Supplemental Material For

Design and Synthesis of Benzopyran-based Inhibitors of Hypoxia-Inducible Factor-1 Pathway with Improved Water Solubility

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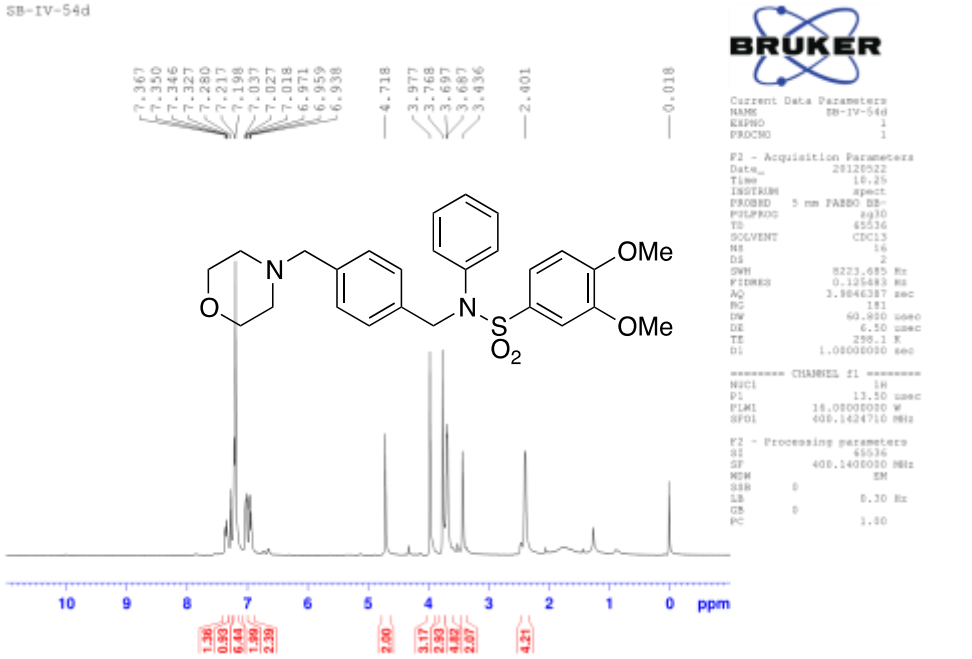
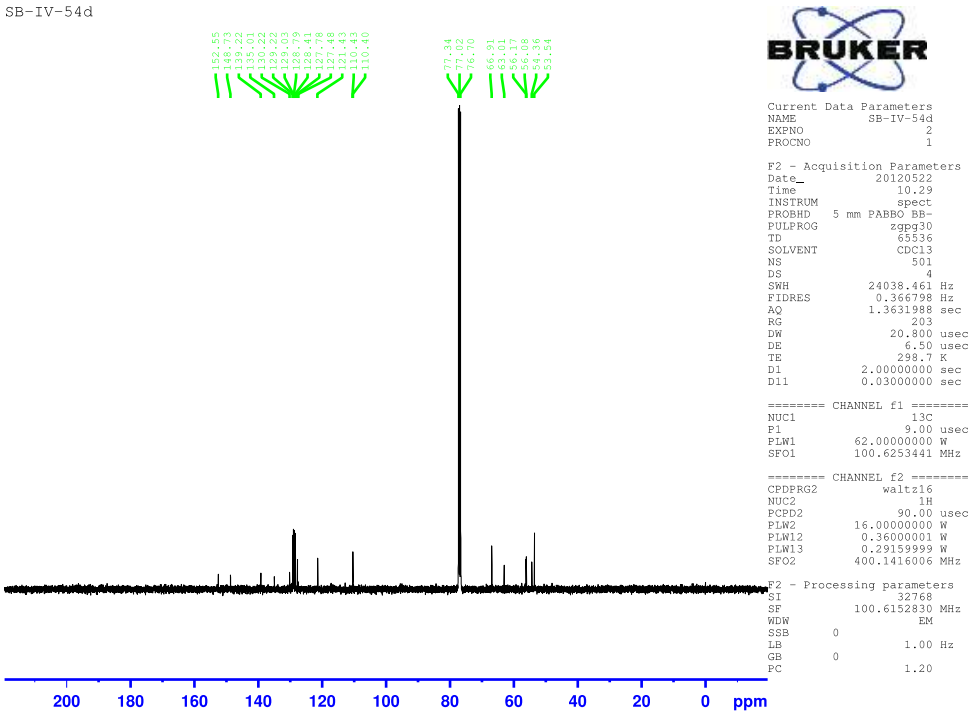
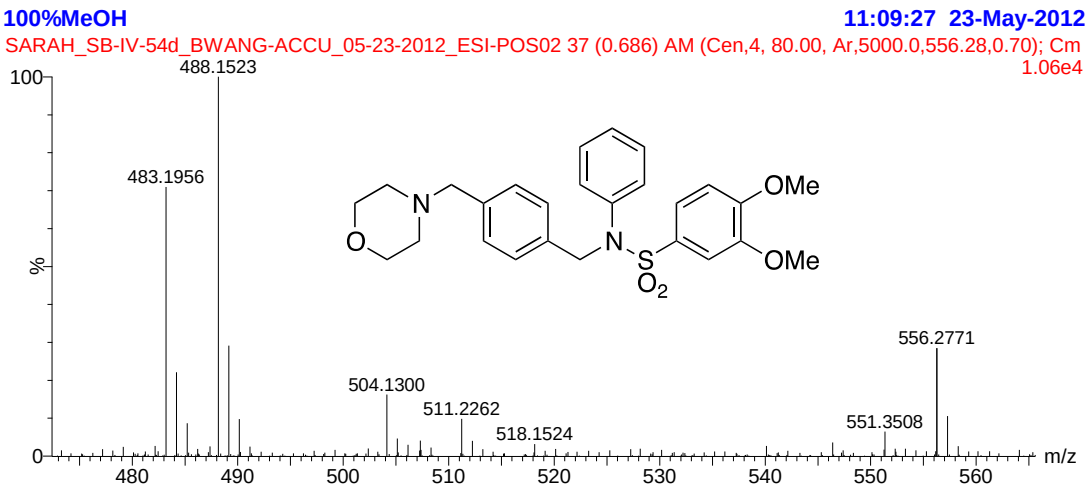
Contents

3,4-Dimethoxy-*N*-(4-(morpholinomethyl)benzyl)-*N*-phenylbenzenesulfonamide (3a)







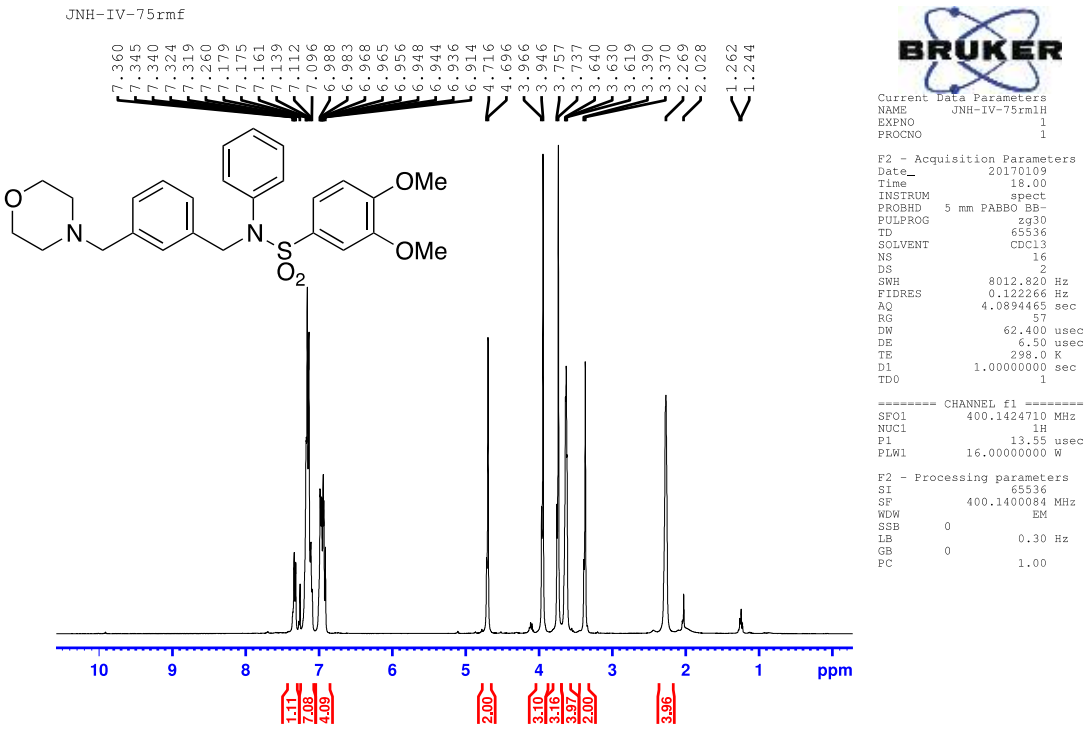
Elemental Composition Report

Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
6053 formula(e) evaluated with 64 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-200 H: 1-200 N: 1-15 O: 1-100 S: 0-50

Minimum:				-1.5			
Maximum:		5.0	20.0	50.0			
Mass	Calc. Mass	mDa		PPM	DBE	i-FIT	Formula
483.1956	483.1954	0.2	0.4	12.5	12.4		C26 H31 N2 O5 S

3,4-Dimethoxy-*N*-(3-(morpholinomethyl)benzyl)-N-phenylbenzenesulfonamide (3b)

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Current Data Parameters
NAME       JNH-IV-75rm1H
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170109
Time               18.00
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ             4.0894465 sec
RG                   57
DW               62.400 usec
DE                6.50 usec
TE                298.0 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         400.1424710 MHz
NUC1                   1H
P1                 13.55 usec
PLW1         16.00000000 W

F2 - Processing parameters
SI                65536
SF           400.1400084 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
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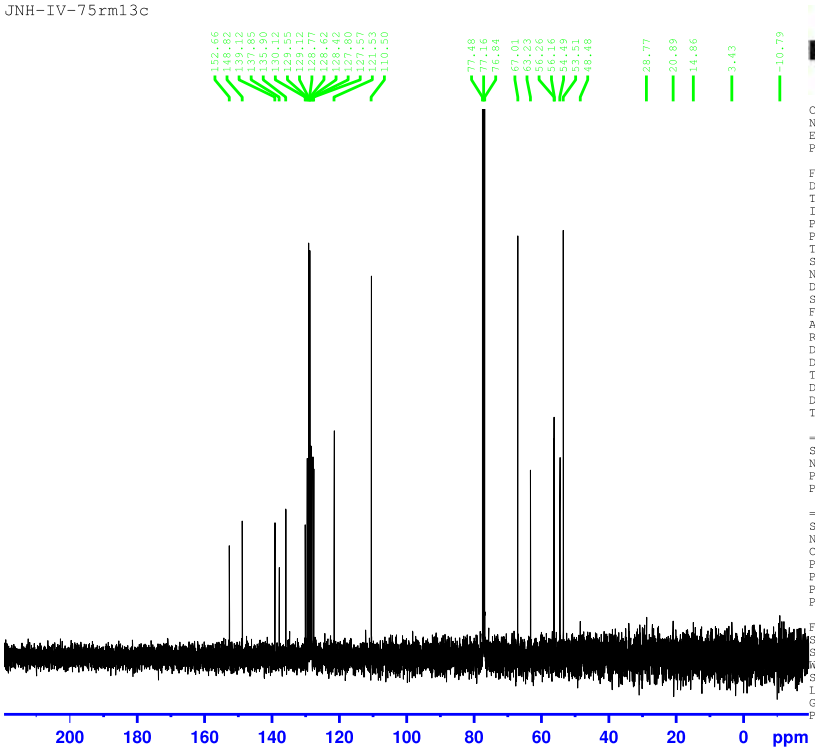


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EXPNO                  1
PROCNO                 1

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INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  106
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                  203
DW               20.800 usec
DE                6.50 usec
TE                298.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         100.6253441 MHz
NUC1                  13C
P1                 9.25 usec
PLW1         62.00000000 W

======== CHANNEL f2 ========
SFO2         400.1416006 MHz
NUC2                   1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         16.00000000 W
PLW12         0.36267000 W
PLW13         0.29376000 W

F2 - Processing parameters
SI                32768
SF           100.6152753 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
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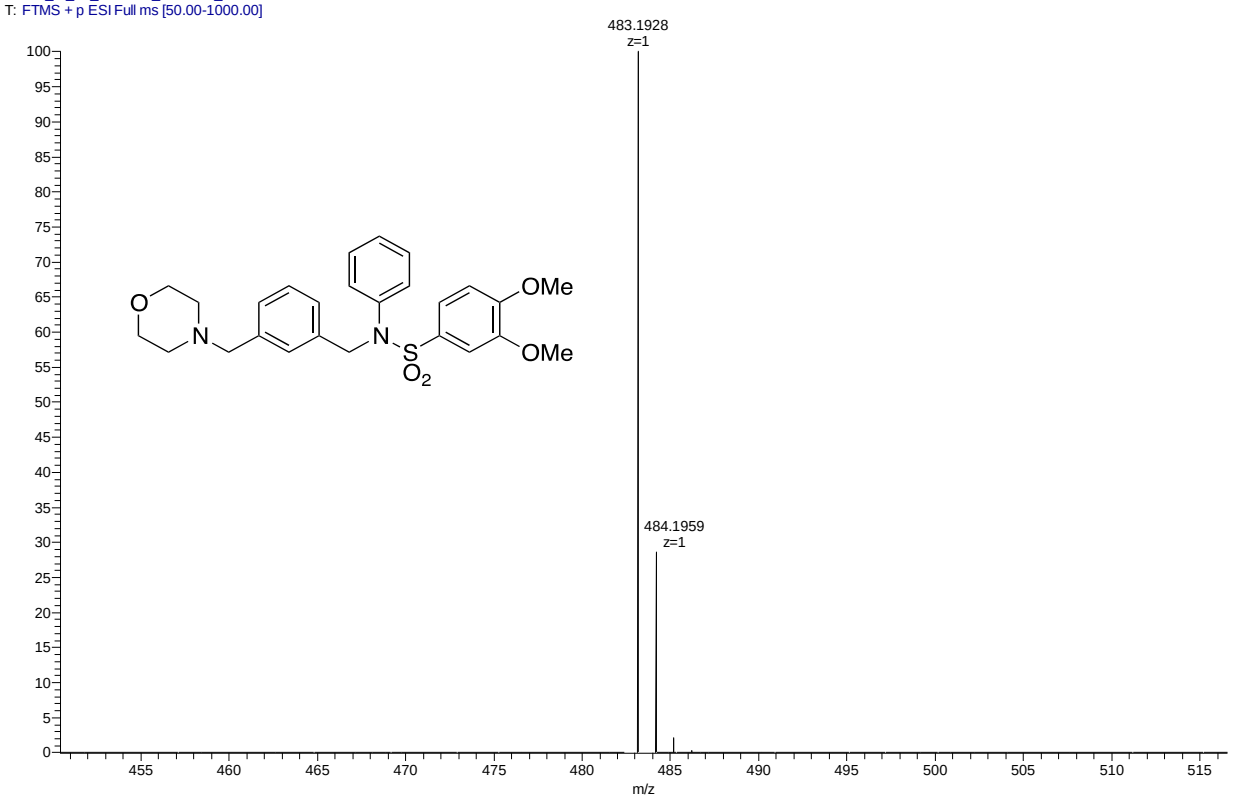
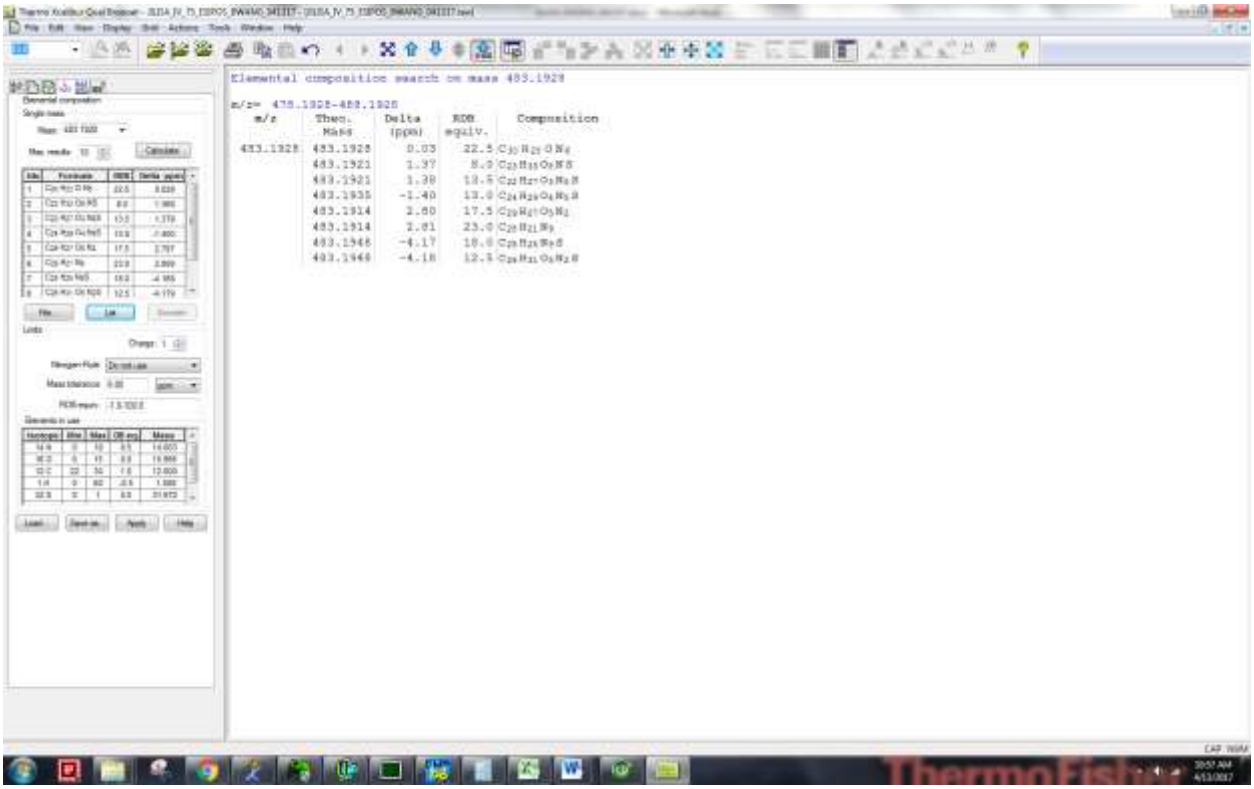
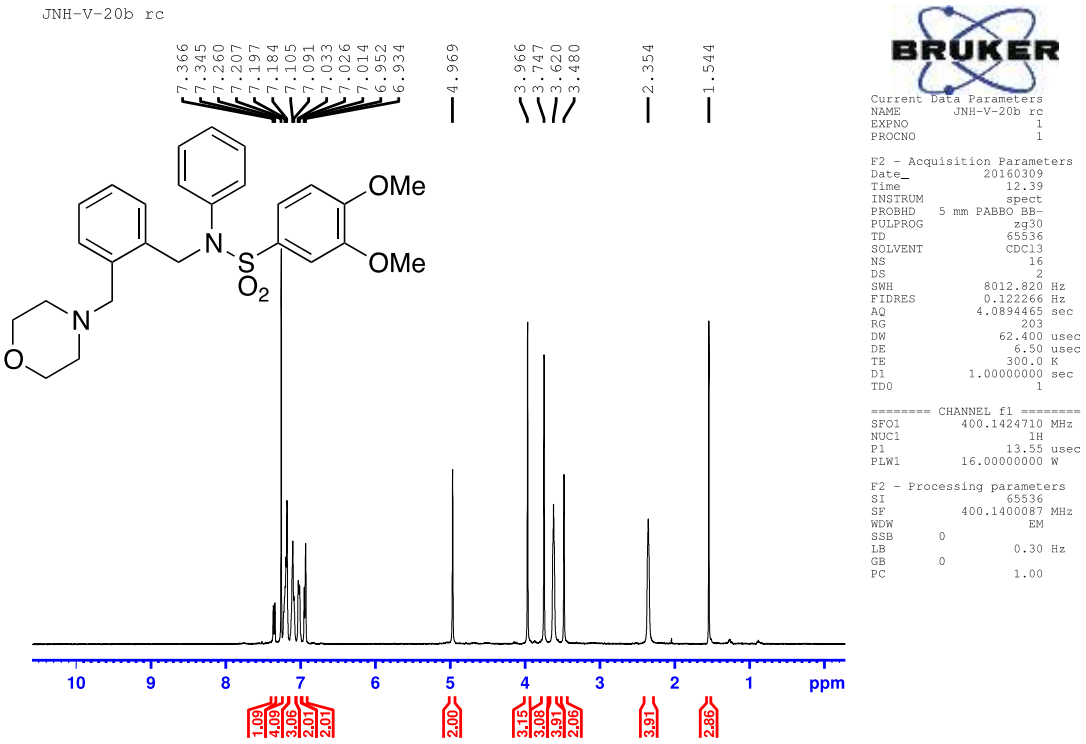
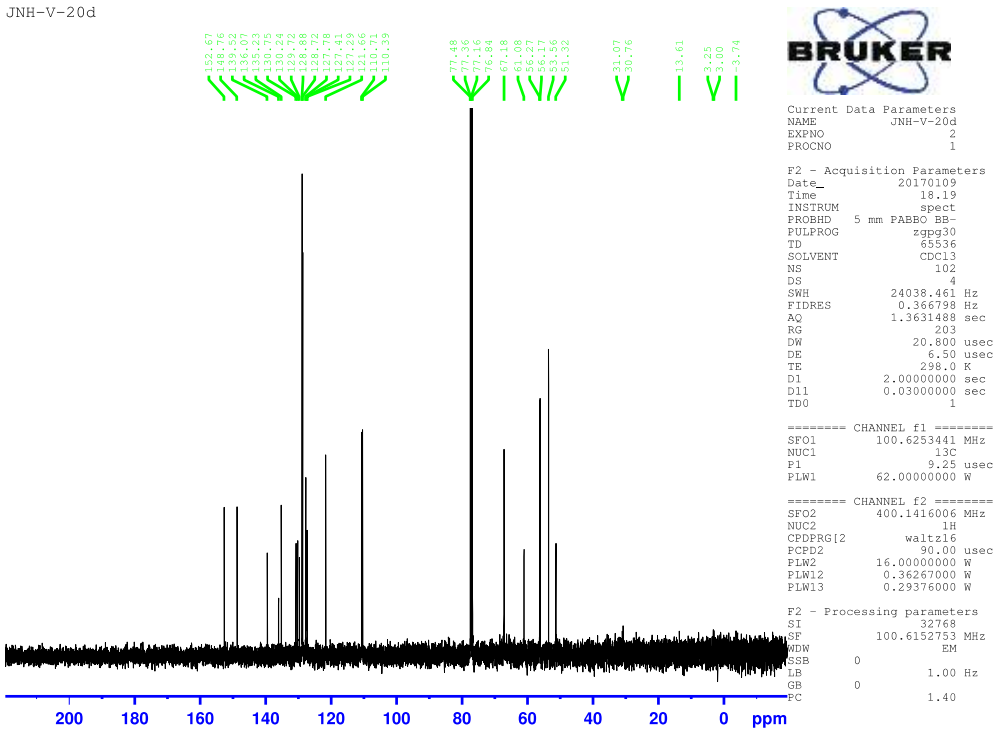
T: FTMS + p ESI Full ms [50.00-1000.00]



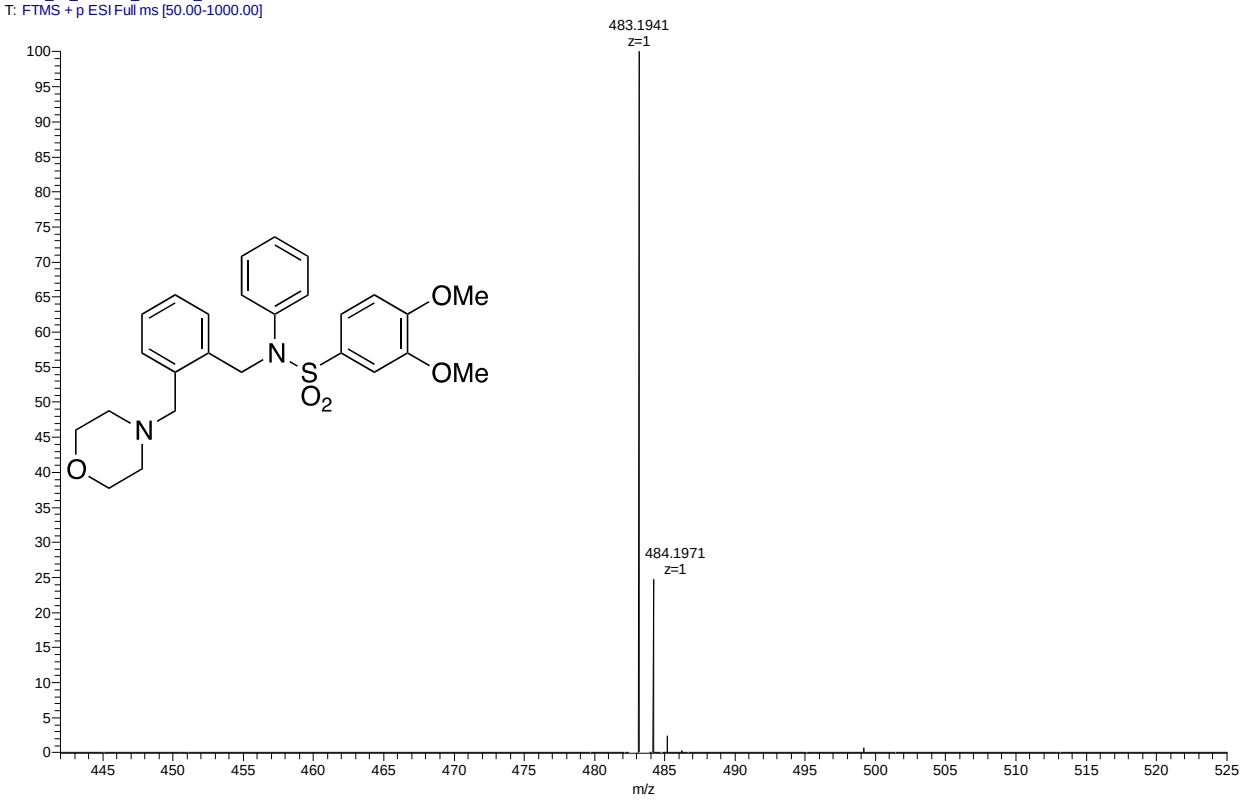


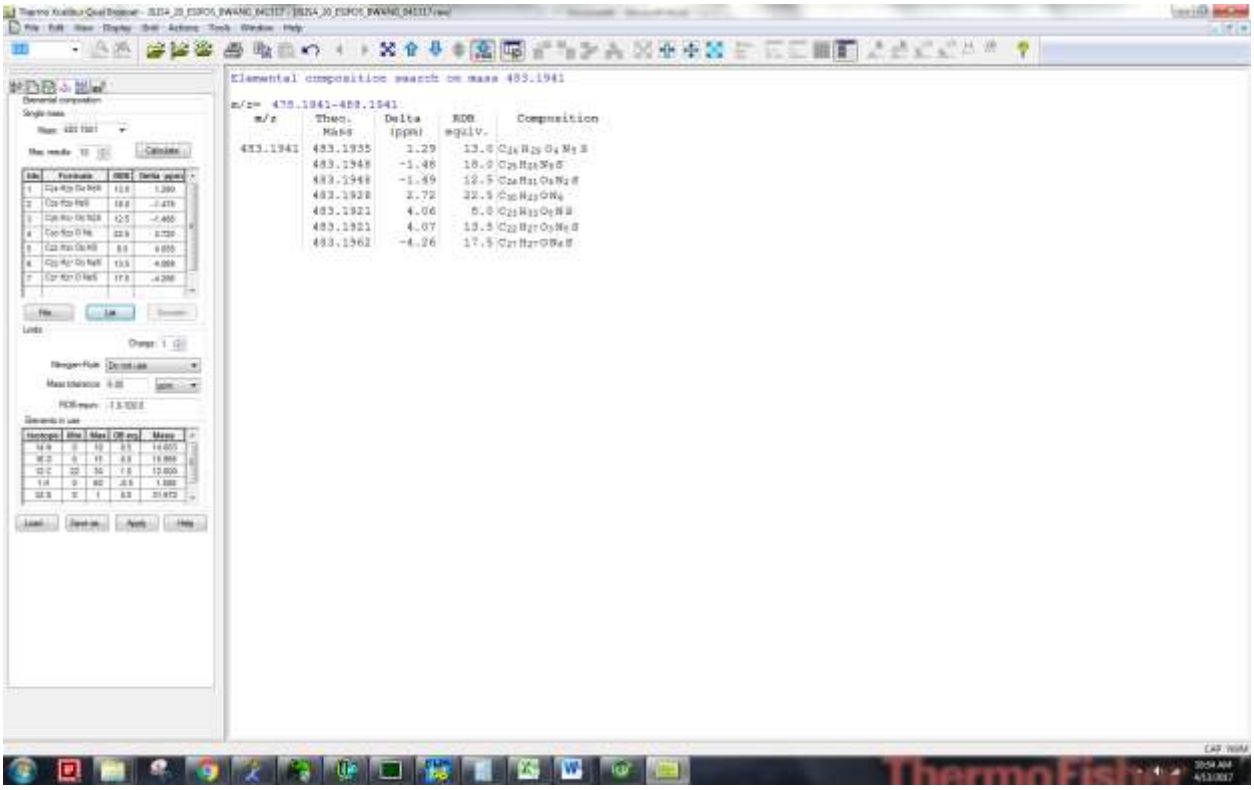
3,4-Dimethoxy-*N*-(2-(morpholinomethyl)benzyl)-*N*-phenylbenzenesulfonamide (3c)





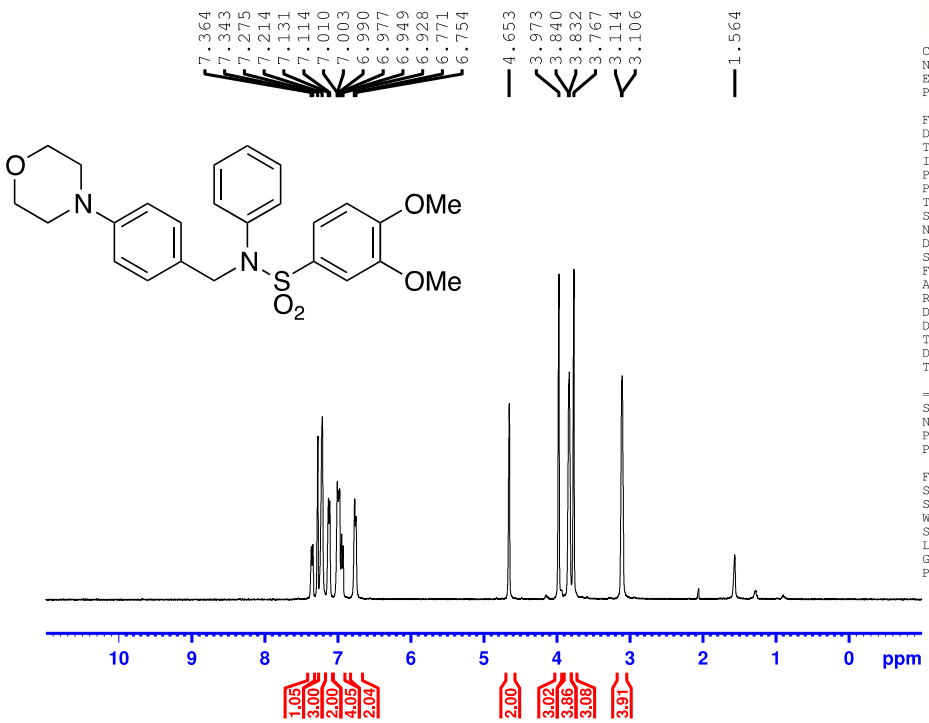
JILISA_20_ESIPOS_BWANG_041317 #129 RT: 1.82 AV: 1 NL: 6.68E6
T: FTMS + p ESI Full ms [50.00-1000.00]





3,4-Dimethoxy-*N*-(4-morpholinobenzyl)-*N*-phenylbenzenesulfonamide (3d)

SB-V-88r1

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PROCNO                        1

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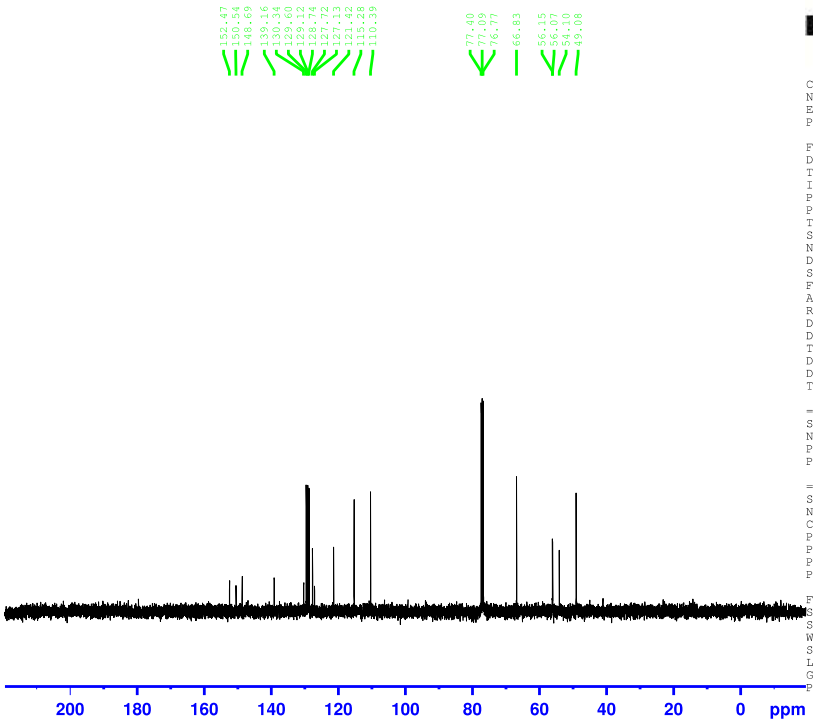
Time                     13.43
INSTRUM                  spect
PROBHD     5 mm PABBO BB-
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         12
DS                          2
SWH                  8012.820 Hz
FIDRES               0.122266 Hz
AQ                   4.0894465 sec
RG                        203
DW                       62.400 usec
DE                        6.50 usec
TE                       298.0 K
D1                  1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
SFO1               400.1424710 MHz
NUC1                         1H
P1                        13.50 usec
PLW1               16.00000000 W

F2 - Processing parameters
SI                      65536
SF                 400.1400000 MHz
WDW                        EM
SSB          0
LB                        0.30 Hz
GB           0
PC                        1.00
```

SB-V-88c

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Current Data Parameters
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EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_               20130219
Time                     18.19
INSTRUM                  spect
PROBHD     5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                         30
DS                          4
SWH                 24038.461 Hz
FIDRES               0.366798 Hz
AQ                   1.3631488 sec
RG                        203
DW                       20.800 usec
DE                        6.50 usec
TE                       298.2 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                           1

======== CHANNEL f1 ========
SFO1               100.6253441 MHz
NUC1                        13C
P1                         9.00 usec
PLW1               62.00000000 W

======== CHANNEL f2 ========
SFO2               400.1416006 MHz
NUC2                         1H
CPDPRG[2                waltz16
PCPD2                     90.00 usec
PLW2               16.00000000 W
PLW12               0.36000001 W
PLW13               0.29159999 W

F2 - Processing parameters
SI                      32768
SF                 100.6152830 MHz
WDW                        EM
SSB          0
LB                        1.00 Hz
GB           0
PC                        1.40
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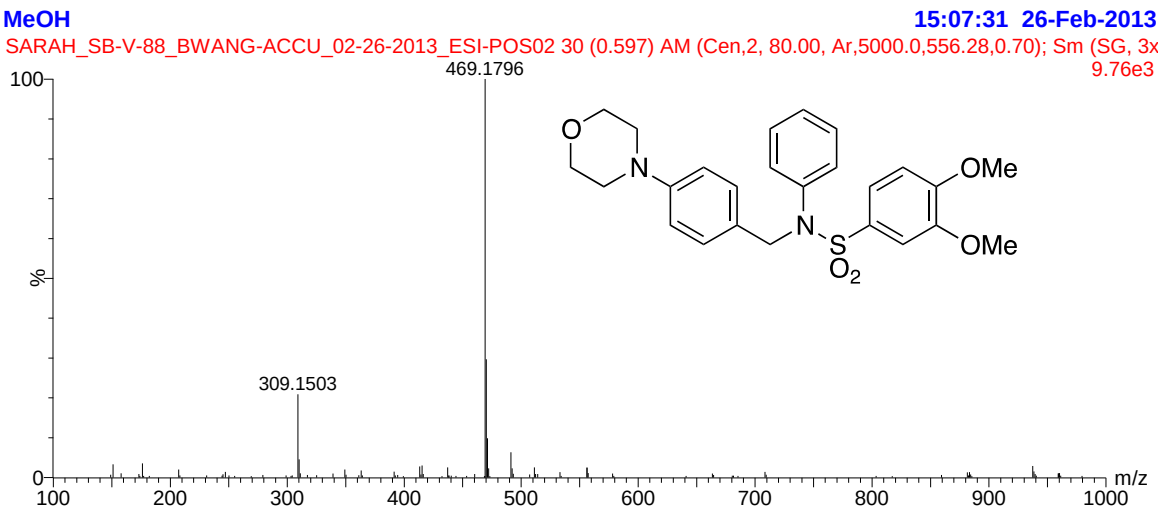


Elemental Composition Report

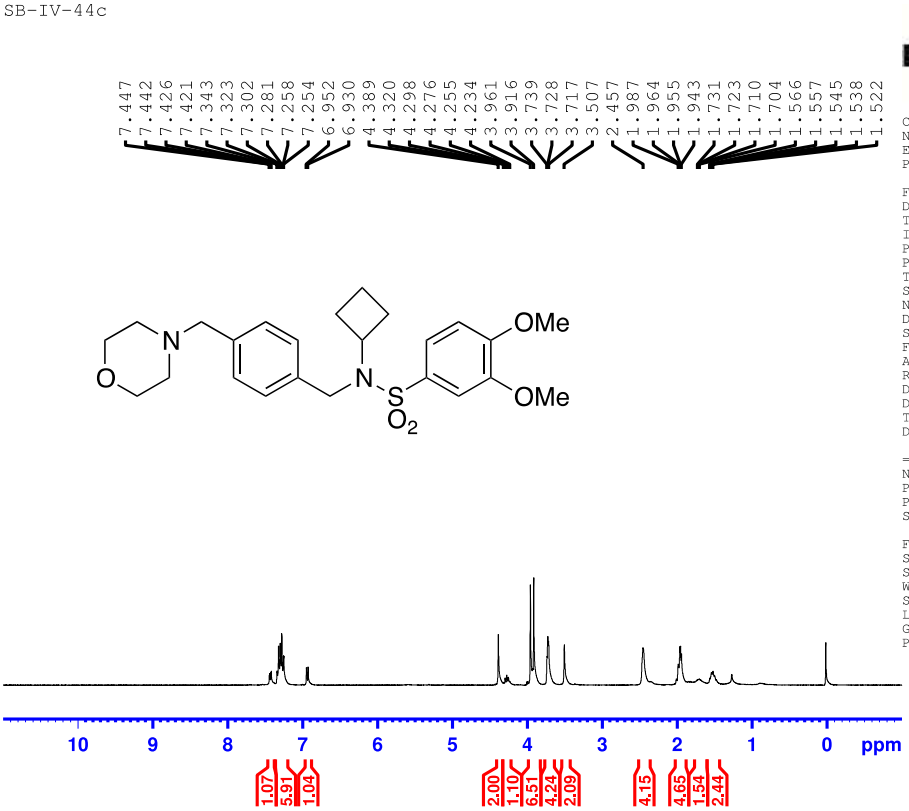
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
2331 formula(e) evaluated with 5 results within limits (up to 100 closest results for each mass)
Elements Used:
C: 1-150 H: 1-150 N: 1-6 O: 1-30 S: 1-10

Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa		PPM	DBE	i-FIT	Formula
469.1796	469.1797	-0.1	-0.2	12.5	0.3		C25 H29 N2 O5 S

N-Cyclobutyl-3,4-dimethoxy-*N*-(4-(morpholinomethyl)benzyl)benzenesulfonamide (4a)

SB-IV-44c

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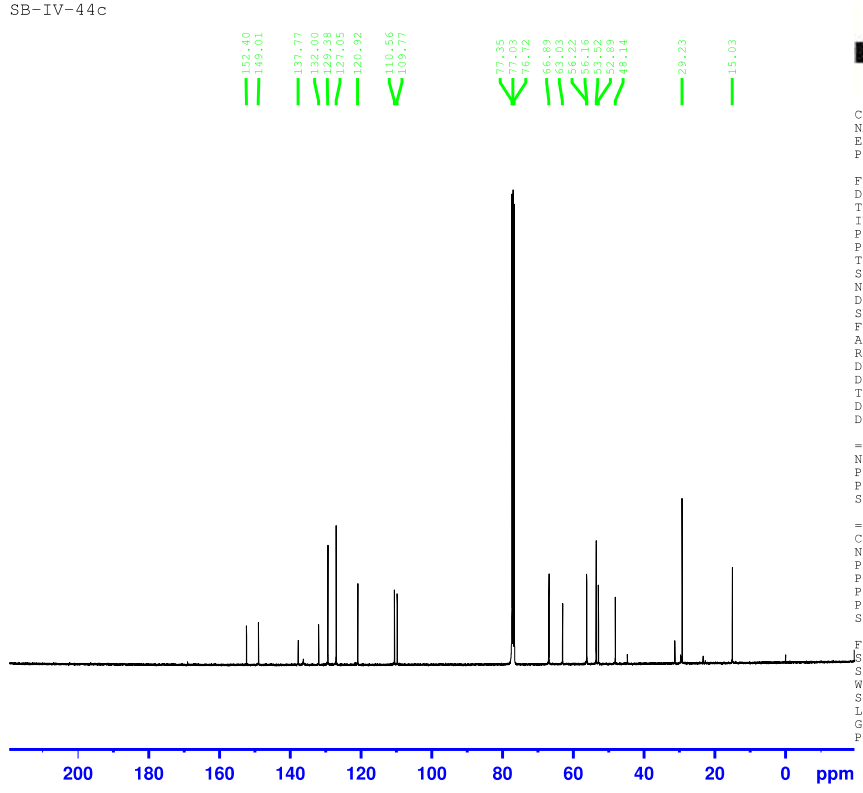
Current Data Parameters
NAME                  SB-IV-44c
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_               20120430
Time                   15.43
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                 8223.685 Hz
FIDRES              0.125483 Hz
AQ                  3.9846387 sec
RG                      203
DW                    60.800 usec
DE                     6.50 usec
TE                    298.1 K
D1                 1.00000000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                     13.50 usec
PLW1              16.00000000 W
SFO1             400.1424710 MHz

F2 - Processing parameters
SI                        65536
SF                400.1400000 MHz
WDW                         EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

SB-IV-44c

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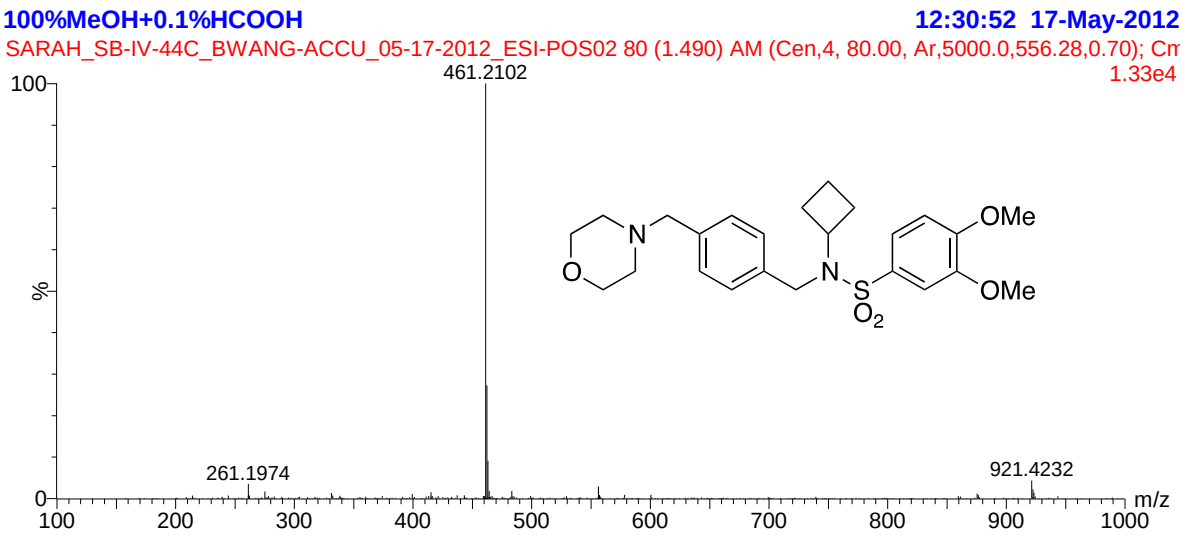
Current Data Parameters
NAME                  SB-IV-44c
EXPNO                         3
PROCNO                        1

F2 - Acquisition Parameters
Date_               20120515
Time                   23.52
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                    10240
DS                        4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631988 sec
RG                      203
DW                    20.800 usec
DE                     6.50 usec
TE                    300.0 K
D1                 2.00000000 sec
D11                0.03000000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                      9.00 usec
PLW1              62.00000000 W
SFO1             100.6253441 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                      1H
PCPD2                  90.00 usec
PLW2              16.00000000 W
PLW12              0.36000001 W
PLW13              0.29159999 W
SFO2             400.1416006 MHz

F2 - Processing parameters
SI                        32768
SF               100.6152830 MHz
WDW                         EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```



Elemental Composition Report

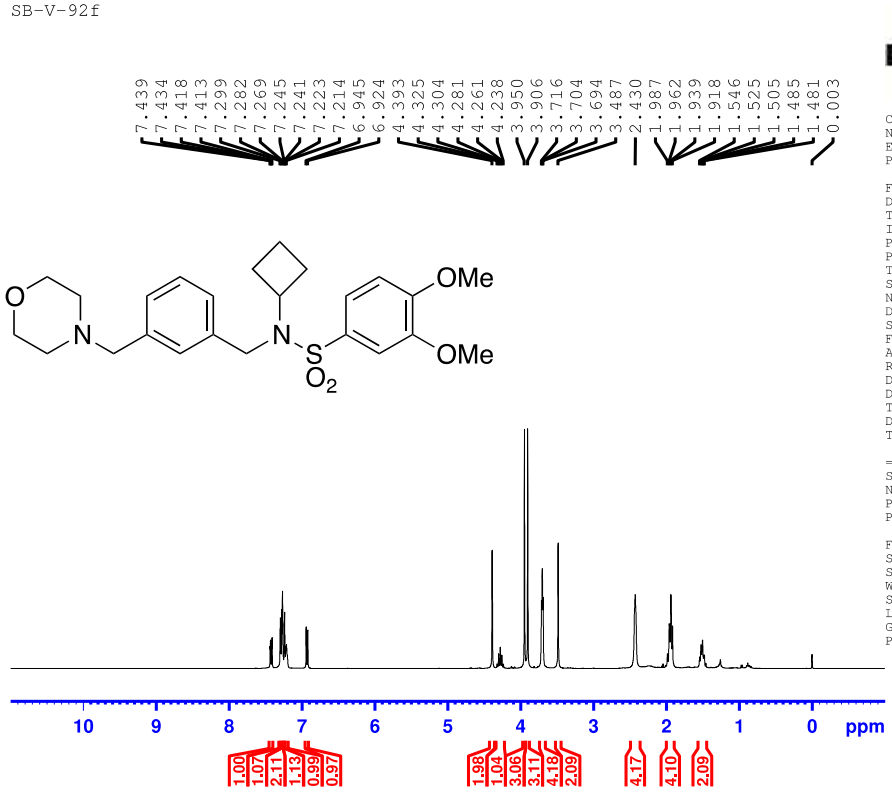
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
4674 formula(e) evaluated with 14 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-100 H: 1-100 N: 1-15 O: 1-100 S: 0-6

Minimum:				-1.5		
Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
461.2102	461.2110	-0.8	-1.7	9.5	5.9	C24 H33 N2 O5 S

N-Cyclobutyl-3,4-dimethoxy-*N*-(3-(morpholinomethyl)benzyl)benzenesulfonamide (4b)

SB-V-92f



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EXPNO 1
PROCNO 1

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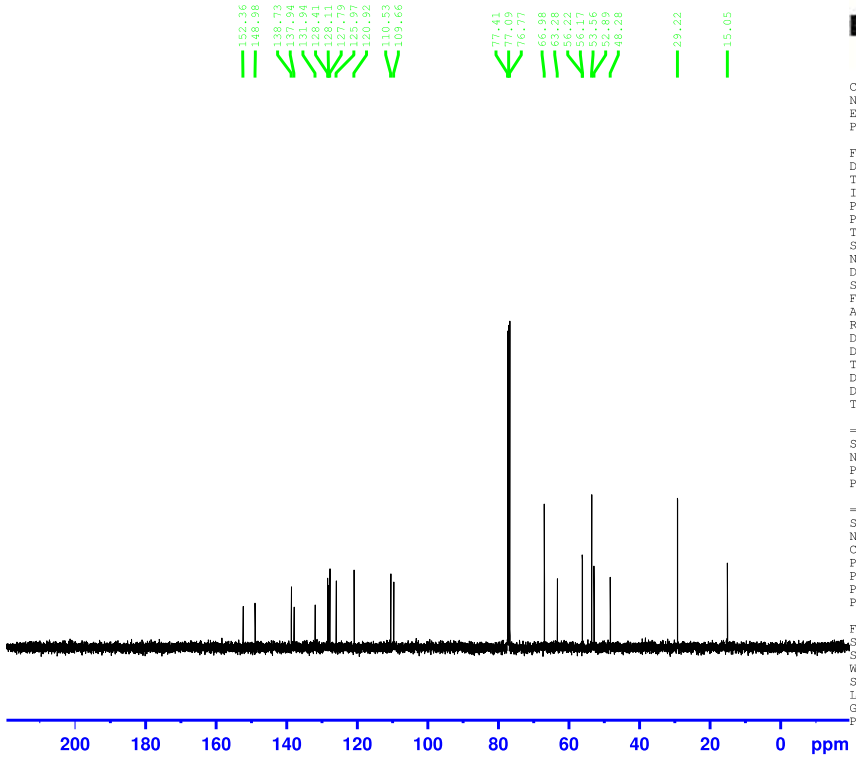
Time 20.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 57
DW 62.400 usec
DE 6.50 usec
TE 293.7 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1424710 MHz
NUC1 1H
P1 13.50 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1400000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

SB-V-92f



Current Data Parameters
NAME SB-V-92f
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
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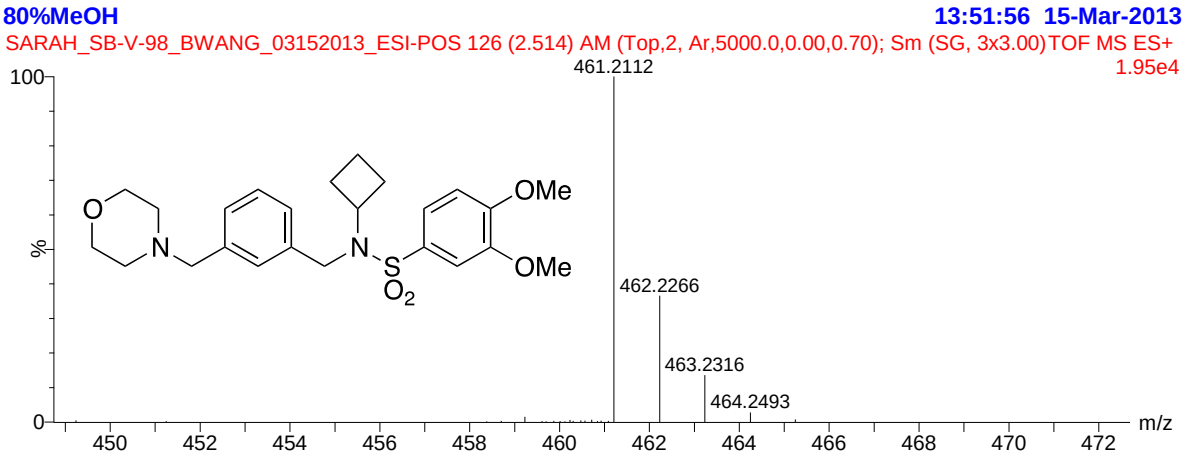
Time 20.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 30
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 294.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6253441 MHz
NUC1 13C
P1 9.00 usec
PLW1 62.00000000 W

======== CHANNEL f2 ========
SFO2 400.1416006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.36000001 W
PLW13 0.29159999 W

F2 - Processing parameters
SI 32768
SF 100.6152830 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Elemental Composition Report

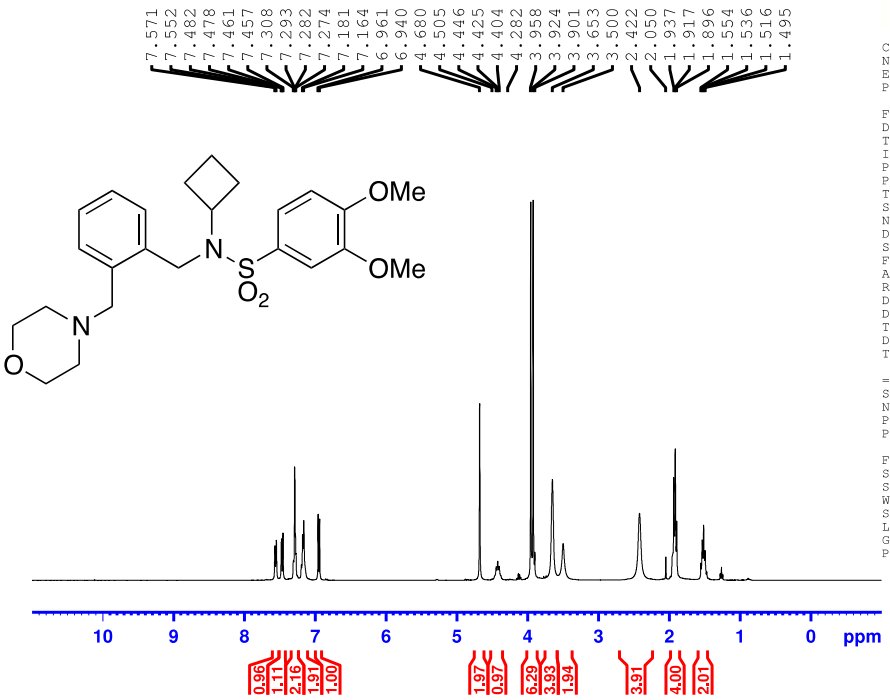
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
4668 formula(e) evaluated with 10 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-150 H: 1-150 N: 1-30 O: 1-60 S: 1-10

Minimum:				-1.5		
Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
461.2112	461.2110	0.2	0.4	9.5	243.0	C24 H33 N2 O5 S

N-Cyclobutyl-3,4-dimethoxy-*N*-(2-(morpholinomethyl)benzyl)benzenesulfonamide (4c)

SB-V-91cR



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Current Data Parameters
NAME                  SB-V-91cR
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
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Time                      21.14
INSTRUM                   spect
PROBHD     5 mm PABBO BB-
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                          16
DS                           2
SWH                   8012.820 Hz
FIDRES                0.122266 Hz
AQ                    4.0894465 sec
RG                          57
DW                       62.400 usec
DE                        6.50 usec
TE                       293.9 K
D1                    1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
SFO1                400.1424710 MHz
NUC1                        1H
P1                       13.50 usec
PLW1                16.00000000 W

F2 - Processing parameters
SI                       65536
SF                  400.1400000 MHz
WDW                         EM
SSB                  0
LB                        0.30 Hz
GB                   0
PC                        1.00
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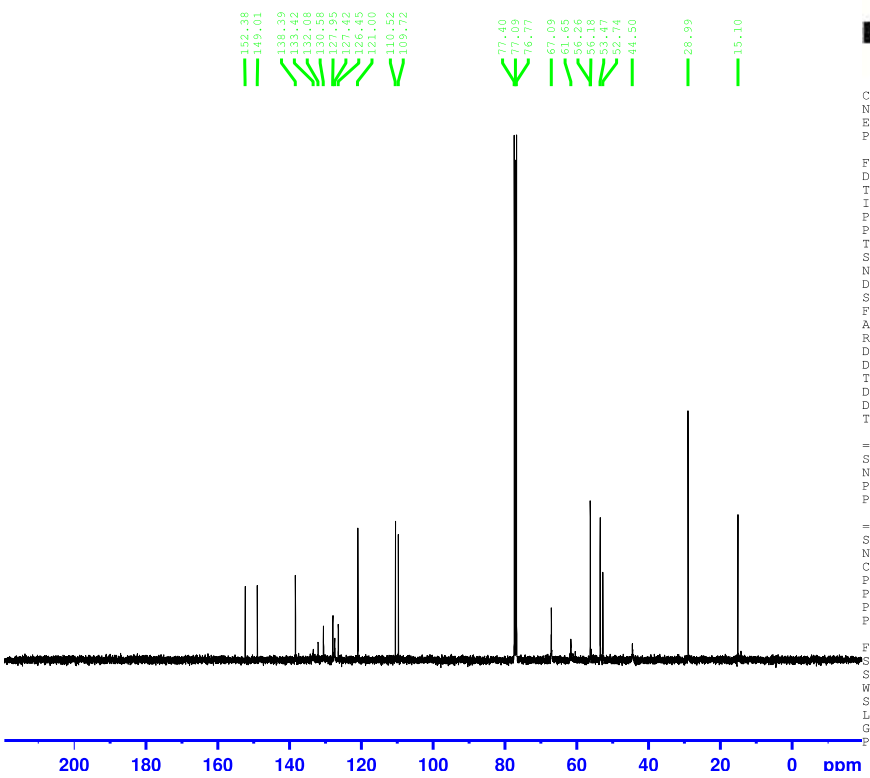
SB-V-91cR



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Current Data Parameters
NAME                  SB-V-91cR
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20130311
Time                      21.18
INSTRUM                   spect
PROBHD     5 mm PABBO BB-
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                         191
DS                           4
SWH                  24038.461 Hz
FIDRES                0.366798 Hz
AQ                    1.3631488 sec
RG                         203
DW                       20.800 usec
DE                        6.50 usec
TE                       294.5 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                           1

======== CHANNEL f1 ========
SFO1                100.6253441 MHz
NUC1                        13C
P1                        9.00 usec
PLW1                62.00000000 W

======== CHANNEL f2 ========
SFO2                400.1416006 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                    90.00 usec
PLW2                16.00000000 W
PLW12                0.36000001 W
PLW13                0.29159999 W

F2 - Processing parameters
SI                       32768
SF                  100.6152830 MHz
WDW                         EM
SSB                  0
LB                        1.00 Hz
GB                   0
PC                        1.40
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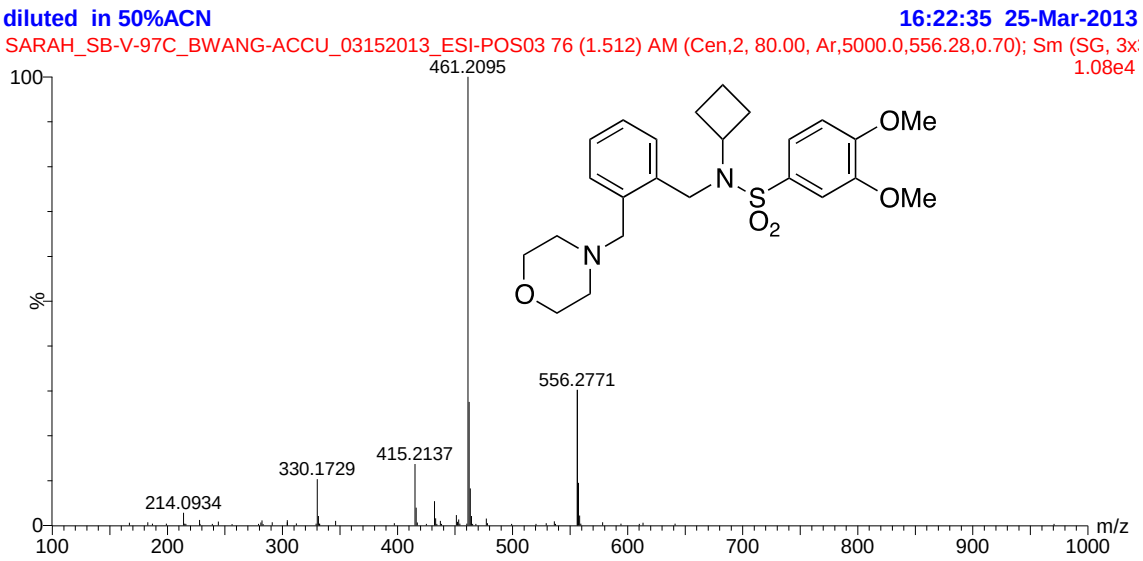


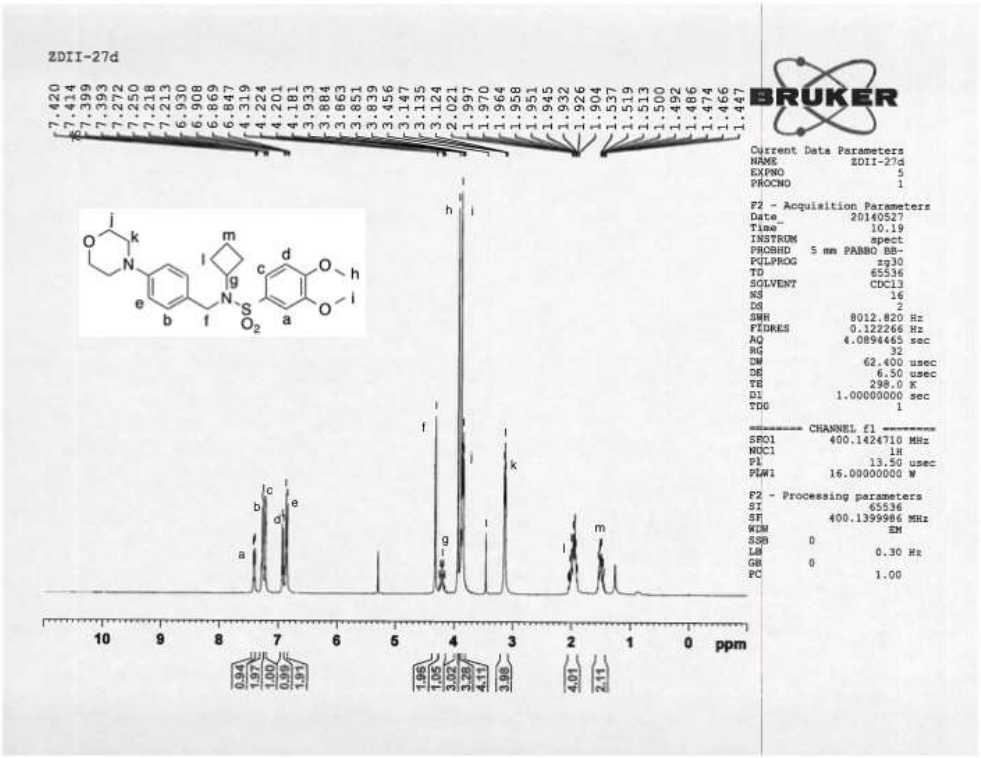
Elemental Composition Report

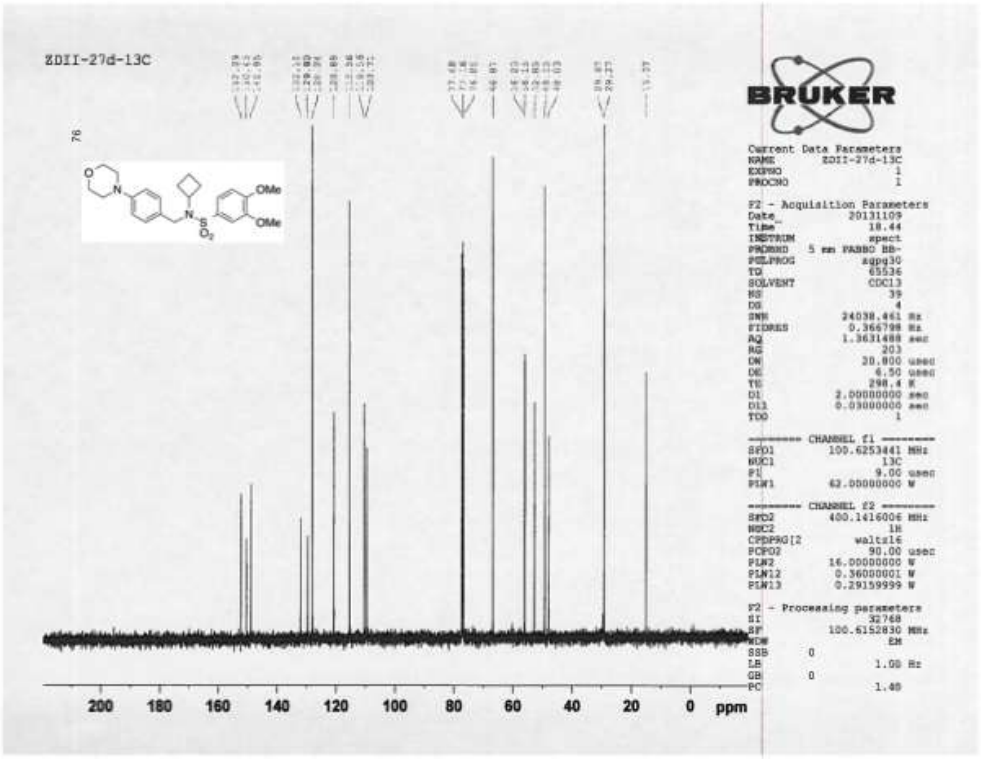
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
4668 formula(e) evaluated with 21 results within limits (up to 100 closest results for each mass)
Elements Used:
C: 1-150 H: 1-150 N: 1-30 O: 1-60 S: 1-10

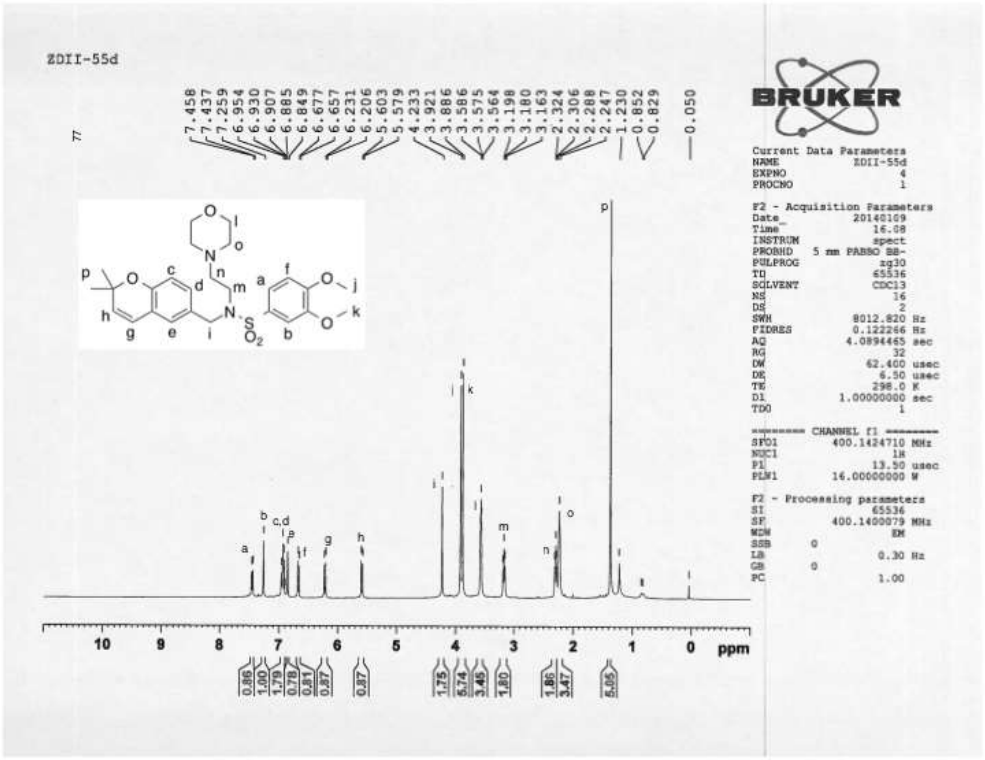
Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa		PPM	DBE	i-FIT	Formula
461.2095	461.2110	-1.5	-3.3	9.5	11.1		C24 H33 N2 O5 S

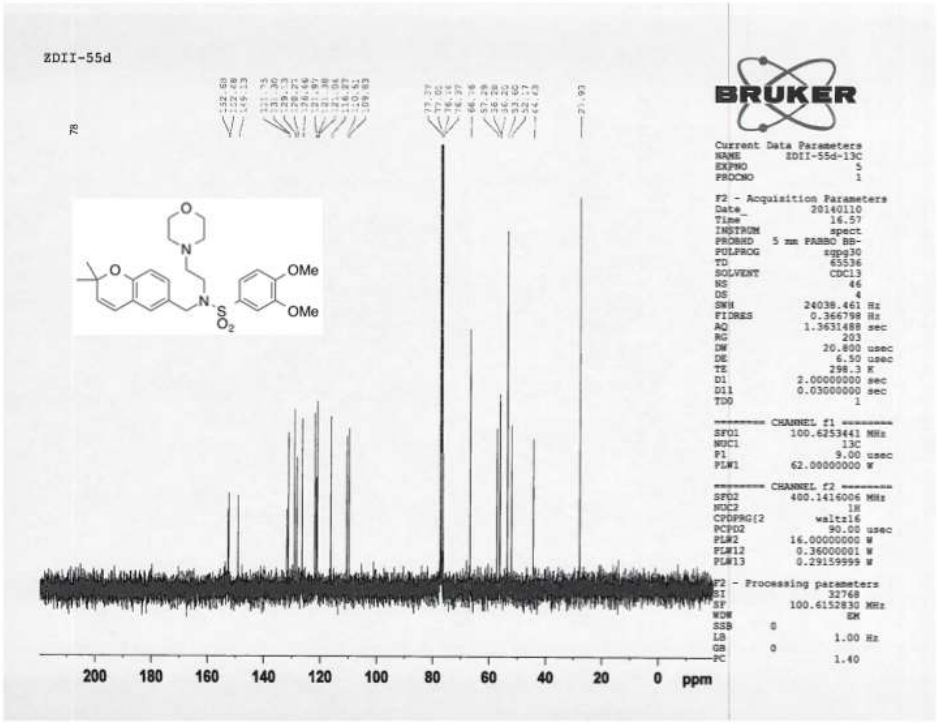
***N*-Cyclobutyl-3,4-dimethoxy-N-(4-morpholinobenzyl)benzenesulfonamide (4d)**



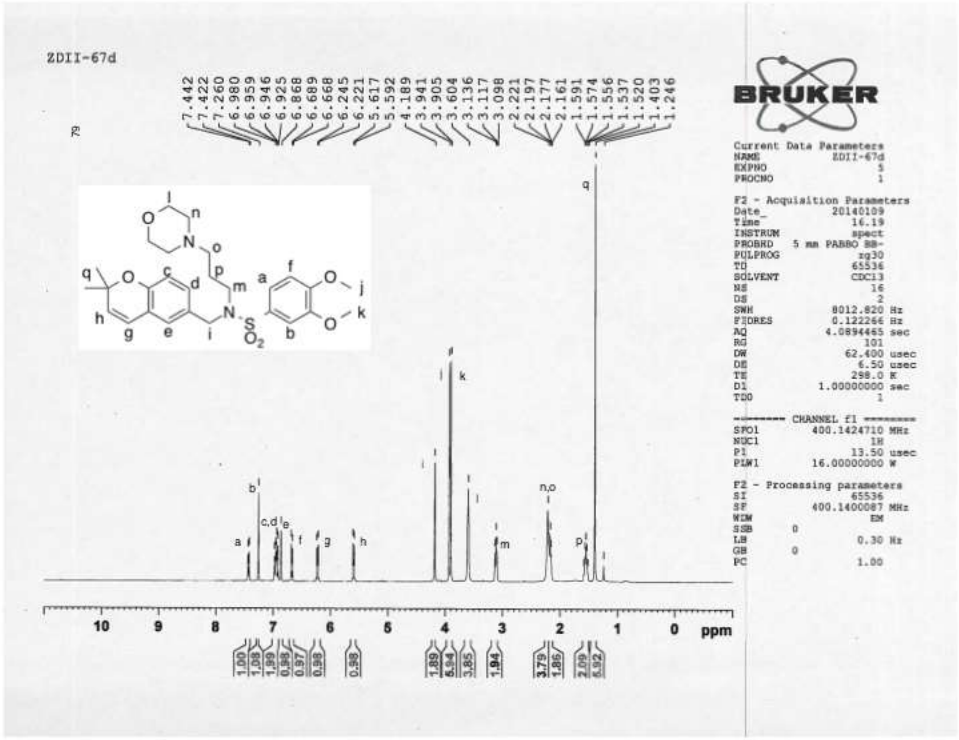


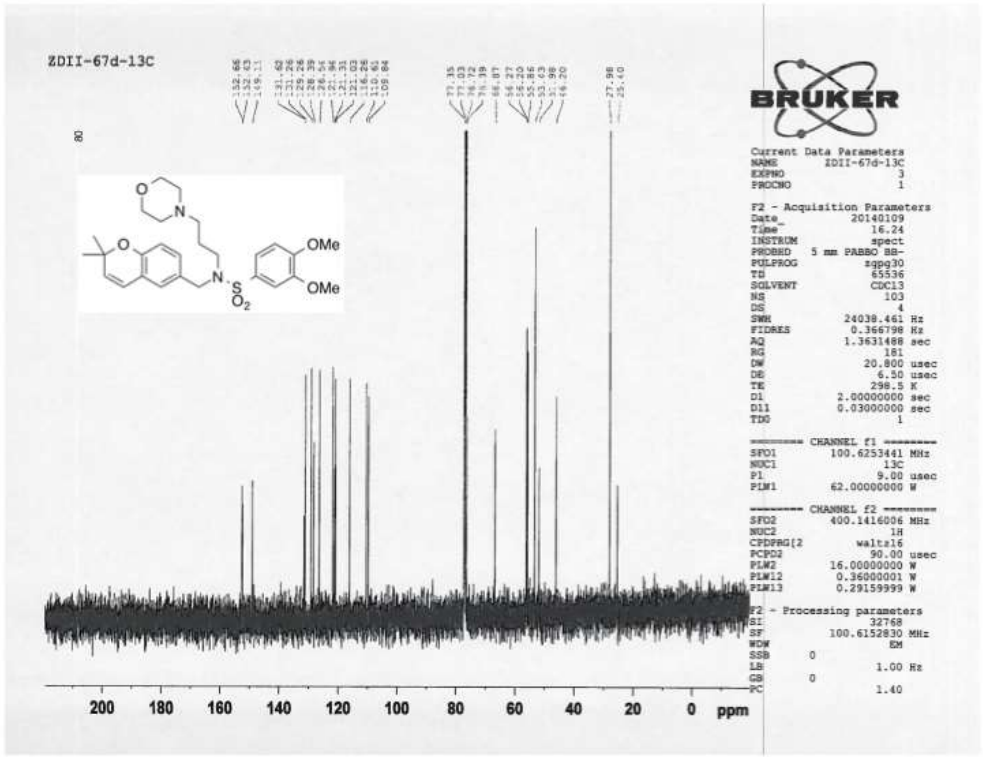
_N_-((2,2-Dimethyl-2H-chromen-6-yl)methyl)-3,4-dimethoxy-N-(2-morpholinoethyl)benzenesulfonamide (5a)



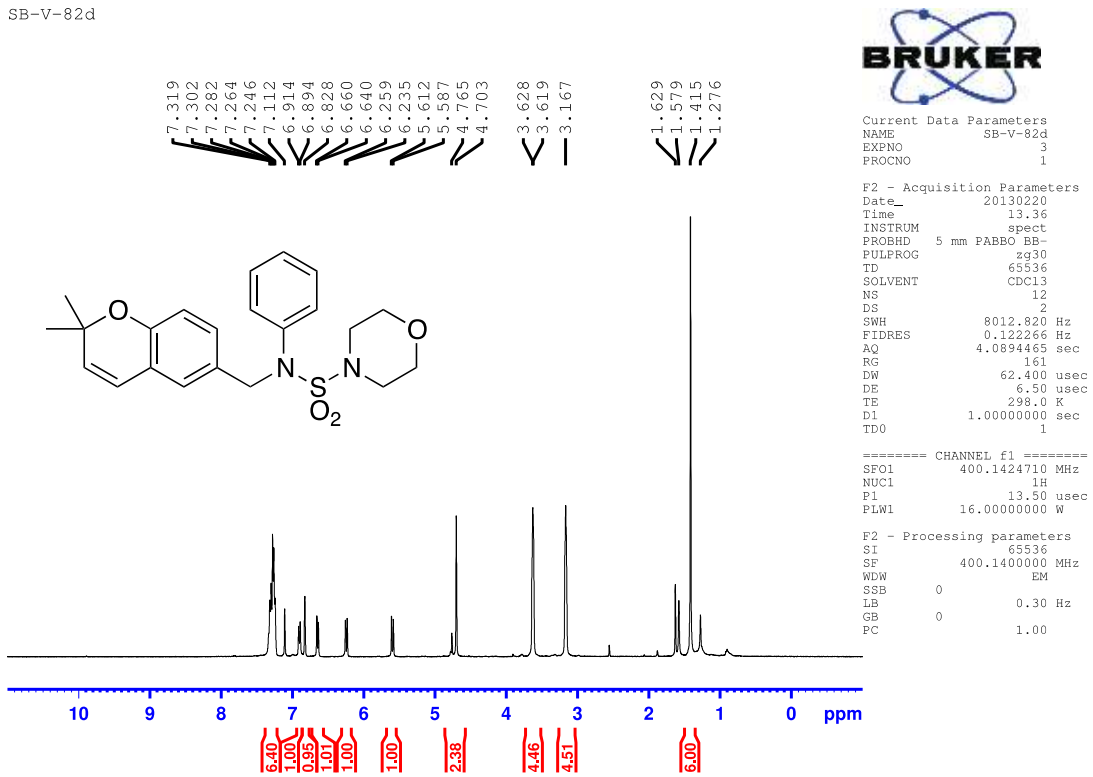


***N*-((2,2-Dimethyl-2H-chromen-6-yl)methyl)-3,4-dimethoxy-N-(3-morpholinopropyl)benzenesulfonamide (5b)**





N-((2,2-Dimethyl-2*H*-chromen-6-yl)methyl)-*N*-phenylmorpholine-4-sulfonamide (6a)



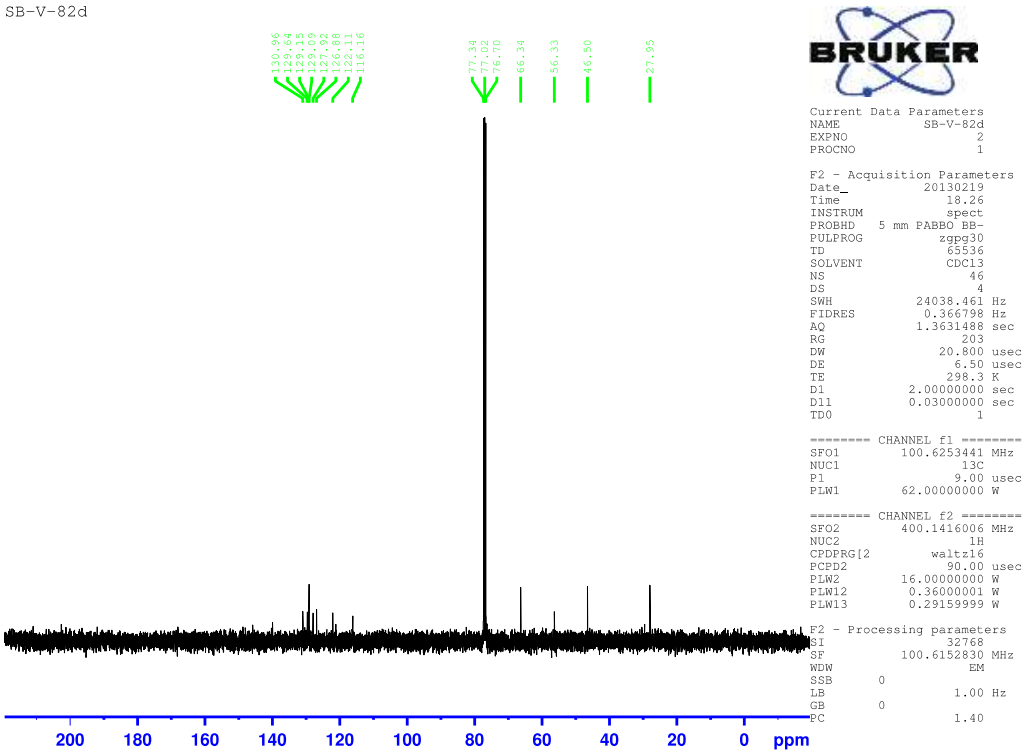
BRUKER

```
Current Data Parameters
NAME              SB-V-82d
EXPNO                    3
PROCNO                   1

F2 - Acquisition Parameters
Date_              20130220
Time                 13.36
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG                zq30
TD                    65536
SOLVENT               CDC13
NS                       12
DS                        2
SWH                8012.820 Hz
FIDRES            0.122266 Hz
AQ                4.0894465 sec
RG                      161
DW                   62.400 usec
DE                    6.50 usec
TE                   298.0 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            400.1424710 MHz
NUC1                    1H
P1                   13.50 usec
PLW1           16.00000000 W

F2 - Processing parameters
SI                    65536
SF              400.1400000 MHz
WDW                     EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    1.00
```



BRUKER

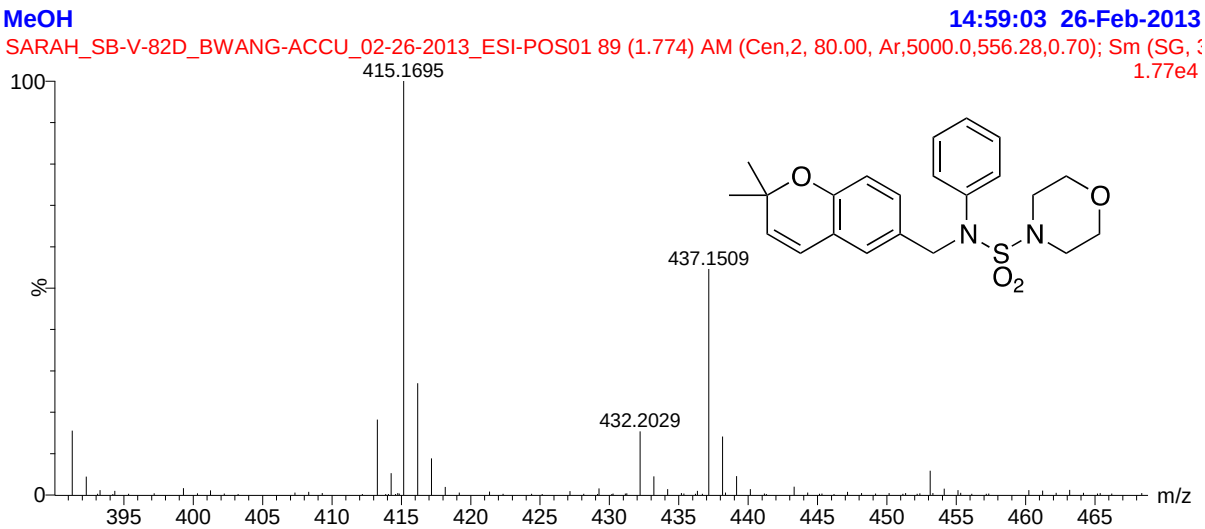
```
Current Data Parameters
NAME              SB-V-82d
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_              20130219
Time                 18.26
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT               CDC13
NS                       46
DS                        4
SWH               24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631488 sec
RG                      203
DW                   20.800 usec
DE                    6.50 usec
TE                   298.3 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            100.6253441 MHz
NUC1                    13C
P1                    9.00 usec
PLW1           62.00000000 W

======== CHANNEL f2 ========
SFO2            400.1416006 MHz
NUC2                    1H
CPDPRG[2           waltz16
PCPD2                90.00 usec
PLW2           16.00000000 W
PLW12           0.36000001 W
PLW13           0.29159999 W

F2 - Processing parameters
SI                    32768
SF              100.6152830 MHz
WDW                     EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```



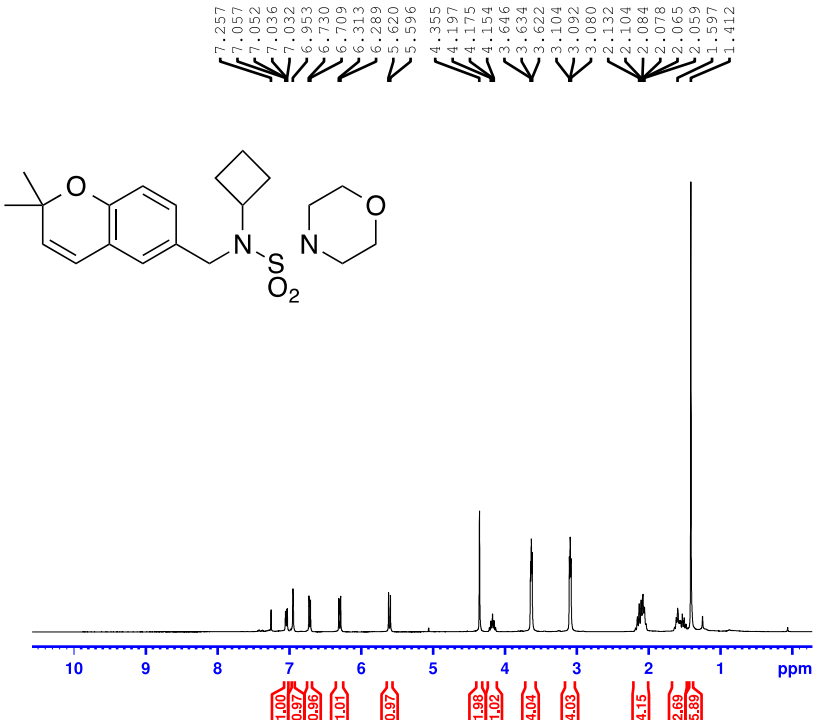
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
1658 formula(e) evaluated with 7 results within limits (up to 100 closest results for each mass)
Elements Used:
C: 1-150 H: 1-150 N: 1-6 O: 1-30 S: 1-10

Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa		PPM	DBE	i-FIT	Formula
415.1695	415.1692	0.3	0.7	10.5	1.3		C22 H27 N2 O4 S

_N_-Cyclobutyl-_N_-((2,2-dimethyl-2_H_-chromen-6-yl)methyl)morpholine-4-sulfonamide (6b)



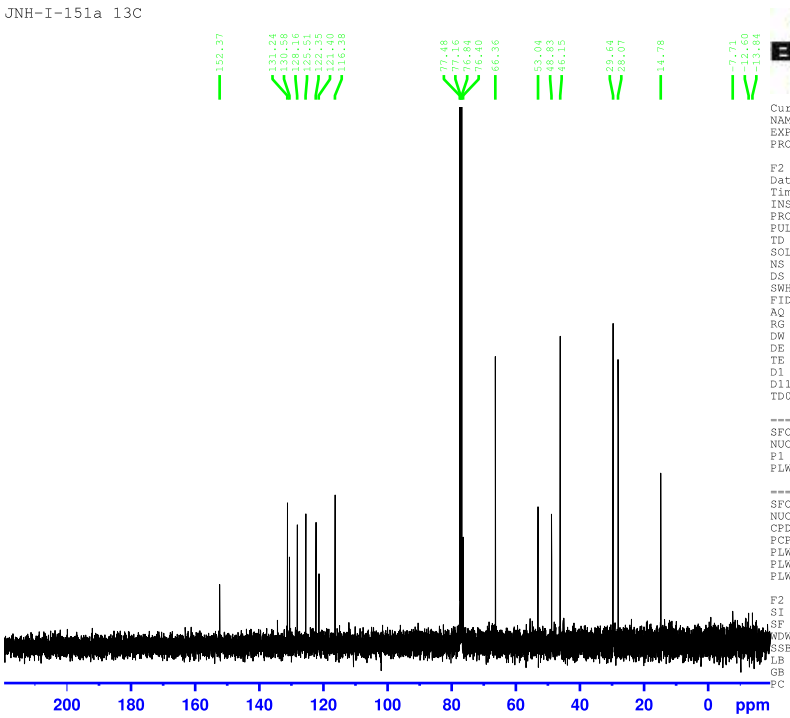
BRUKER

```
Current Data Parameters
NAME          JNH-I-151a
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_          20130721
Time              15.22
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES            0.122266 Hz
AQ             4.0894465 sec
RG                 90.5
DW                62.400 usec
DE                 6.50 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.1424710 MHz
NUC1                  1H
P1                 13.50 usec
PLW1          16.00000000 W

F2 - Processing parameters
SI                 65536
SF            400.1400094 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



BRUKER

```
Current Data Parameters
NAME          JNH-I-151a
EXPNO                  2
PROCNO                 1

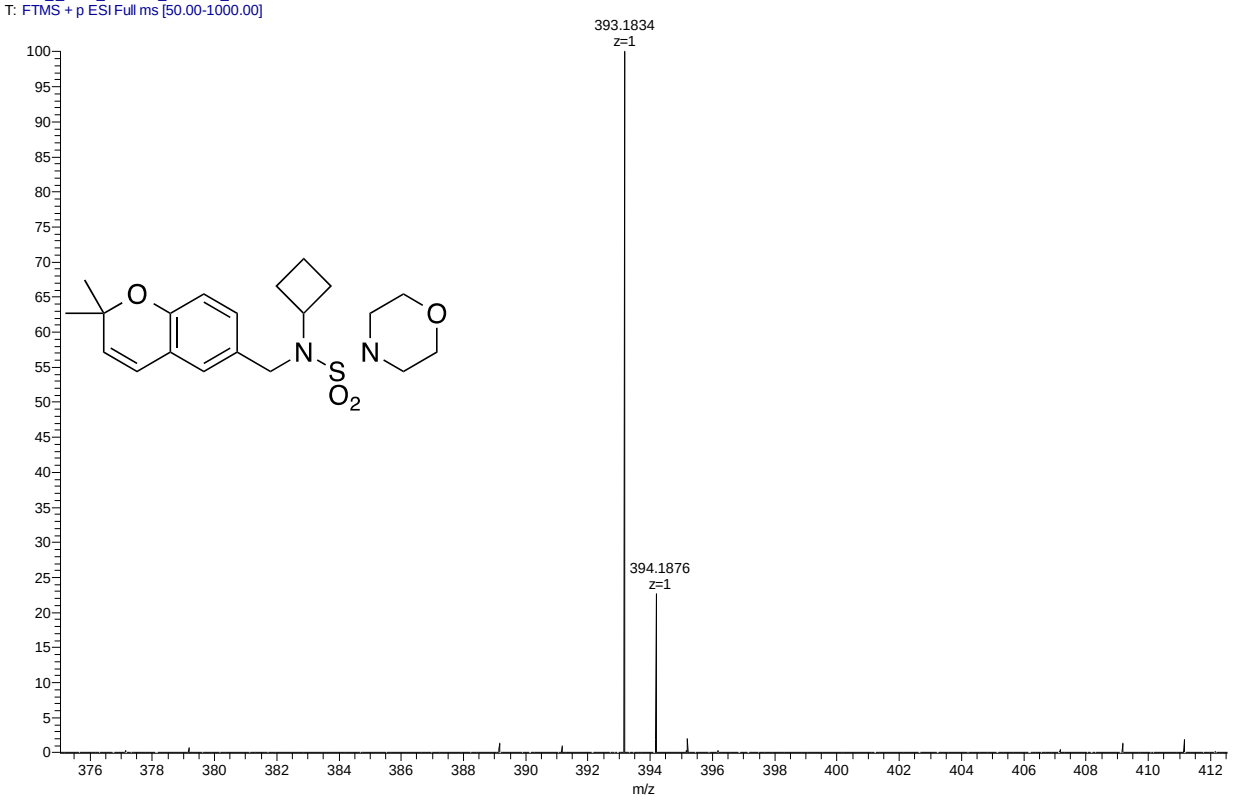
F2 - Acquisition Parameters
Date_          20170109
Time              17.57
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   84
DS                    4
SWH           24038.461 Hz
FIDRES            0.366798 Hz
AQ             1.3631488 sec
RG                  203
DW                20.800 usec
DE                 6.50 usec
TE                298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

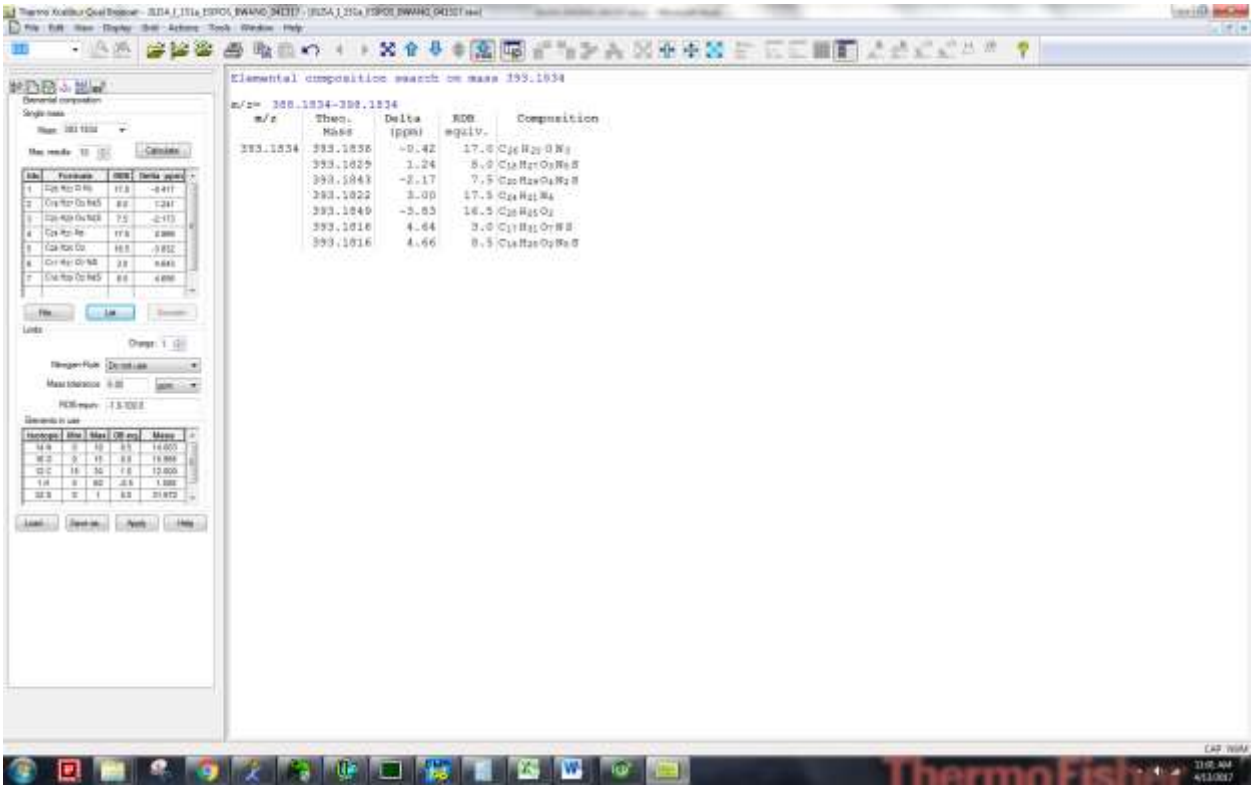
======== CHANNEL f1 ========
SFO1          100.6253441 MHz
NUC1                  13C
P1                 9.25 usec
PLW1          62.00000000 W

======== CHANNEL f2 ========
SFO2          400.1416006 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2          16.00000000 W
PLW12          0.36267000 W
PLW13          0.29376000 W

F2 - Processing parameters
SI                 32768
SF            100.6152701 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

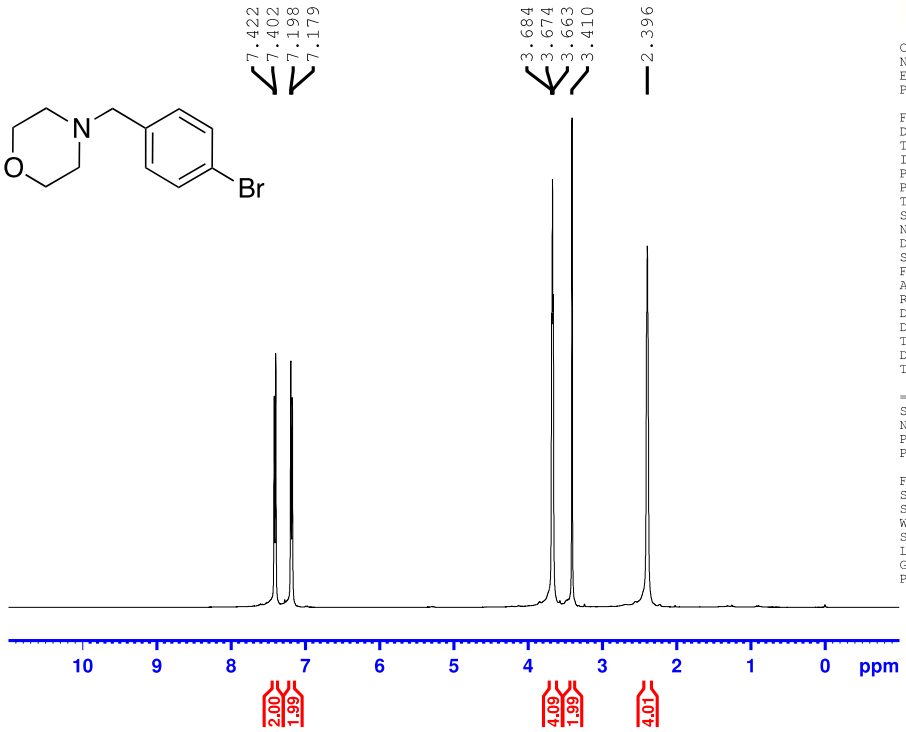
JILISA_I_151a_ESIPOS_BWANG_041317 #107-119 RT: 1.52-1.68 AV: 13 NL: 3.73E6
T: FTMS + p ESI Full ms [50.00-1000.00]





4-(4-Bromobenzyl)morpholine (8a)

SB-IV-110



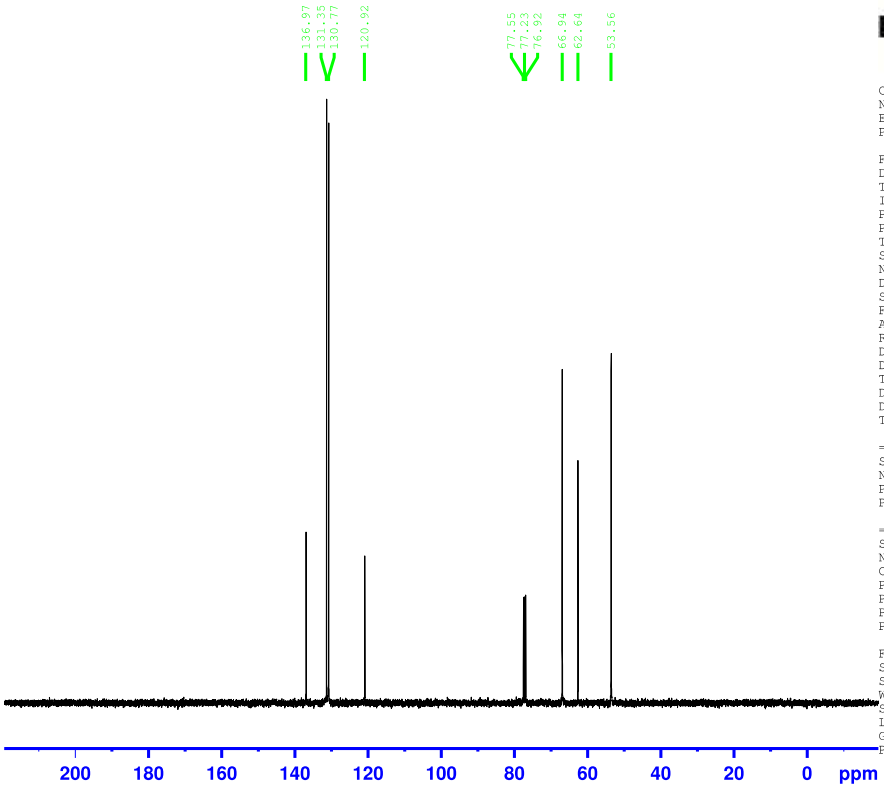

```
Current Data Parameters
NAME                 SB-IV-110
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_               20120726
Time                   13.24
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        6
DS                        2
SWH                8012.820 Hz
FIDRES                0.122266 Hz
AQ                 4.0894465 sec
RG                     50.8
DW                    62.400 usec
DE                     6.50 usec
TE                    299.0 K
D1                 1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1          400.1424710 MHz
NUC1                      1H
P1                    13.50 usec
PLW1          16.00000000 W

F2 - Processing parameters
SI                    65536
SF               400.1400000 MHz
WDW                      EM
SSB                   0
LB                    0.30 Hz
GB                    0
PC                    1.00
```

SB-IV-110



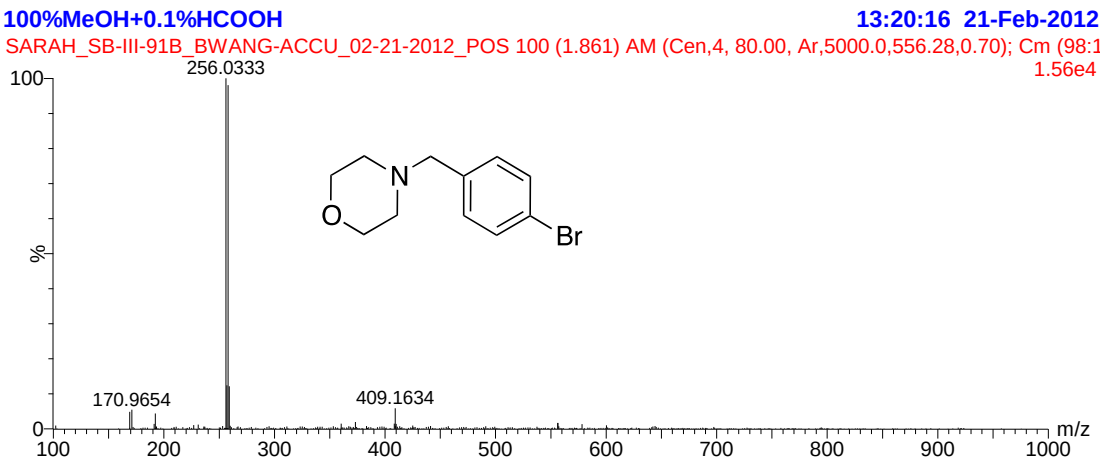

```
Current Data Parameters
NAME                 SB-IV-110
EXPNO                        2
PROCNO                       1

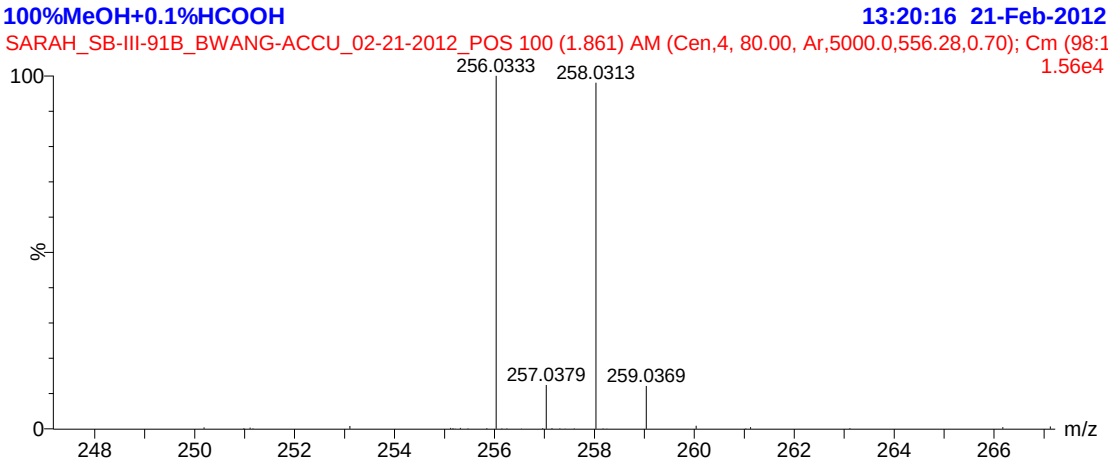
F2 - Acquisition Parameters
Date_               20120726
Time                   13.26
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                       27
DS                        4
SWH               24038.461 Hz
FIDRES                0.366798 Hz
AQ                 1.3631488 sec
RG                      203
DW                    20.800 usec
DE                     6.50 usec
TE                    299.4 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1          100.6253441 MHz
NUC1                     13C
P1                     9.00 usec
PLW1          62.00000000 W

======== CHANNEL f2 ========
SFO2          400.1416006 MHz
NUC2                      1H
CPDPRG[2           waltz16
PCPD2                 90.00 usec
PLW2          16.00000000 W
PLW12          0.36000001 W
PLW13          0.29159999 W

F2 - Processing parameters
SI                    32768
SF               100.6152830 MHz
WDW                      EM
SSB                   0
LB                    1.00 Hz
GB                    0
PC                    1.40
```



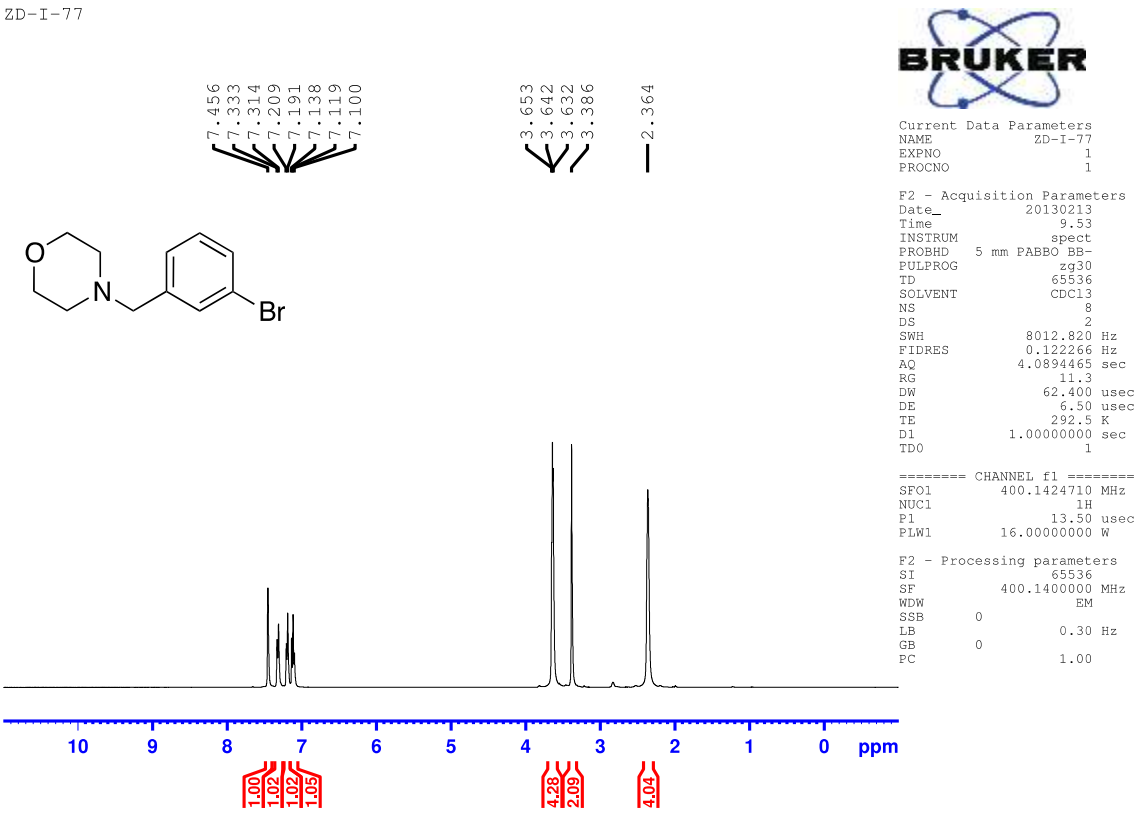


Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
106 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-100 H: 1-100 N: 1-15 O: 1-20 Br: 1-5

Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa		PPM	DBE	i-FIT	Formula
256.0333	256.0337	-0.4	-1.6	4.5	1.6		C11 H15 N O Br

3-(2-Bromobenzyl)morpholine (8b)

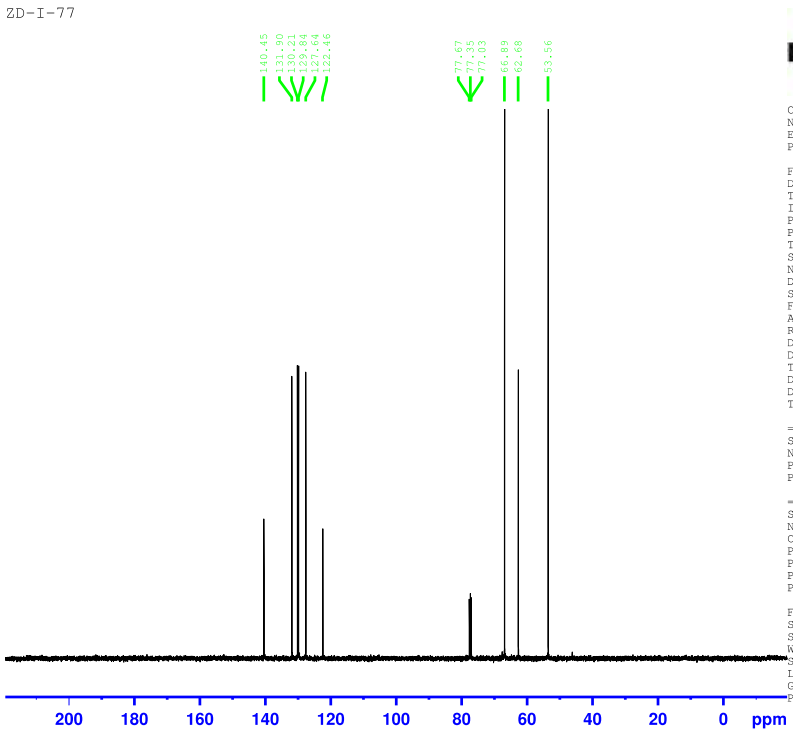



```
Current Data Parameters
NAME                  ZD-I-77
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20130213
Time                    9.53
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                         8
DS                         2
SWH                 8012.820 Hz
FIDRES              0.122266 Hz
AQ                  4.0894465 sec
RG                       11.3
DW                     62.400 usec
DE                      6.50 usec
TE                     292.5 K
D1                  1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1           400.1424710 MHz
NUC1                      1H
P1                     13.50 usec
PLW1           16.00000000 W

F2 - Processing parameters
SI                     65536
SF           400.1400000 MHz
WDW                       EM
SSB         0
LB                      0.30 Hz
GB          0
PC                      1.00
```



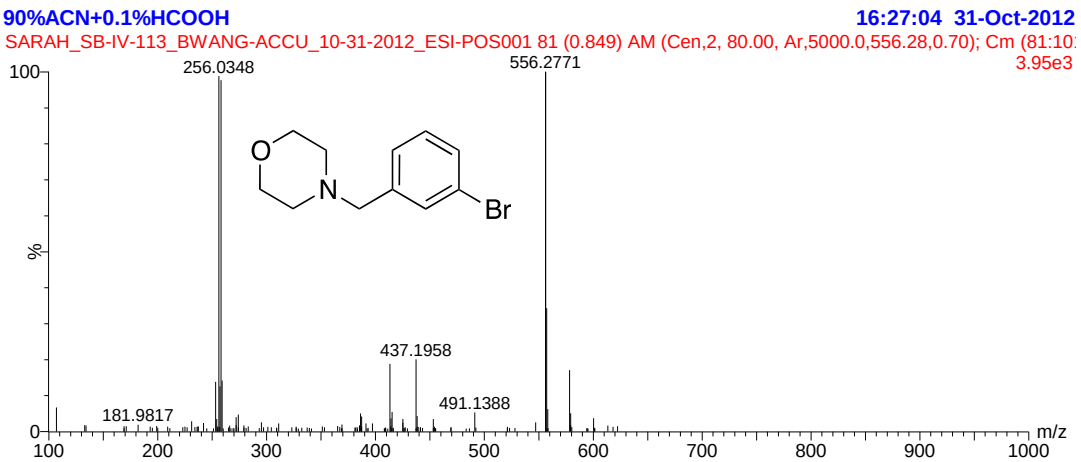

```
Current Data Parameters
NAME                  ZD-I-77
EXPNO                       2
PROCNO                      1

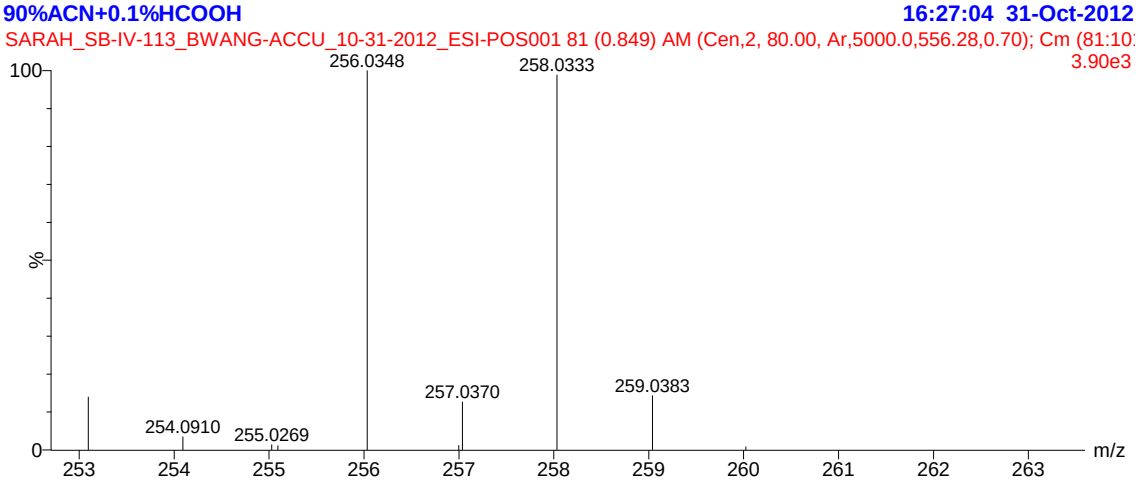
F2 - Acquisition Parameters
Date_              20130213
Time                    9.55
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG              zgpg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631488 sec
RG                       203
DW                     20.800 usec
DE                      6.50 usec
TE                     293.0 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1           100.6253441 MHz
NUC1                      13C
P1                      9.00 usec
PLW1           62.00000000 W

======== CHANNEL f2 ========
SFO2           400.1416006 MHz
NUC2                      1H
CPDPRG[2             waltz16
PCPD2                  90.00 usec
PLW2           16.00000000 W
PLW12           0.36000001 W
PLW13           0.29159999 W

F2 - Processing parameters
SI                     32768
SF           100.6152830 MHz
WDW                       EM
SSB         0
LB                      1.00 Hz
GB          0
PC                      1.40
```





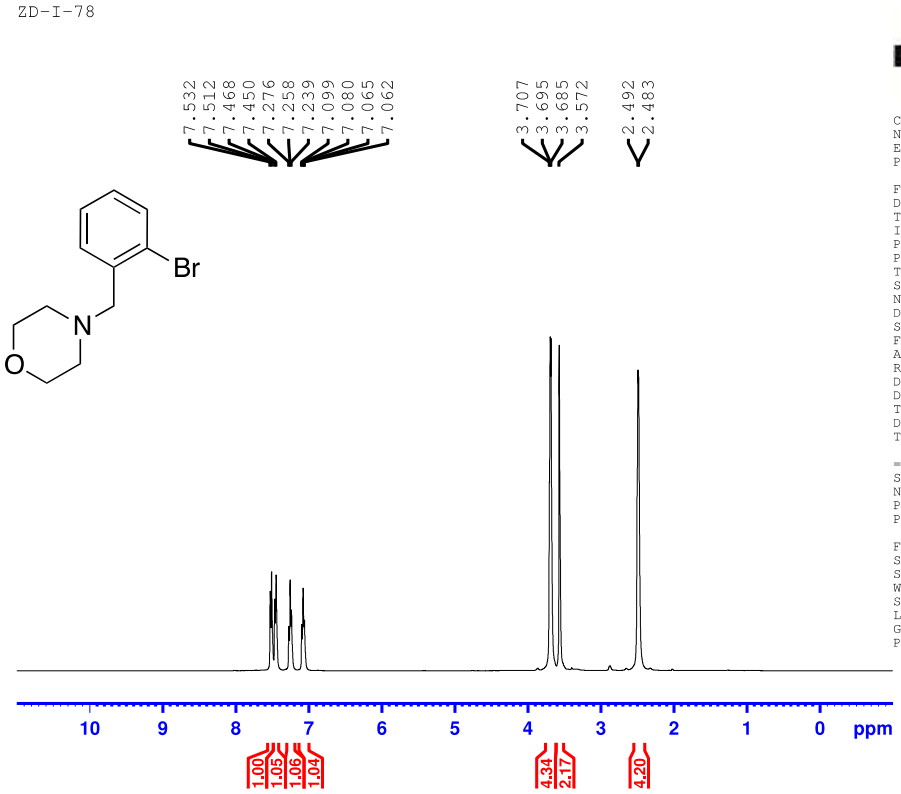
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
106 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-200 H: 1-200 N: 1-20 O: 1-30 Br: 1-5

Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa		PPM	DBE	i-FIT	Formula
256.0348	256.0337	1.1	4.3	4.5	0.7		C11 H15 N O Br

4-(2-Bromobenzyl)morpholine (8c)

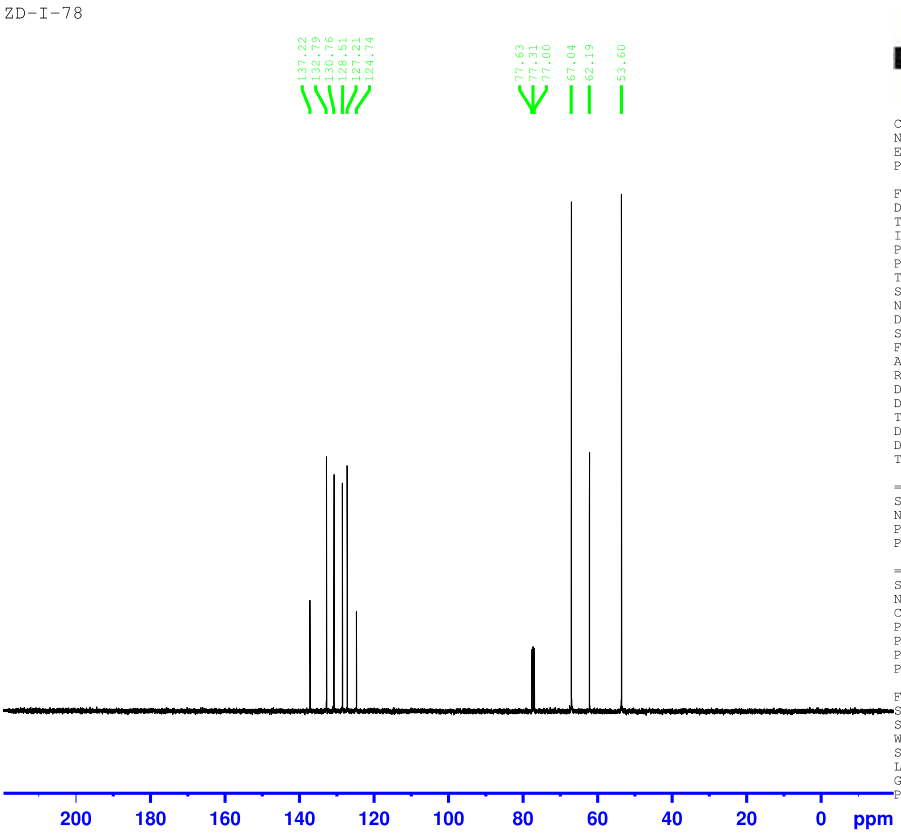



```
Current Data Parameters
NAME                  ZD-I-78
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20130213
Time                   9.57
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        9
DS                        2
SWH                8012.820 Hz
FIDRES            0.122266 Hz
AQ                4.0894465 sec
RG                     11.3
DW                   62.400 usec
DE                    6.50 usec
TE                   292.6 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1             400.1424710 MHz
NUC1                     1H
P1                    13.50 usec
PLW1            16.00000000 W

F2 - Processing parameters
SI                    65536
SF               400.1400000 MHz
WDW                      EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    1.00
```



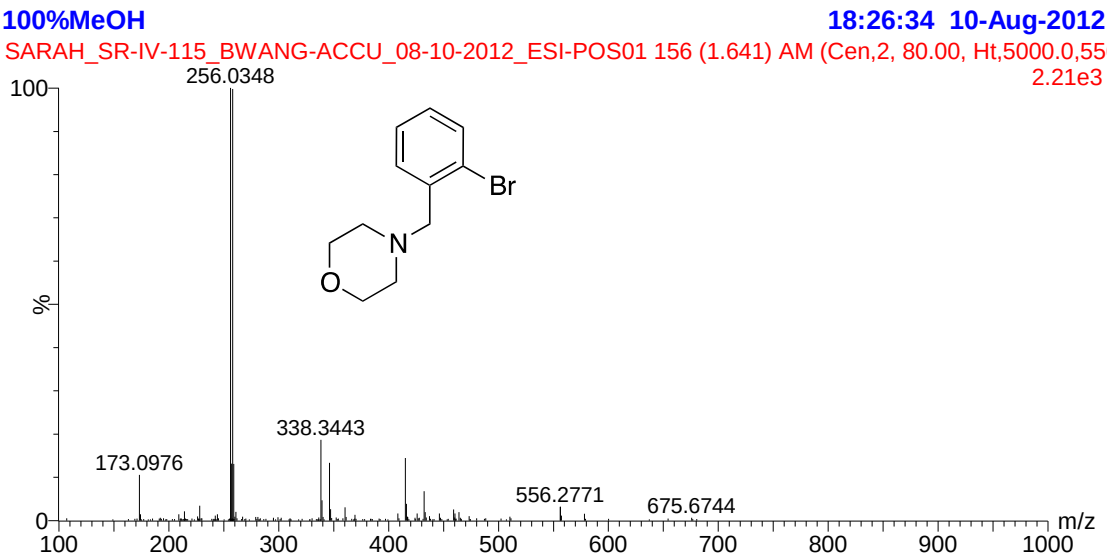

```
Current Data Parameters
NAME                  ZD-I-78
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20130213
Time                   9.58
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        4
SWH               24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631488 sec
RG                      203
DW                   20.800 usec
DE                    6.50 usec
TE                   293.1 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1             100.6253441 MHz
NUC1                     13C
P1                    9.00 usec
PLW1            62.00000000 W

======== CHANNEL f2 ========
SFO2             400.1416006 MHz
NUC2                     1H
CPDPRG[2          waltz16
PCPD2                90.00 usec
PLW2            16.00000000 W
PLW12            0.36000001 W
PLW13            0.29159999 W

F2 - Processing parameters
SI                    32768
SF               100.6152830 MHz
WDW                      EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```



Elemental Composition Report

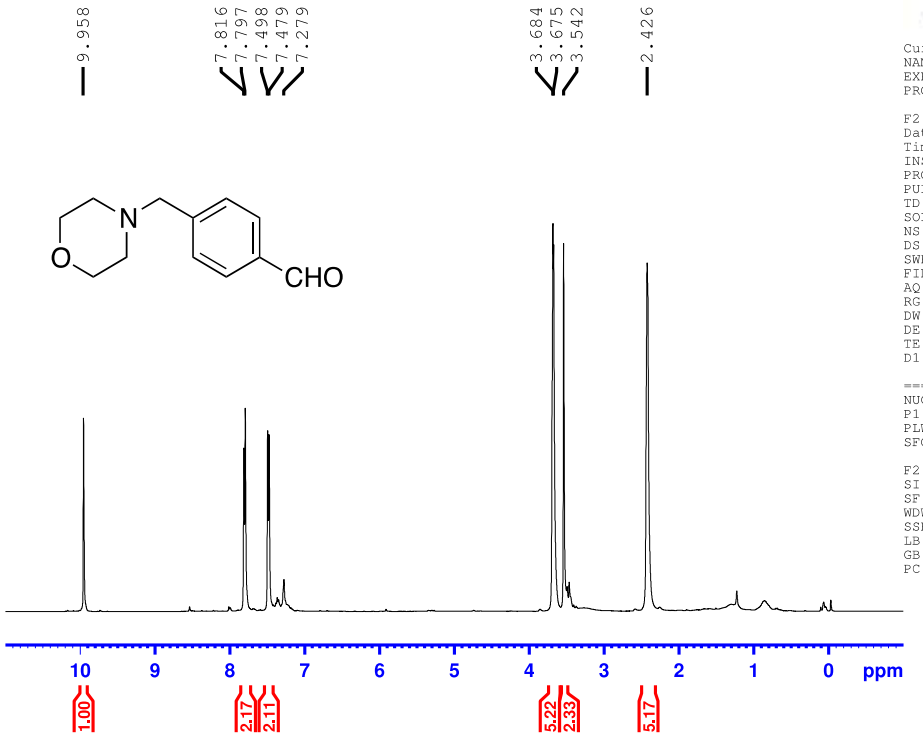
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
106 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-200 H: 1-200 N: 1-15 O: 1-100 Br: 1-5

Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa		PPM	DBE	i-FIT	Formula
256.0348	256.0337	1.1	4.3	4.5	0.5		C11 H15 N O Br

4-(Morpholinomethyl)benzaldehyde (9a)

SB-IV-30



BRUKER

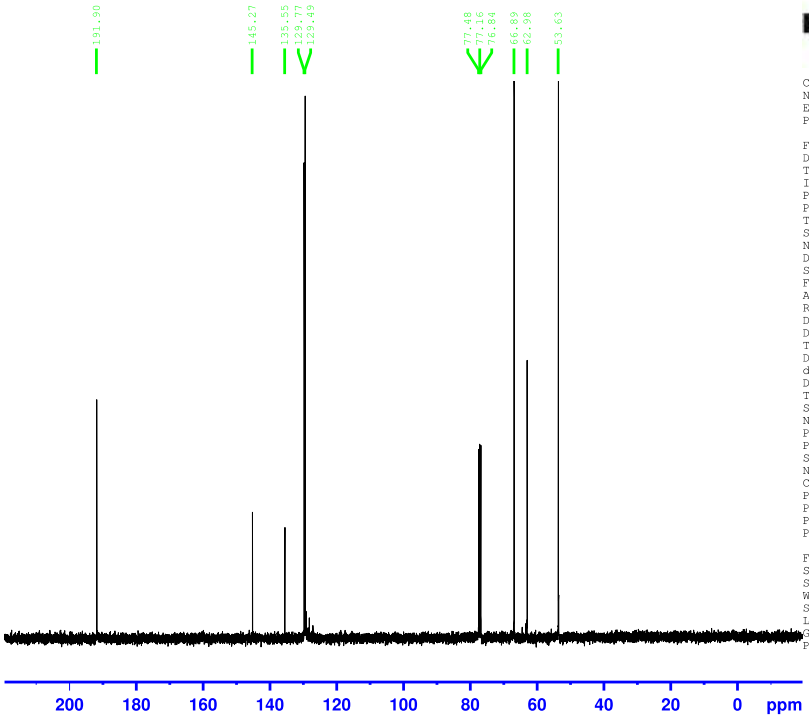
```
Current Data Parameters
NAME                  SB-IV-30
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20120420
Time                 15.49
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH               8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9846387 sec
RG                     20.2
DW                 60.800 usec
DE                   6.50 usec
TE                  298.2 K
D1              1.00000000 sec

======== CHANNEL f1 ========
NUC1                    1H
P1                   13.50 usec
PLW1          16.00000000 W
SFO1          400.1424710 MHz

F2 - Processing parameters
SI                    65536
SF            400.1400000 MHz
WDW                     EM
SSB       0
LB                   0.30 Hz
GB        0
PC                   1.00
```

SB-IV-30

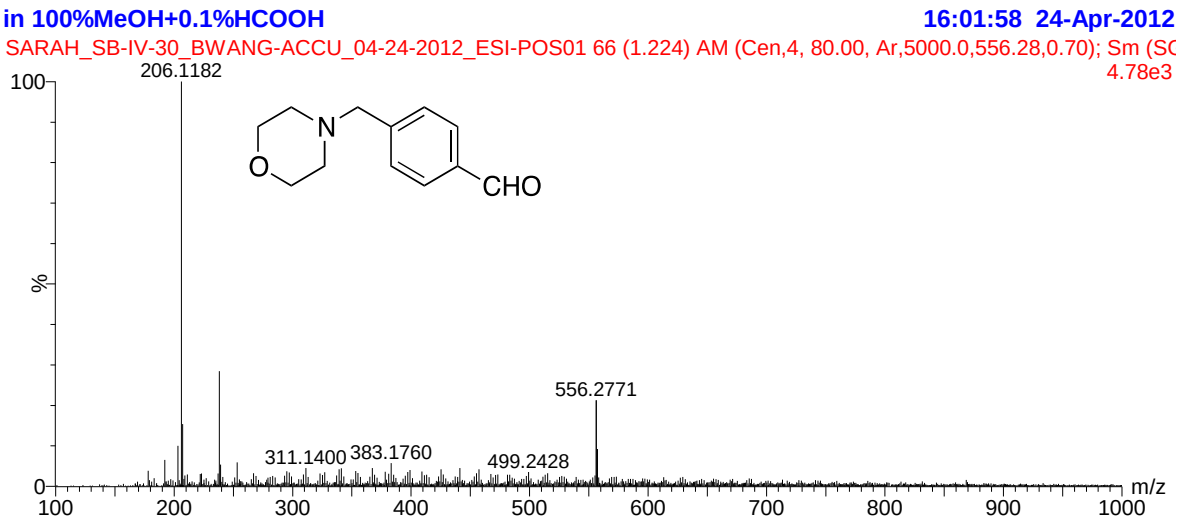


BRUKER

```
Current Data Parameters
NAME                  SB-IV-30
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_              20120420
Time                 15.51
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                     29
DS                      4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631488 sec
RG                     203
DW                 20.800 usec
DE                   6.50 usec
TE                  298.4 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                     1
SFO1          100.6253441 MHz
NUC1                   13C
P1                    9.00 usec
PLW1          62.00000000 W
SFO2          400.1416006 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2                90.00 usec
PLW2          16.00000000 W
PLW12          0.36000001 W
PLW13          0.29159999 W

F2 - Processing parameters
SI                    32768
SF            100.6152830 MHz
WDW                     EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

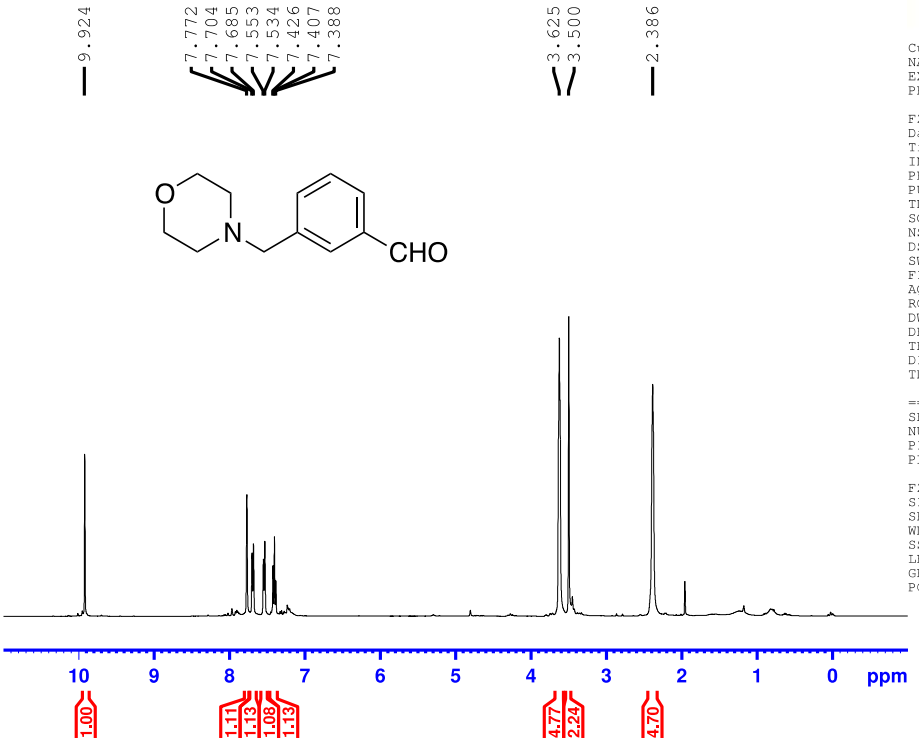


Elemental Composition Report
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
181 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-100 H: 1-100 N: 1-15 O: 1-35 80Se: 0-1

Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa		PPM	DBE	i-FIT	Formula
206.1182	206.1181	0.1	0.5	5.5	5.0	C12 H16 N O2	

3-(Morpholinomethyl)benzaldehyde (9b)

SB-V-80b



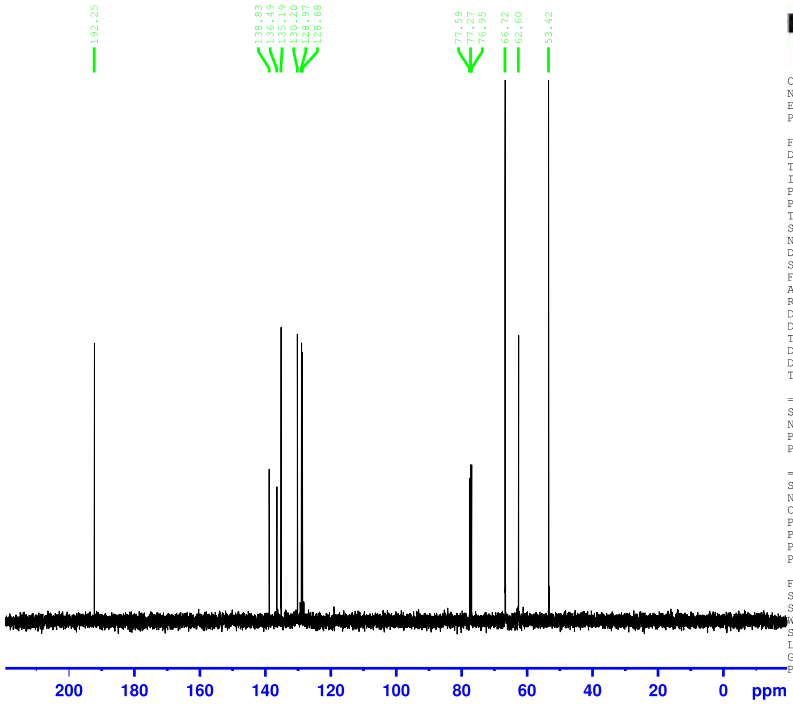

```
Current Data Parameters
NAME                 SB-V-80b
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20130216
Time                   18.32
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       12
DS                        2
SWH                8012.820 Hz
FIDRES                0.122266 Hz
AQ                 4.0894465 sec
RG                       18
DW                    62.400 usec
DE                     6.50 usec
TE                    298.0 K
D1                 1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1               400.1424710 MHz
NUC1                       1H
P1                      13.50 usec
PLW1               16.00000000 W

F2 - Processing parameters
SI                        65536
SF                 400.1400000 MHz
WDW                        EM
SSB             0
LB                      0.30 Hz
GB              0
PC                      1.00
```

SB-V-80b



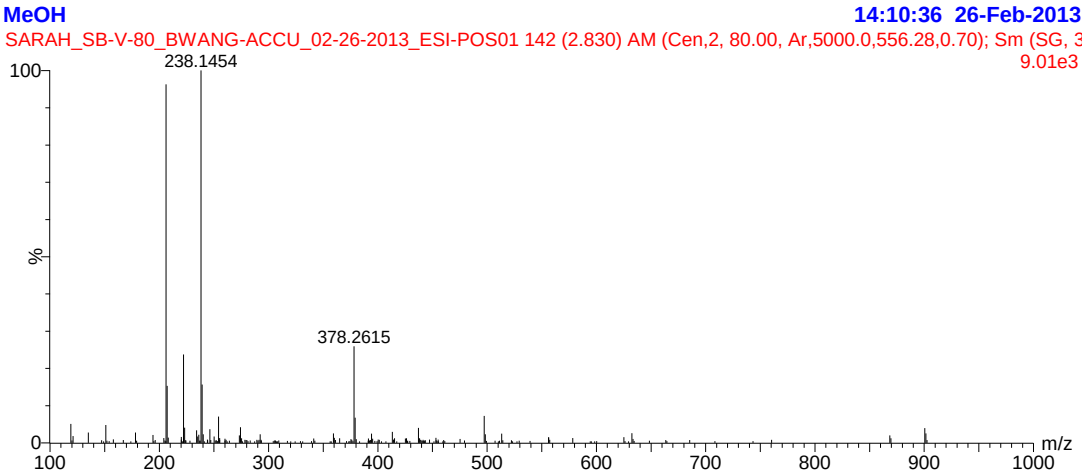

```
Current Data Parameters
NAME                 SB-V-80b
EXPNO                       2
PROCNO                      1

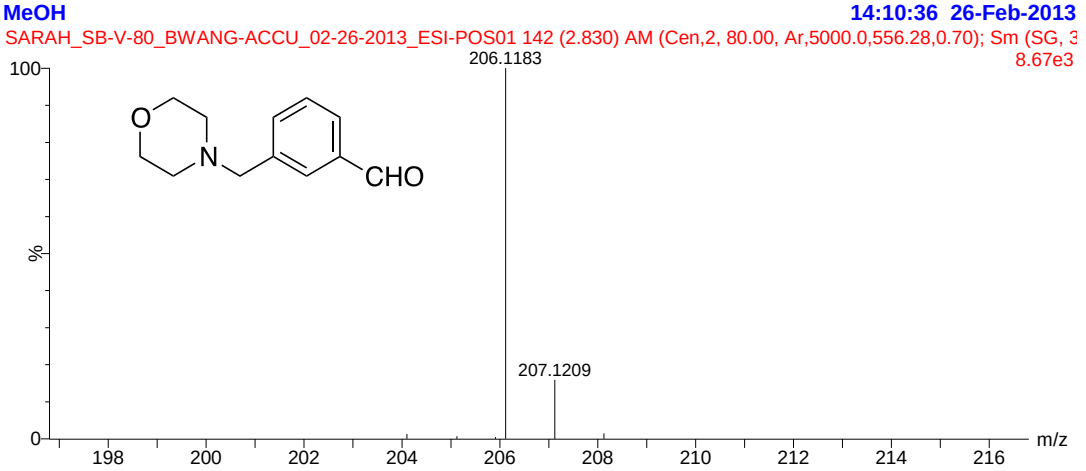
F2 - Acquisition Parameters
Date_               20130216
Time                   18.34
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                        5
DS                        4
SWH               24038.461 Hz
FIDRES                0.366798 Hz
AQ                 1.3631488 sec
RG                      203
DW                    20.800 usec
DE                     6.50 usec
TE                    298.3 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1               100.6253441 MHz
NUC1                       13C
P1                      9.00 usec
PLW1               62.00000000 W

======== CHANNEL f2 ========
SFO2               400.1416006 MHz
NUC2                       1H
CPDPRG[2             waltz16
PCPD2                  90.00 usec
PLW2               16.00000000 W
PLW12               0.36000001 W
PLW13               0.29159999 W

F2 - Processing parameters
SI                        32768
SF                 100.6152830 MHz
WDW                        EM
SSB             0
LB                      1.00 Hz
GB              0
PC                      1.40
```





Elemental Composition Report

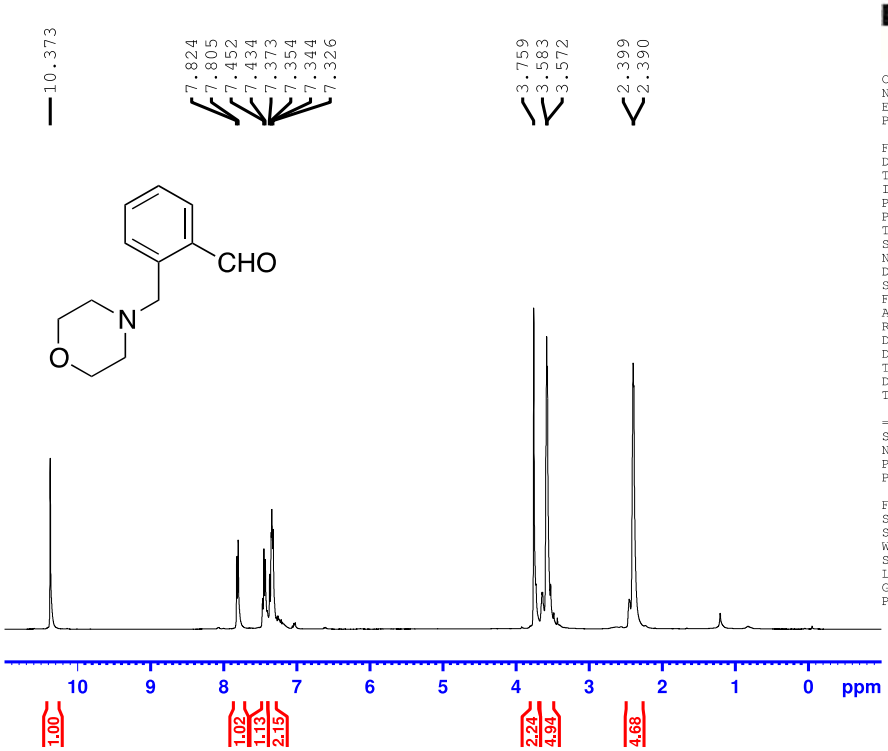
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
105 formula(e) evaluated with 1 results within limits (up to 100 closest results for each mass)
Elements Used:
C: 1-150 H: 1-150 N: 1-6 O: 1-30

Minimum:				-1.5		
Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
206.1183	206.1181	0.2	1.0	5.5	8.5	C12 H16 N O2

2-(Morpholinomethyl)benzaldehyde (9c)

SB-V-17c1



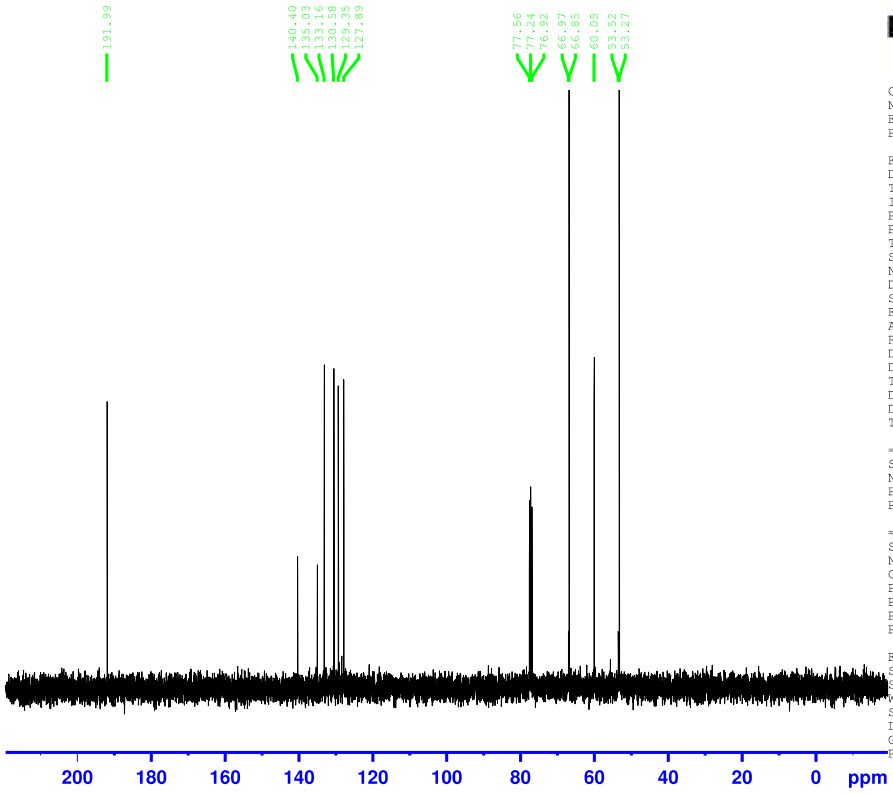

```
Current Data Parameters
NAME                  SB-V-17c1
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                20121120
Time                     11.38
INSTRUM                  spect
PROBHD    5 mm PABBO BB-
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         16
DS                          2
SWH                   8012.820 Hz
FIDRES                0.122266 Hz
AQ                    4.0894465 sec
RG                         36
DW                       62.400 usec
DE                        6.50 usec
TE                       298.0 K
D1                    1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
SFO1                400.1424710 MHz
NUC1                        1H
P1                       13.50 usec
PLW1                16.00000000 W

F2 - Processing parameters
SI                          65536
SF                    400.1400000 MHz
WDW                            EM
SSB                 0
LB                            0.30 Hz
GB                  0
PC                            1.00
```

SB-V-17c1



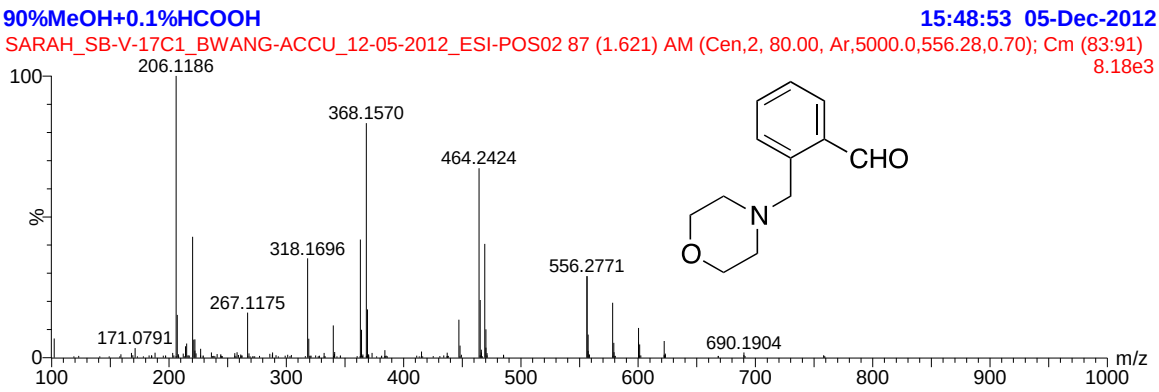

```
Current Data Parameters
NAME                  SB-V-17c1
EXPNO                         3
PROCNO                        1

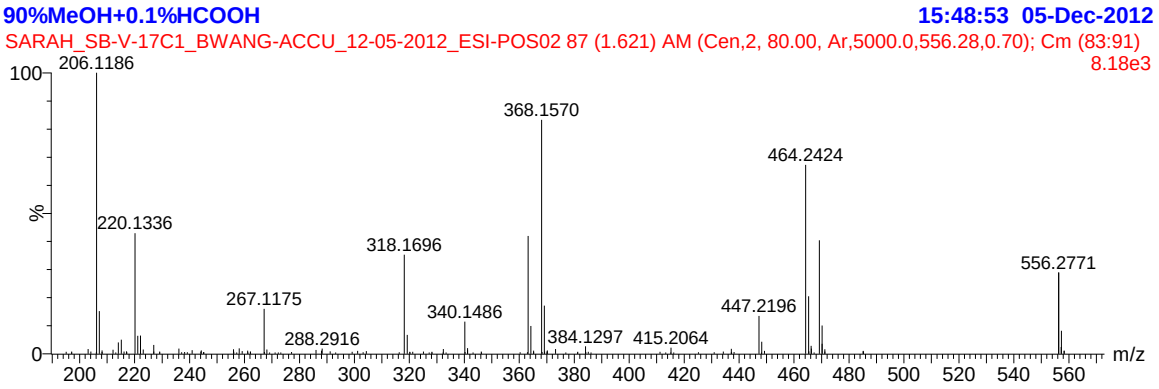
F2 - Acquisition Parameters
Date_                20121120
Time                     11.42
INSTRUM                  spect
PROBHD    5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                         11
DS                          4
SWH                  24038.461 Hz
FIDRES                0.366798 Hz
AQ                    1.3631488 sec
RG                        203
DW                       20.800 usec
DE                        6.50 usec
TE                       298.1 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                           1

======== CHANNEL f1 ========
SFO1                100.6253441 MHz
NUC1                        13C
P1                        9.00 usec
PLW1                62.00000000 W

======== CHANNEL f2 ========
SFO2                400.1416006 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                    90.00 usec
PLW2                16.00000000 W
PLW12                0.36000001 W
PLW13                0.29159999 W

F2 - Processing parameters
SI                          32768
SF                    100.6152830 MHz
WDW                            EM
SSB                 0
LB                            1.00 Hz
GB                  0
PC                            1.40
```





Elemental Composition Report

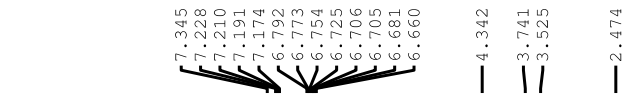
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

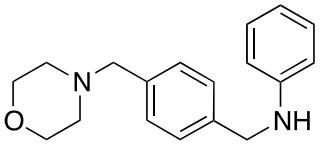
Monoisotopic Mass, Odd and Even Electron Ions
145 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-200 H: 1-200 N: 1-20 O: 1-30

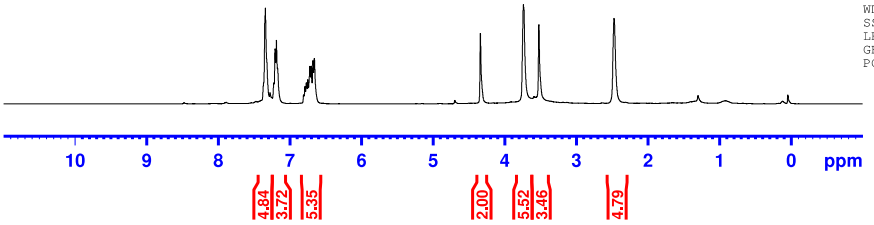
Minimum:				-1.5		
Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
206.1186	206.1181	0.5	2.4	5.5	5.5	C12 H16 N O2

N-(4-(morpholinomethyl)benzyl)aniline (10a)

SB-IV-37a







BRUKER

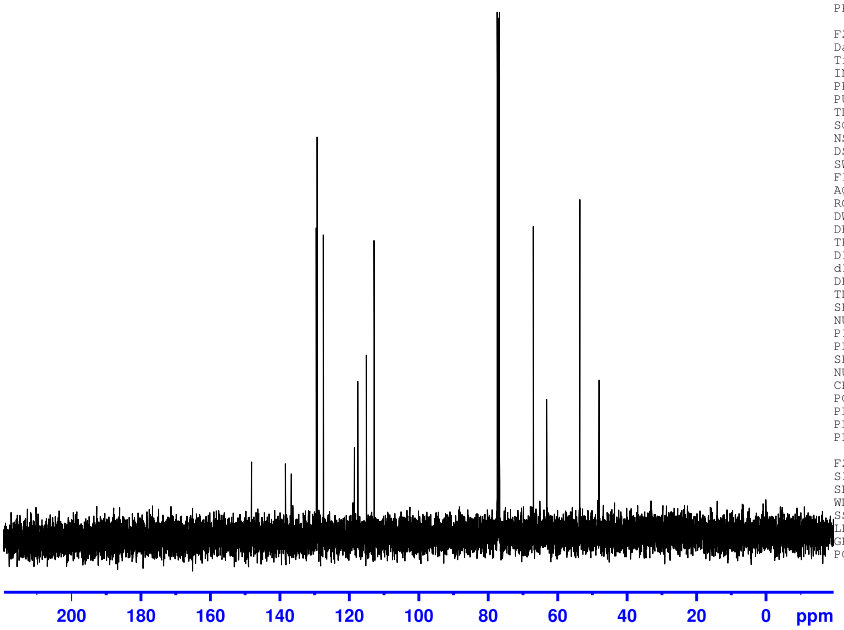
```
Current Data Parameters
NAME                  SB-IV-37a
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20120426
Time                      11.04
INSTRUM                   spect
PROBHD    5 mm PABBO BB-
PULPROG                    zg30
TD                        65536
SOLVENT                   CDCl3
NS                            7
DS                            2
SWH                    8223.685 Hz
FIDRES                 0.125483 Hz
AQ                     3.9846387 sec
RG                         40.3
DW                       60.800 usec
DE                        6.50 usec
TE                       298.2 K
D1                    1.00000000 sec

======== CHANNEL f1 ========
NUC1                         1H
P1                        13.50 usec
PLW1                16.00000000 W
SFO1                400.1424710 MHz

F2 - Processing parameters
SI                        65536
SF                  400.1400000 MHz
WDW                          EM
SSB               0
LB                        0.30 Hz
GB                0
PC                        1.00
```

SB-IV-37a

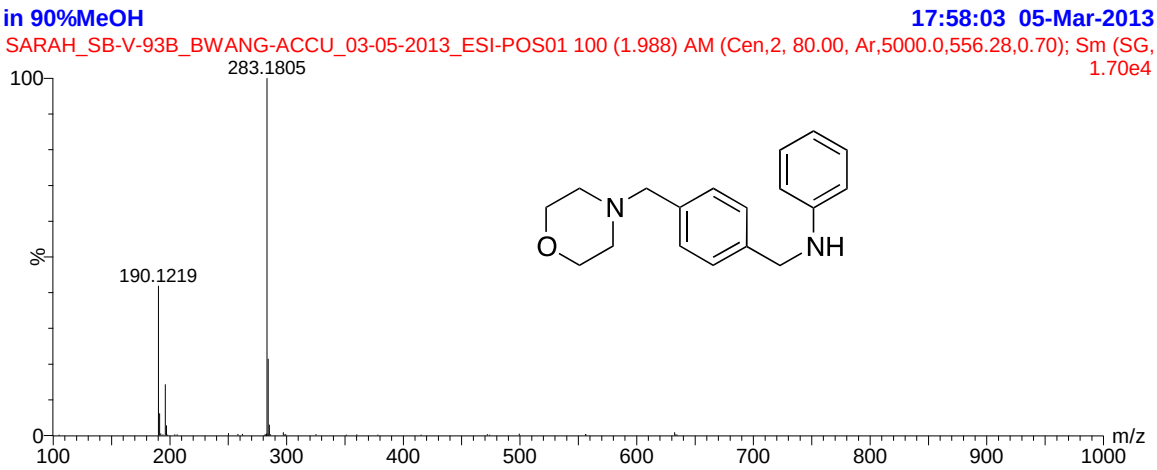


BRUKER

```
Current Data Parameters
NAME                  SB-IV-37a
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20120426
Time                      11.06
INSTRUM                   spect
PROBHD    5 mm PABBO BB-
PULPROG                 zgpg30
TD                        65536
SOLVENT                   CDCl3
NS                           22
DS                            4
SWH                24038.461 Hz
FIDRES                 0.366798 Hz
AQ                     1.3631488 sec
RG                          203
DW                       20.800 usec
DE                        6.50 usec
TE                       298.3 K
D1                    2.00000000 sec
d11                   0.03000000 sec
DELTA                 1.89999998 sec
TD0                           1
SFO1                100.6253441 MHz
NUC1                         13C
P1                        9.00 usec
PLW1                62.00000000 W
SFO2                400.1416006 MHz
NUC2                         1H
CPDPRG[2                waltz16
PCPD2                    90.00 usec
PLW2                16.00000000 W
PLW12                0.36000001 W
PLW13                0.29159999 W

F2 - Processing parameters
SI                        32768
SF                  100.6152830 MHz
WDW                          EM
SSB               0
LB                        1.00 Hz
GB                0
PC                        1.40
```



Elemental Composition Report

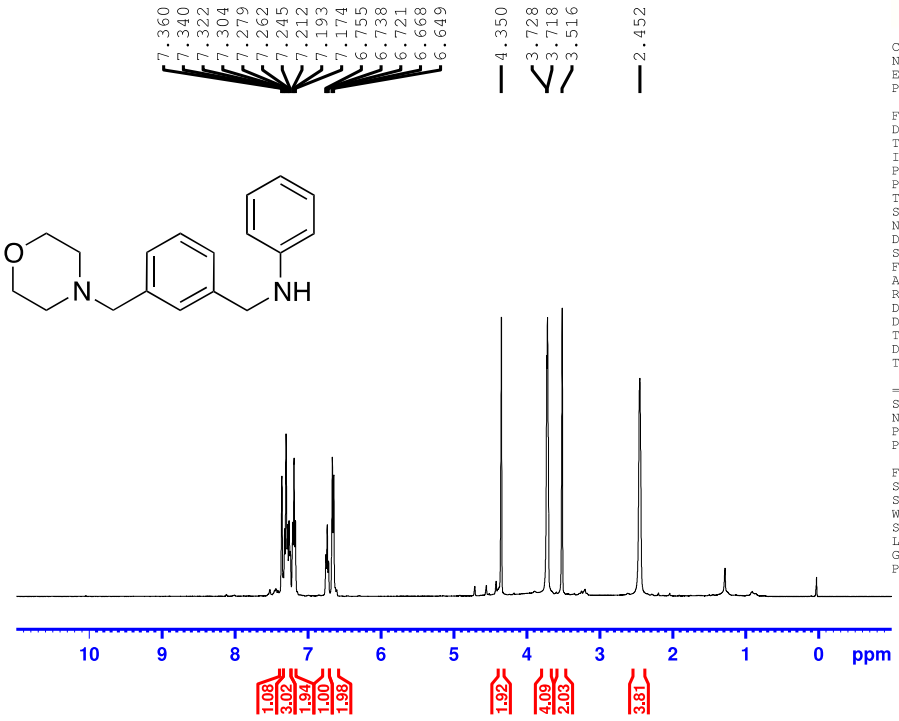
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
363 formula(e) evaluated with 2 results within limits (up to 100 closest results for each mass)
Elements Used:
C: 1-150 H: 1-150 N: 1-30 O: 1-60

Minimum:				-1.5		
Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
283.1805	283.1810	-0.5	-1.8	8.5	12.4	C18 H23 N2 O
	283.1815	-1.0	-3.5	1.5	741.3	C3 H19 N14 O2

N-(3-(Morpholinomethyl)benzyl)aniline (10b)

SB-V-107d



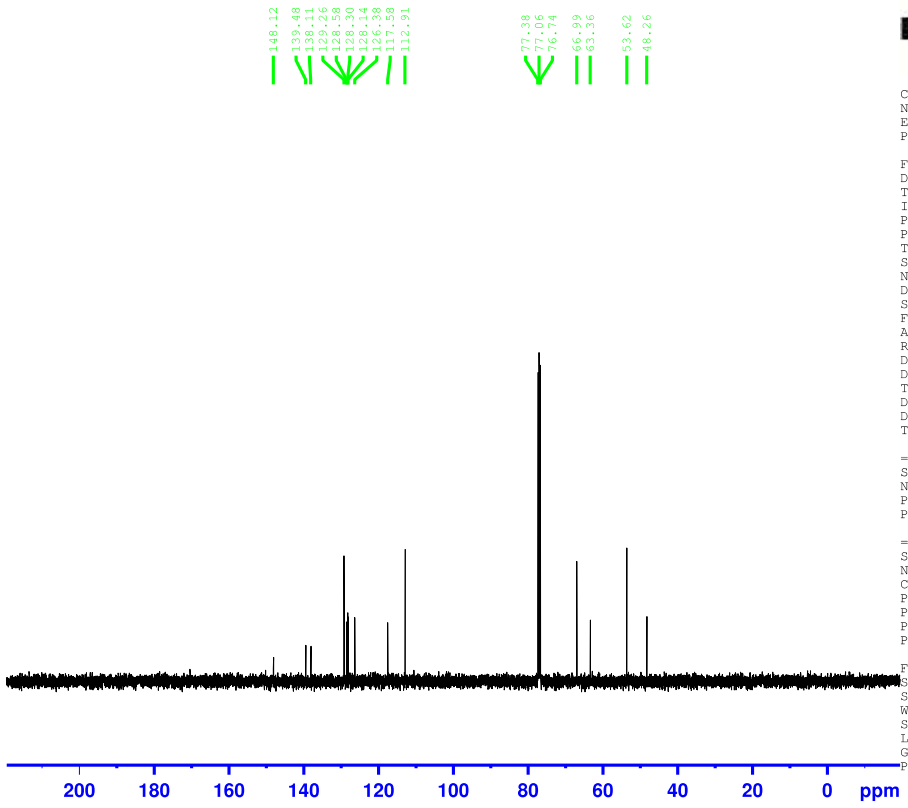

```
Current Data Parameters
NAME                  SB-V-107d
EXPNO                         3
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20130319
Time                      13.06
INSTRUM                   spect
PROBHD    5 mm PABBO BB-
PULPROG                    zg30
TD                        65536
SOLVENT                   CDCl3
NS                            6
DS                            2
SWH                    8012.820 Hz
FIDRES                 0.122266 Hz
AQ                     4.0894465 sec
RG                          101
DW                       62.400 usec
DE                        6.50 usec
TE                       294.2 K
D1                  1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
SFO1                400.1424710 MHz
NUC1                        1H
P1                       13.50 usec
PLW1                16.00000000 W

F2 - Processing parameters
SI                        65536
SF                  400.1400000 MHz
WDW                          EM
SSB                 0
LB                        0.30 Hz
GB                  0
PC                        1.00
```

SB-V-107d



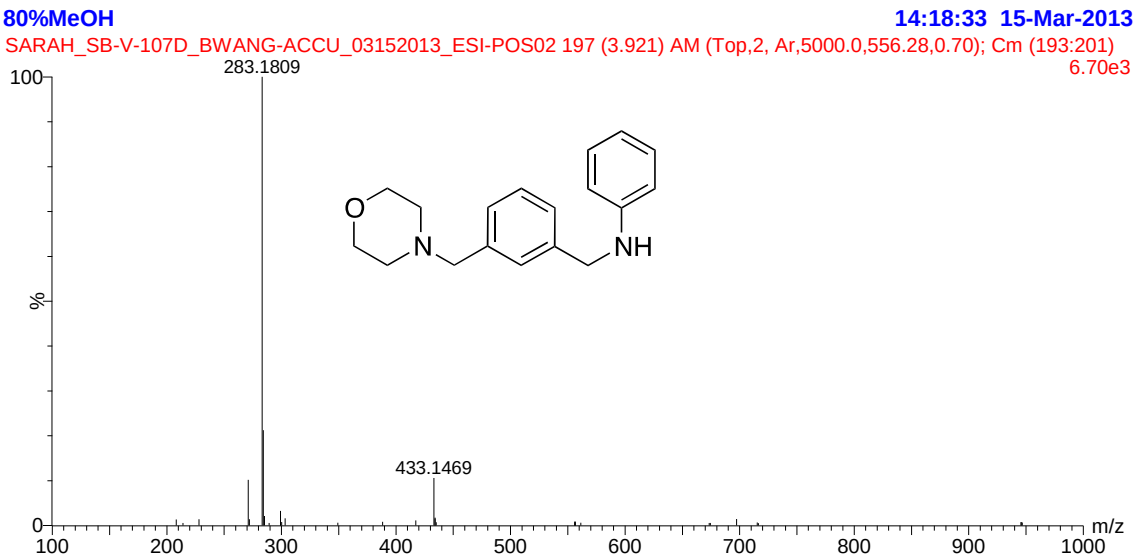

```
Current Data Parameters
NAME                  SB-V-107d
EXPNO                         4
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20130319
Time                      13.08
INSTRUM                   spect
PROBHD    5 mm PABBO BB-
PULPROG                  zgpg30
TD                        65536
SOLVENT                   CDCl3
NS                           30
DS                            4
SWH                   24038.461 Hz
FIDRES                 0.366798 Hz
AQ                     1.3631488 sec
RG                          203
DW                       20.800 usec
DE                        6.50 usec
TE                       294.8 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                           1

======== CHANNEL f1 ========
SFO1                100.6253441 MHz
NUC1                        13C
P1                        9.00 usec
PLW1                62.00000000 W

======== CHANNEL f2 ========
SFO2                400.1416006 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                    90.00 usec
PLW2                16.00000000 W
PLW12                0.36000001 W
PLW13                0.29159999 W

F2 - Processing parameters
SI                        32768
SF                  100.6152830 MHz
WDW                          EM
SSB                 0
LB                        1.00 Hz
GB                  0
PC                        1.40
```



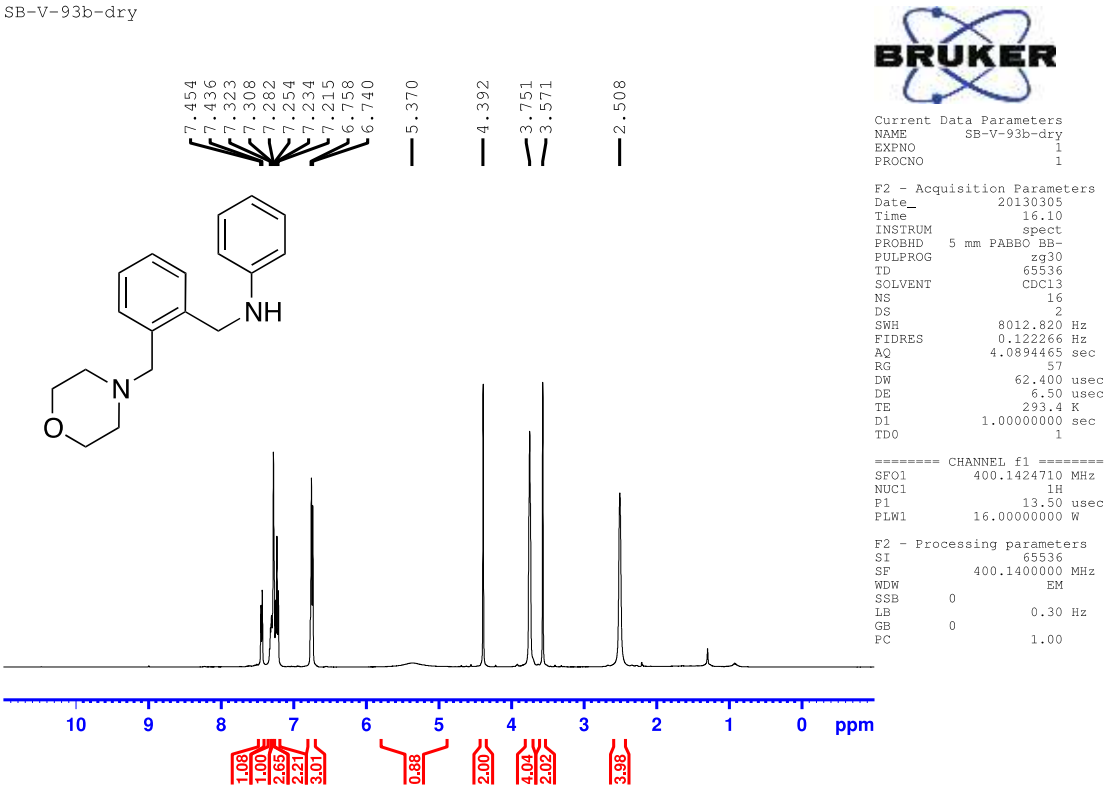
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
363 formula(e) evaluated with 3 results within limits (up to 100 closest results for each mass)
Elements Used:
C: 1-150 H: 1-150 N: 1-30 O: 1-60

Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa		PPM	DBE	i-FIT	Formula
283.1809	283.1810	-0.1	-0.4	8.5	1.7		C18 H23 N2 O

N-(2-(Morpholinomethyl)benzyl)aniline (10c)

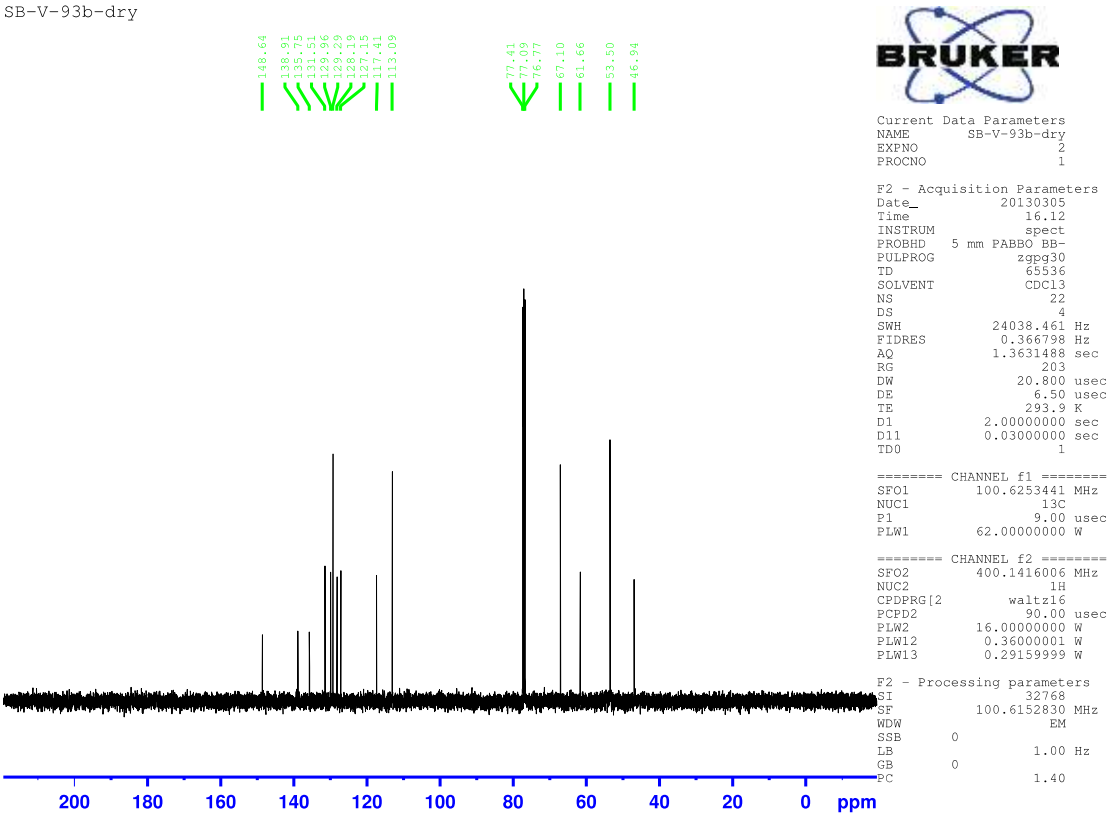



```
Current Data Parameters
NAME        SB-V-93b-dry
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130305
Time               16.10
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                    57
DW                62.400 usec
DE                 6.50 usec
TE                293.4 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1424710 MHz
NUC1                   1H
P1                 13.50 usec
PLW1         16.00000000 W

F2 - Processing parameters
SI                 65536
SF          400.1400000 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



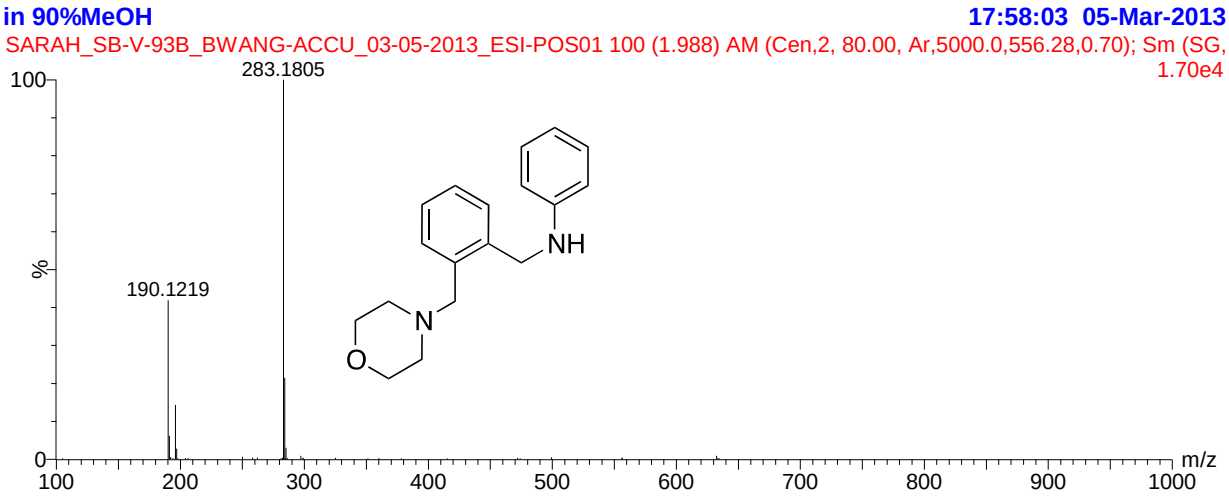

```
Current Data Parameters
NAME        SB-V-93b-dry
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130305
Time               16.12
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    22
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631488 sec
RG                   203
DW                20.800 usec
DE                 6.50 usec
TE                293.9 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6253441 MHz
NUC1                   13C
P1                 9.00 usec
PLW1         62.00000000 W

======== CHANNEL f2 ========
SFO2         400.1416006 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2         16.00000000 W
PLW12         0.36000001 W
PLW13         0.29159999 W

F2 - Processing parameters
SI                 32768
SF          100.6152830 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



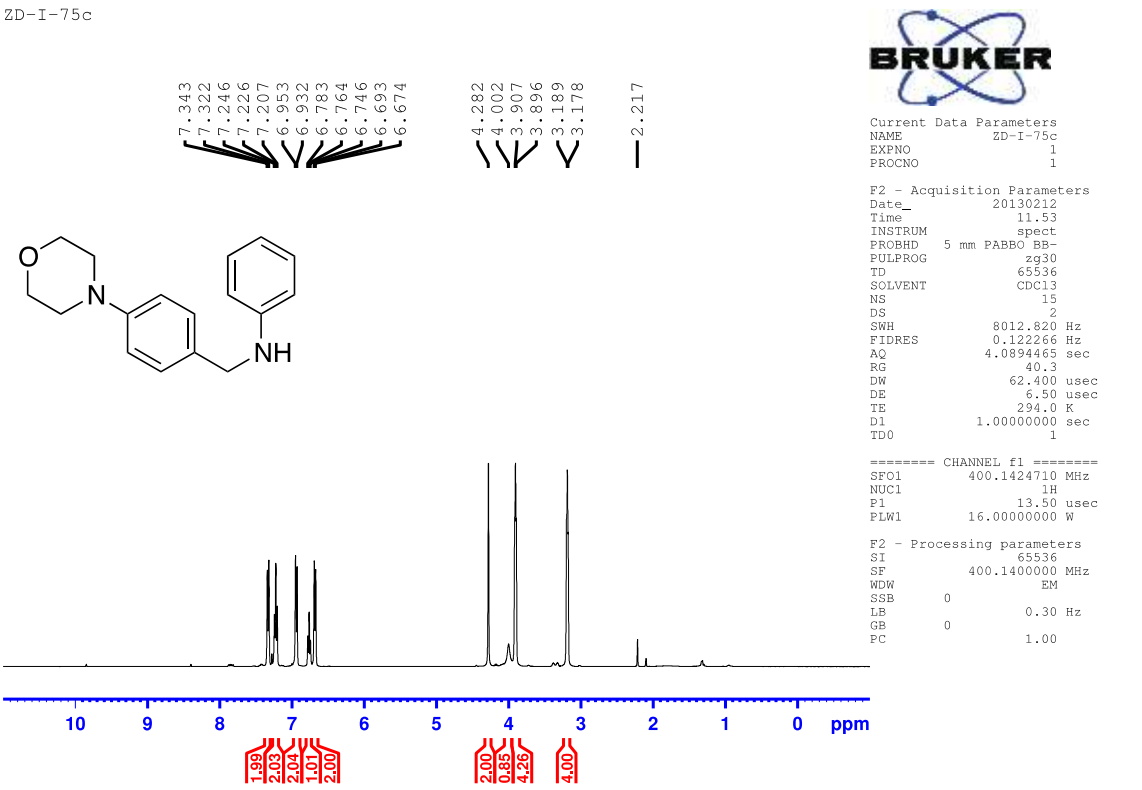
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
363 formula(e) evaluated with 2 results within limits (up to 100 closest results for each mass)
Elements Used:
C: 1-150 H: 1-150 N: 1-30 O: 1-60

Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa		PPM	DBE	i-FIT	Formula
283.1805	283.1810	-0.5	-1.8	8.5	12.4		C18 H23 N2 O

N-(4-Morpholinobenzyl)aniline (10d)

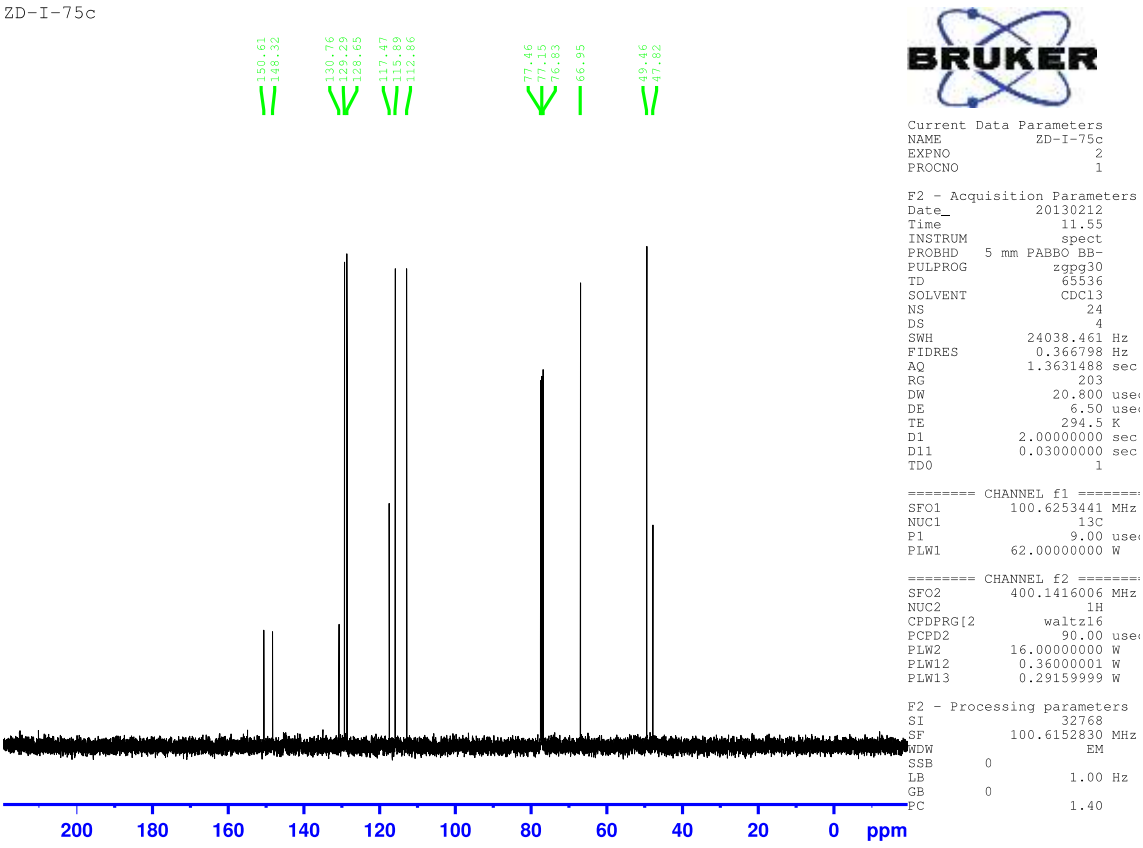


Current Data Parameters
NAME ZD-I-75c
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130212
Time 11.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 15
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 40.3
DW 62.400 usec
DE 6.50 usec
TE 294.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1424710 MHz
NUC1 1H
P1 13.50 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1400000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



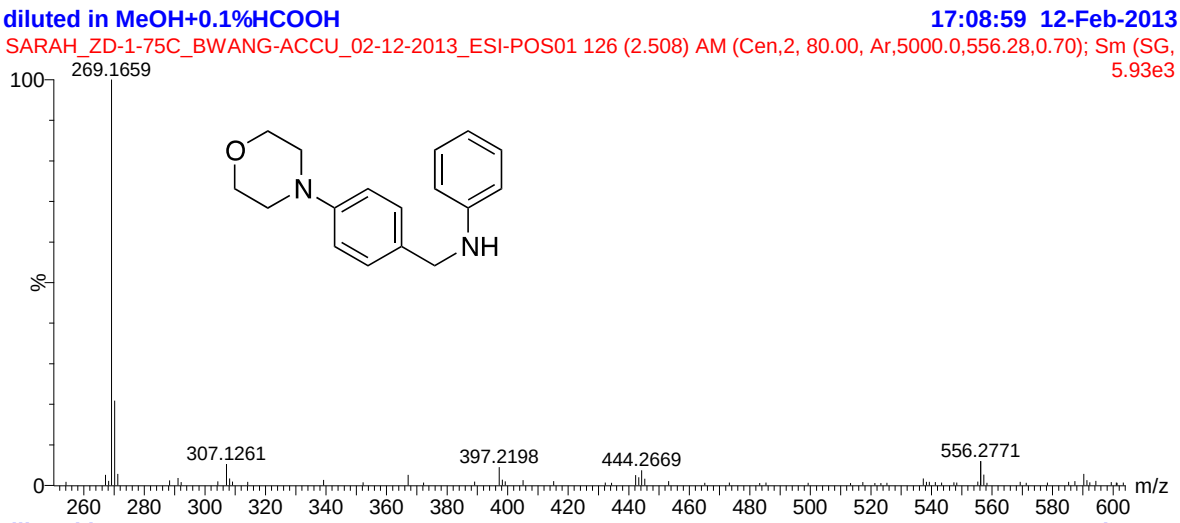
Current Data Parameters
NAME ZD-I-75c
EXPNO 2
PROCNO 1

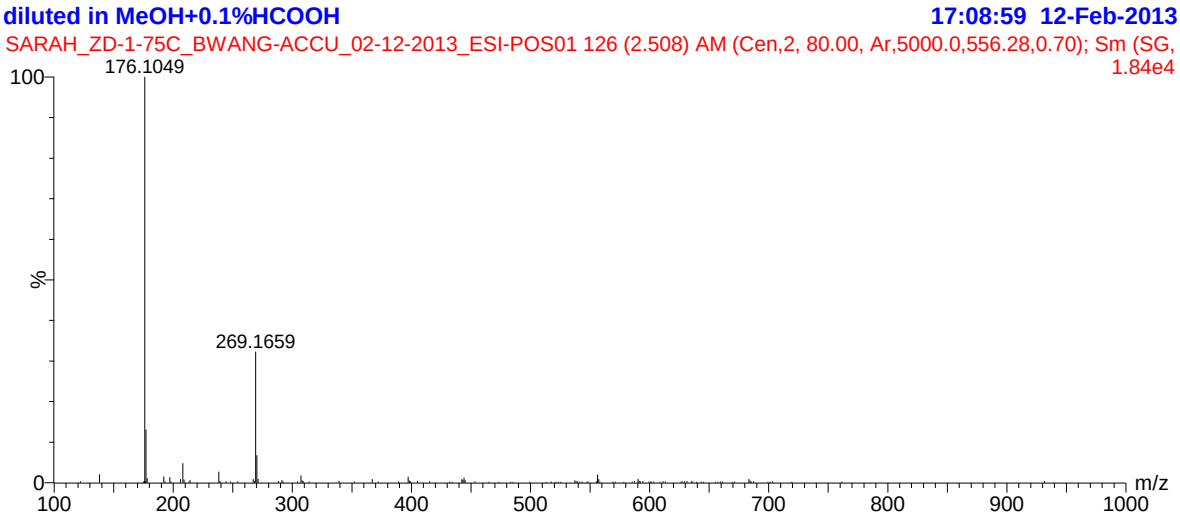
F2 - Acquisition Parameters
Date_ 20130212
Time 11.55
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 24
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 use
DE 6.50 use
TE 294.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6253441 MHz
NUC1 13C
P1 9.00 use
PLW1 62.00000000 W

======== CHANNEL f2 ========
SFO2 400.1416006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 use
PLW2 16.00000000 W
PLW12 0.36000001 W
PLW13 0.29159999 W

F2 - Processing parameters
SI 32768
SF 100.6152830 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





Elemental Composition Report

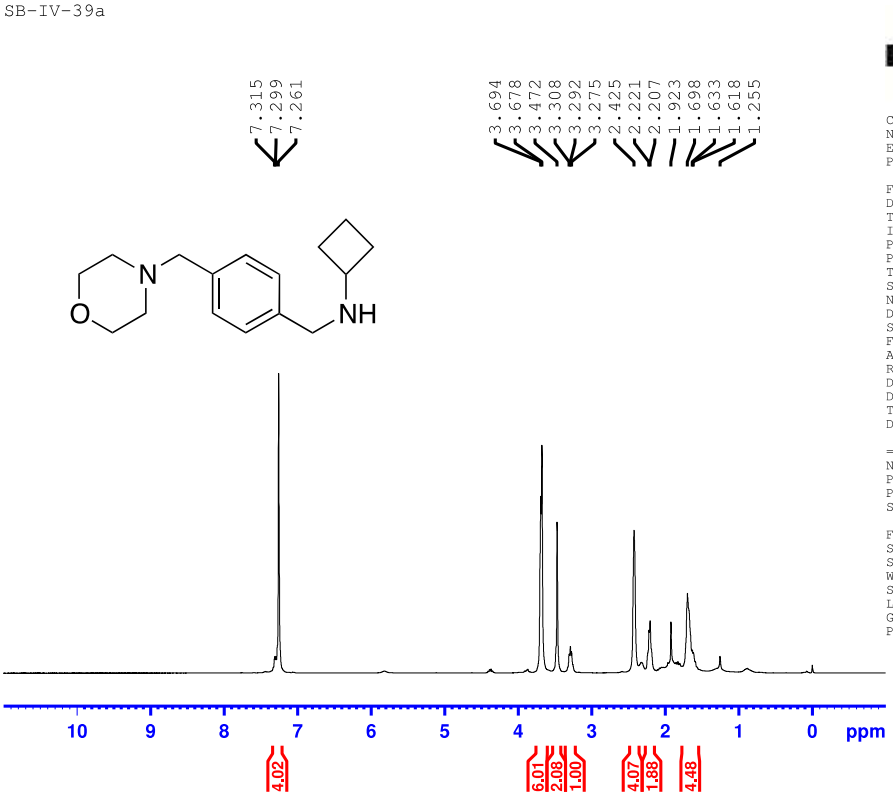
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
313 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-150 H: 1-150 N: 1-30 O: 1-30

Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa		PPM		DBE	i-FIT	Formula
269.1659	269.1654	0.5	1.9	8.5	n/a			C17H21N2O

N-(4-(Morpholinomethyl)benzyl)cyclobutanamine (11a)

SB-IV-39a



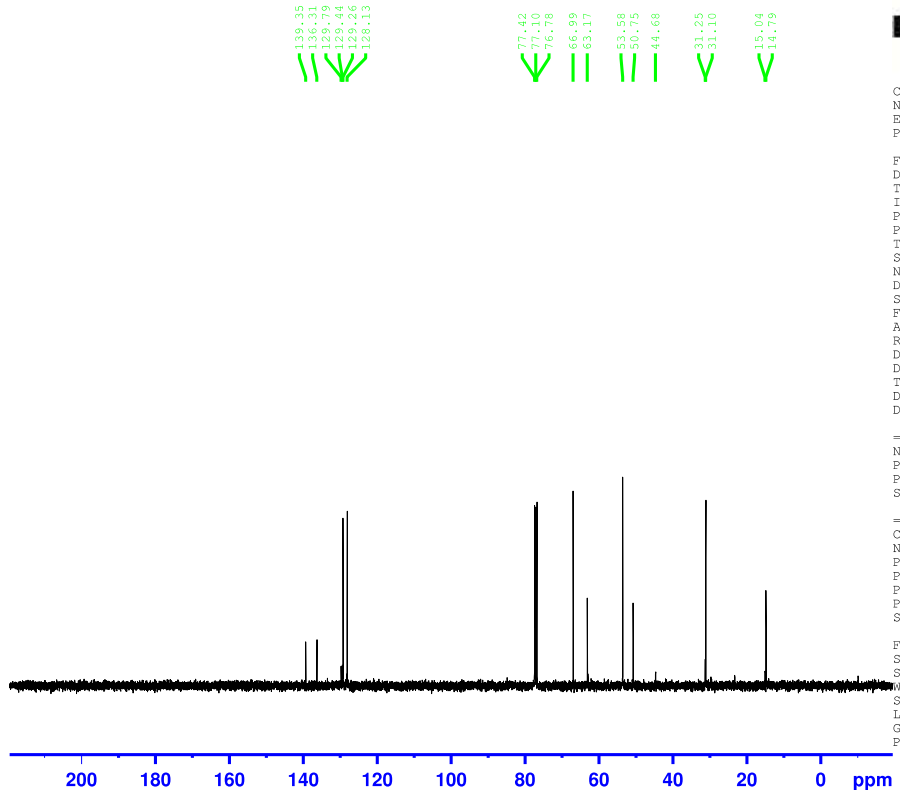

```
Current Data Parameters
NAME                  SB-IV-39a
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20120425
Time                      16.37
INSTRUM                   spect
PROBHD    5 mm PABBO BB-
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                          16
DS                           2
SWH                   8223.685 Hz
FIDRES                0.125483 Hz
AQ                    3.9846387 sec
RG                         25.4
DW                       60.800 usec
DE                        6.50 usec
TE                       298.1 K
D1                  1.00000000 sec

======== CHANNEL f1 ========
NUC1                         1H
P1                        13.50 usec
PLW1                16.00000000 W
SFO1                400.1424710 MHz

F2 - Processing parameters
SI                       65536
SF                  400.1400000 MHz
WDW                         EM
SSB          0
LB                        0.30 Hz
GB           0
PC                        1.00
```

SB-IV-39a



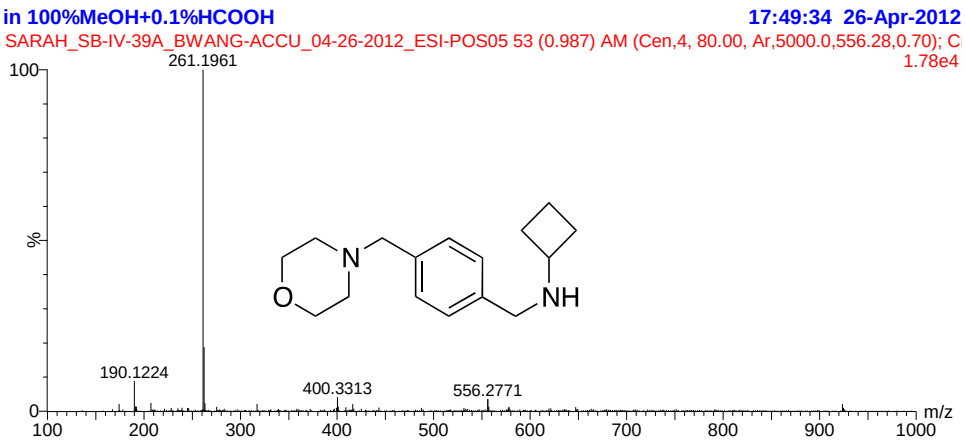

```
Current Data Parameters
NAME                  SB-IV-39a
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20120425
Time                      16.40
INSTRUM                   spect
PROBHD    5 mm PABBO BB-
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                          26
DS                           4
SWH                  24038.461 Hz
FIDRES                0.366798 Hz
AQ                    1.3631988 sec
RG                         203
DW                       20.800 usec
DE                        6.50 usec
TE                       298.2 K
D1                  2.00000000 sec
D11                 0.03000000 sec

======== CHANNEL f1 ========
NUC1                        13C
P1                         9.00 usec
PLW1                62.00000000 W
SFO1               100.6253441 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                         1H
PCPD2                     90.00 usec
PLW2                16.00000000 W
PLW12                0.36000001 W
PLW13                0.29159999 W
SFO2               400.1416006 MHz

F2 - Processing parameters
SI                       32768
SF                 100.6152830 MHz
WDW                         EM
SSB          0
LB                        1.00 Hz
GB           0
PC                        1.40
```



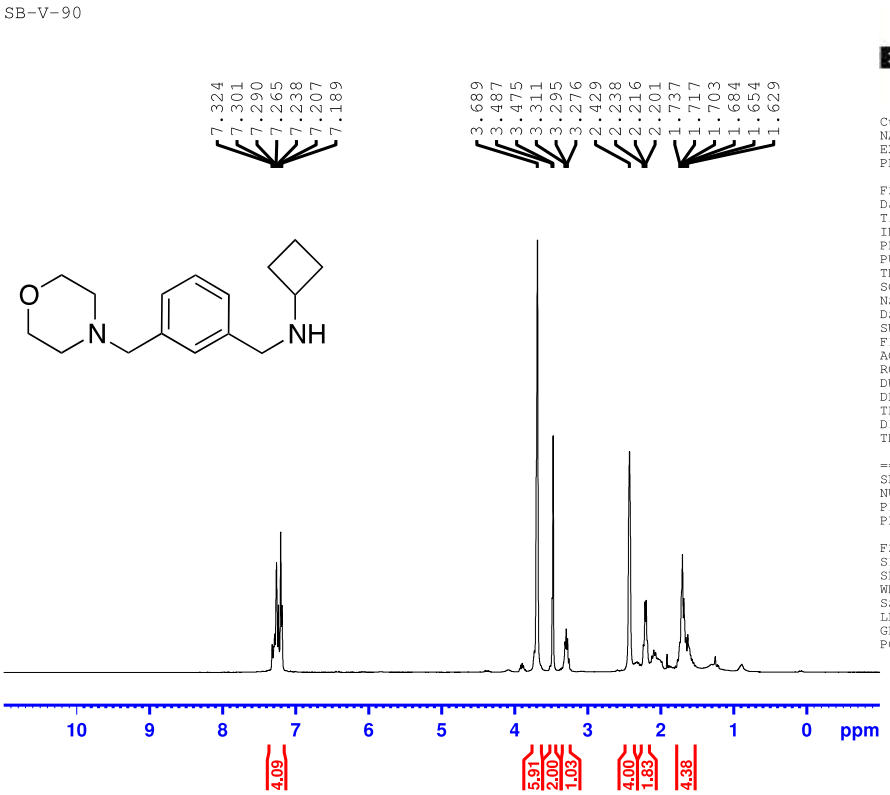
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
284 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-100 H: 1-100 N: 1-15 O: 1-100

Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa		PPM	DBE	i-FIT	Formula
261.1961	261.1967	-0.6	-2.3	5.5	7.3		C16 H25 N2 O

N-(3-(Morpholinomethyl)benzyl)cyclobutanamine (11b)

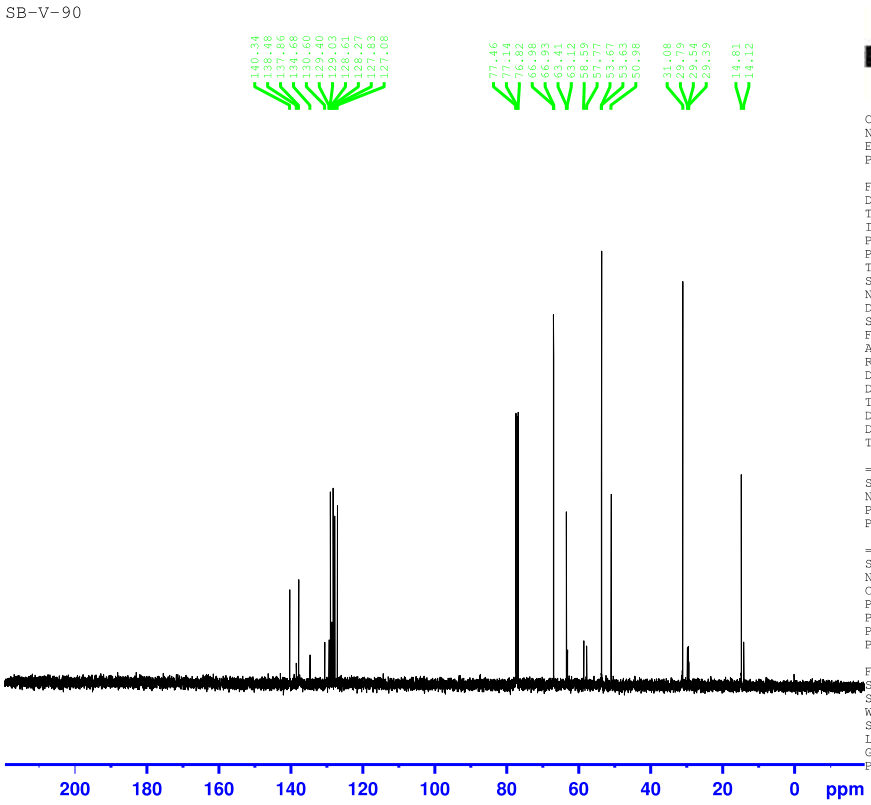



```
Current Data Parameters
NAME                  SB-V-90
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20130221
Time                   16.24
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 8012.820 Hz
FIDRES              0.122266 Hz
AQ                  4.0894465 sec
RG                       28.5
DW                     62.400 usec
DE                      6.50 usec
TE                     298.1 K
D1                1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1              400.1424710 MHz
NUC1                        1H
P1                      13.50 usec
PLW1             16.00000000 W

F2 - Processing parameters
SI                     65536
SF                400.1400000 MHz
WDW                       EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      1.00
```



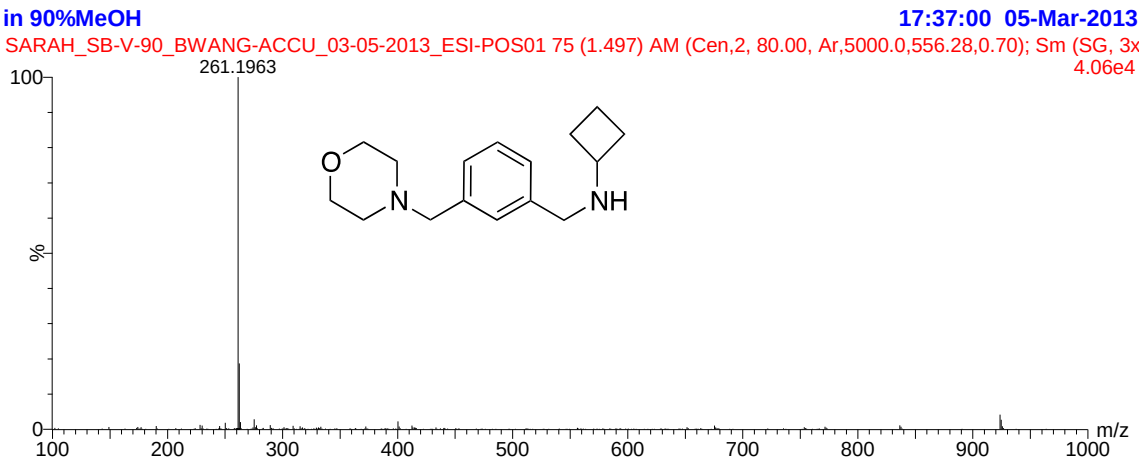

```
Current Data Parameters
NAME                  SB-V-90
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_               20130221
Time                   16.27
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                zgpg30
TD                     65536
SOLVENT                CDCl3
NS                        25
DS                         4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631488 sec
RG                       203
DW                     20.800 usec
DE                      6.50 usec
TE                     298.3 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1              100.6253441 MHz
NUC1                       13C
P1                      9.00 usec
PLW1              62.00000000 W

======== CHANNEL f2 ========
SFO2              400.1416006 MHz
NUC2                        1H
CPDPRG[2             waltz16
PCPD2                  90.00 usec
PLW2              16.00000000 W
PLW12              0.36000001 W
PLW13              0.29159999 W

F2 - Processing parameters
SI                     32768
SF                100.6152830 MHz
WDW                       EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
```



Elemental Composition Report

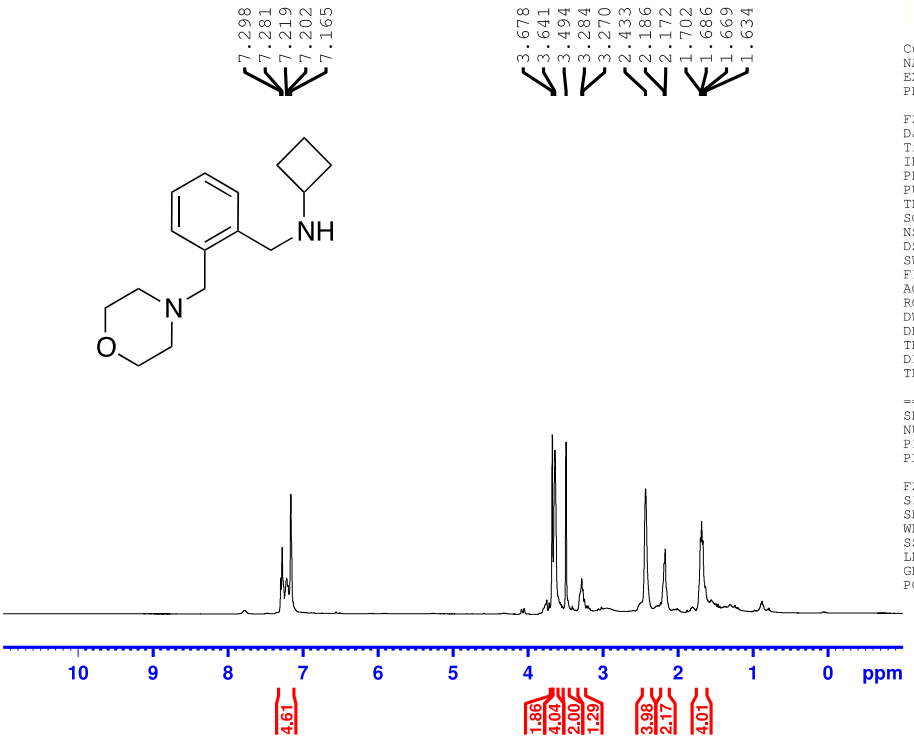
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
286 formula(e) evaluated with 2 results within limits (up to 100 closest results for each mass)
Elements Used:
C: 1-150 H: 1-150 N: 1-30 O: 1-60

Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa		PPM	DBE	i-FIT	Formula
261.1963	261.1967	-0.4	-1.5	5.5	2.5		C16 H25 N2 O

N-(2-(Morpholinomethyl)benzyl)cyclobutanamine (11c)

SB-V-91



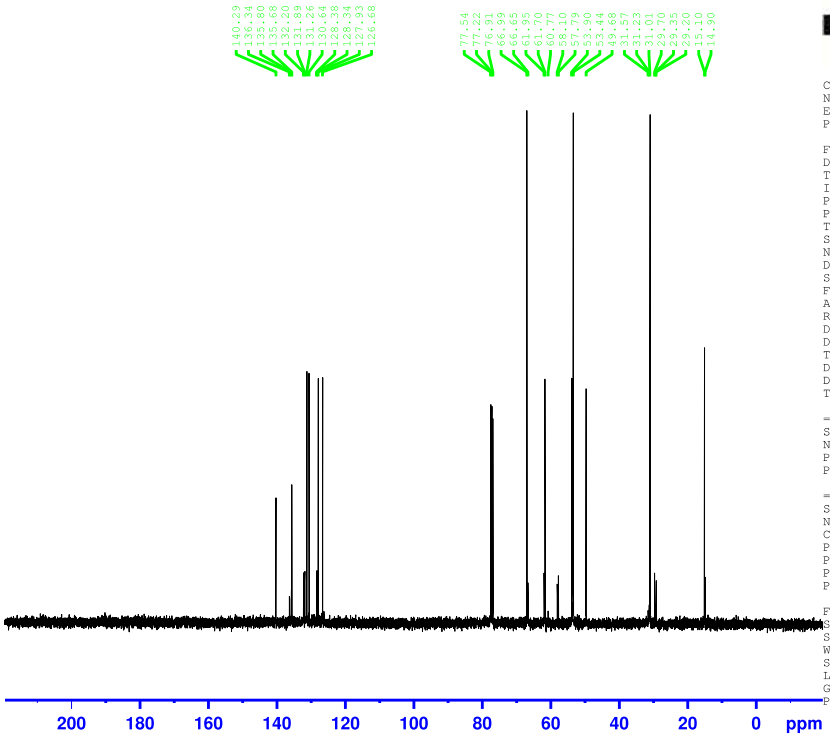

```
Current Data Parameters
NAME              SB-V-91
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20130221
Time                16.29
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      9
DS                      2
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894465 sec
RG                     16
DW                62.400 usec
DE                 6.50 usec
TE                297.9 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         400.1424710 MHz
NUC1                   1H
P1                 13.50 usec
PLW1         16.00000000 W

F2 - Processing parameters
SI                  65536
SF           400.1400000 MHz
WDW                    EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

SB-V-91



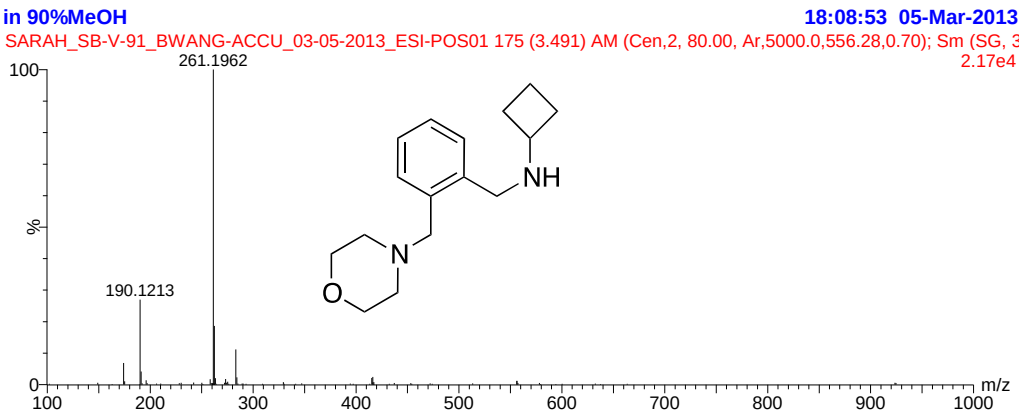

```
Current Data Parameters
NAME              SB-V-91
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20130221
Time                16.31
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                     21
DS                      4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631488 sec
RG                    203
DW                20.800 usec
DE                 6.50 usec
TE                298.4 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         100.6253441 MHz
NUC1                  13C
P1                 9.00 usec
PLW1         62.00000000 W

======== CHANNEL f2 ========
SFO2         400.1416006 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2         16.00000000 W
PLW12         0.36000001 W
PLW13         0.29159999 W

F2 - Processing parameters
SI                  32768
SF           100.6152830 MHz
WDW                    EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



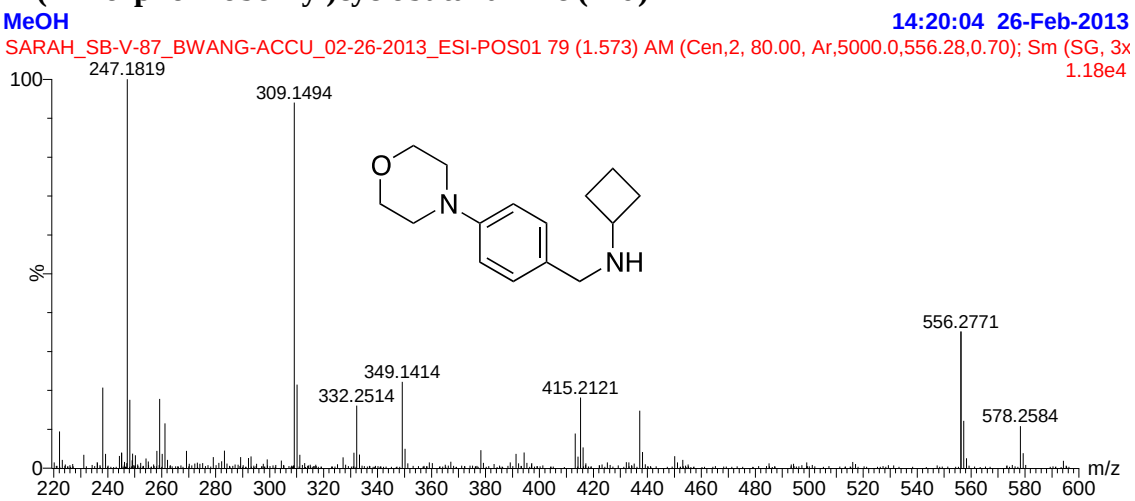
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
286 formula(e) evaluated with 2 results within limits (up to 100 closest results for each mass)
Elements Used:
C: 1-150 H: 1-150 N: 1-30 O: 1-60

Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa		PPM	DBE	i-FIT	Formula
261.1962	261.1967	-0.5	-1.9	5.5	1.6		C16 H25 N2 O

***N*-(4-Morpholinobenzyl)cyclobutanamine (11d)**



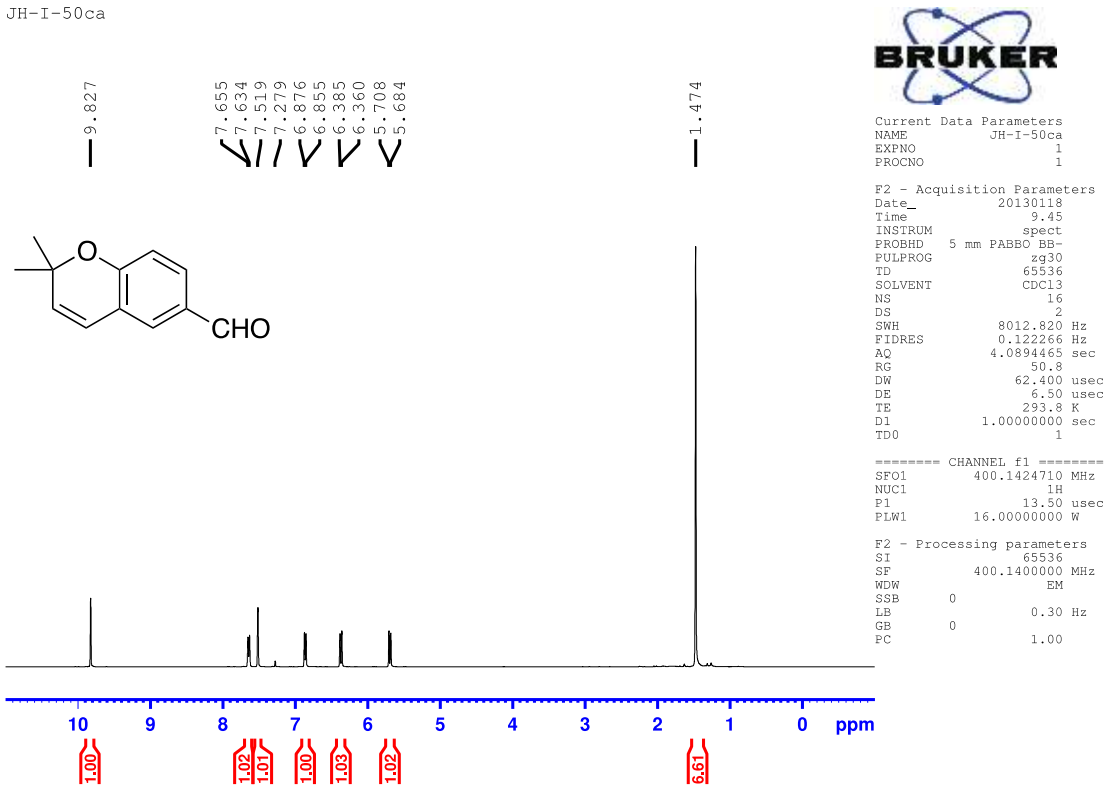
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
153 formula(e) evaluated with 1 results within limits (up to 100 closest results for each mass)
Elements Used:
C: 1-150 H: 1-150 N: 1-6 O: 1-30

Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa		PPM	DBE	i-FIT	Formula
247.1819	247.1810	0.9	3.6	5.5	70.6		C15 H23 N2 O

2,2-Dimethyl-2*H*-chromene-6-carbaldehyde (12)



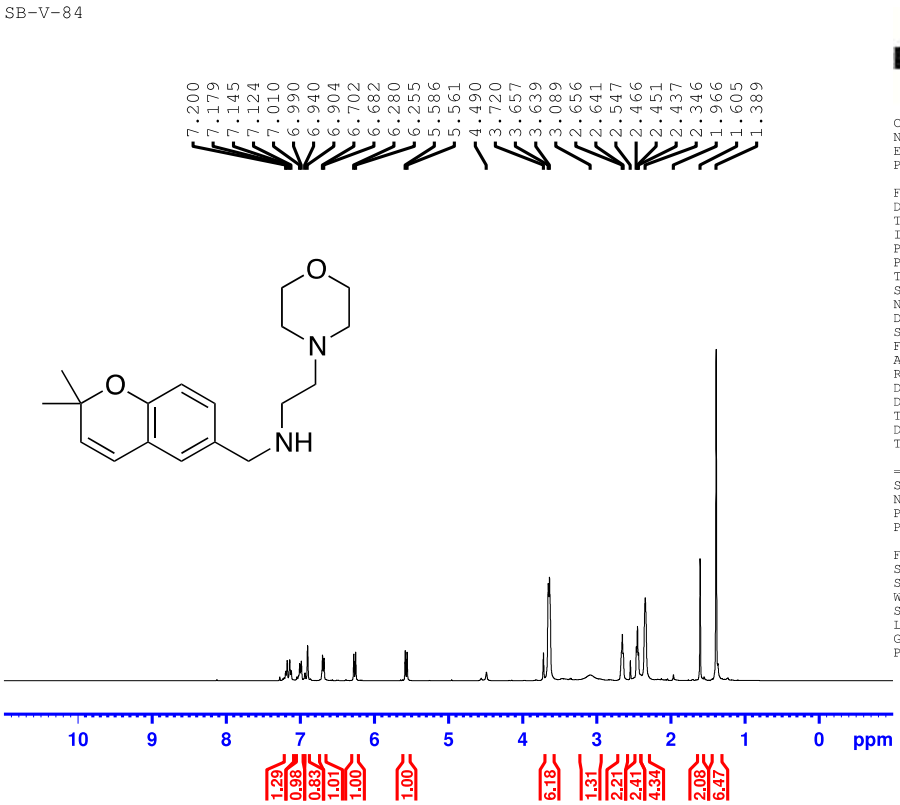

```
Current Data Parameters
NAME            JH-I-50ca
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20130118
Time                9.45
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894465 sec
RG                  50.8
DW                62.400 usec
DE                 6.50 usec
TE                293.8 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.1424710 MHz
NUC1                  1H
P1                 13.50 usec
PLW1         16.00000000 W

F2 - Processing parameters
SI                 65536
SF            400.1400000 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

N-((2,2-Dimethyl-2*H*-chromen-6-yl)methyl)-2-morpholinoethanamine (13a)

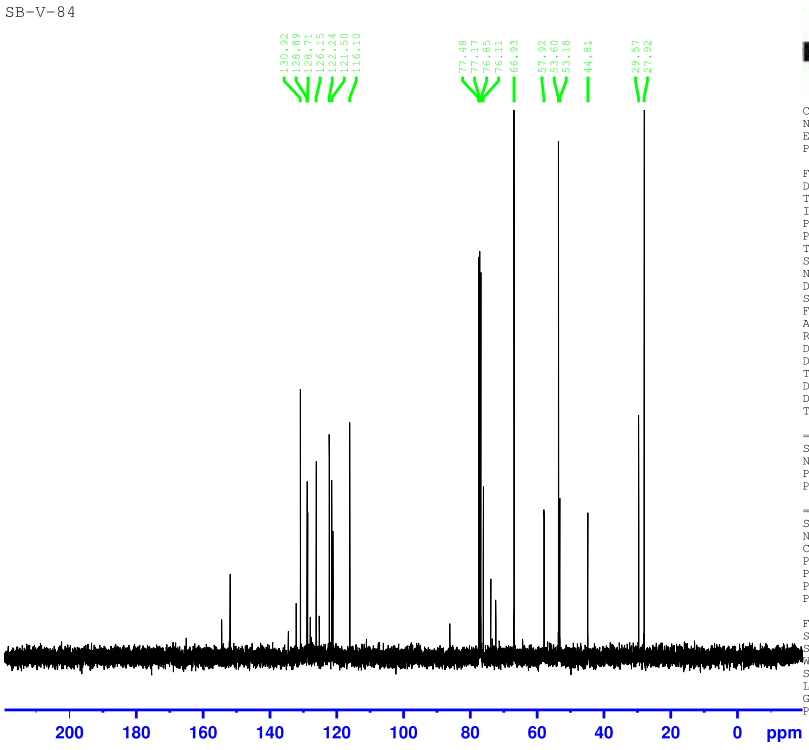



```
Current Data Parameters
NAME                  SB-V-84
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20130216
Time                   15.50
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       10
DS                        2
SWH                8012.820 Hz
FIDRES                0.122266 Hz
AQ                 4.0894465 sec
RG                       18
DW                    62.400 usec
DE                     6.50 usec
TE                    298.0 K
D1                 1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1             400.1424710 MHz
NUC1                       1H
P1                     13.50 usec
PLW1            16.00000000 W

F2 - Processing parameters
SI                        65536
SF               400.1400000 MHz
WDW                         EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```



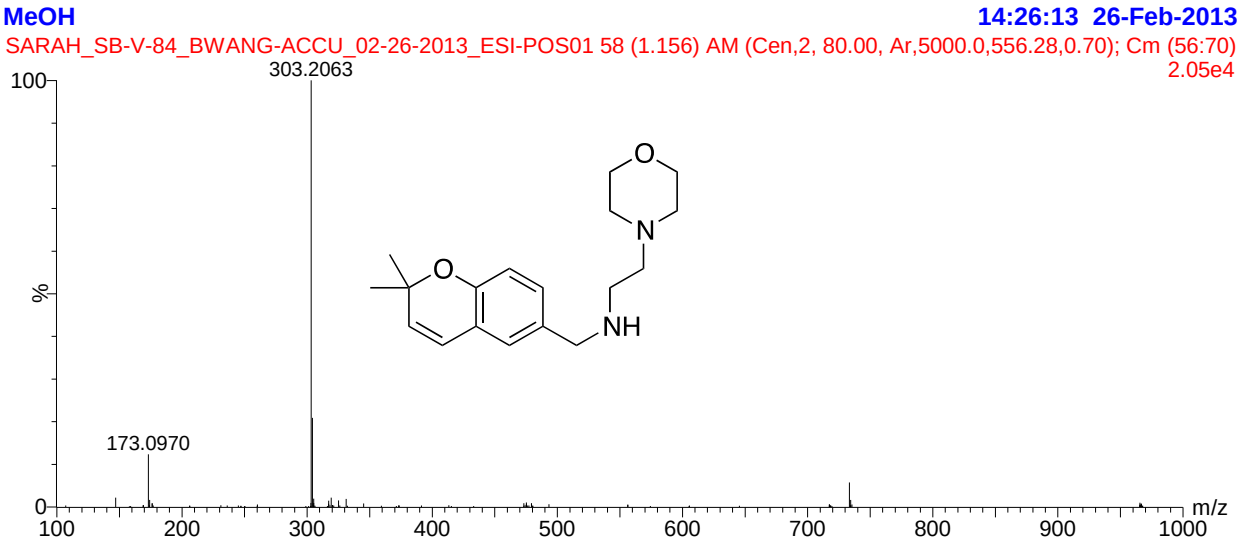

```
Current Data Parameters
NAME                  SB-V-84
EXPNO                       2
PROCNO                      1

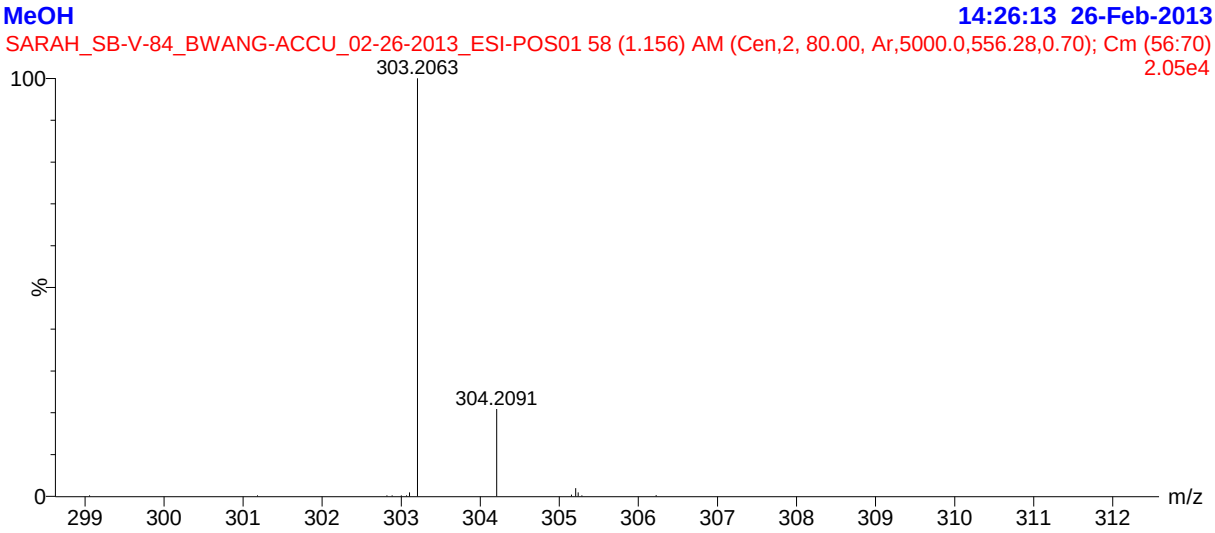
F2 - Acquisition Parameters
Date_              20130216
Time                   15.53
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                       15
DS                        4
SWH               24038.461 Hz
FIDRES                0.366798 Hz
AQ                 1.3631488 sec
RG                      203
DW                    20.800 usec
DE                     6.50 usec
TE                    298.5 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1             100.6253441 MHz
NUC1                       13C
P1                      9.00 usec
PLW1            62.00000000 W

======== CHANNEL f2 ========
SFO2             400.1416006 MHz
NUC2                       1H
CPDPRG[2             waltz16
PCPD2                  90.00 usec
PLW2            16.00000000 W
PLW12            0.36000001 W
PLW13            0.29159999 W

F2 - Processing parameters
SI                        32768
SF               100.6152830 MHz
WDW                         EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```





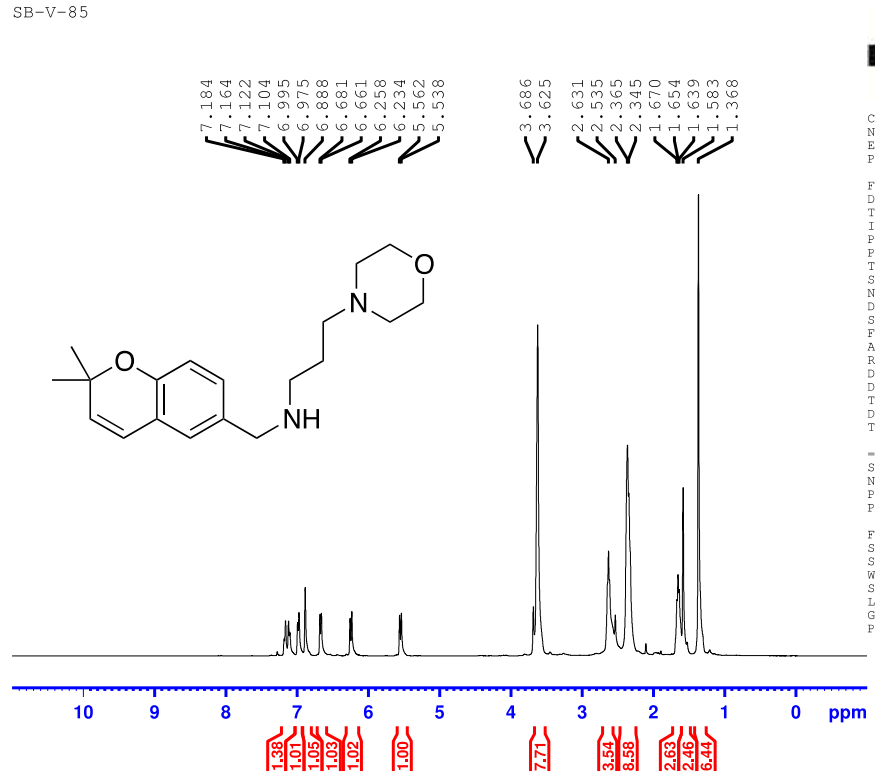
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
234 formula(e) evaluated with 1 results within limits (up to 100 closest results for each mass)
Elements Used:
C: 1-150 H: 1-150 N: 1-6 O: 1-30

Minimum:				-1.5		
Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
303.2063	303.2073	-1.0	-3.3	6.5	22.6	C18 H27 N2 O2

N-((2,2-Dimethyl-2*H*-chromen-6-yl)methyl)-3-morpholinopropan-1-amine (13b)

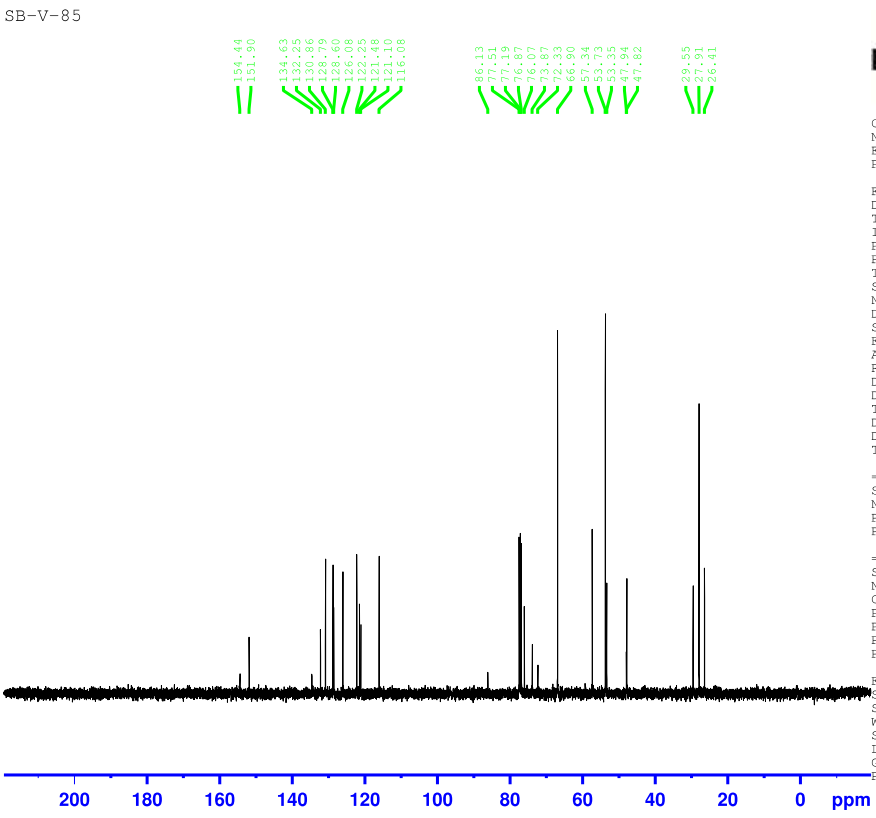



```
Current Data Parameters
NAME                  SB-V-85
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20130216
Time                  15.55
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       12
DS                        2
SWH                8012.820 Hz
FIDRES            0.122266 Hz
AQ                4.0894465 sec
RG                       18
DW                  62.400 usec
DE                   6.50 usec
TE                   297.7 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1           400.1424710 MHz
NUC1                     1H
P1                    13.50 usec
PLW1           16.00000000 W

F2 - Processing parameters
SI                    65536
SF             400.1400000 MHz
WDW                      EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```



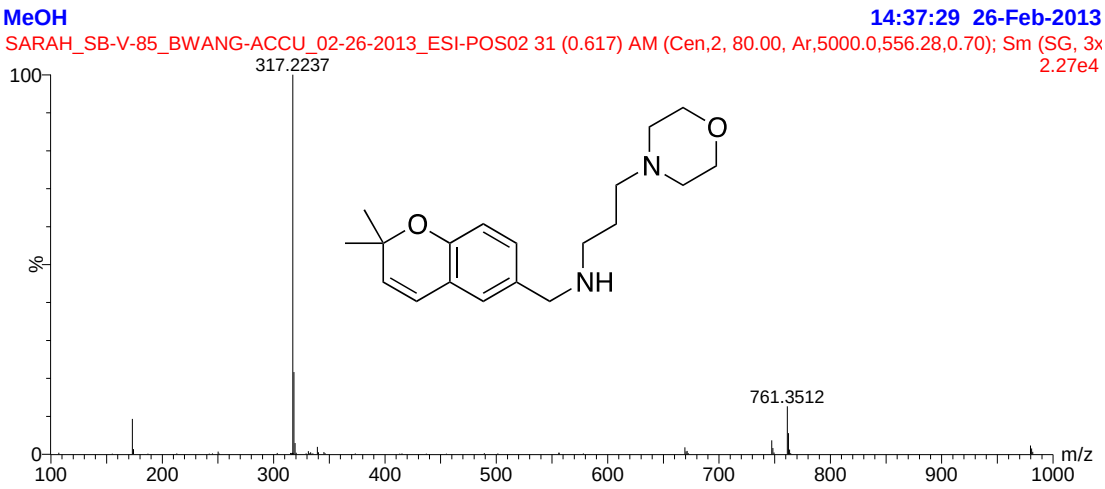

```
Current Data Parameters
NAME                  SB-V-85
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20130216
Time                  15.57
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                       19
DS                        4
SWH               24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631488 sec
RG                      203
DW                  20.800 usec
DE                   6.50 usec
TE                   298.6 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1           100.6253441 MHz
NUC1                     13C
P1                    9.00 usec
PLW1           62.00000000 W

======== CHANNEL f2 ========
SFO2           400.1416006 MHz
NUC2                     1H
CPDPRG[2             waltz16
PCPD2                90.00 usec
PLW2           16.00000000 W
PLW12           0.36000001 W
PLW13           0.29159999 W

F2 - Processing parameters
SI                    32768
SF             100.6152830 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```



Elemental Composition Report

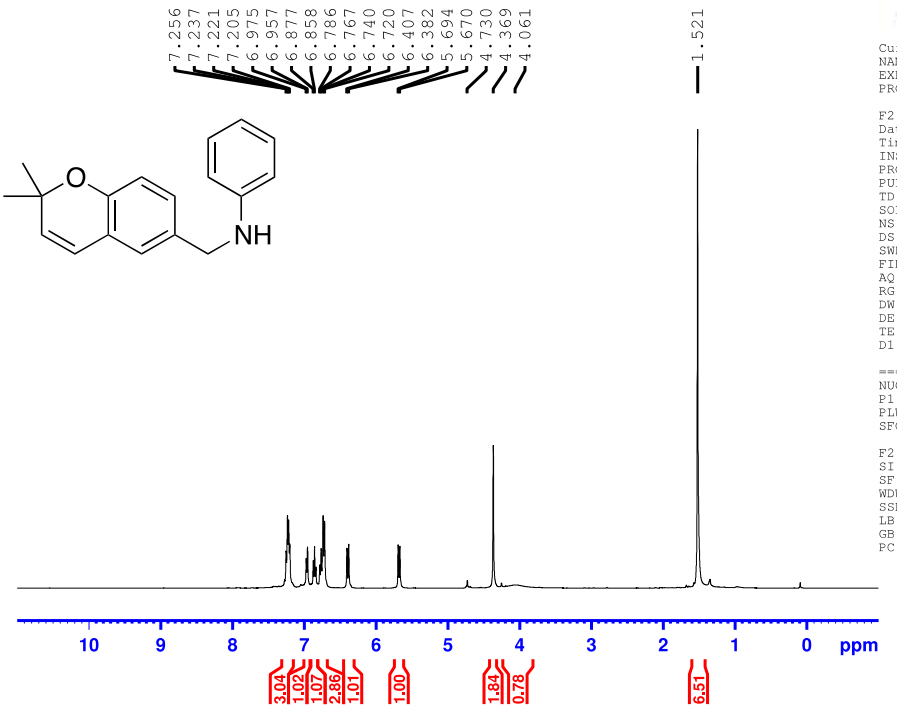
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
255 formula(e) evaluated with 1 results within limits (up to 100 closest results for each mass)
Elements Used:
C: 1-150 H: 1-150 N: 1-6 O: 1-30

Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa		PPM	DBE	i-FIT	Formula
317.2237	317.2229	0.8	2.5	6.5	3.5		C19 H29 N2 O2

N-((2,2-Dimethyl-2*H*-chromen-6-yl)methyl)aniline (14a)

SB-IV-53



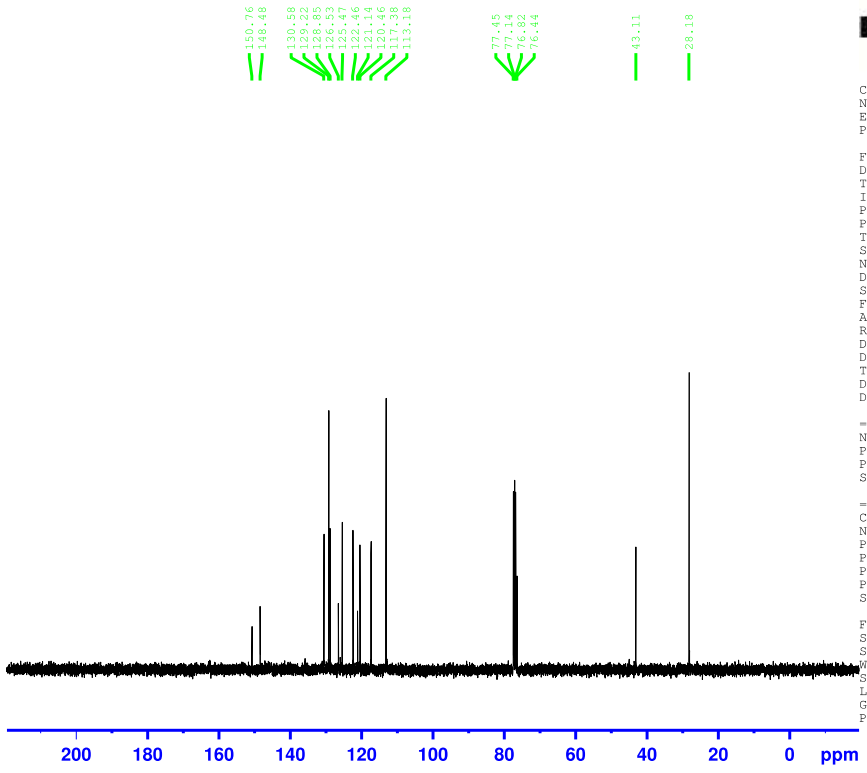

```
Current Data Parameters
NAME                  SB-IV-53
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20120509
Time                    12.26
INSTRUM                 spect
PROBHD    5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 8223.685 Hz
FIDRES              0.125483 Hz
AQ                  3.9846387 sec
RG                       28.5
DW                     60.800 usec
DE                      6.50 usec
TE                     298.2 K
D1                  1.00000000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                      13.50 usec
PLW1               16.00000000 W
SFO1              400.1424710 MHz

F2 - Processing parameters
SI                         65536
SF                400.1400000 MHz
WDW                           EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      1.00
```

SB-IV-53

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Current Data Parameters
NAME                  SB-IV-53
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_              20120509
Time                    12.28
INSTRUM                 spect
PROBHD    5 mm PABBO BB-
PULPROG              zgpg30
TD                     65536
SOLVENT                CDCl3
NS                        20
DS                         4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631988 sec
RG                       203
DW                     20.800 usec
DE                      6.50 usec
TE                     298.3 K
D1                  2.00000000 sec
D11                 0.03000000 sec

======== CHANNEL f1 ========
NUC1                       13C
P1                      9.00 usec
PLW1               62.00000000 W
SFO1              100.6253441 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  90.00 usec
PLW2               16.00000000 W
PLW12               0.36000001 W
PLW13               0.29159999 W
SFO2              400.1416006 MHz

F2 - Processing parameters
SI                         32768
SF                100.6152830 MHz
WDW                           EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
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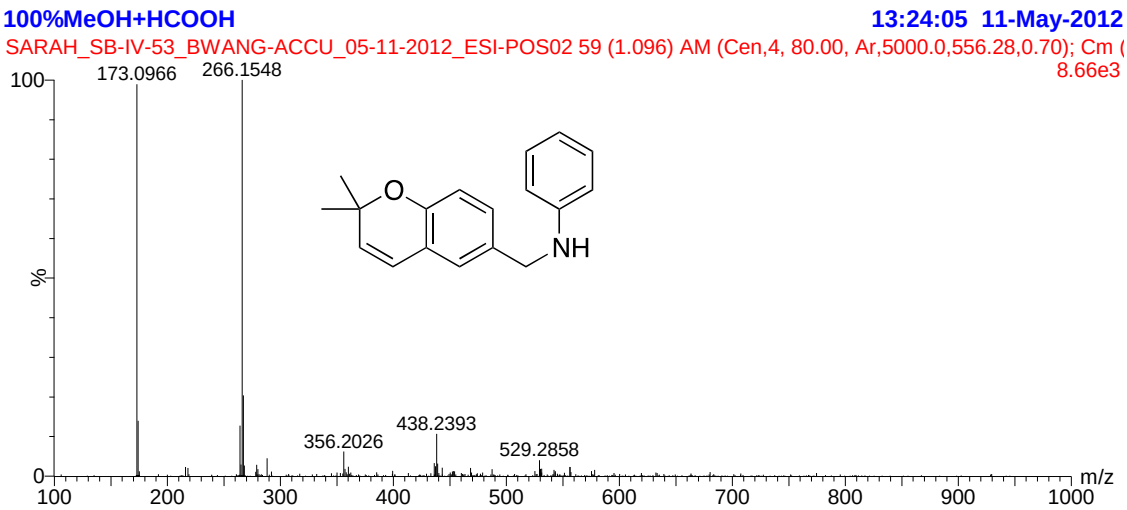


Elemental Composition Report

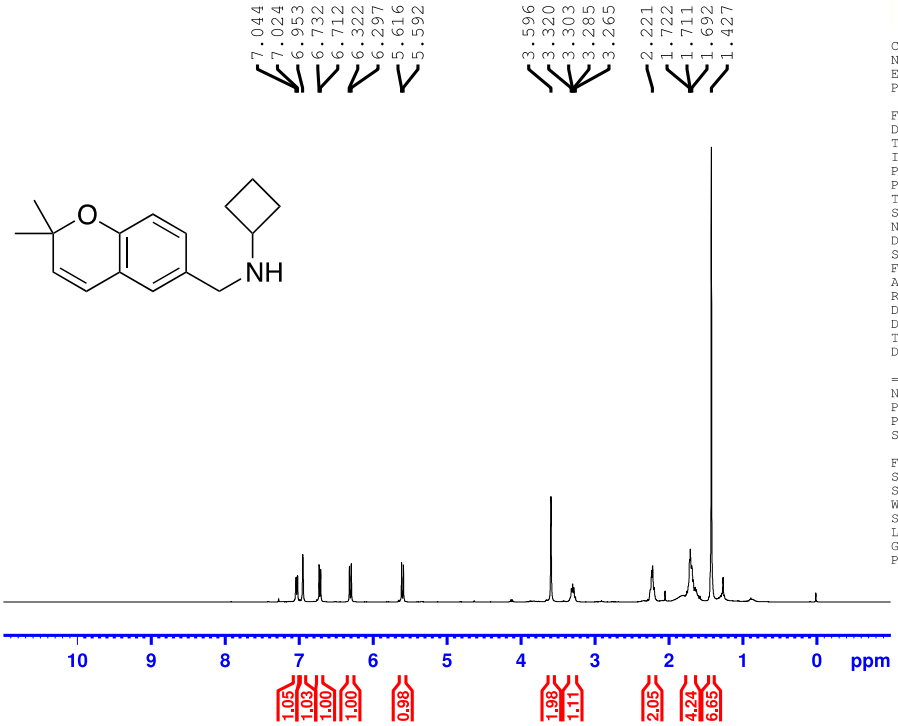
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
293 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-100 H: 1-100 N: 1-15 O: 1-100

Minimum:				-1.5		
Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
266.1548	266.1545	0.3	1.1	9.5	3.1	C18 H20 N O

N-((2,2-Dimethyl-2*H*-chromen-6-yl)methyl)cyclobutanamine (14b)

SB-IV-9a



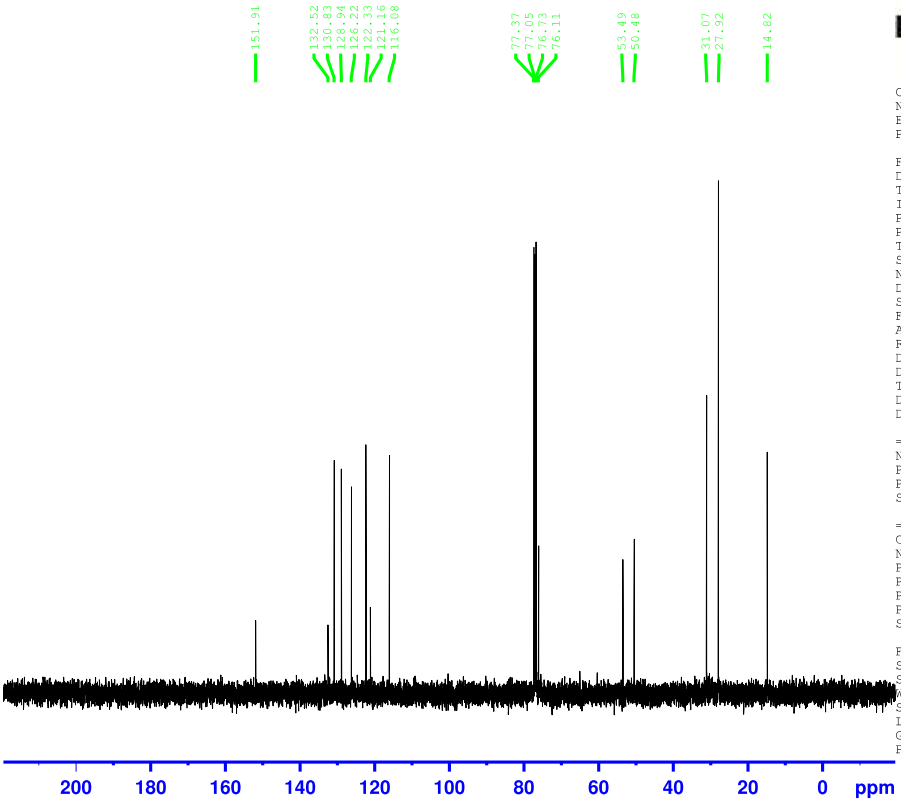

```
Current Data Parameters
NAME                  SB-IV-9a
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_               20120405
Time                   16.15
INSTRUM                spect
PROBHD     5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9846387 sec
RG                       32
DW                   60.800 usec
DE                    6.50 usec
TE                   298.1 K
D1                 1.00000000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                     13.50 usec
PLW1              16.00000000 W
SFO1             400.1424710 MHz

F2 - Processing parameters
SI                        65536
SF                400.1400000 MHz
WDW                        EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

SB-IV-9a



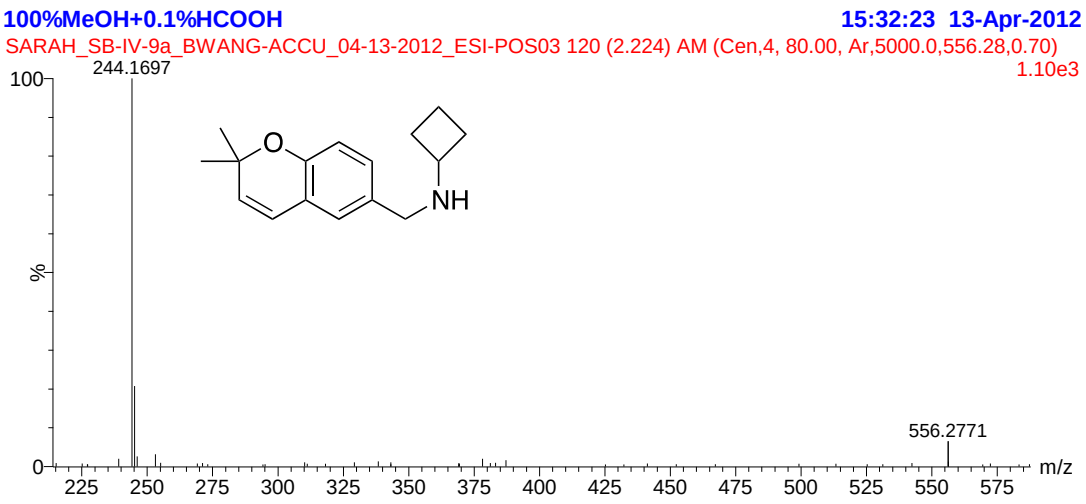

```
Current Data Parameters
NAME                  SB-IV-9a
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_               20120405
Time                   16.18
INSTRUM                spect
PROBHD     5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                       21
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631988 sec
RG                      203
DW                   20.800 usec
DE                    6.50 usec
TE                   298.6 K
D1                 2.00000000 sec
D11                0.03000000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                      9.00 usec
PLW1              62.00000000 W
SFO1             100.6253441 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                      1H
PCPD2                  90.00 usec
PLW2              16.00000000 W
PLW12              0.36000001 W
PLW13              0.29159999 W
SFO2             400.1416006 MHz

F2 - Processing parameters
SI                        32768
SF                100.6152830 MHz
WDW                        EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```



Elemental Composition Report

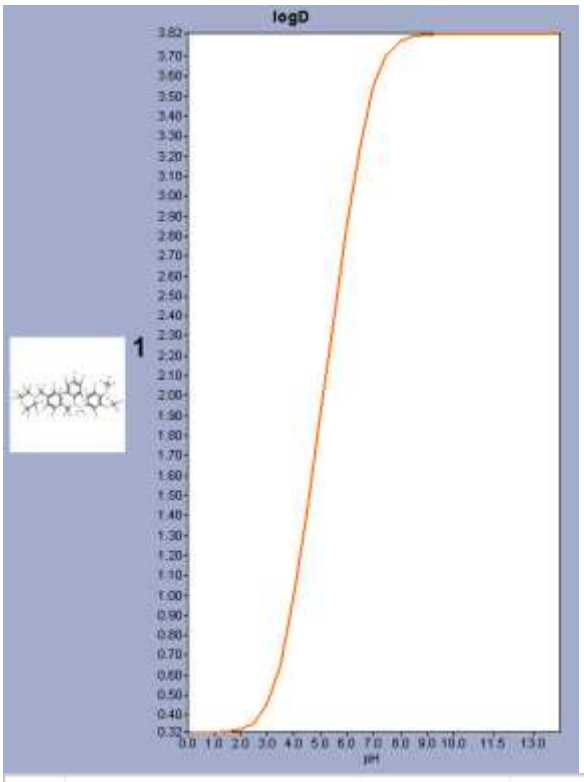
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

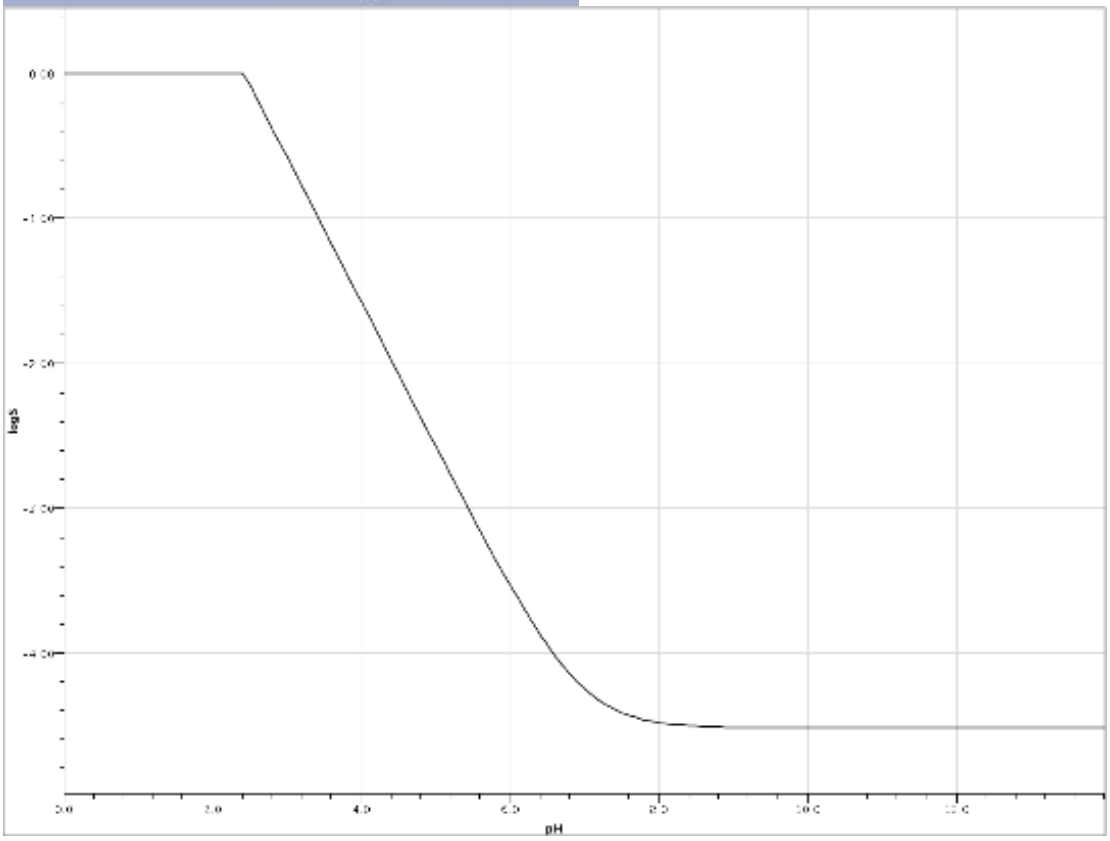
Monoisotopic Mass, Even Electron Ions
227 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-100 H: 1-100 N: 1-15 O: 1-20

Minimum:			-1.5			
Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
244.1697	244.1701	-0.4	-1.6	6.5	2.7	C16 H22 N O

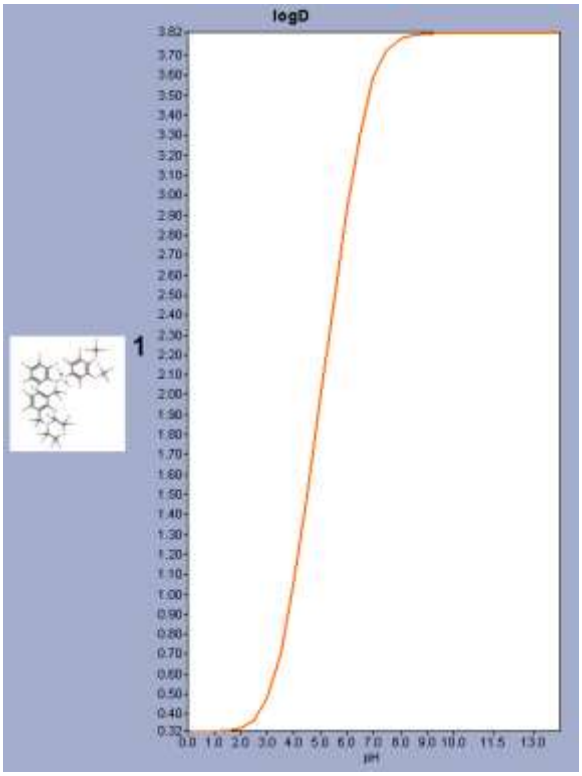
Graphical Representations of calculated log*D* and log*S* values for **3a-6b**

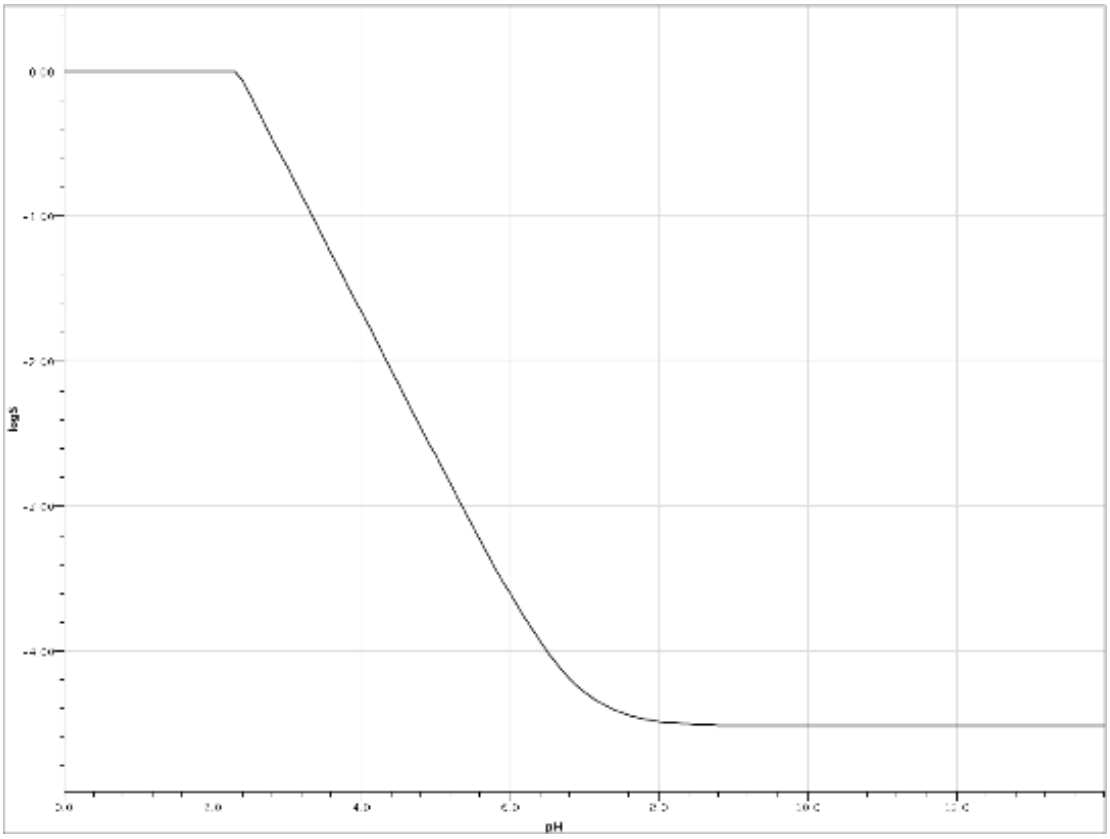
3a



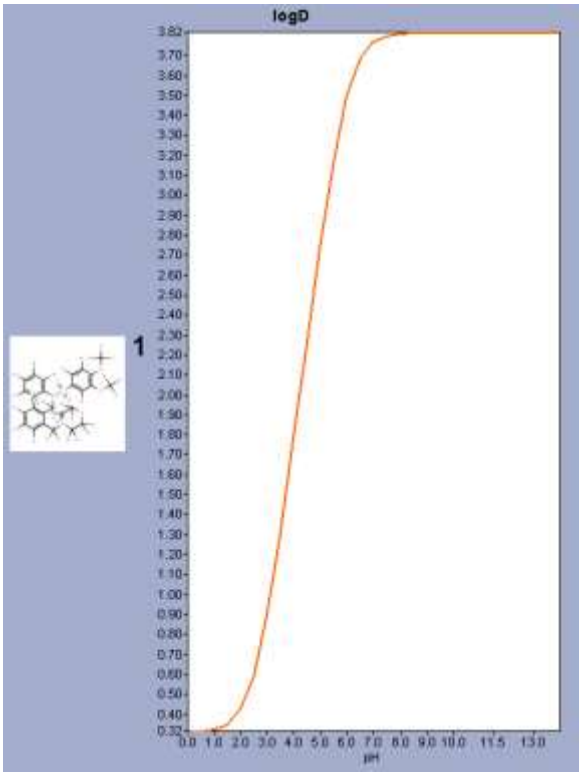


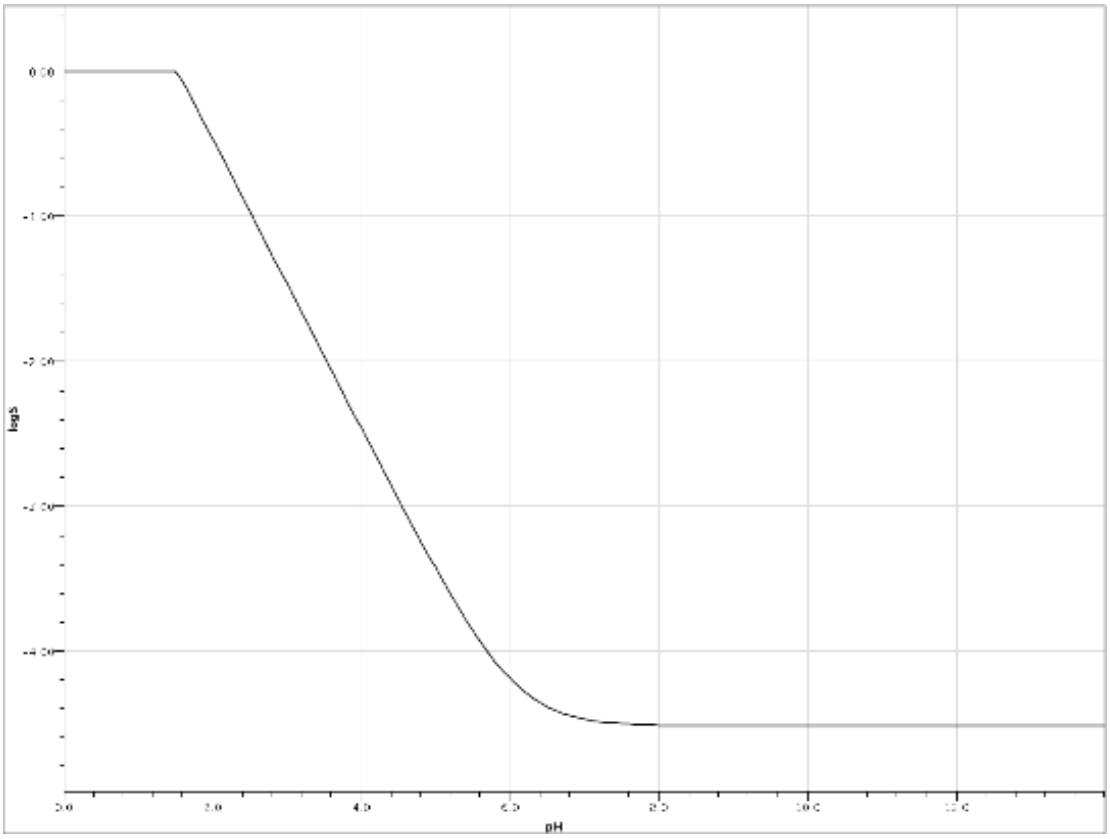
3b



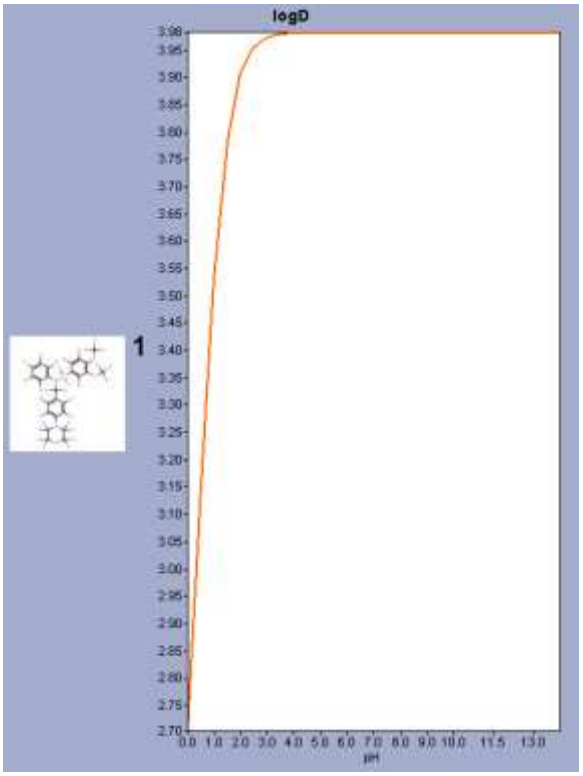


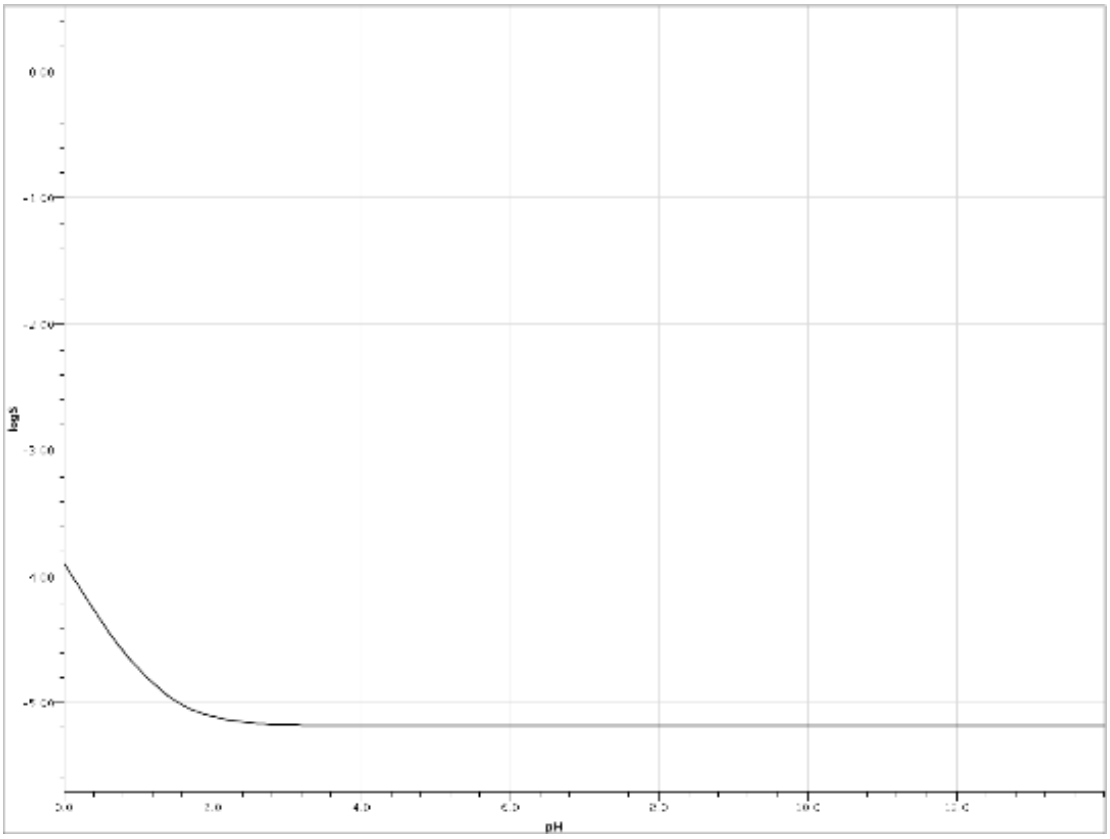
3c



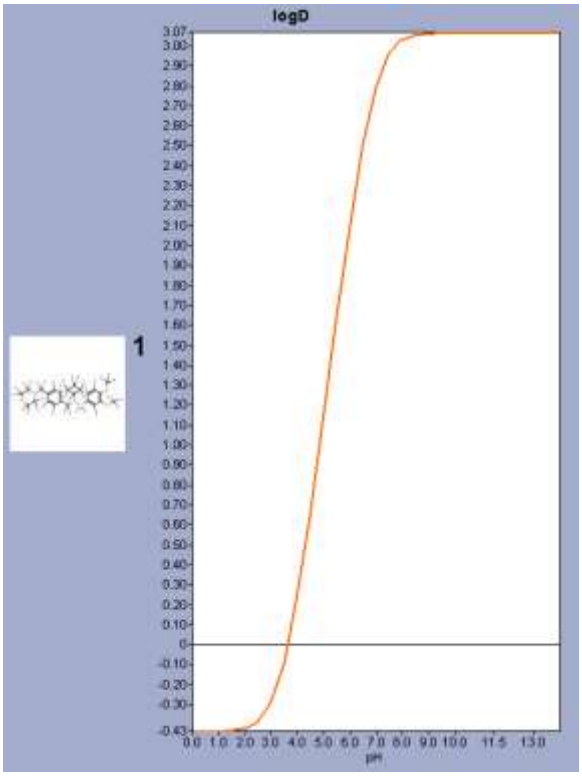


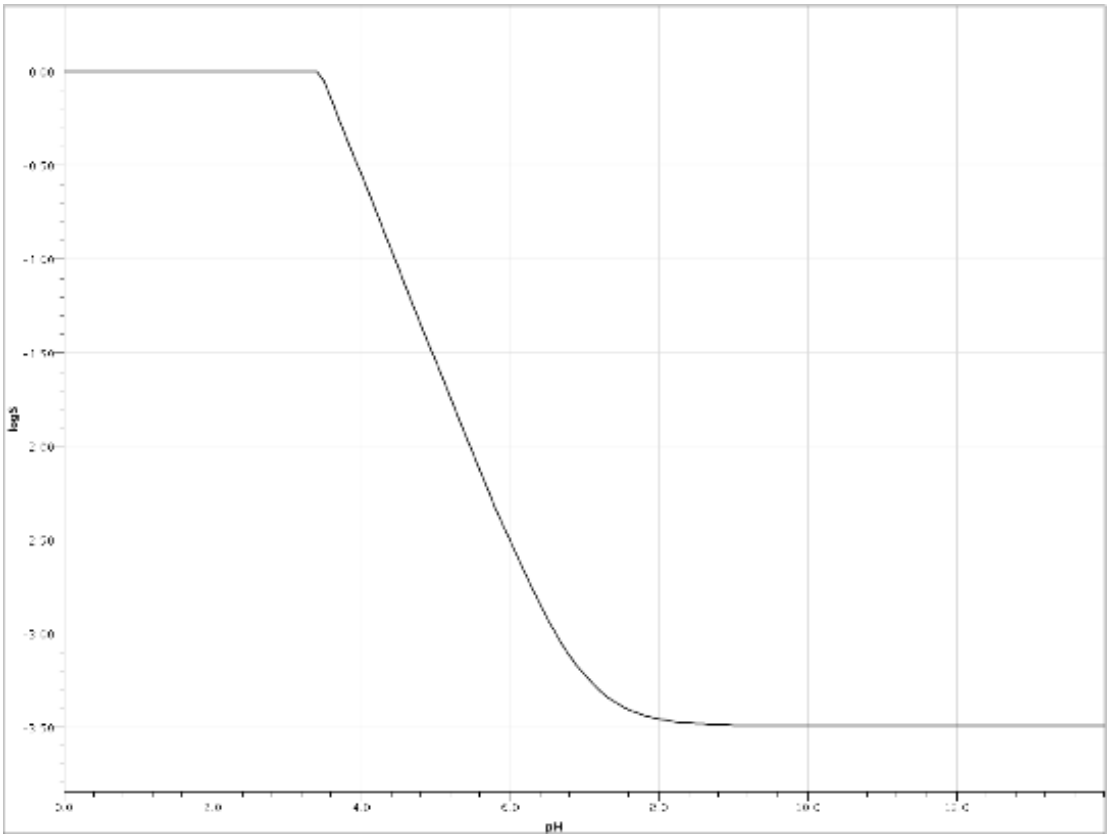
3d



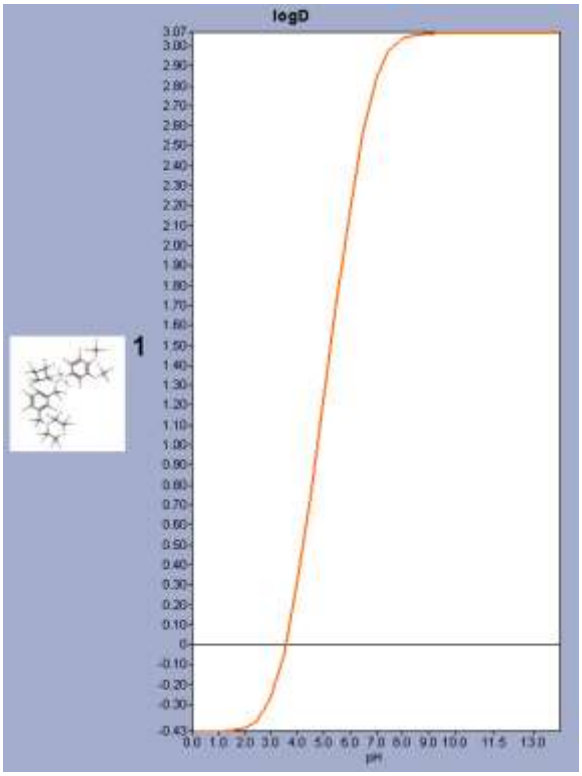


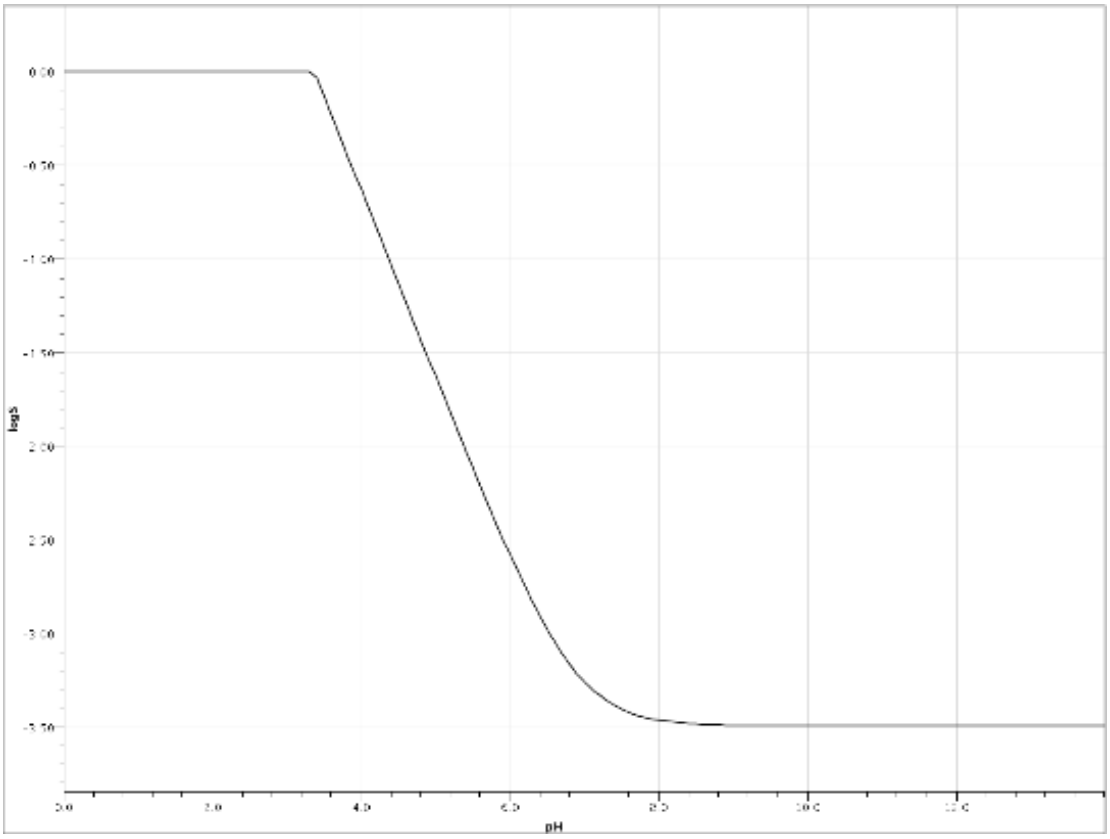
4a





4b





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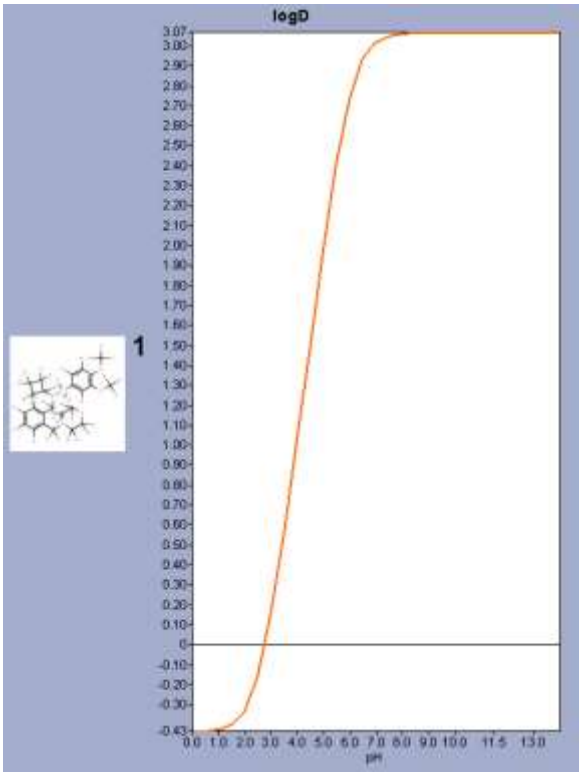
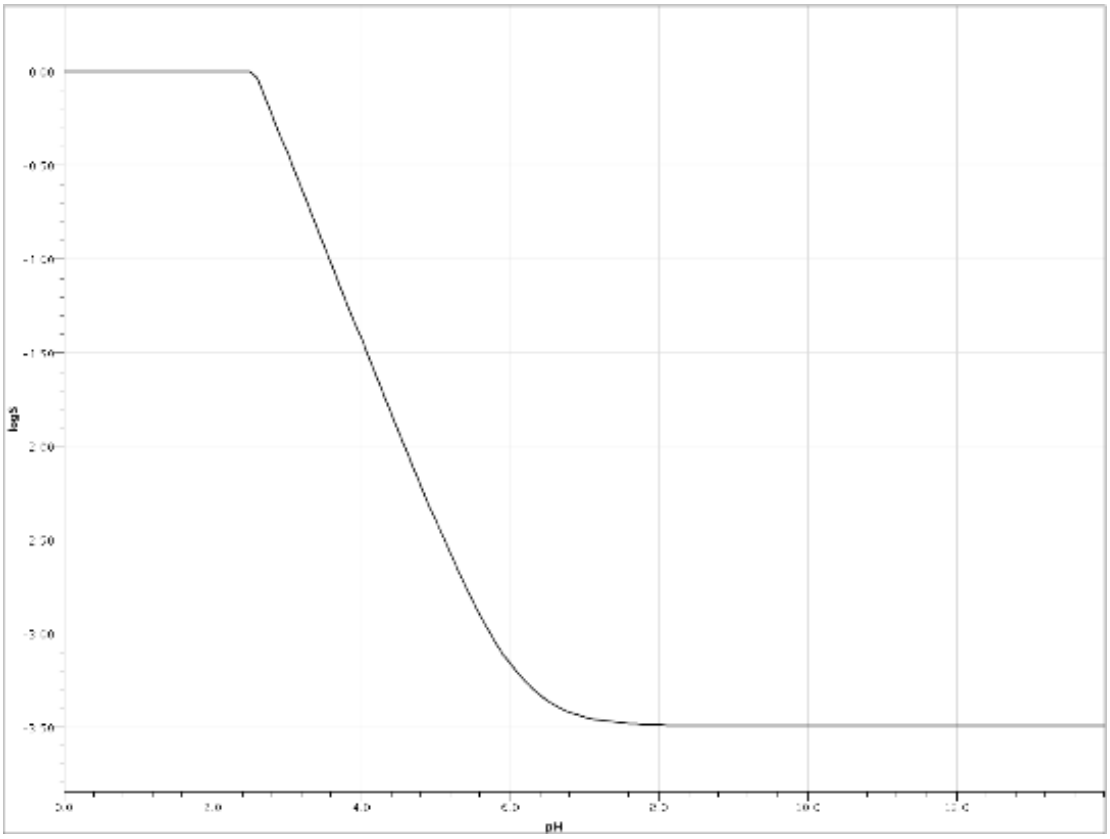
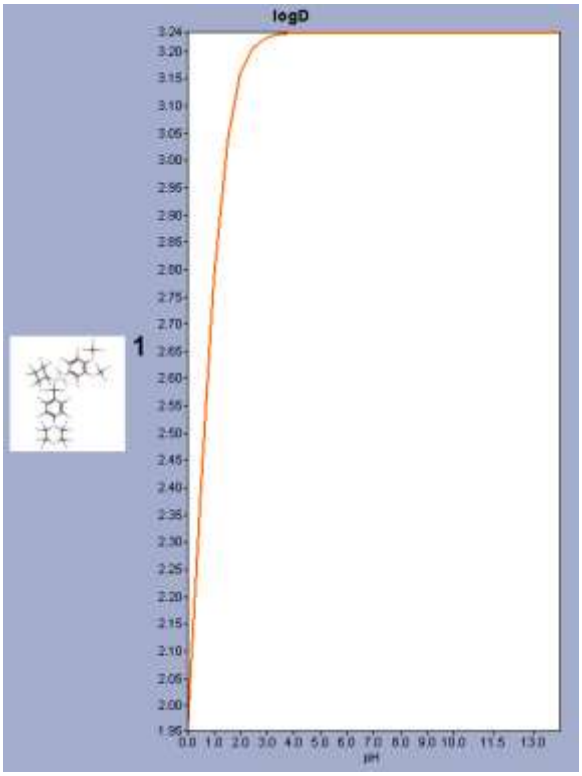
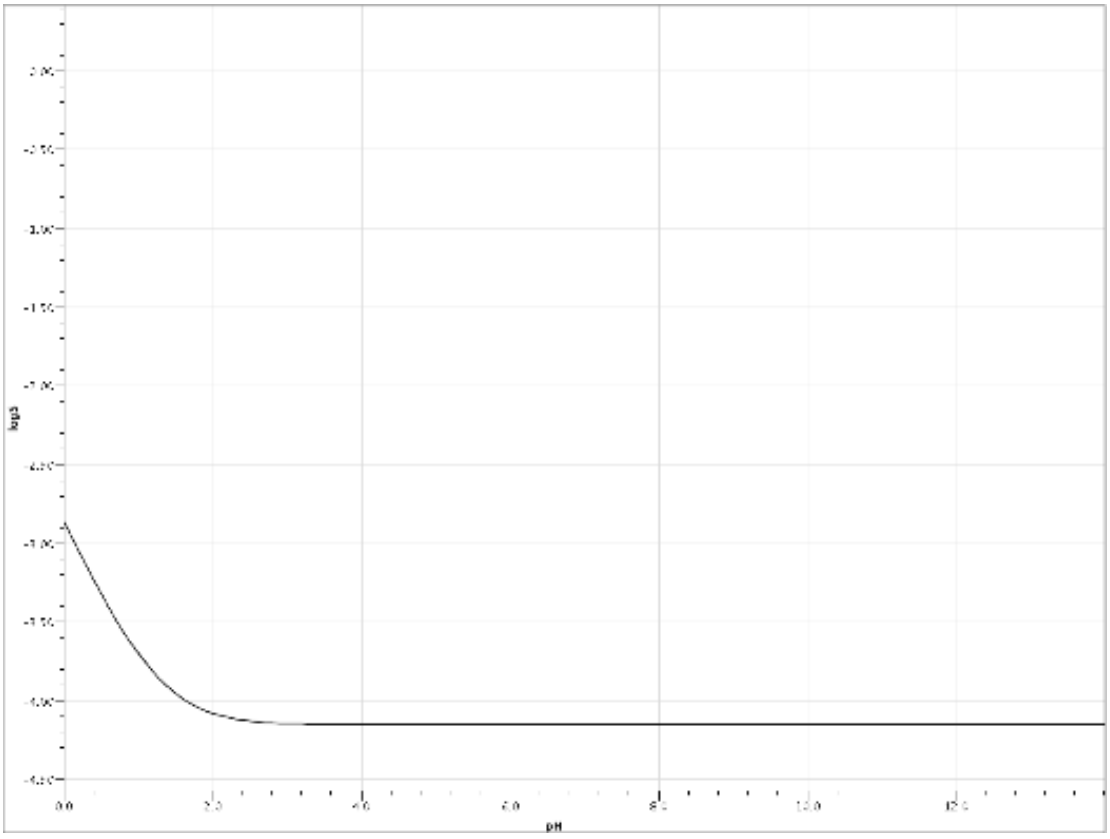


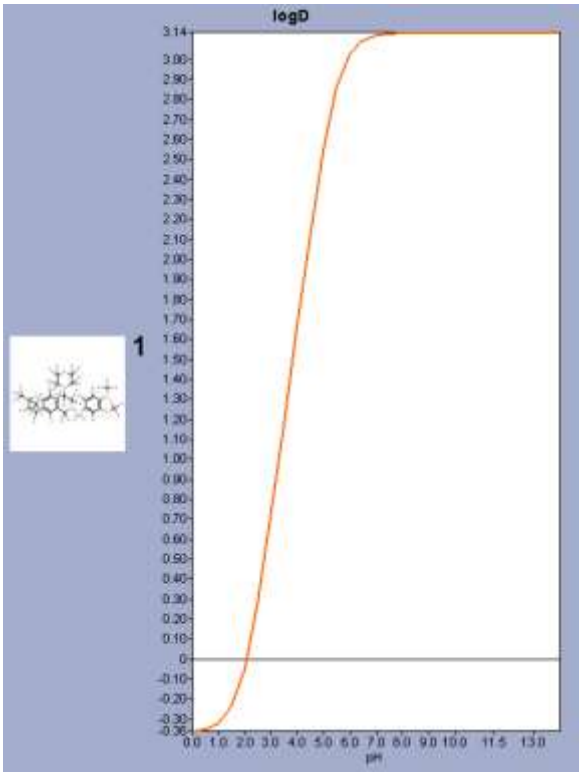


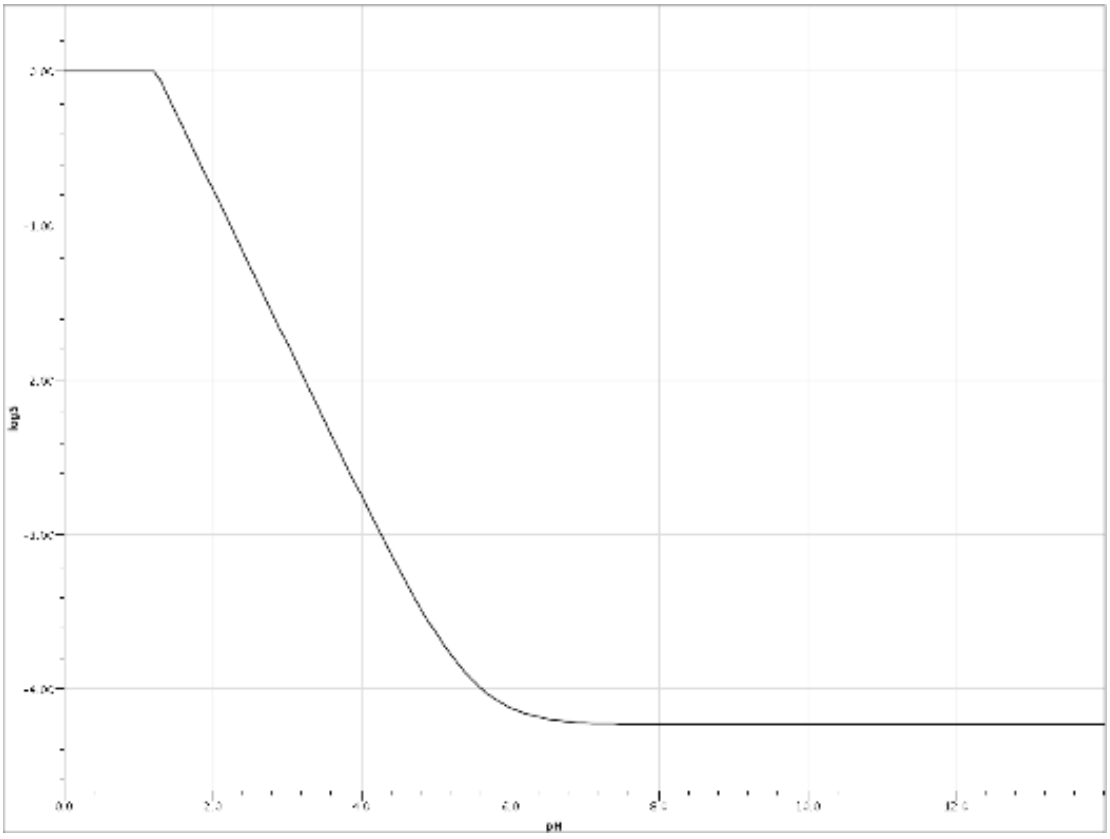
4d



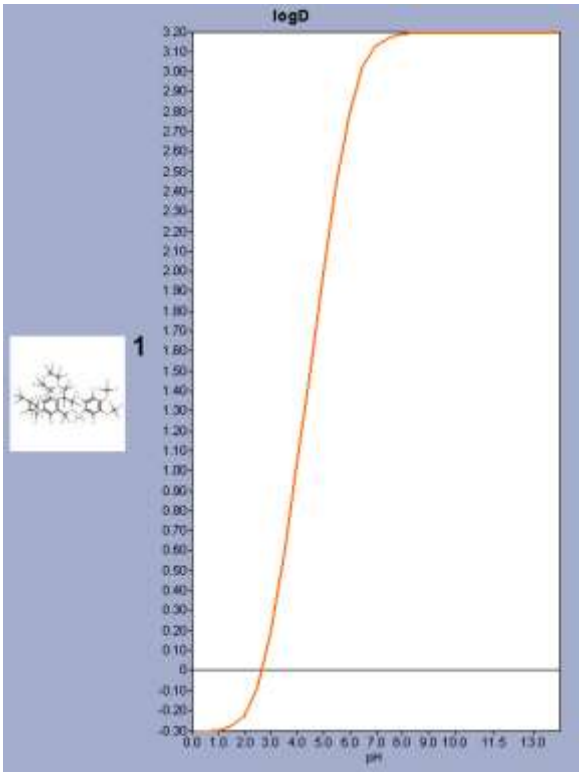


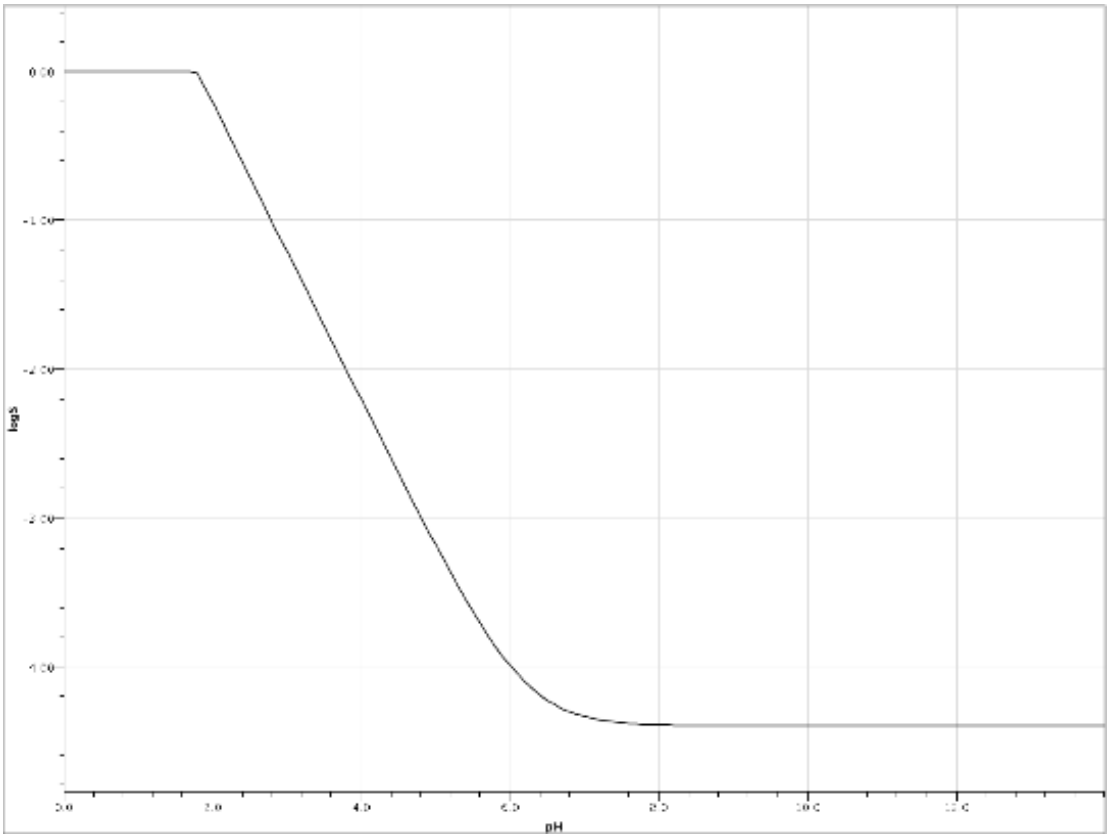
5a



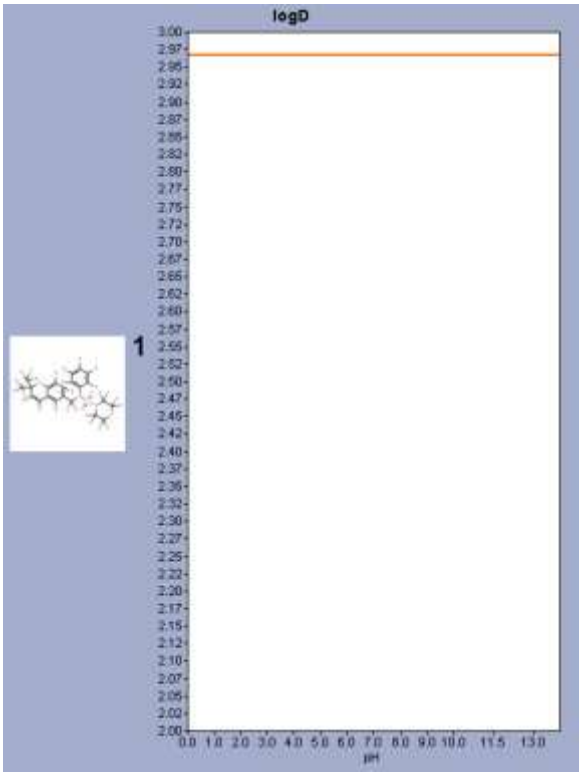


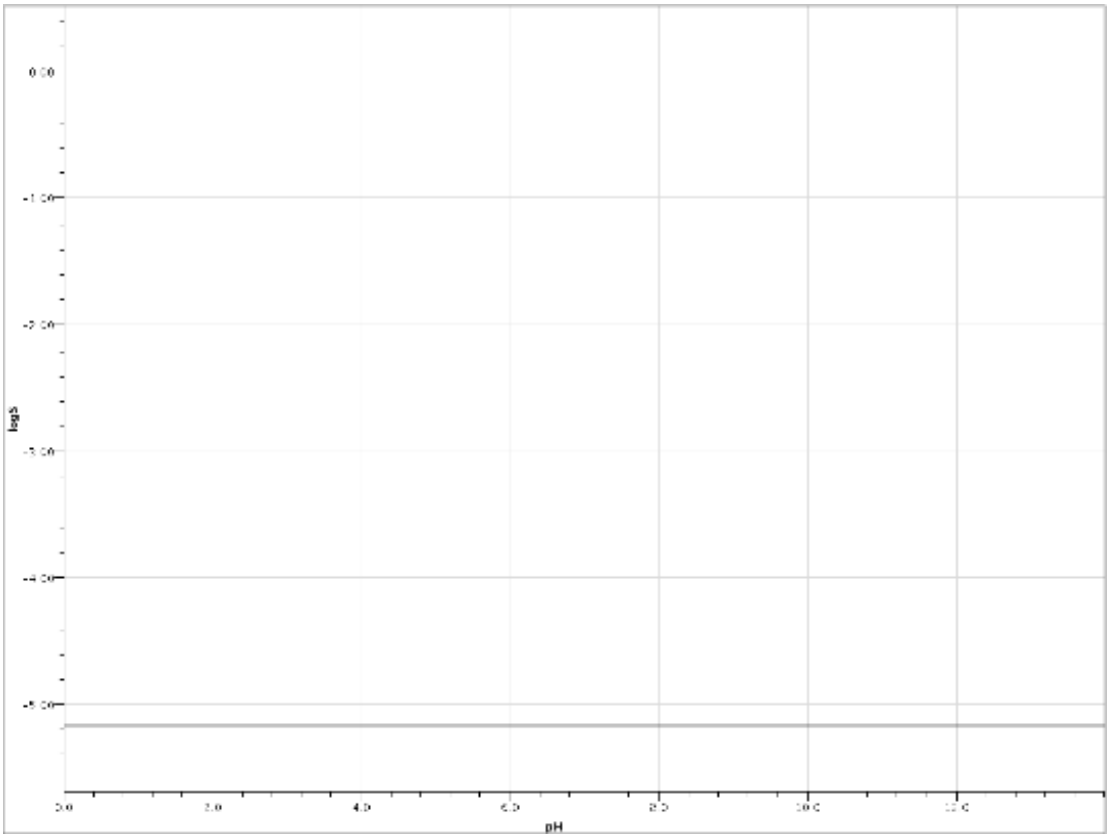
5b





6a





6b