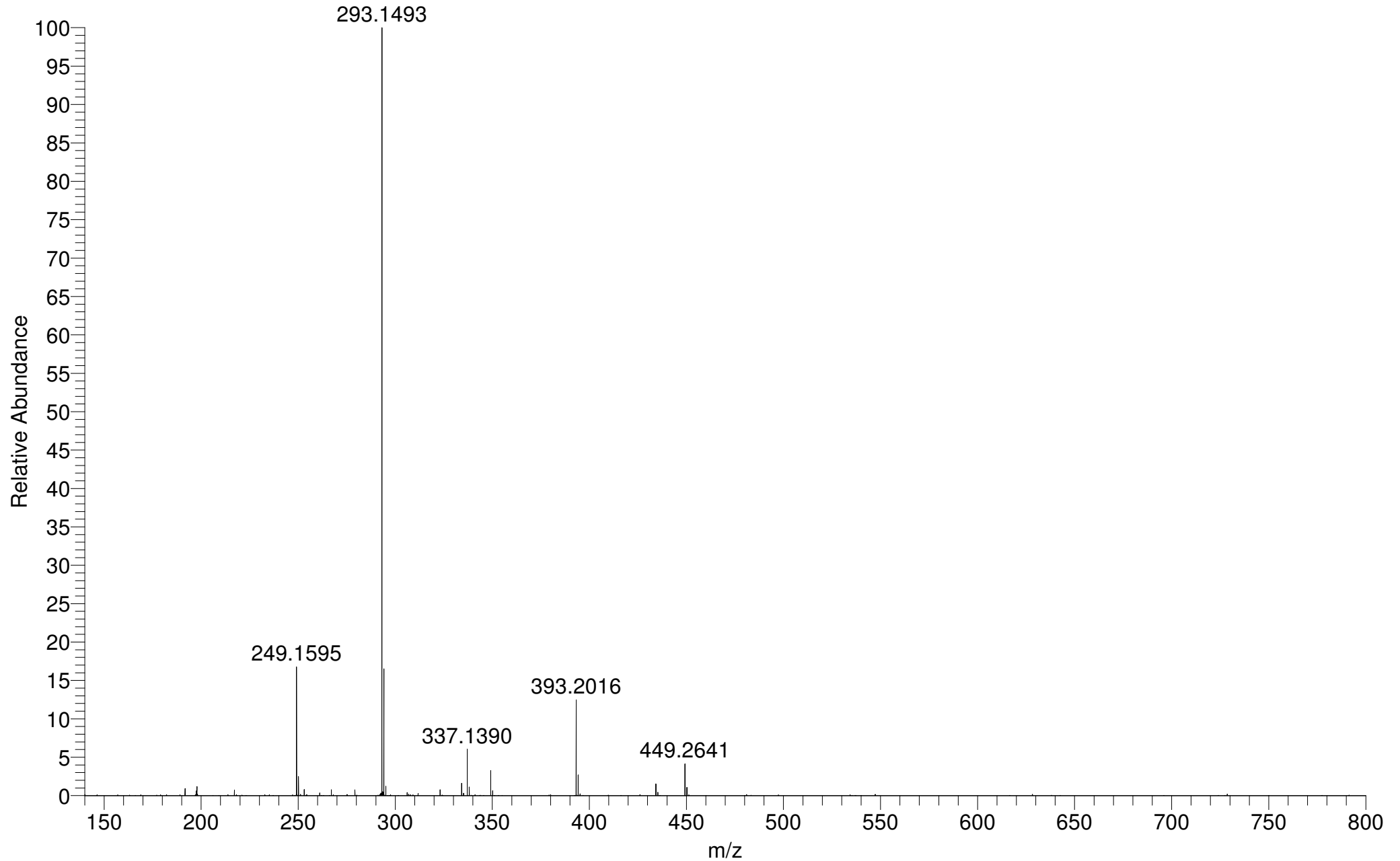
Compound 48

aet7-27 MW=347?
ASAP

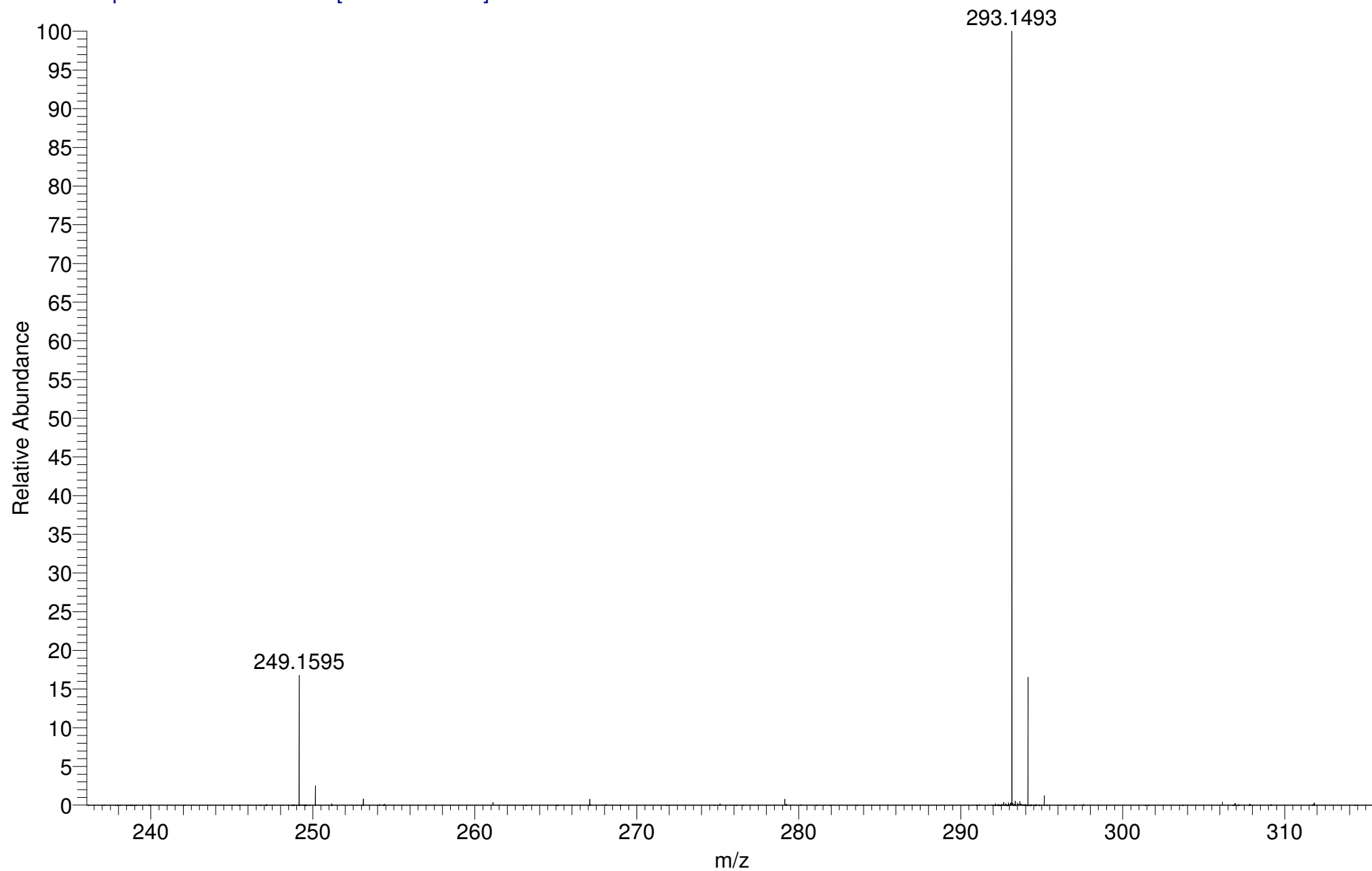
EPSRC National Centre Swansea
LTQ Orbitrap XL

adam throup
13/12/2011 14:15:40

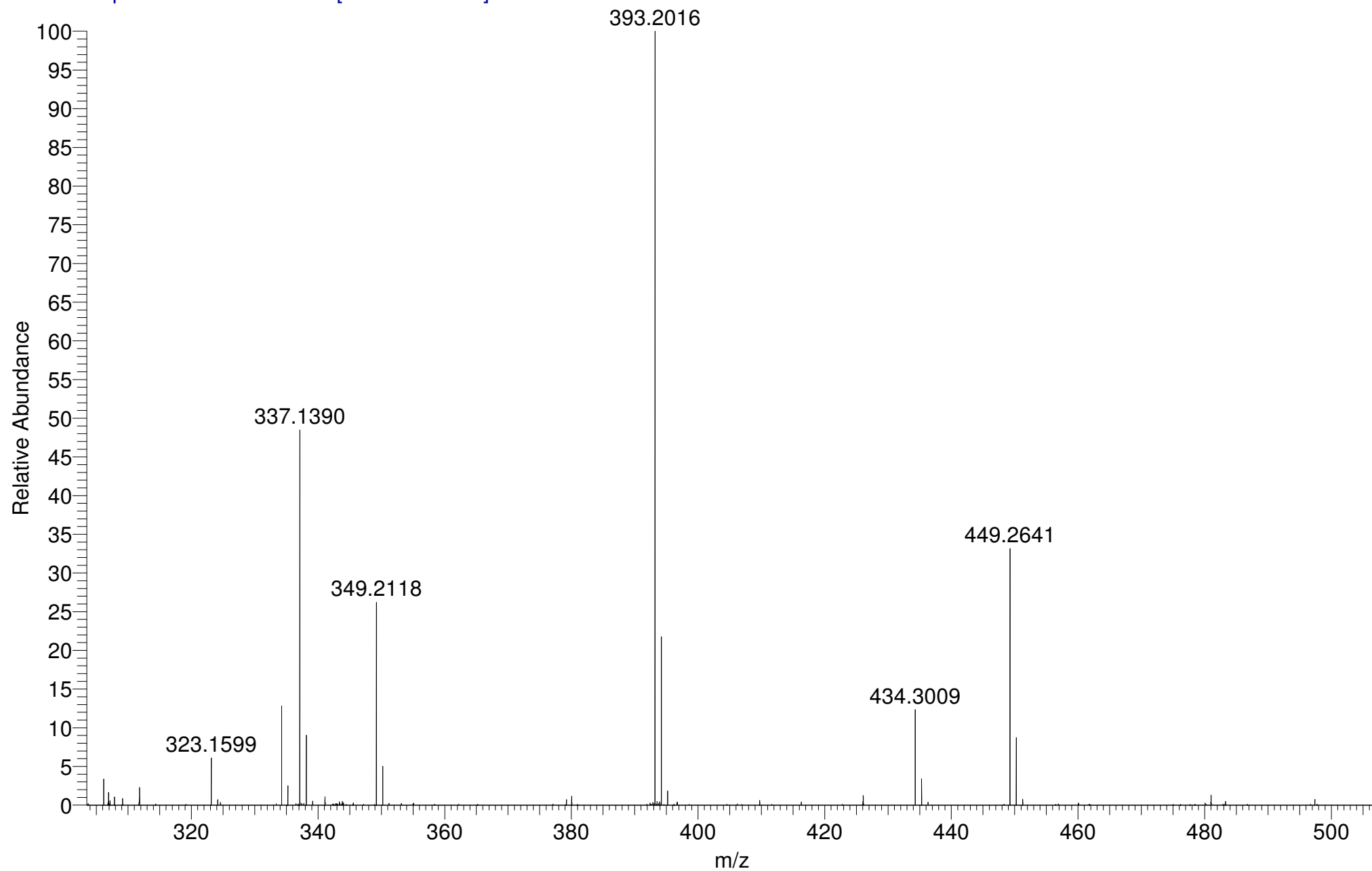
BRASHE169-OC-HASP #17 RT: 0.62 AV: 1 SM: 7G NL: 3.86E8
T: FTMS + p APCI corona Full ms [140.00-800.00]

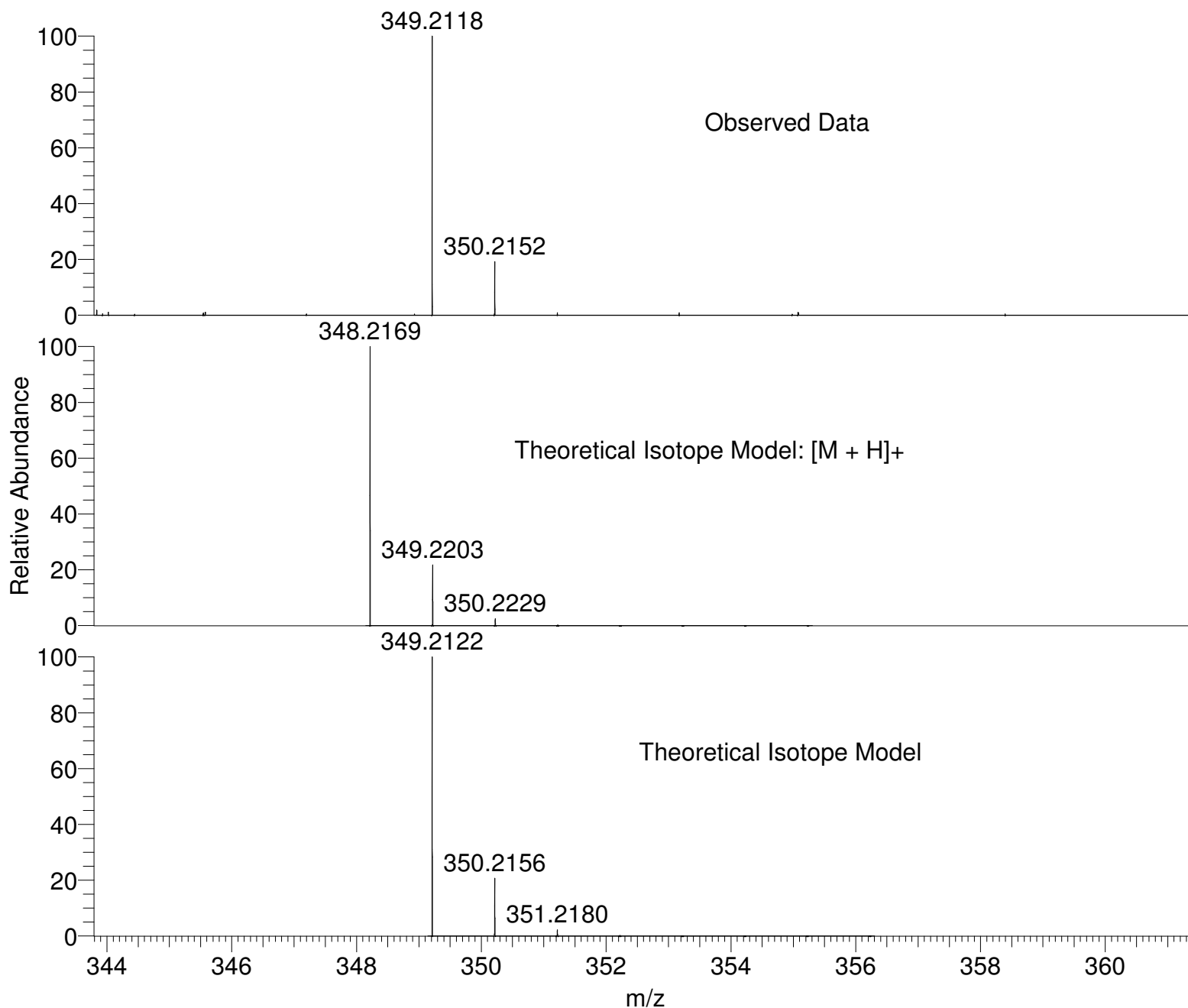


BRASHE169-OC-HASP #17 RT: 0.62 AV: 1 SM: 7G NL: 3.86E8
T: FTMS + p APCI corona Full ms [140.00-800.00]



BRASHE169-OC-HASP #17 RT: 0.62 AV: 1 SM: 7G NL: 4.81E7
T: FTMS + p APCI corona Full ms [140.00-800.00]





NL:
1.26E7
BRASHE169-OC-HASP#17
RT: 0.62 AV: 1 T: FTMS + p
APCI corona Full ms
[140.00-800.00]

NL:
1.86E4
C₂₀H₂₉NO₄H:
C₂₀H₃₀N₁O₄
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

NL:
1.87E4
C₁₉H₂₉N₂O₄:
C₁₉H₂₉N₂O₄
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

Isotope: Min. .. Max.
 12 C 0....40
 1 H 0....60
 14 N 0....10
 16 O 0....10
 23 Na 0....0
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3.. 100
 Fits: 200

N-Rule: Do not use
 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
349.2118	349.2122	-1.1	6.5	C ₁₉ H ₂₉ O ₄ N ₂
	349.2108	2.7	7.0	C ₁₇ H ₂₇ O ₃ N ₅
	349.2135	-4.9	11.5	C ₂₀ H ₂₅ N ₆

aet7-39 MW=574?
(DCM)/MeOH + NH4OAc

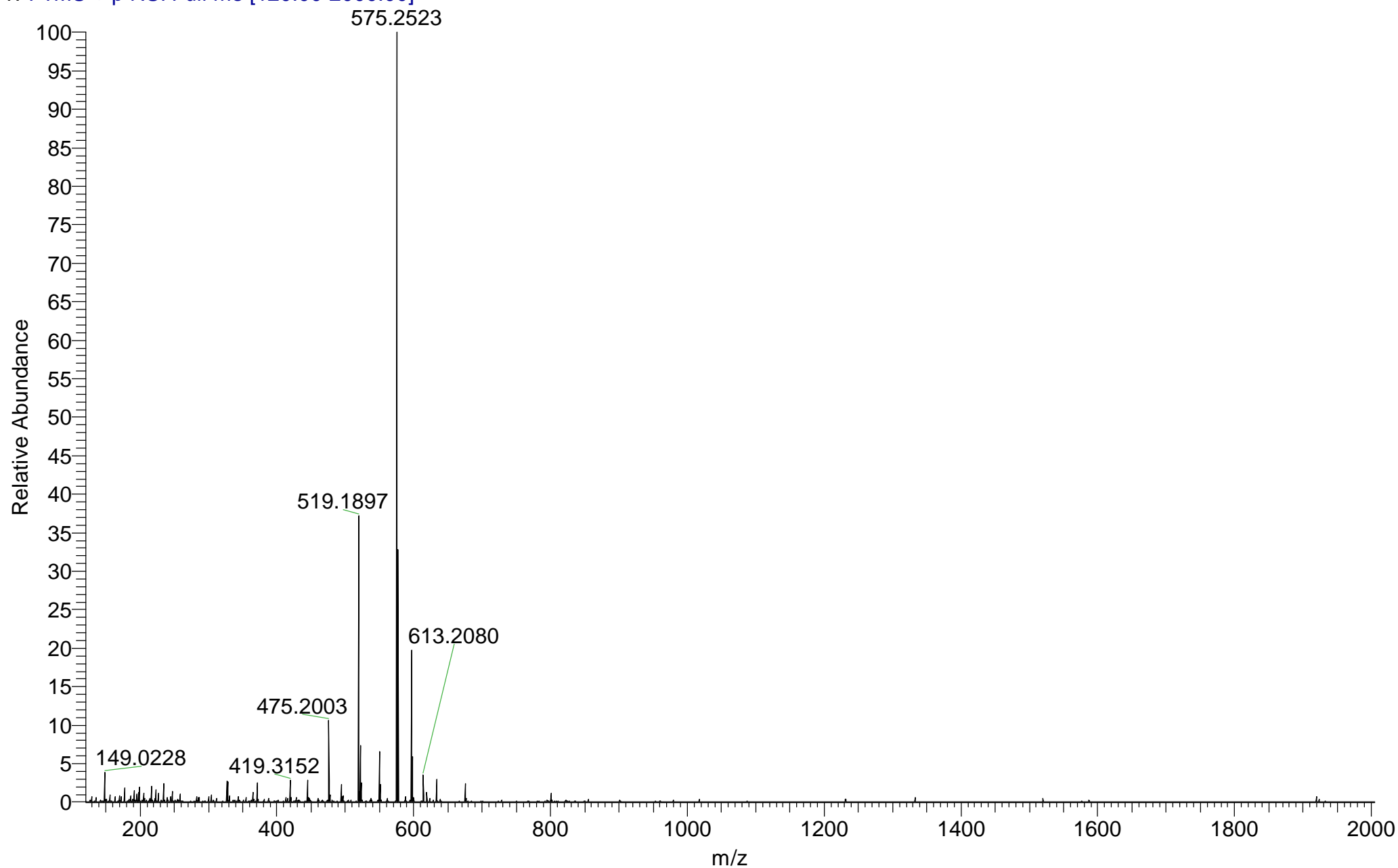
Compound 51

EPSRC National Centre Swansea
LTQ Orbitrap XL

adam throup
13/01/2012 14:33:35

BRASHE178-OV-HNESP #21-34 RT: 0.88-1.26 AV: 14 NL: 5.08E6

T: FTMS + p NSI Full ms [120.00-2000.00]



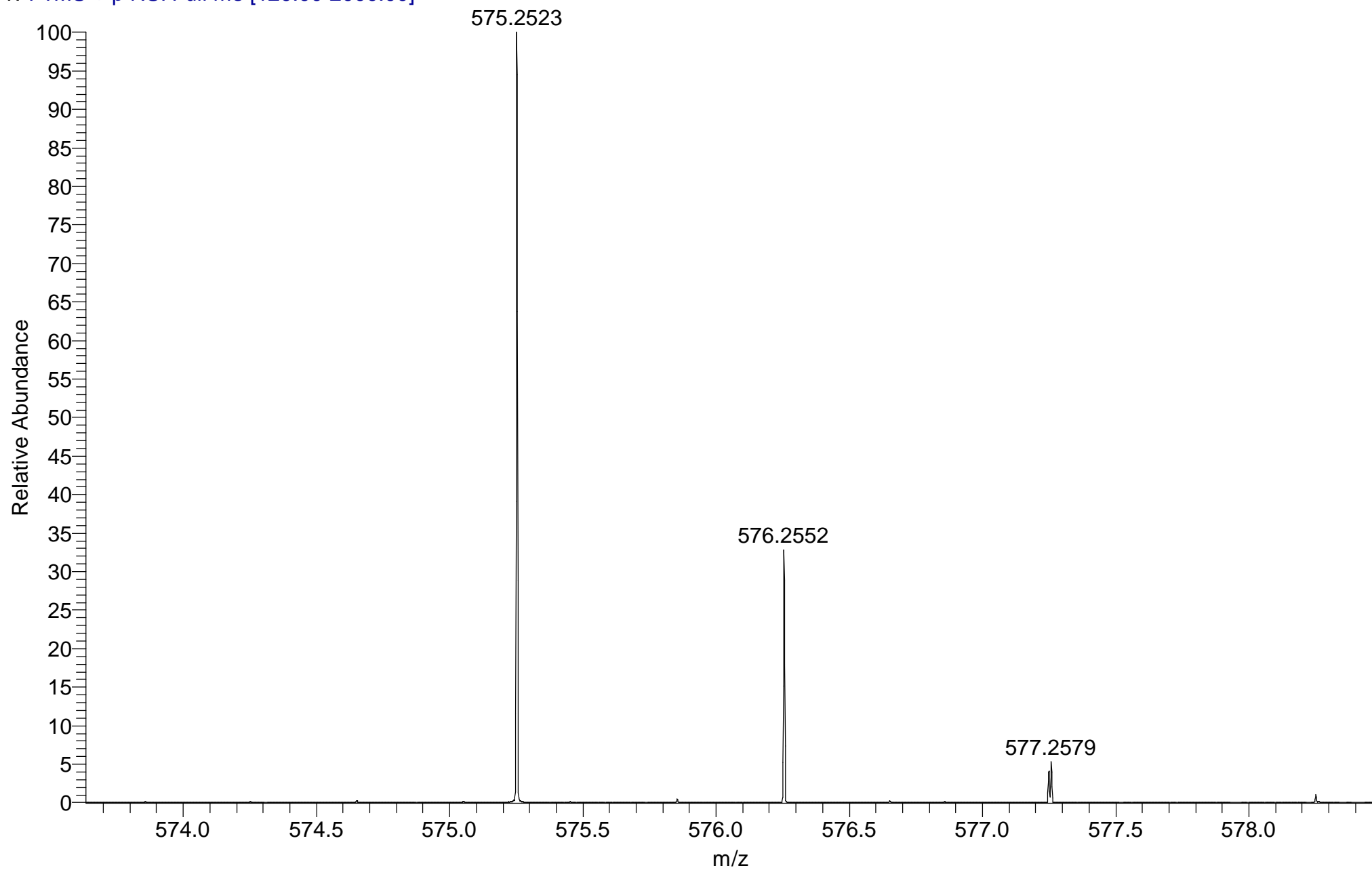
aet7-39 MW=574?
(DCM)/MeOH + NH₄OAc

EPSRC National Centre Swansea
LTQ Orbitrap XL

adam throup
13/01/2012 14:33:35

BRASHE178-OV-HNESP #21-34 RT: 0.88-1.26 AV: 14 NL: 5.08E6

T: FTMS + p NSI Full ms [120.00-2000.00]



Isotope: Min. .. Max.
 14 N 0....10
 16 O 0....15
 12 C 0....30
 1 H 0....60
 23 Na 0....0
 32 S 0....2
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3..100
 Fits: 100

N-Rule: Do not use
 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
575.2523	575.2521	0.4	6.5	C ₂₇ H ₄₃ O ₁₁ S ₁
	575.2521	0.4	12.0	C ₂₆ H ₃₇ O ₆ N ₇ S ₁
	575.2519	0.7	3.5	C ₁₉ H ₃₉ O ₁₄ N ₆
	575.2527	-0.8	2.5	C ₂₀ H ₄₃ O ₉ N ₆ S ₂
	575.2514	1.6	-2.5	C ₁₉ H ₄₇ O ₁₃ N ₂ S ₂
	575.2514	1.6	3.0	C ₁₈ H ₄₁ O ₈ N ₉ S ₂
	575.2532	-1.6	8.5	C ₂₀ H ₃₅ O ₁₀ N ₁₀
	575.2532	-1.6	3.0	C ₂₁ H ₄₁ O ₁₅ N ₃
	575.2534	-1.9	11.5	C ₂₈ H ₃₉ O ₇ N ₄ S ₁
	575.2507	2.8	7.0	C ₂₅ H ₄₁ O ₁₀ N ₃ S ₁
	575.2507	2.8	12.5	C ₂₄ H ₃₅ O ₅ N ₁₀ S ₁
	575.2539	-2.8	-1.0	C ₁₄ H ₄₁ O ₁₃ N ₉ S ₁
	575.2505	3.1	4.0	C ₁₇ H ₃₇ O ₁₃ N ₉
	575.2541	-3.1	7.5	C ₂₁ H ₃₉ O ₅ N ₁₀ S ₂
	575.2541	-3.1	2.0	C ₂₂ H ₄₅ O ₁₀ N ₃ S ₂
	575.2501	3.9	-2.0	C ₁₇ H ₄₅ O ₁₂ N ₅ S ₂
	575.2546	-3.9	8.0	C ₂₂ H ₃₇ O ₁₁ N ₇
	575.2547	-4.2	16.5	C ₂₉ H ₃₅ O ₃ N ₈ S ₁
	575.2547	-4.2	11.0	C ₂₉ H ₄₁ O ₈ N ₁ S ₁
	575.2496	4.8	16.0	C ₃₀ H ₃₇ O ₁ N ₇ S ₂

aet7-47 MW=616?
(DCM)/MeOH + NH4OAc

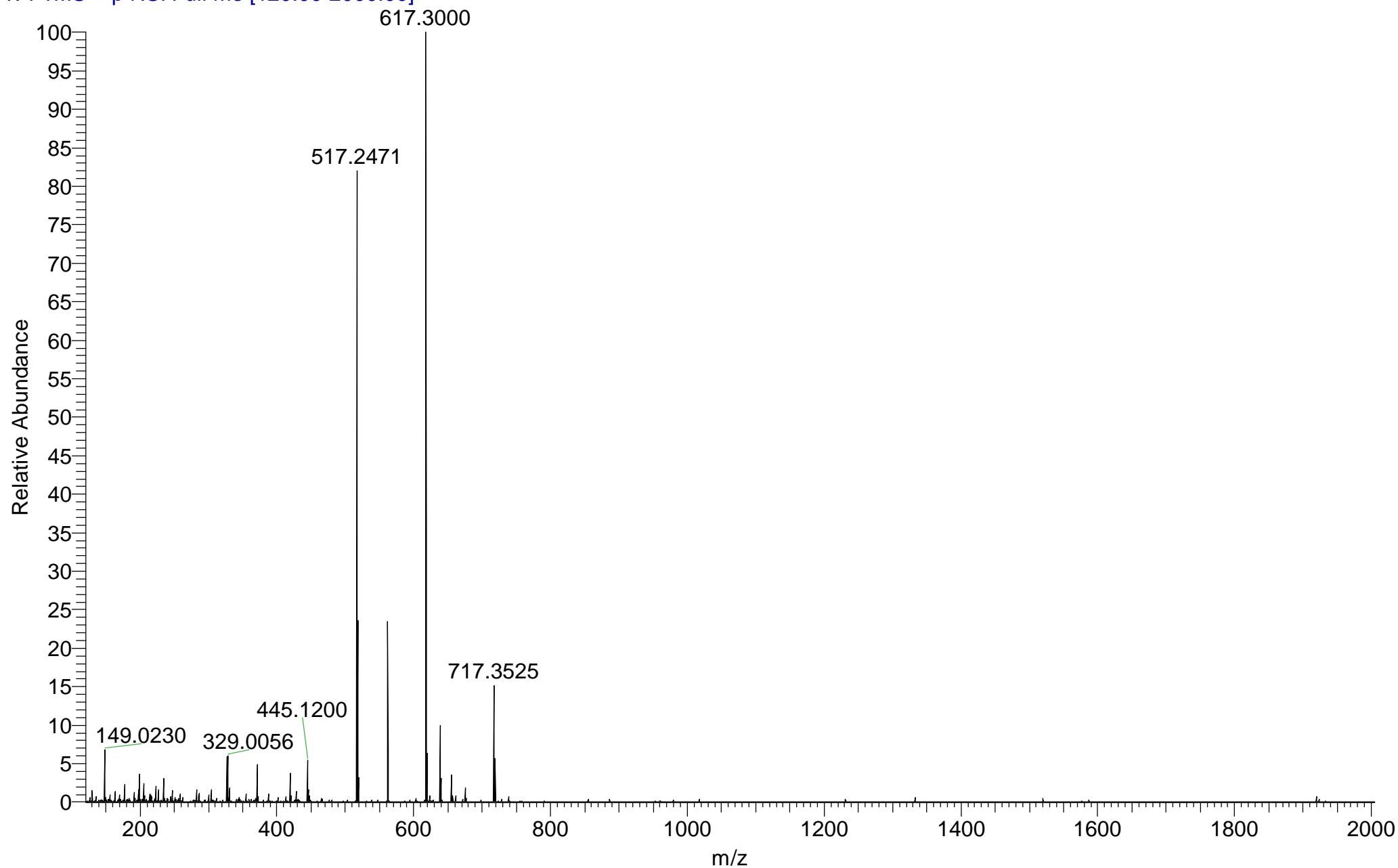
Compound 52

EPSRC National Centre Swansea
LTQ Orbitrap XL

adam throup
13/01/2012 14:40:48

BRASHE180-OV-HNESP #20-33 RT: 0.87-1.26 AV: 14 NL: 2.51E6

T: FTMS + p NSI Full ms [120.00-2000.00]



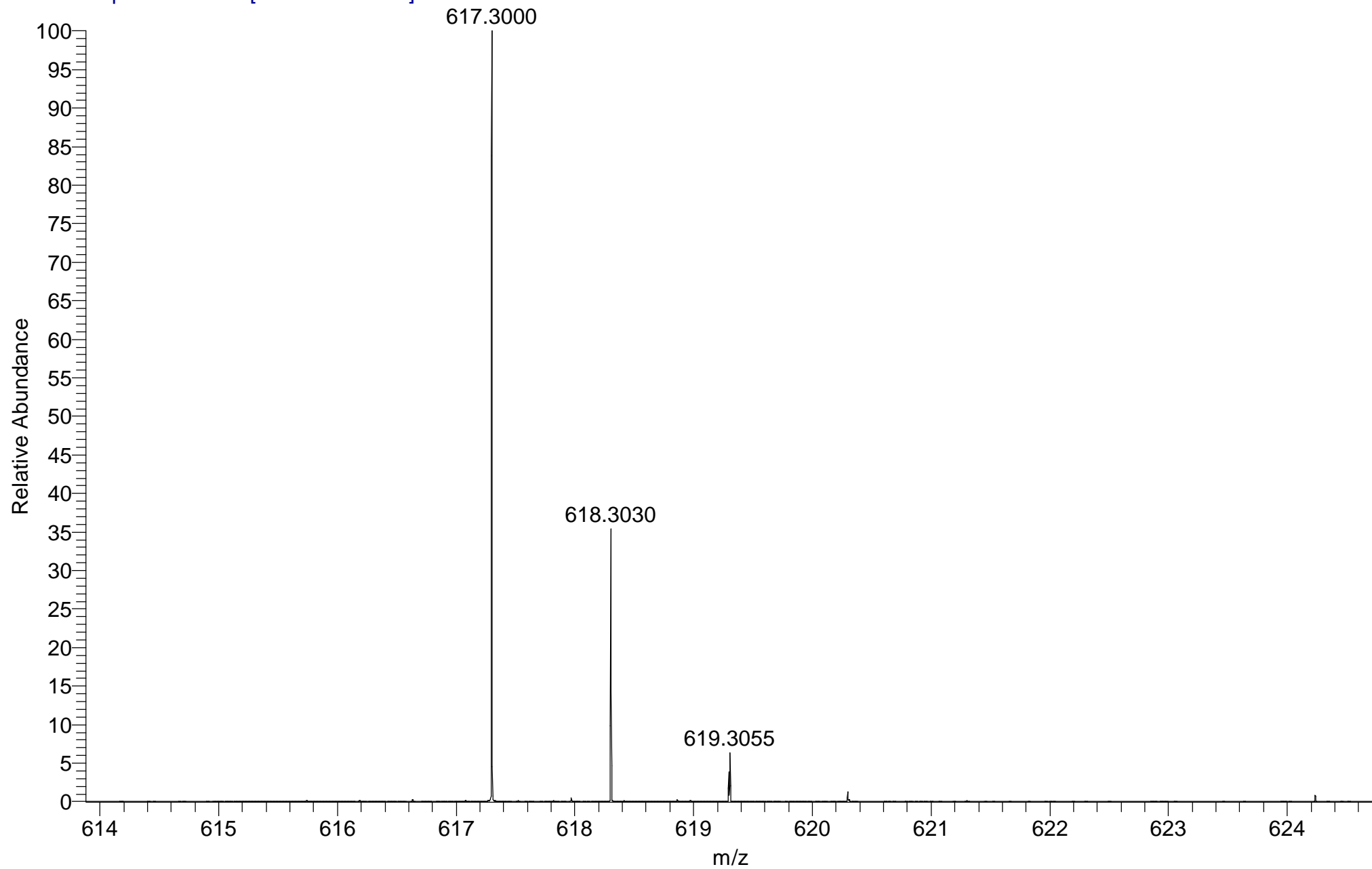
aet7-47 MW=616?
(DCM)/MeOH + NH₄OAc

EPSRC National Centre Swansea
LTQ Orbitrap XL

adam throup
13/01/2012 14:40:48

BRASHE180-OV-HNESP #20-33 RT: 0.87-1.26 AV: 14 NL: 2.51E6

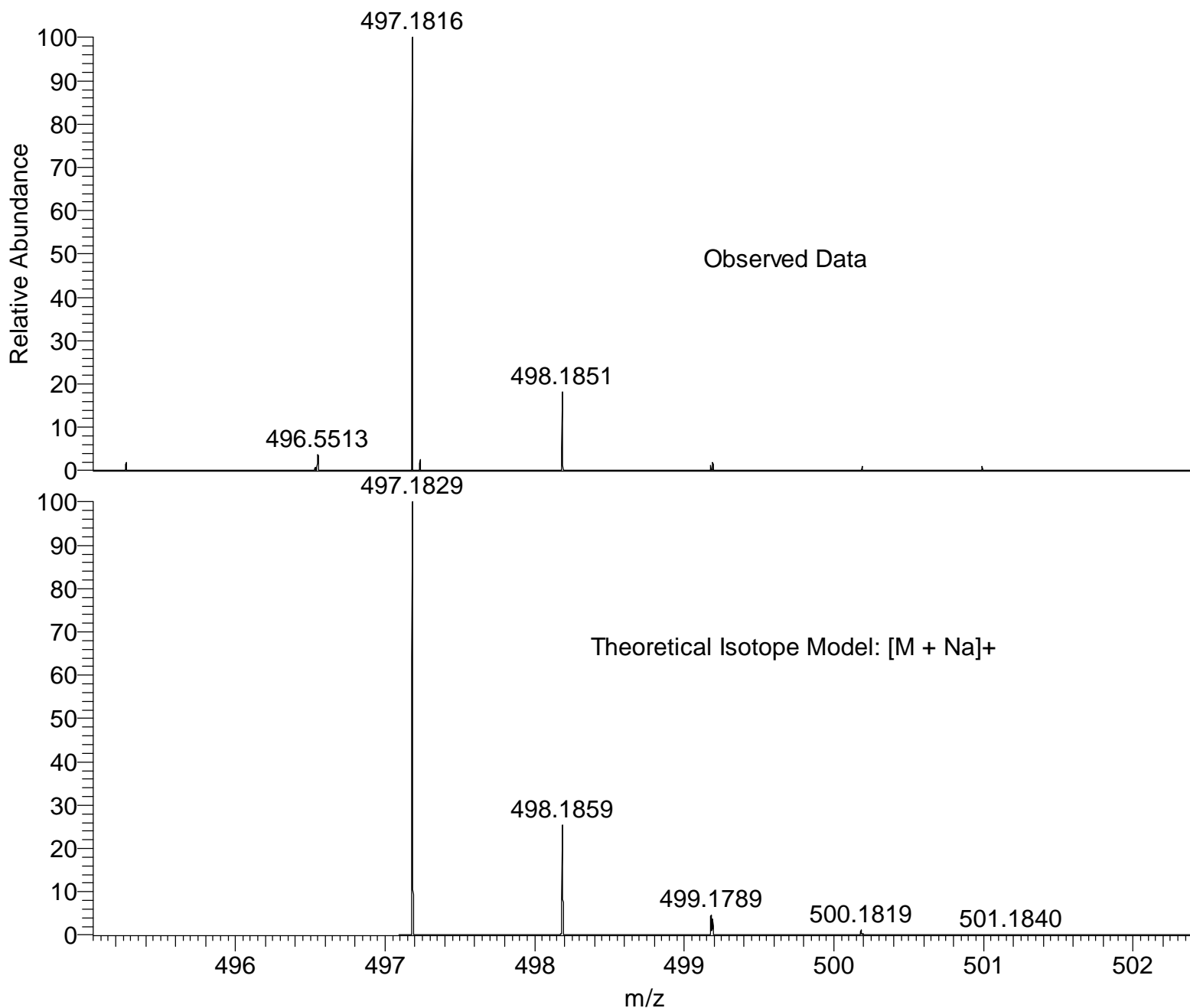
T: FTMS + p NSI Full ms [120.00-2000.00]



Isotope: Min. .. Max.
 14 N 0....10
 16 O 0....15
 12 C 0....40
 1 H 0....60
 23 Na 0....0
 32 S 0....2
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3..100
 Fits: 100

N-Rule: Do not use
 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
617.3000	617.3002	-0.3	8.5	C ₂₃ H ₄₁ O ₁₀ N ₁₀
	617.3002	-0.3	3.0	C ₂₄ H ₄₇ O ₁₅ N ₃
	617.2997	0.5	2.5	C ₂₃ H ₄₉ O ₉ N ₆ S ₂
	617.2997	0.6	21.0	C ₃₇ H ₃₉ O ₄ N ₅
	617.3003	-0.6	11.5	C ₃₁ H ₄₅ O ₇ N ₄ S ₁
	617.2992	1.3	15.0	C ₃₇ H ₄₇ O ₃ N ₁ S ₂
	617.3009	-1.4	-1.0	C ₁₇ H ₄₇ O ₁₃ N ₉ S ₁
	617.2990	1.6	6.5	C ₃₀ H ₄₉ O ₁₁ S ₁
	617.3010	-1.6	26.0	C ₃₈ H ₃₅ N ₉
	617.2990	1.6	12.0	C ₂₉ H ₄₃ O ₆ N ₇ S ₁
	617.3010	-1.6	20.5	C ₃₉ H ₄₁ O ₅ N ₂
	617.3010	-1.7	7.5	C ₂₄ H ₄₅ O ₅ N ₁₀ S ₂
	617.3010	-1.7	2.0	C ₂₅ H ₅₁ O ₁₀ N ₃ S ₂
	617.2988	1.9	3.5	C ₂₂ H ₄₅ O ₁₄ N ₆
	617.3015	-2.4	8.0	C ₂₅ H ₄₃ O ₁₁ N ₇
	617.2984	2.7	-2.5	C ₂₂ H ₅₃ O ₁₃ N ₂ S ₂
	617.2984	2.7	3.0	C ₂₁ H ₄₇ O ₈ N ₉ S ₂
	617.2983	2.7	16.0	C ₃₆ H ₄₃ O ₈ N ₁
	617.3017	-2.7	16.5	C ₃₂ H ₄₁ O ₃ N ₈ S ₁
	617.2983	2.7	21.5	C ₃₅ H ₃₇ O ₃ N ₈
	617.3017	-2.7	11.0	C ₃₃ H ₄₇ O ₈ N ₁ S ₁
	617.3019	-3.0	19.5	C ₄₀ H ₄₅ N ₂ S ₂
	617.2978	3.5	15.5	C ₃₅ H ₄₅ O ₂ N ₄ S ₂
	617.3022	-3.6	-1.5	C ₁₉ H ₄₉ O ₁₄ N ₆ S ₁
	617.2977	3.8	7.0	C ₂₈ H ₄₇ O ₁₀ N ₃ S ₁
	617.3023	-3.8	25.5	C ₄₀ H ₃₇ O ₁ N ₆
	617.2977	3.8	12.5	C ₂₇ H ₄₁ O ₅ N ₁₀ S ₁
	617.3024	-3.8	7.0	C ₂₆ H ₄₇ O ₆ N ₇ S ₂
	617.3024	-3.9	1.5	C ₂₇ H ₅₃ O ₁₁ S ₂
	617.2975	4.1	4.0	C ₂₀ H ₄₃ O ₁₃ N ₉
	617.3028	-4.6	7.5	C ₂₇ H ₄₅ O ₁₂ N ₄



NL:
1.20E5
BRASHE179-OV-HNESP#25
RT: 1.02 AV: 1 T: FTMS + p
NSI Full ms [120.00-2000.00]

NL:
1.69E4
C₂₃ H₃₀ N₄ O₅ SNa:
C₂₃ H₃₀ N₄ O₅ S₁ Na₁
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

Isotope: Min. .. Max.
 14 N 0....10
 16 O 0....15
 12 C 0....30
 1 H 0....60
 23 Na 0....1
 32 S 0....2
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3..100
 Fits: 100

N-Rule: Do not use
 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
497.1816	497.1816	0.1	5.5	C ₂₂ H ₃₄ O ₉ Na ₁ S ₁
	497.1816	0.1	11.0	C ₂₁ H ₂₈ O ₄ N ₇ Na ₁ S ₁
	497.1815	0.2	12.5	C ₂₈ H ₃₃ O ₄ S ₂
	497.1818	-0.3	14.0	C ₂₉ H ₃₂ O ₁ N ₁ Na ₁ S ₂
	497.1814	0.4	2.5	C ₁₄ H ₃₀ O ₁₂ N ₆ Na ₁
	497.1813	0.6	9.5	C ₂₀ H ₂₉ O ₇ N ₆ S ₁
	497.1819	-0.7	18.5	C ₂₈ H ₂₅ O ₅ N ₄
	497.1820	-0.8	0.0	C ₁₄ H ₃₅ O ₁₀ N ₅ S ₂
	497.1811	1.0	1.0	C ₁₃ H ₃₁ O ₁₅ N ₅
	497.1822	-1.2	20.0	C ₂₉ H ₂₄ O ₂ N ₅ Na ₁
	497.1823	-1.3	1.5	C ₁₅ H ₃₄ O ₇ N ₆ Na ₁ S ₂
	497.1809	1.4	2.0	C ₁₃ H ₃₂ O ₆ N ₉ Na ₁ S ₂
	497.1809	1.4	15.0	C ₂₈ H ₂₈ O ₆ N ₁ Na ₁
	497.1809	1.5	20.5	C ₂₇ H ₂₂ O ₁ N ₈ Na ₁
	497.1825	-1.7	6.0	C ₁₄ H ₂₇ O ₁₁ N ₉
	497.1806	1.9	0.5	C ₁₂ H ₃₃ O ₉ N ₈ S ₂
	497.1806	2.0	13.5	C ₂₇ H ₂₉ O ₉
	497.1806	2.0	19.0	C ₂₆ H ₂₃ O ₄ N ₇
	497.1826	-2.1	14.5	C ₂₁ H ₂₅ O ₃ N ₁₀ S ₁
	497.1826	-2.1	9.0	C ₂₂ H ₃₁ O ₈ N ₃ S ₁
	497.1827	-2.3	7.5	C ₁₅ H ₂₆ O ₈ N ₁₀ Na ₁
	497.1827	-2.3	2.0	C ₁₆ H ₃₂ O ₁₃ N ₃ Na ₁
	497.1804	2.4	14.5	C ₂₇ H ₃₀ N ₄ Na ₁ S ₂
	497.1828	-2.4	17.5	C ₂₉ H ₂₉ N ₄ S ₂
	497.1829	-2.6	10.5	C ₂₃ H ₃₀ O ₅ N ₄ Na ₁ S ₁
	497.1802	2.8	6.0	C ₂₀ H ₃₂ O ₈ N ₃ Na ₁ S ₁
	497.1802	2.8	11.5	C ₁₉ H ₂₆ O ₃ N ₁₀ Na ₁ S ₁
	497.1801	2.9	13.0	C ₂₆ H ₃₁ O ₃ N ₃ S ₂
	497.1800	3.1	3.0	C ₁₂ H ₂₈ O ₁₁ N ₉ Na ₁
	497.1800	3.3	4.5	C ₁₉ H ₃₃ O ₁₁ N ₂ S ₁
	497.1800	3.3	10.0	C ₁₈ H ₂₇ O ₆ N ₉ S ₁

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
497.1833	497.1833	-3.4	23.5	C ₂₉ H ₂₁ O ₁ N ₈
497.1833	497.1833	-3.4	18.0	C ₃₀ H ₂₇ O ₆ N ₁
497.1833	497.1833	-3.5	5.0	C ₁₅ H ₃₁ O ₆ N ₉ S ₂
497.1833	497.1833	-3.5	-0.5	C ₁₆ H ₃₇ O ₁₁ N ₂ S ₂
497.1834	497.1834	-3.7	-2.0	C ₉ H ₃₂ O ₁₁ N ₉ Na ₁ S ₁
497.1798	497.1798	3.7	1.5	C ₁₁ H ₂₉ O ₁₄ N ₈
497.1836	497.1836	-4.0	6.5	C ₁₆ H ₃₀ O ₃ N ₁₀ Na ₁ S ₂
497.1836	497.1836	-4.0	1.0	C ₁₇ H ₃₆ O ₈ N ₃ Na ₁ S ₂
497.1796	497.1796	4.1	-3.0	C ₁₂ H ₃₆ O ₁₀ N ₅ Na ₁ S ₂
497.1795	497.1795	4.1	15.5	C ₂₆ H ₂₆ O ₅ N ₄ Na ₁
497.1838	497.1838	-4.4	5.5	C ₁₆ H ₂₉ O ₁₂ N ₆
497.1793	497.1793	4.7	14.0	C ₂₅ H ₂₇ O ₈ N ₃
497.1793	497.1793	4.7	19.5	C ₂₄ H ₂₁ O ₃ N ₁₀
497.1840	497.1840	-4.8	14.0	C ₂₃ H ₂₇ O ₄ N ₇ S ₁
497.1840	497.1840	-4.8	8.5	C ₂₄ H ₃₃ O ₉ S ₁
497.1841	497.1841	-5.0	7.0	C ₁₇ H ₂₈ O ₉ N ₇ Na ₁
497.1841	497.1841	-5.0	1.5	C ₁₈ H ₃₄ O ₁₄ Na ₁

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
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Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
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aet7-49 MW=516?
(DCM)/MeOH + NH4OAc

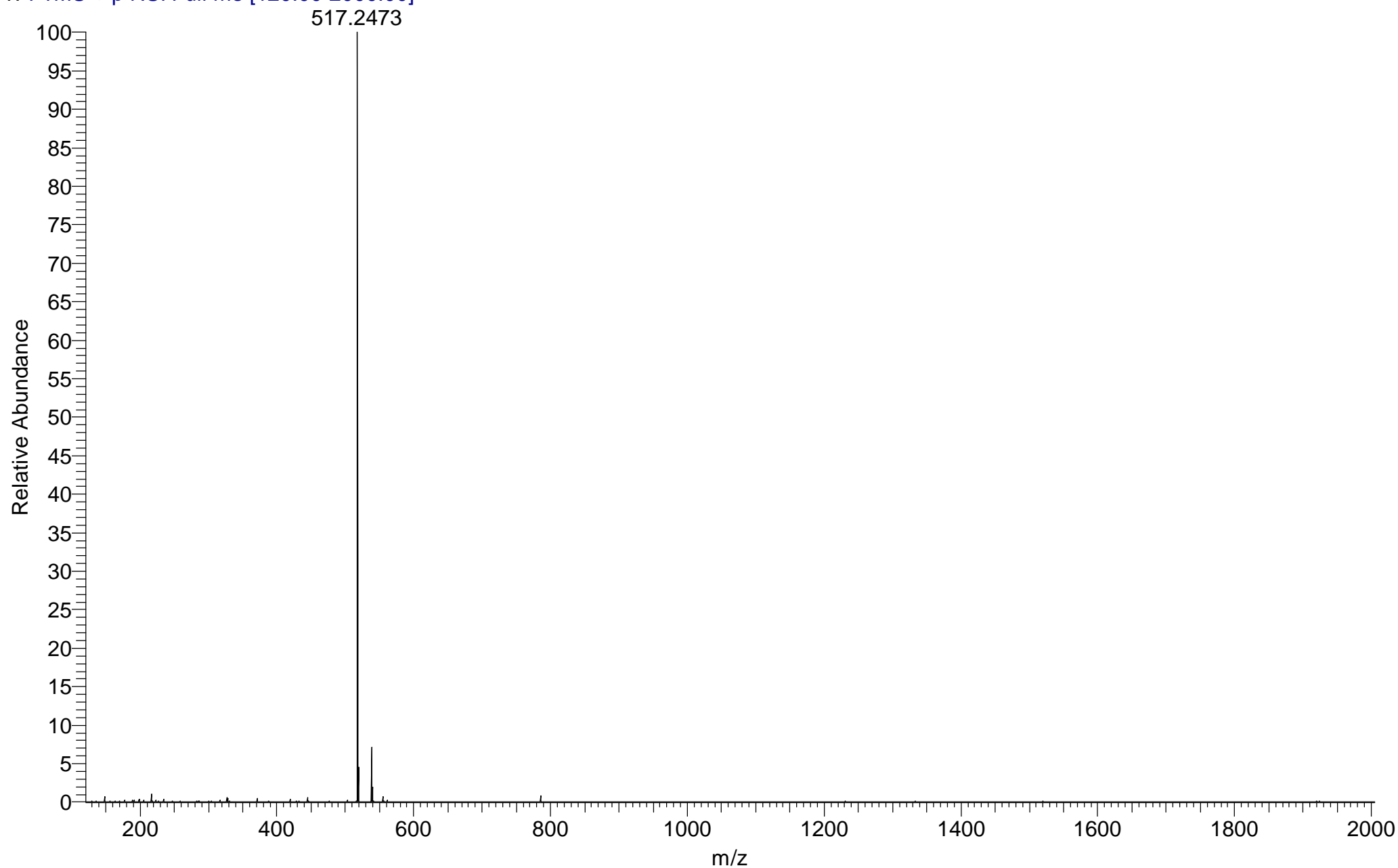
Compound 54

EPSRC National Centre Swansea
LTQ Orbitrap XL

adam throup
13/01/2012 14:44:24

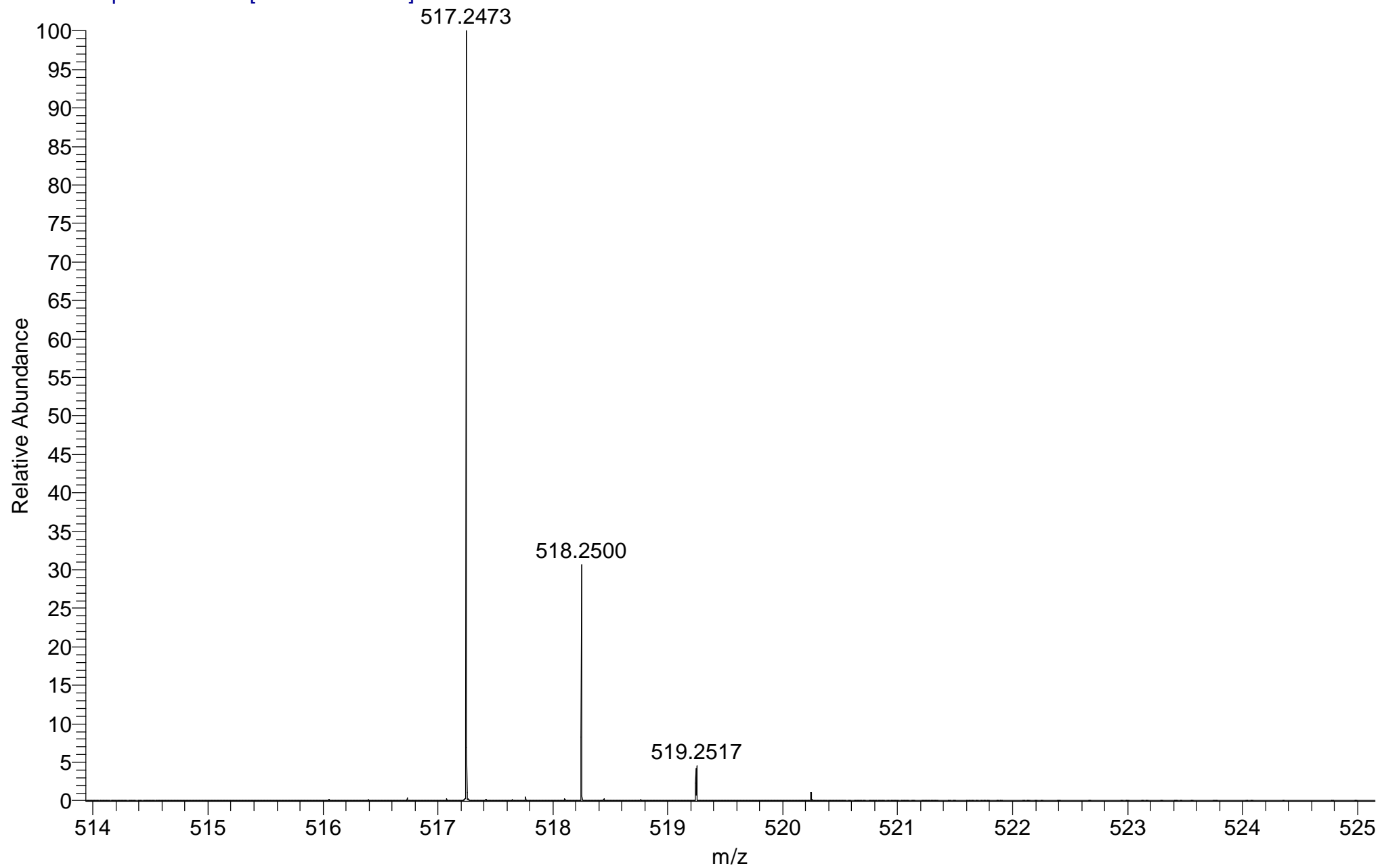
BRASHE181-OV-HNESP #21-33 RT: 0.89-1.24 AV: 13 NL: 2.30E7

T: FTMS + p NSI Full ms [120.00-2000.00]



BRASHE181-OV-HNESP #21-33 RT: 0.89-1.24 AV: 13 NL: 2.30E7

T: FTMS + p NSI Full ms [120.00-2000.00]



Isotope: Min. .. Max.
 14 N 0....10
 16 O 0....15
 12 C 0....40
 1 H 0....60
 23 Na 0....0
 32 S 0....2
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3..100
 Fits: 100

N-Rule: Do not use
 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
517.2473	517.2473	0.1	1.5	C ₁₈ H ₄₁ O ₇ N ₆ S ₂
	517.2472	0.1	20.0	C ₃₂ H ₃₁ O ₂ N ₅
	517.2477	-0.8	7.5	C ₁₈ H ₃₃ O ₈ N ₁₀
	517.2477	-0.8	2.0	C ₁₉ H ₃₉ O ₁₃ N ₃
	517.2468	1.0	14.0	C ₃₂ H ₃₉ O ₁ N ₁ S ₂
	517.2479	-1.2	10.5	C ₂₆ H ₃₇ O ₅ N ₄ S ₁
	517.2466	1.4	5.5	C ₂₅ H ₄₁ O ₉ S ₁
	517.2466	1.4	11.0	C ₂₄ H ₃₅ O ₄ N ₇ S ₁
	517.2464	1.7	2.5	C ₁₇ H ₃₇ O ₁₂ N ₆
	517.2484	-2.2	-2.0	C ₁₂ H ₃₉ O ₁₁ N ₉ S ₁
	517.2486	-2.5	19.5	C ₃₄ H ₃₃ O ₃ N ₂
	517.2486	-2.5	6.5	C ₁₉ H ₃₇ O ₃ N ₁₀ S ₂
	517.2486	-2.5	1.0	C ₂₀ H ₄₃ O ₈ N ₃ S ₂
	517.2459	2.7	2.0	C ₁₆ H ₃₉ O ₆ N ₉ S ₂
	517.2459	2.7	15.0	C ₃₁ H ₃₅ O ₆ N ₁
	517.2459	2.7	20.5	C ₃₀ H ₂₉ O ₁ N ₈
	517.2491	-3.4	7.0	C ₂₀ H ₃₅ O ₉ N ₇
	517.2491	-3.4	1.5	C ₂₁ H ₄₁ O ₁₄
	517.2454	3.6	14.5	C ₃₀ H ₃₇ N ₄ S ₂
	517.2493	-3.8	15.5	C ₂₇ H ₃₃ O ₁ N ₈ S ₁
	517.2493	-3.8	10.0	C ₂₈ H ₃₉ O ₆ N ₁ S ₁
	517.2452	4.0	6.0	C ₂₃ H ₃₉ O ₈ N ₃ S ₁
	517.2452	4.0	11.5	C ₂₂ H ₃₃ O ₃ N ₁₀ S ₁
	517.2451	4.3	3.0	C ₁₅ H ₃₅ O ₁₁ N ₉
	517.2498	-4.8	-2.5	C ₁₄ H ₄₁ O ₁₂ N ₆ S ₁

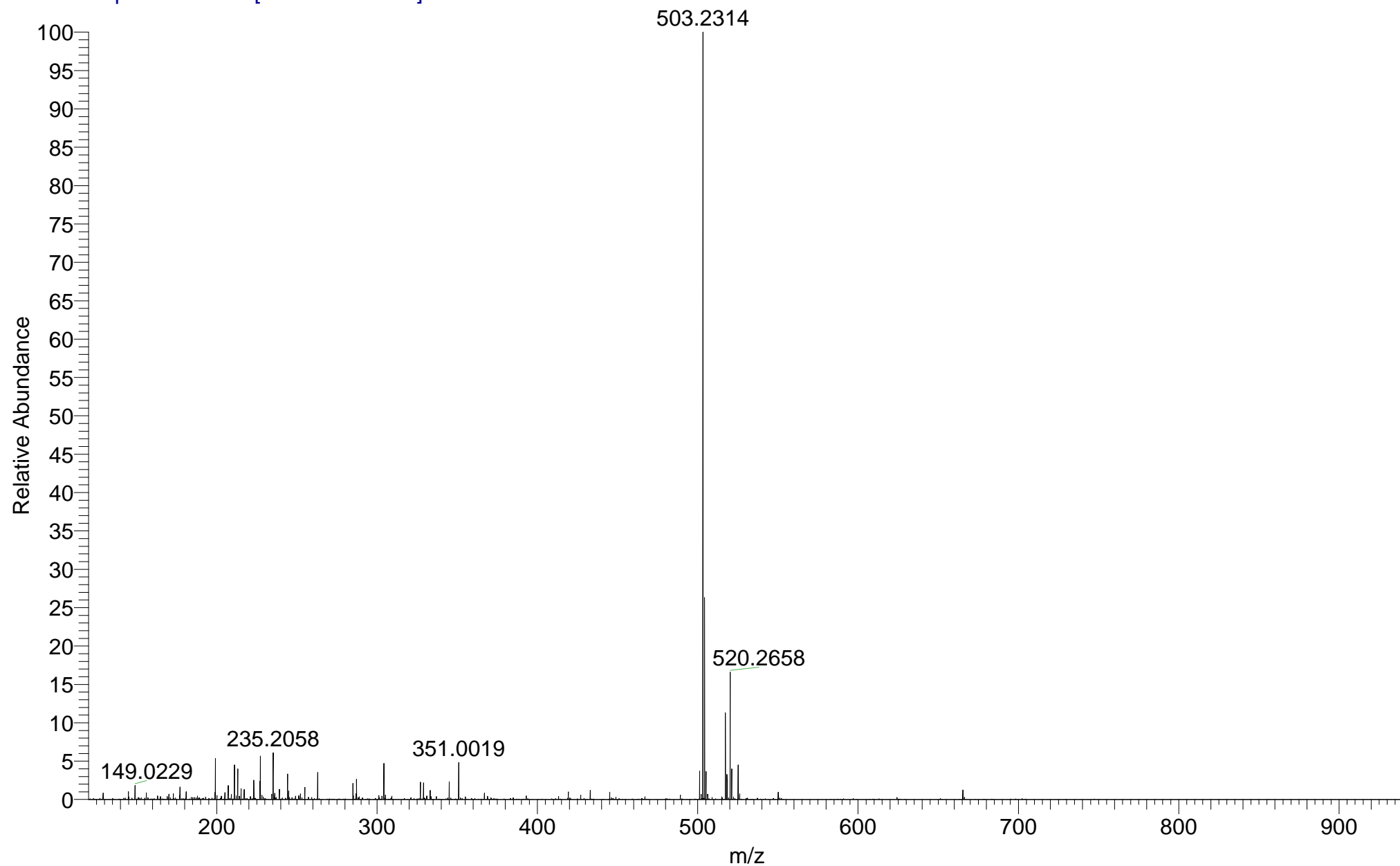
15-187
(MeOH)/MeOH+NH4OAc
C25H34N4O5S

Compound 55

EPSRC National Facility Swansea
LTQ Orbitrap XL

BRASHE
22/02/2017 15:50:57

BRASHE_O88TR_A #39-52 RT: 0.66-1.04 AV: 14 SM: 7G NL: 3.12E6
T: FTMS + p NSI Full ms [120.00-1935.00]

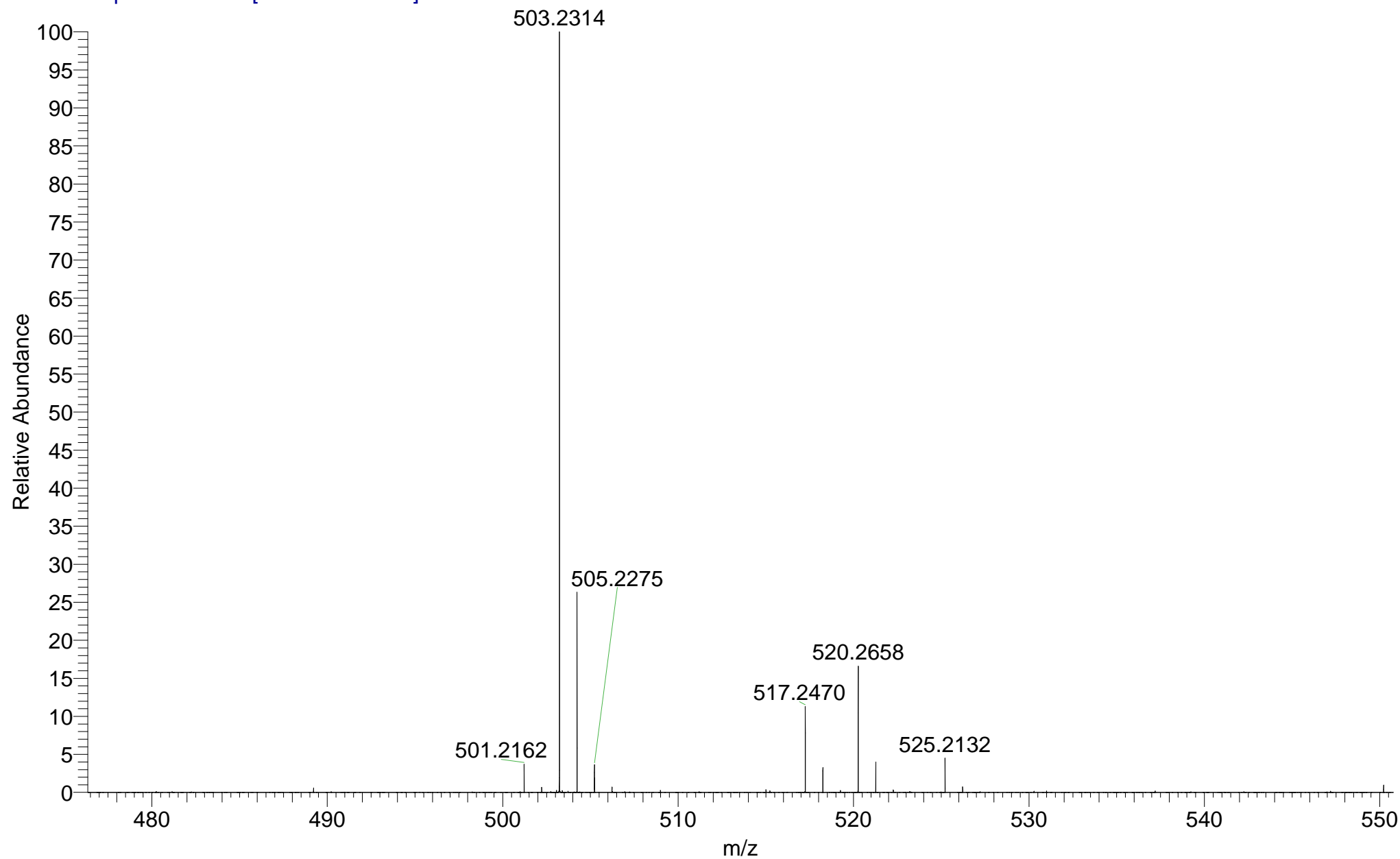


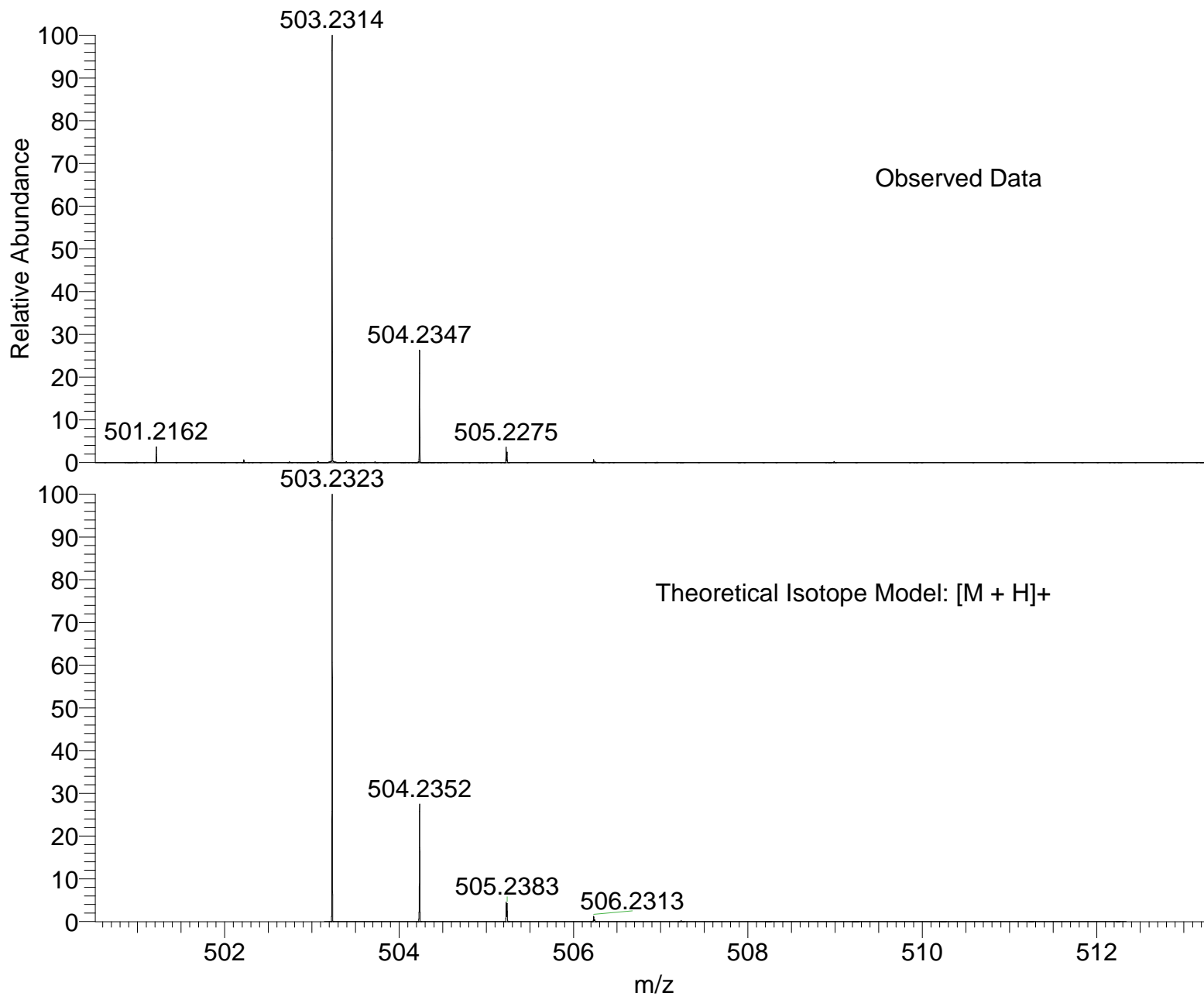
15-187
(MeOH)/MeOH+NH4OAc
C25H34N4O5S

EPSRC National Facility Swansea
LTQ Orbitrap XL

BRASHE
22/02/2017 15:50:57

BRASHE_O88TR_A #39-52 RT: 0.66-1.04 AV: 14 SM: 7G NL: 3.12E6
T: FTMS + p NSI Full ms [120.00-1935.00]





NL:
3.12E6
BRASHE_O88TR_A#39-52
RT: 0.66-1.04 AV: 14 T: FTMS
+ p NSI Full ms
[120.00-1935.00]

NL:
1.65E4
C₂₅ H₃₄ N₄ O₅ SH:
C₂₅ H₃₅ N₄ O₅ S₁
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

Isotope: Min. .. Max.
 14 N 0....15
 16 O 0....15
 12 C 0....60
 1 H 0....70
 23 Na 0....0
 32 S 0....5
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3.. 100
 Fits: 150

N-Rule: Do not use
 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
503.2314	503.2314	-0.1	-1.5	C ₉ H ₃₅ O ₁₀ N ₁₂ S ₁
	503.2316	-0.4	20.0	C ₃₁ H ₂₉ O ₂ N ₅
	503.2316	-0.4	7.0	C ₁₆ H ₃₃ O ₂ N ₁₃ S ₂
	503.2316	-0.4	1.5	C ₁₇ H ₃₉ O ₇ N ₆ S ₂
	503.2311	0.5	1.0	C ₁₆ H ₄₁ O ₁ N ₉ S ₄
	503.2311	0.6	14.0	C ₃₁ H ₃₇ O ₁ N ₁ S ₂
	503.2318	-0.8	4.5	C ₂₅ H ₄₃ O ₄ S ₃
	503.2310	0.9	-2.0	C ₈ H ₃₇ O ₄ N ₁₅ S ₃
	503.2309	0.9	5.5	C ₂₄ H ₃₉ O ₉ S ₁
	503.2309	0.9	11.0	C ₂₃ H ₃₃ O ₄ N ₇ S ₁
	503.2307	1.3	2.5	C ₁₆ H ₃₅ O ₁₂ N ₆
	503.2307	1.3	8.0	C ₁₅ H ₂₉ O ₇ N ₁₃
	503.2321	-1.4	7.5	C ₁₇ H ₃₁ O ₈ N ₁₀
	503.2321	-1.4	2.0	C ₁₈ H ₃₇ O ₁₃ N ₃
	503.2323	-1.7	16.0	C ₂₄ H ₂₉ N ₁₁ S ₁
	503.2323	-1.7	10.5	C ₂₅ H ₃₅ O ₅ N ₄ S ₁
	503.2323	-1.8	-2.5	C ₁₀ H ₃₉ O ₅ N ₁₂ S ₃
	503.2305	1.9	5.0	C ₂₃ H ₄₁ O ₃ N ₃ S ₃
	503.2325	-2.2	0.5	C ₁₈ H ₄₃ O ₂ N ₆ S ₄
	503.2303	2.2	2.0	C ₁₅ H ₃₇ O ₆ N ₉ S ₂
	503.2302	2.3	15.0	C ₃₀ H ₃₃ O ₆ N ₁
	503.2302	2.3	20.5	C ₂₉ H ₂₇ O ₁ N ₈
	503.2301	2.6	-1.0	C ₇ H ₃₃ O ₉ N ₁₅ S ₁
	503.2328	-2.7	-2.0	C ₁₁ H ₃₇ O ₁₁ N ₉ S ₁
	503.2329	-3.0	19.5	C ₃₃ H ₃₁ O ₃ N ₂
	503.2330	-3.1	6.5	C ₁₈ H ₃₅ O ₃ N ₁₀ S ₂
	503.2330	-3.1	1.0	C ₁₉ H ₄₁ O ₈ N ₃ S ₂
	503.2298	3.2	1.5	C ₁₄ H ₃₉ N ₁₂ S ₄
	503.2298	3.2	14.5	C ₂₉ H ₃₅ N ₄ S ₂
	503.2331	-3.4	9.5	C ₂₆ H ₃₉ N ₄ S ₃
	503.2296	3.6	6.0	C ₂₂ H ₃₇ O ₈ N ₃ S ₁

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
	503.2296	3.6	11.5	C ₂₁ H ₃₁ O ₃ N ₁₀ S ₁
	503.2294	4.0	3.0	C ₁₄ H ₃₃ O ₁₁ N ₉
	503.2334	-4.0	12.5	C ₁₈ H ₂₇ O ₄ N ₁₄
	503.2334	-4.0	7.0	C ₁₉ H ₃₃ O ₉ N ₇
	503.2334	-4.0	1.5	C ₂₀ H ₃₉ O ₁₄
	503.2336	-4.4	15.5	C ₂₆ H ₃₁ O ₁ N ₈ S ₁
	503.2336	-4.4	10.0	C ₂₇ H ₃₇ O ₆ N ₁ S ₁
	503.2336	-4.5	-3.0	C ₁₂ H ₄₁ O ₆ N ₉ S ₃
	503.2291	4.5	5.5	C ₂₁ H ₃₉ O ₂ N ₆ S ₃
	503.2338	-4.8	0.0	C ₂₀ H ₄₅ O ₃ N ₃ S ₄
	503.2289	4.9	-3.0	C ₁₄ H ₄₁ O ₁₀ N ₅ S ₂
	503.2289	4.9	2.5	C ₁₃ H ₃₅ O ₅ N ₁₂ S ₂
	503.2289	5.0	15.5	C ₂₈ H ₃₁ O ₅ N ₄
	503.2289	5.0	21.0	C ₂₇ H ₂₅ N ₁₁