

## Supplemental Material For

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

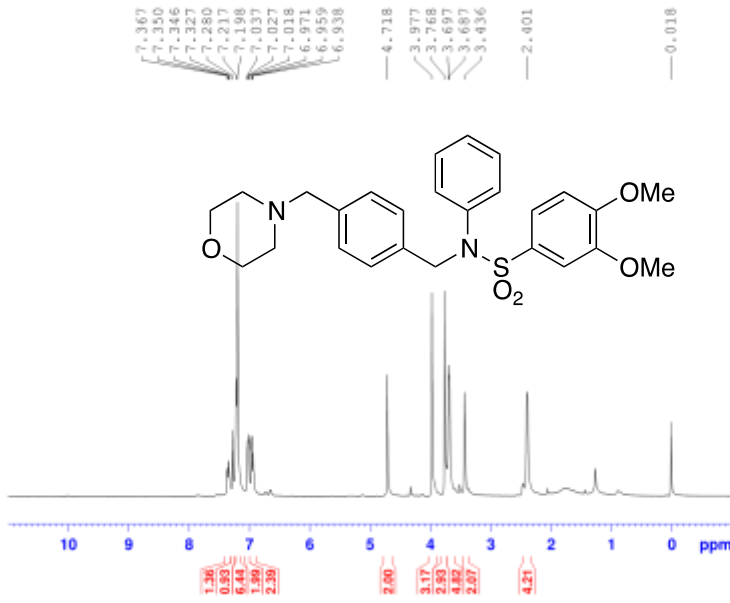
Jalisa H. Ferguson, Zeus De Los Santos, Saroja N. Devi, Stefan Kaluz, Erwin Van Meir, Sarah K. Zingales, Binghe Wang.

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

SB-IV-54d



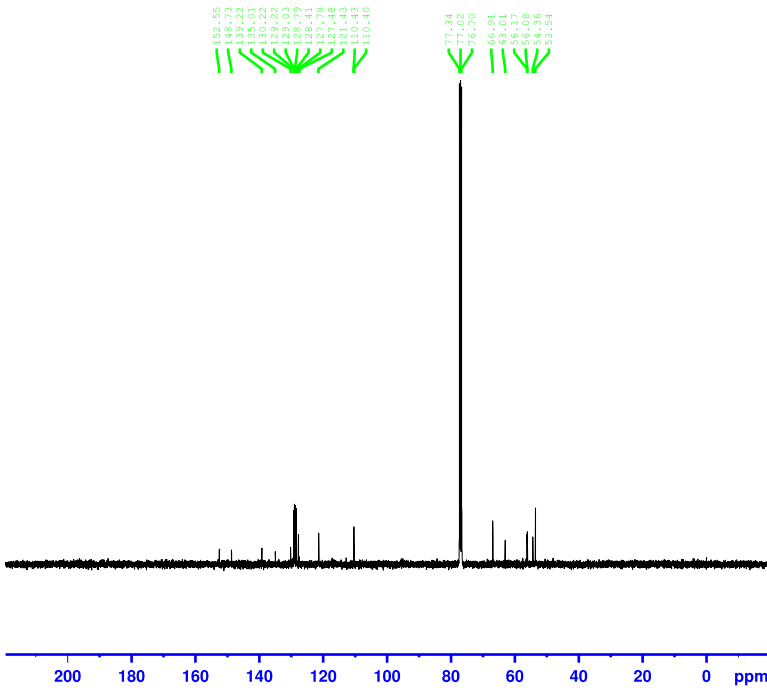
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 PULPROG zg30  
 TD 45536  
 SOLVENT CDCl3  
 NS 501  
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 SWH 823.685 Hz  
 FIDRES 0.125483 Hz  
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 RG 181  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 298.1 K  
 D1 1.0000000 sec

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SB-IV-54d



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 PROCNO 1

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 TD 65536  
 SOLVENT CDCl3  
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 FIDRES 0.366798 Hz  
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 DE 6.50 usec  
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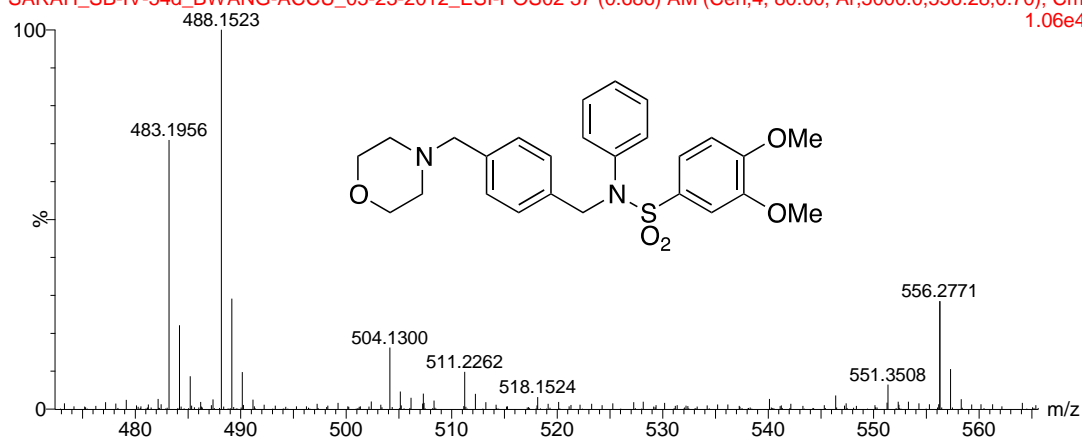
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100%MeOH

11:09:27 23-May-2012

SARAH\_SB-IV-54d\_BWANG-ACCU\_05-23-2012\_ESI-POS02 37 (0.686) AM (Cen,4, 80.00, Ar,5000.0,556.28,0.70); Cm  
1.06e4



### 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:

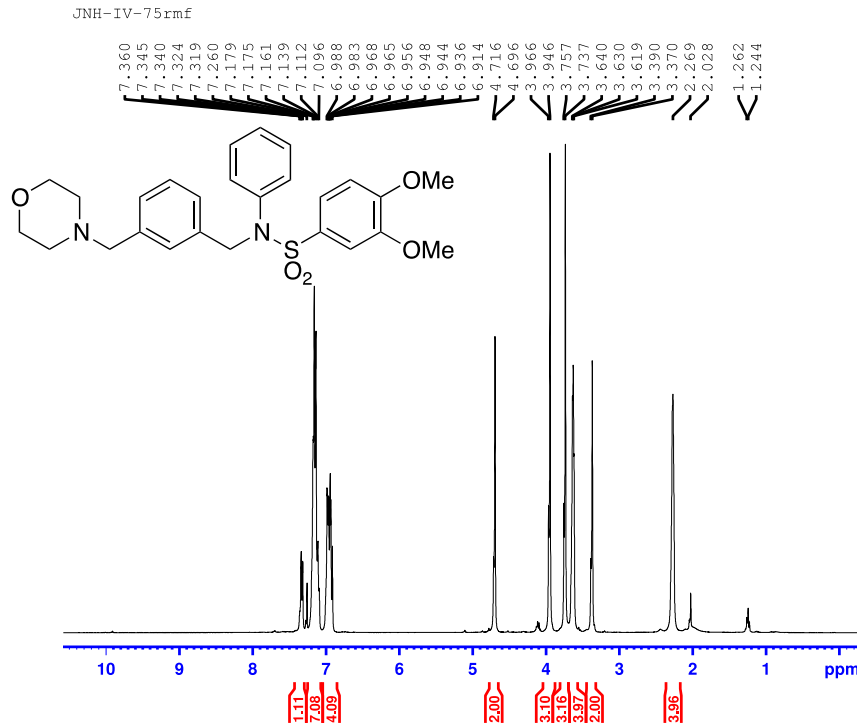
C: 1-200 H: 1-200 N: 1-15 O: 1-100 S: 0-50

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)

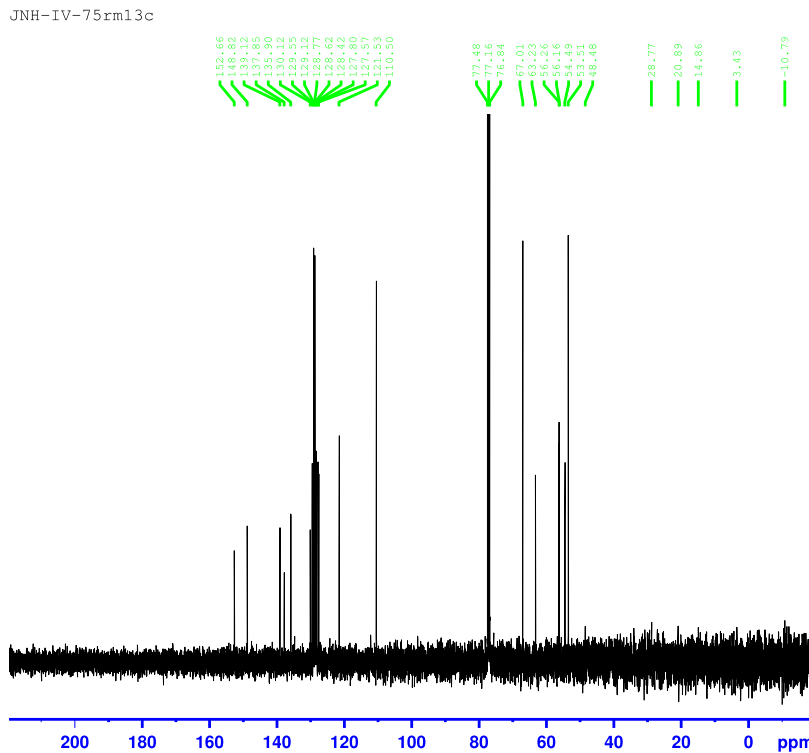


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 SOLVENT CDCl3  
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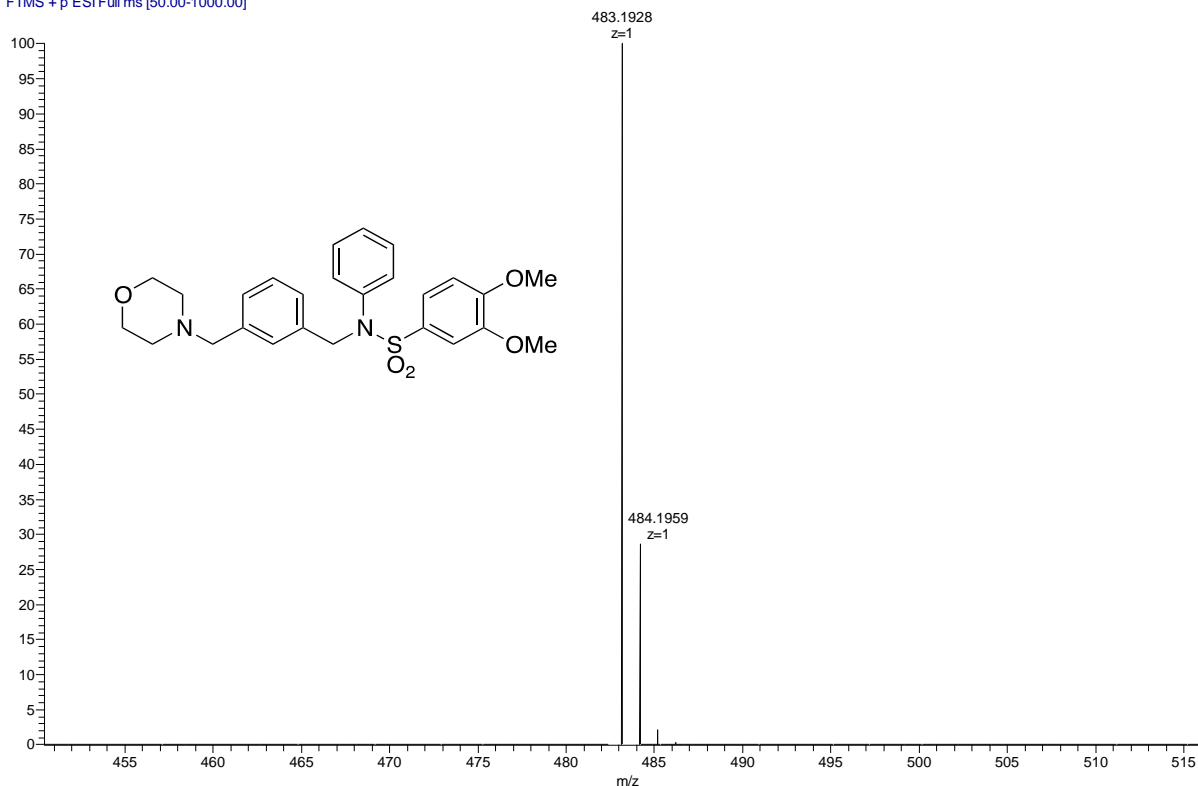
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 SOLVENT CDCl3  
 NS 106  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 203  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

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 PLW13 0.29376000 W

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JILISA\_IV\_75\_ESIPOS\_BWANG\_041317 #83 RT: 1.17 AV: 1 NL: 8.38E6  
 T: FTMS + p ESI Full ms [50.00-1000.00]



Thermo Xcalibur Qual Browser - JILISA\_IV\_75\_ESIPOS\_BWANG\_041317 - JILISA\_IV\_75\_ESIPOS\_BWANG\_041317.html

File Edit View Display Data Actions Tools Windows Help

Elemental composition search on mass 483.1928

m/z= 478.1922-488.1928

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
483.1928	483.1928	0.03	22.5	C <sub>23</sub> H <sub>25</sub> O <sub>3</sub> N <sub>2</sub> S
483.1923	483.1923	1.37	8.0	C <sub>23</sub> H <sub>23</sub> O <sub>3</sub> N <sub>2</sub> S
483.1923	483.1923	1.39	18.5	C <sub>22</sub> H <sub>27</sub> O <sub>3</sub> N <sub>2</sub> S
483.1935	483.1935	-1.40	13.0	C <sub>24</sub> H <sub>25</sub> O <sub>3</sub> N <sub>2</sub> S
483.1934	483.1934	2.00	17.5	C <sub>23</sub> H <sub>25</sub> O <sub>3</sub> N <sub>2</sub> S
483.1934	483.1934	2.01	23.0	C <sub>23</sub> H <sub>21</sub> N <sub>2</sub> S
483.1946	483.1946	-4.17	18.0	C <sub>24</sub> H <sub>23</sub> N <sub>2</sub> S
483.1946	483.1946	-4.18	12.5	C <sub>24</sub> H <sub>21</sub> O <sub>3</sub> N <sub>2</sub> S

General composition  
 Single mass  
 Mass: 483.1928

Rank	Formula	Mass	Delta (ppm)
1	C <sub>23</sub> H <sub>25</sub> O <sub>3</sub> N <sub>2</sub> S	483.1928	0.03
2	C <sub>23</sub> H <sub>23</sub> O <sub>3</sub> N <sub>2</sub> S	483.1923	1.37
3	C <sub>23</sub> H <sub>25</sub> O <sub>3</sub> N <sub>2</sub> S	483.1934	2.00
4	C <sub>23</sub> H <sub>25</sub> O <sub>3</sub> N <sub>2</sub> S	483.1934	2.01
5	C <sub>23</sub> H <sub>21</sub> N <sub>2</sub> S	483.1934	2.01
6	C <sub>24</sub> H <sub>23</sub> N <sub>2</sub> S	483.1946	-4.17
7	C <sub>24</sub> H <sub>21</sub> O <sub>3</sub> N <sub>2</sub> S	483.1946	-4.18

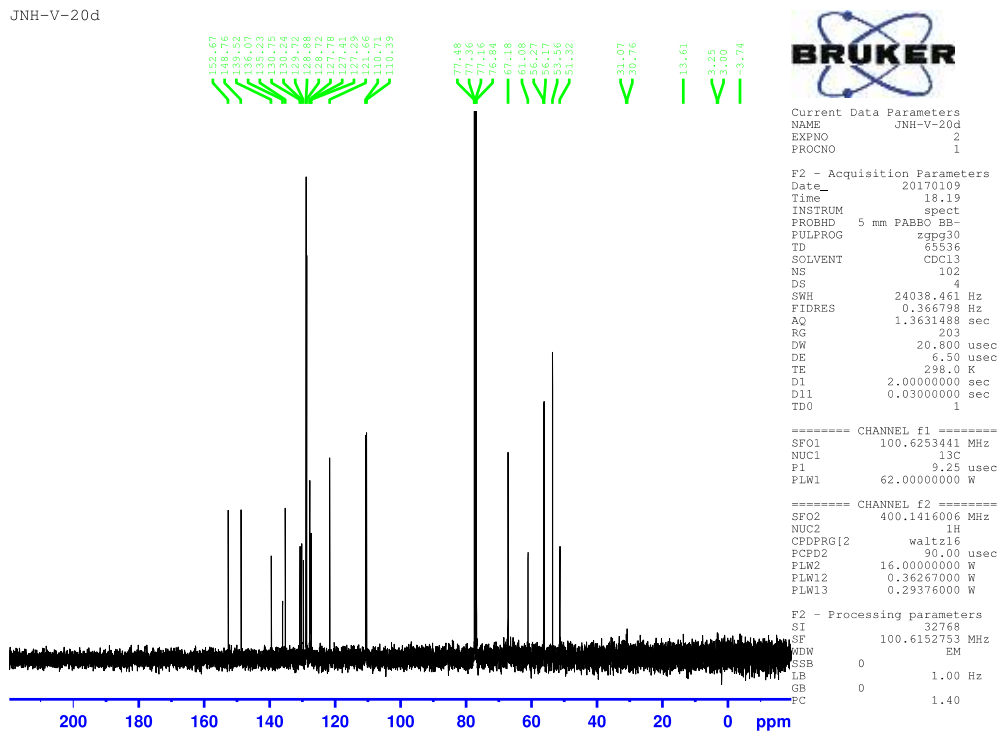
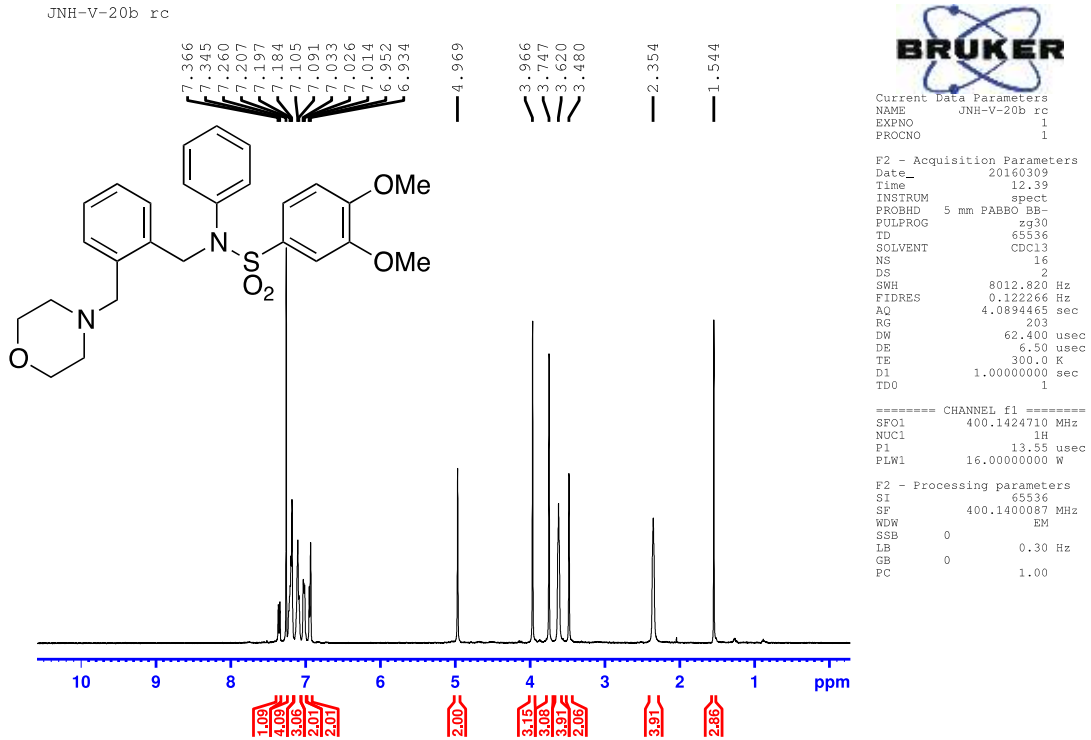
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Search results:

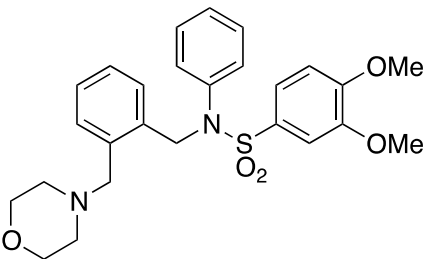
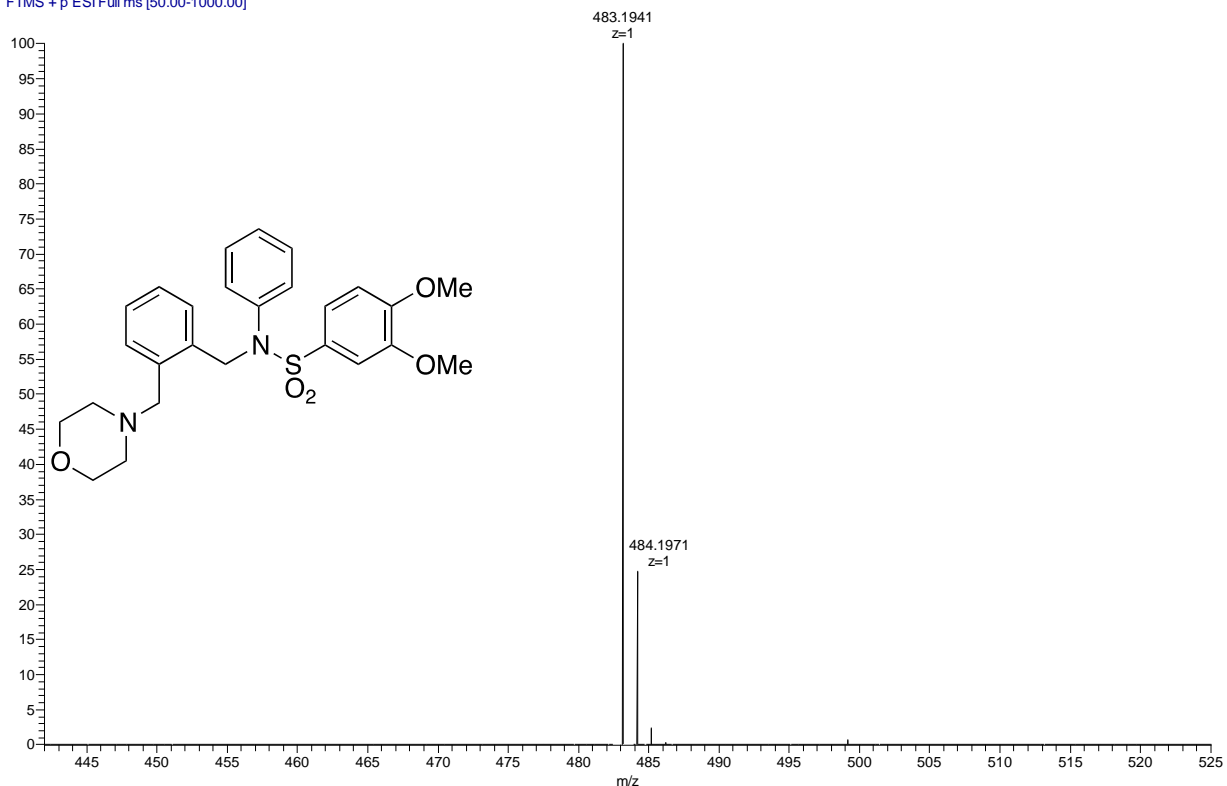
Element	Min	Max	DB	Mass
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H	1.008	1.008	1	1.008
N	14.007	14.007	1	14.007
O	16.003	16.003	1	16.003
S	32.065	32.065	1	32.065

ThermoFisher 3000 AM 4431067

### 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]



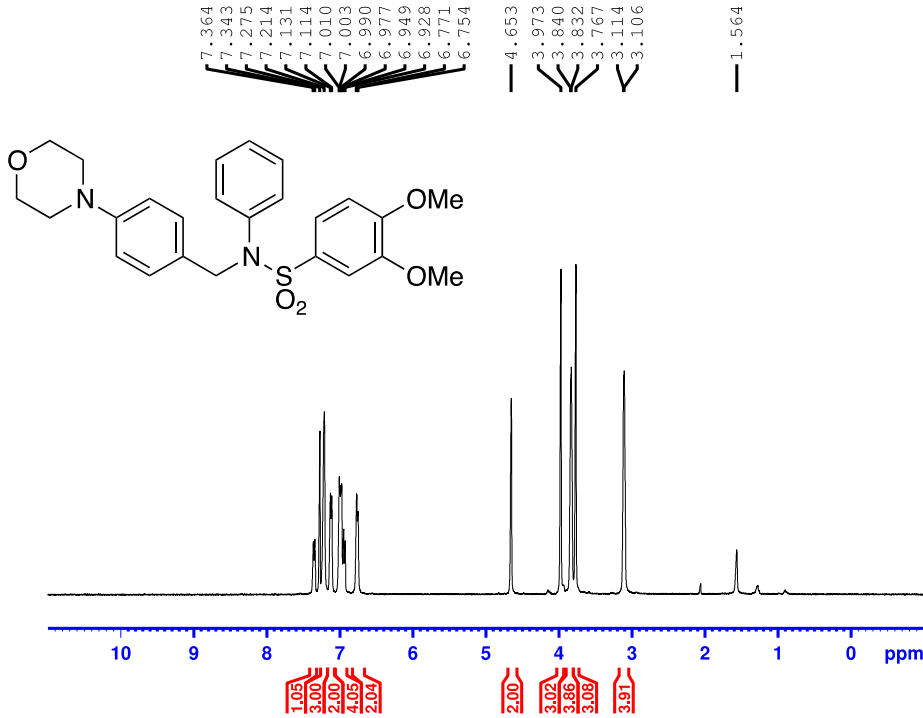
Elemental composition search on mass 483.1941

m/z	Theo. Mass	Delta (ppm)	RDB eq. IV.	Composition
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	483.1948	-1.48	16.0	C <sub>25</sub> H <sub>31</sub> O <sub>4</sub> N <sub>2</sub> S
	483.1958	-1.89	12.5	C <sub>24</sub> H <sub>27</sub> O <sub>4</sub> N <sub>2</sub> S
	483.1928	2.72	32.5	C <sub>30</sub> H <sub>35</sub> O <sub>4</sub> N <sub>2</sub> S
	483.1921	4.06	6.0	C <sub>23</sub> H <sub>29</sub> O <sub>4</sub> N <sub>2</sub> S
	483.1921	4.07	13.5	C <sub>23</sub> H <sub>27</sub> O <sub>4</sub> N <sub>2</sub> S
	483.1962	-4.26	17.5	C <sub>27</sub> H <sub>31</sub> O <sub>4</sub> N <sub>2</sub> S

Additional software interface elements include a table of isotopes in use and various control buttons.

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

SB-V-88r1



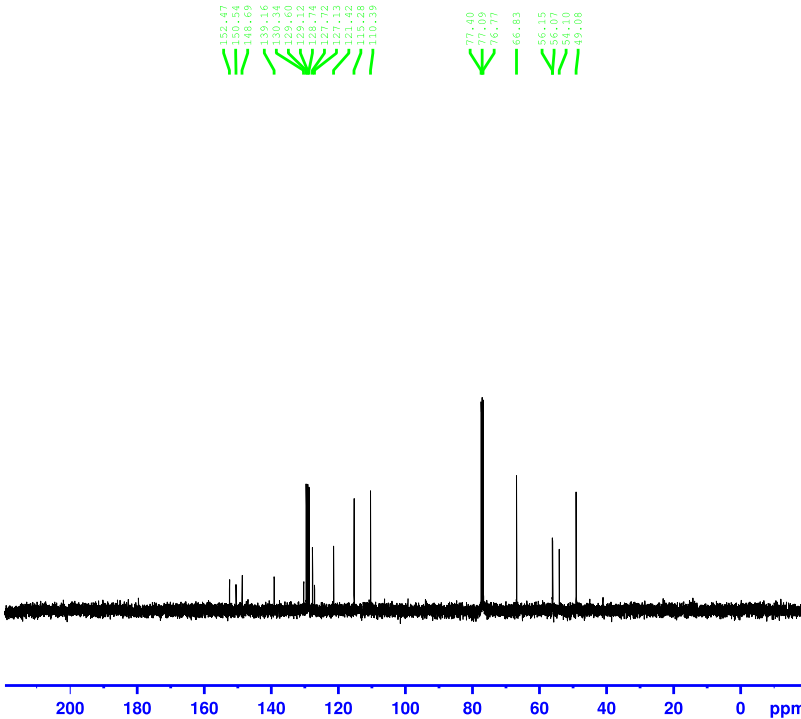
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 SOLVENT CDCl3  
 NS 12  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 203  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 1.0000000 sec  
 TD0 1

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 NUC1 1H  
 P1 13.50 usec  
 PLW1 16.0000000 W

F2 - Processing parameters  
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 WDW EM  
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 GB 0  
 PC 1.00

SB-V-88c



Current Data Parameters  
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 PROCNO 1

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 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 30  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 203  
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 DE 6.50 usec  
 TE 298.2 K  
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 TD0 1

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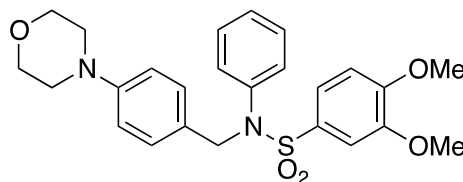
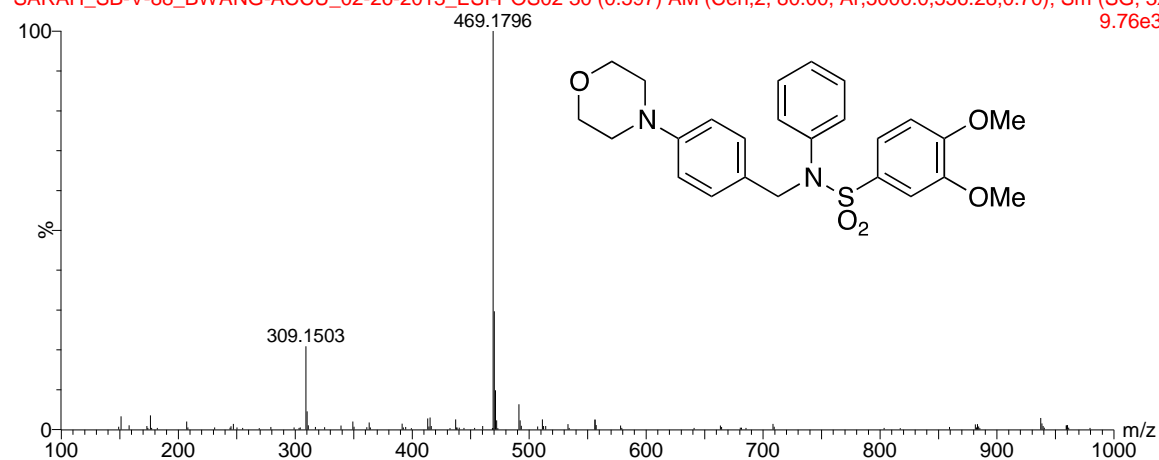
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MeOH

15:07:31 26-Feb-2013

SARAH\_SB-V-88\_BWANG-ACCU\_02-26-2013\_ESI-POS02 30 (0.597) AM (Cen,2, 80.00, Ar,5000.0,556.28,0.70); Sm (SG, 3x 9.76e3



### 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

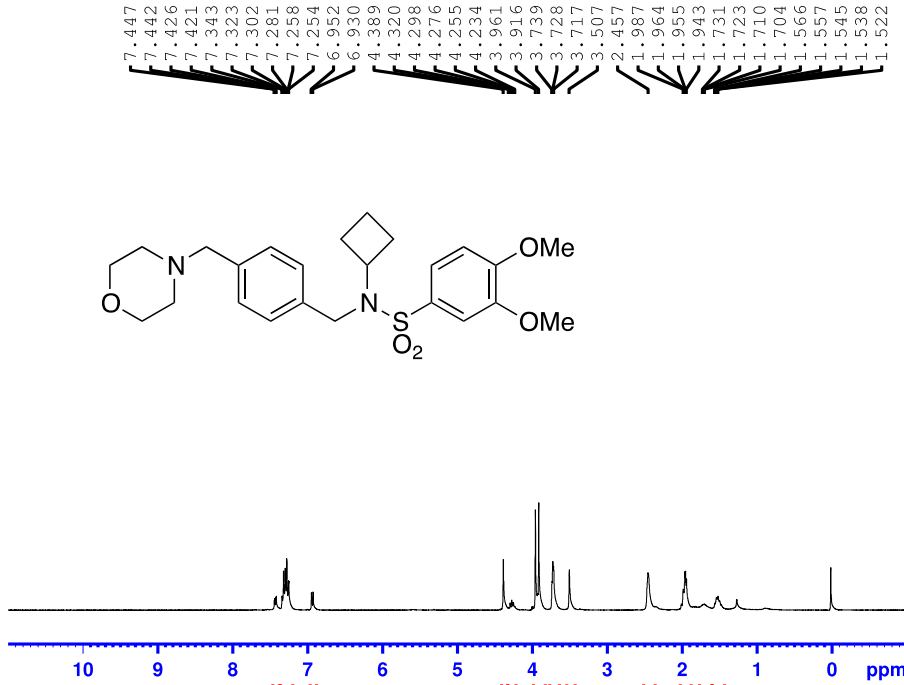
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Maximum: 5.0 5.0 50.0

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



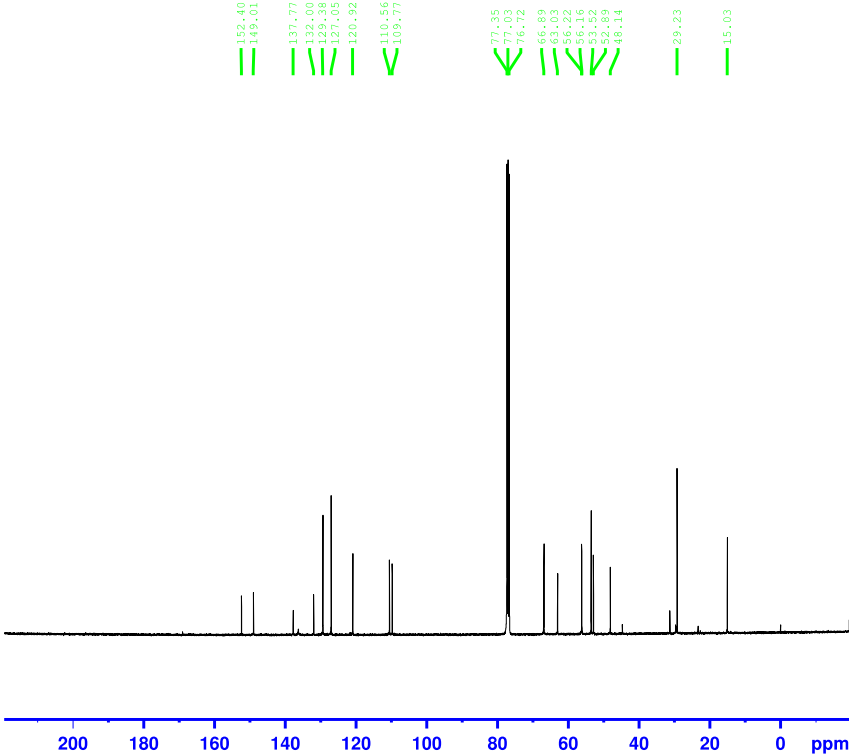
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 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 203  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 298.1 K  
 D1 1.00000000 sec

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 PC 1.00

SB-IV-44c



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 NS 10240  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 203  
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 DE 6.50 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
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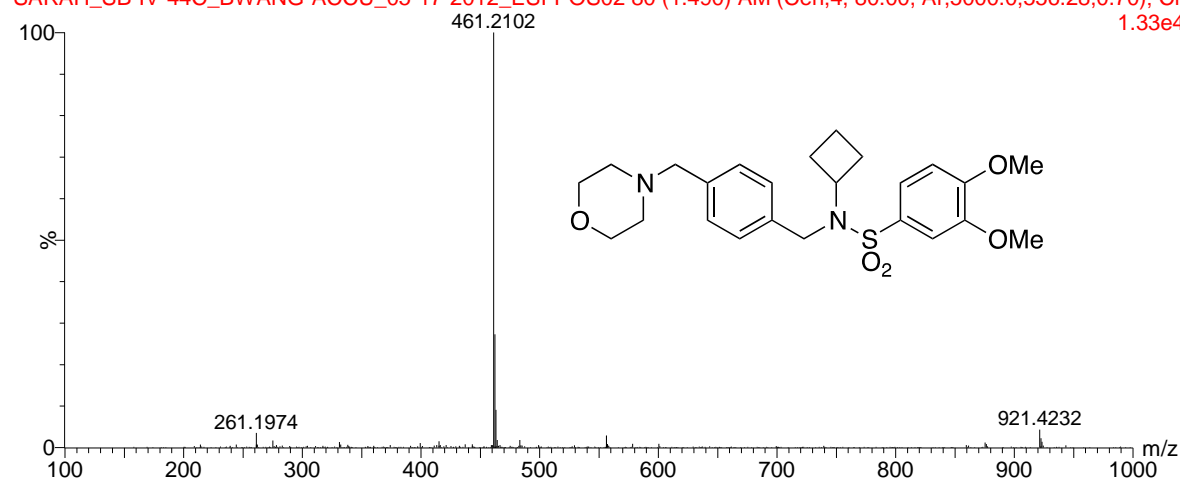
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 PLW13 0.29159999 W  
 SFO2 400.1416006 MHz

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

100%MeOH+0.1%HCOOH

12:30:52 17-May-2012

SARAH\_SB-IV-44C\_BWANG-ACCU\_05-17-2012\_ESI-POS02 80 (1.490) AM (Gen,4, 80.00, Ar,5000.0,556.28,0.70); Cr  
1.33e4



### 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

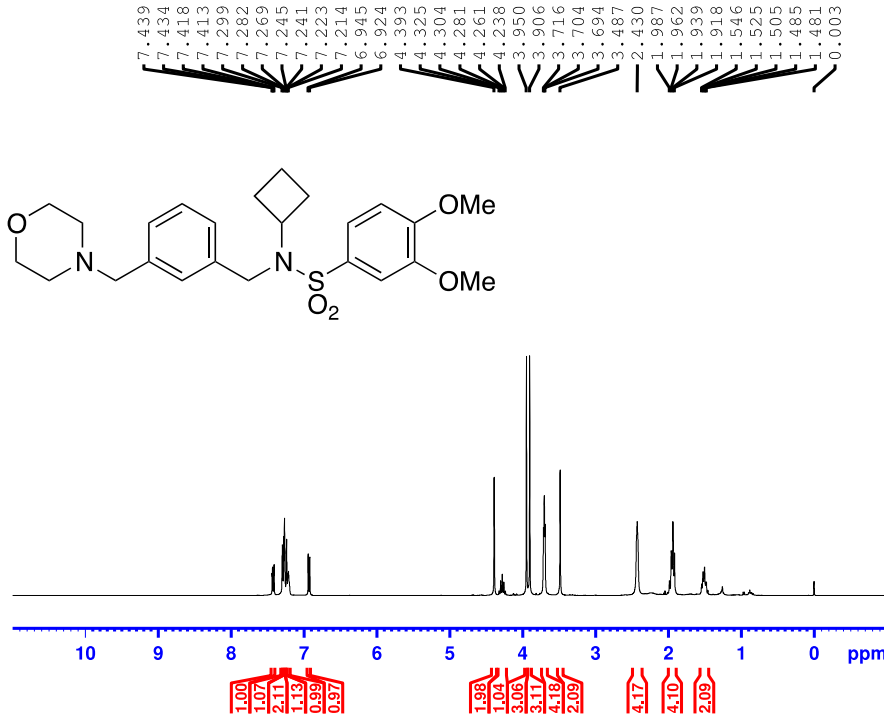
Minimum: -1.5

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



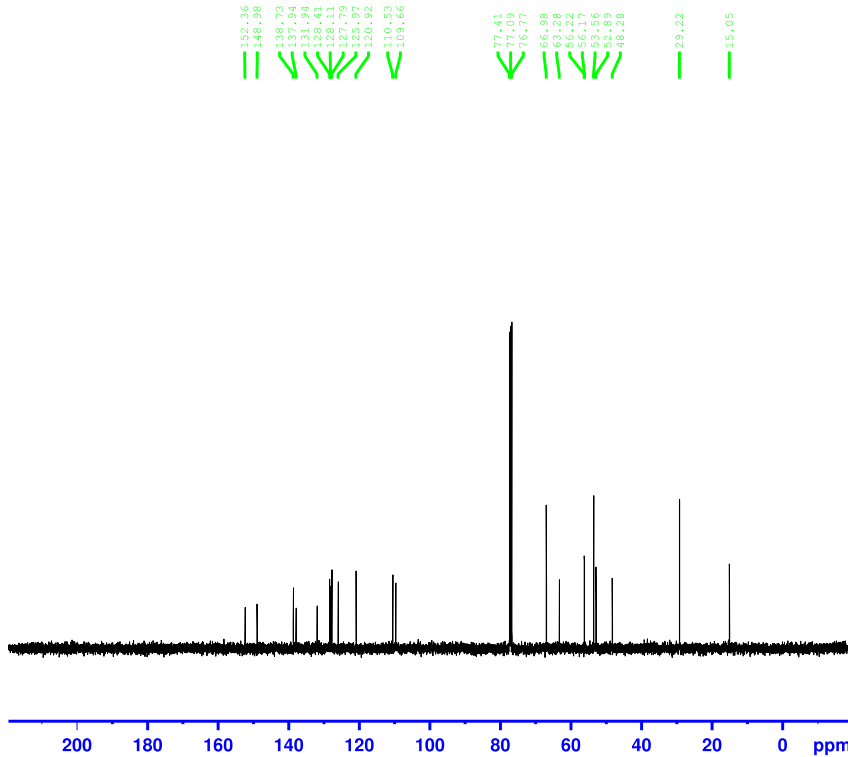
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 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 57  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 293.7 K  
 D1 1.00000000 sec  
 TD0 1

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

F2 - Processing parameters  
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 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

SB-V-92f



Current Data Parameters  
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 PROCNO 1

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 PULPROG zgpg30  
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 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  
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 PLW1 62.00000000 W

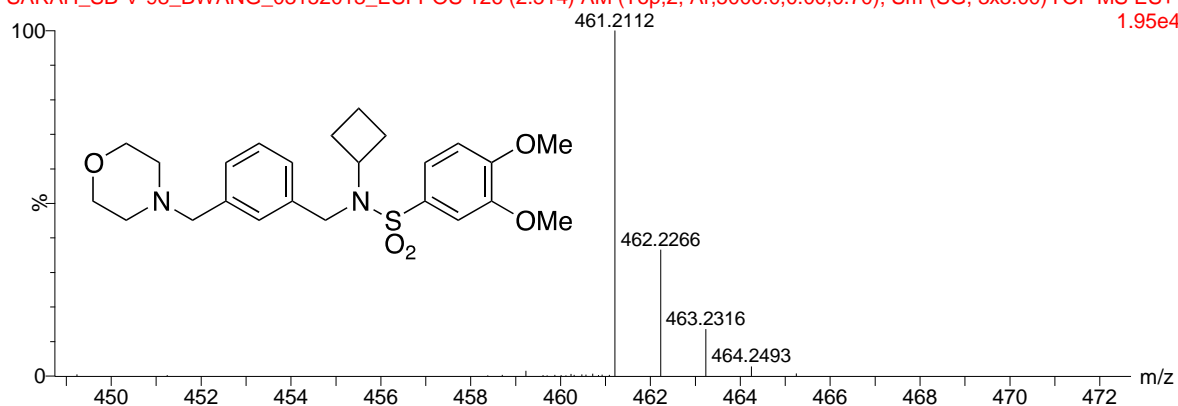
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 PCPD2 90.00 usec  
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 PLW12 0.36000001 W  
 PLW13 0.29159999 W

F2 - Processing parameters  
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 LB 1.00 Hz  
 GB 0  
 PC 1.40

80%MeOH

13:51:56 15-Mar-2013

SARAH\_SB-V-98\_BWANG\_03152013\_ESI-POS 126 (2.514) AM (Top,2, Ar,5000.0,0.00,0.70); Sm (SG, 3x3.00)TOF MS ES+ 1.95e4



### 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

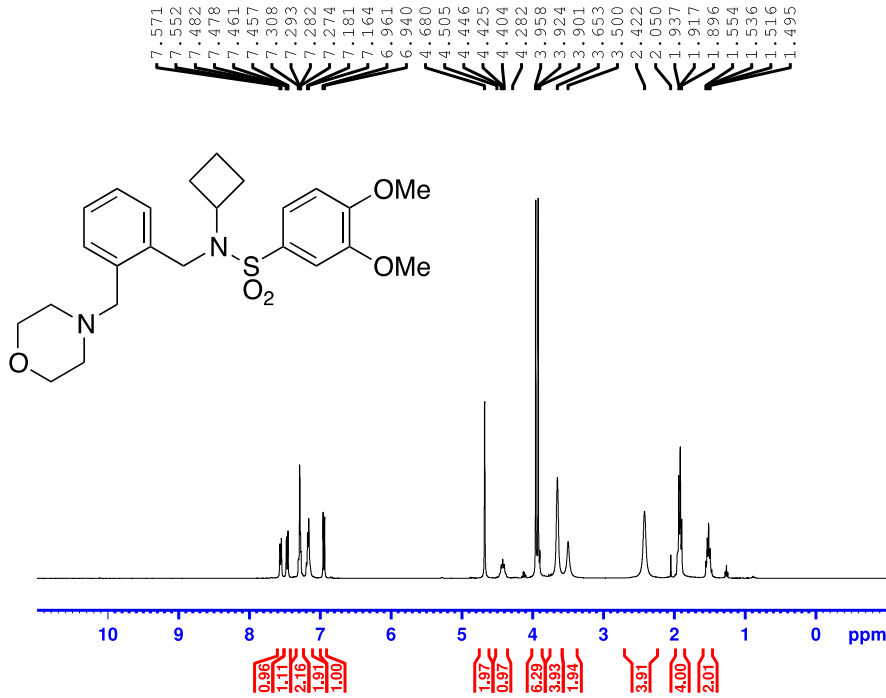
Minimum: -1.5

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	C <sub>24</sub> H <sub>33</sub> N <sub>2</sub> O <sub>5</sub> S

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

SB-V-91cR



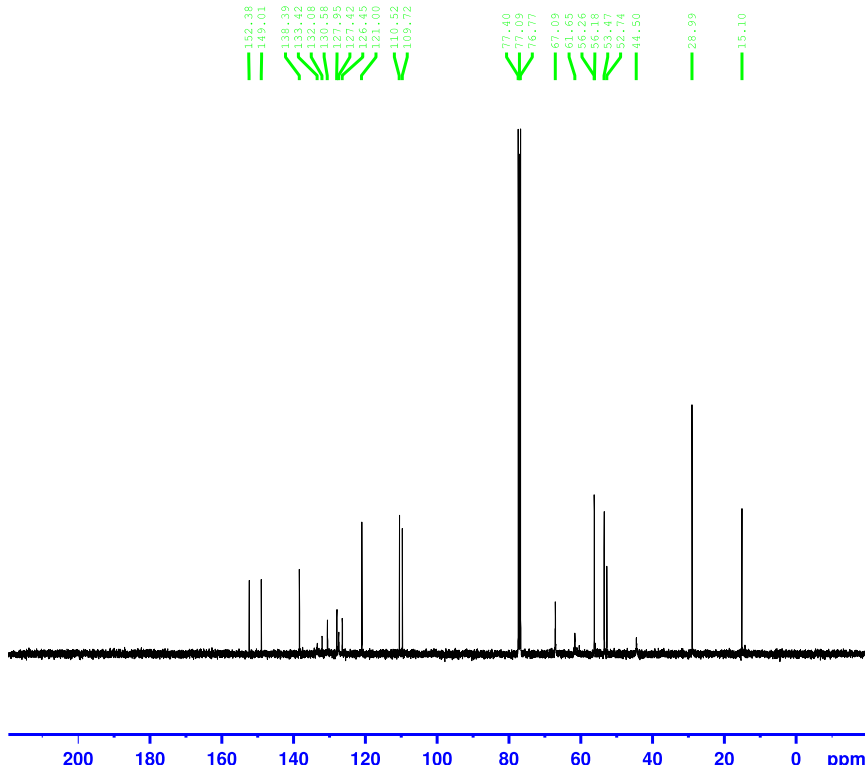
Current Data Parameters  
 NAME SB-V-91cR  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20130311  
 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

SB-V-91cR



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

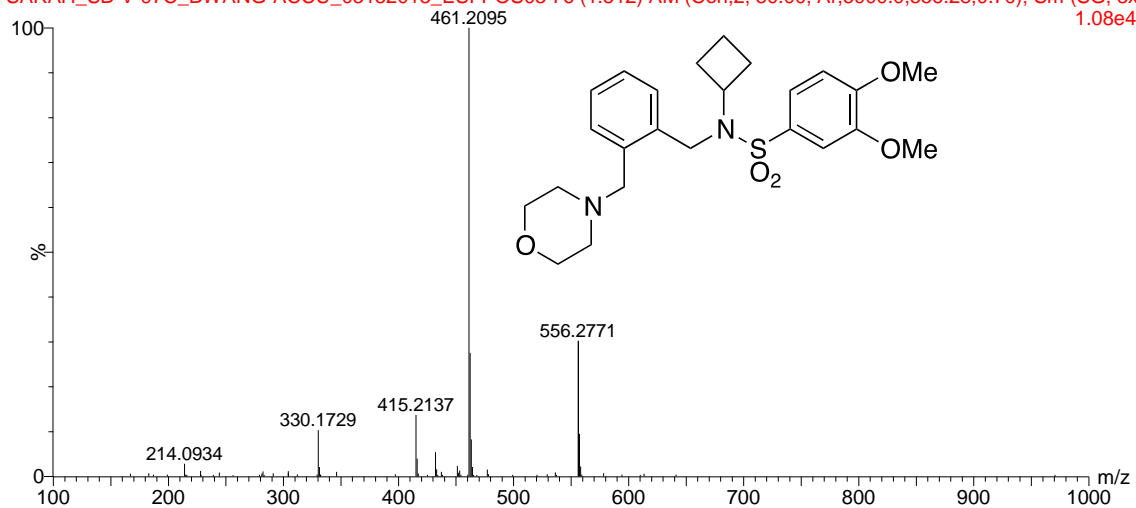
===== CHANNEL f2 =====  
 SFO2 400.1416006 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 16.00000000 W  
 PLW12 0.36000001 W  
 PLW13 0.29159999 W

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

diluted in 50%ACN

16:22:35 25-Mar-2013

SARAH\_SB-V-97C\_BWANG-ACCU\_03152013\_ESI-POS03 76 (1.512) AM (Cen,2, 80.00, Ar,5000.0,556.28,0.70); Sm (SG, 3x  
1.08e4



### 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

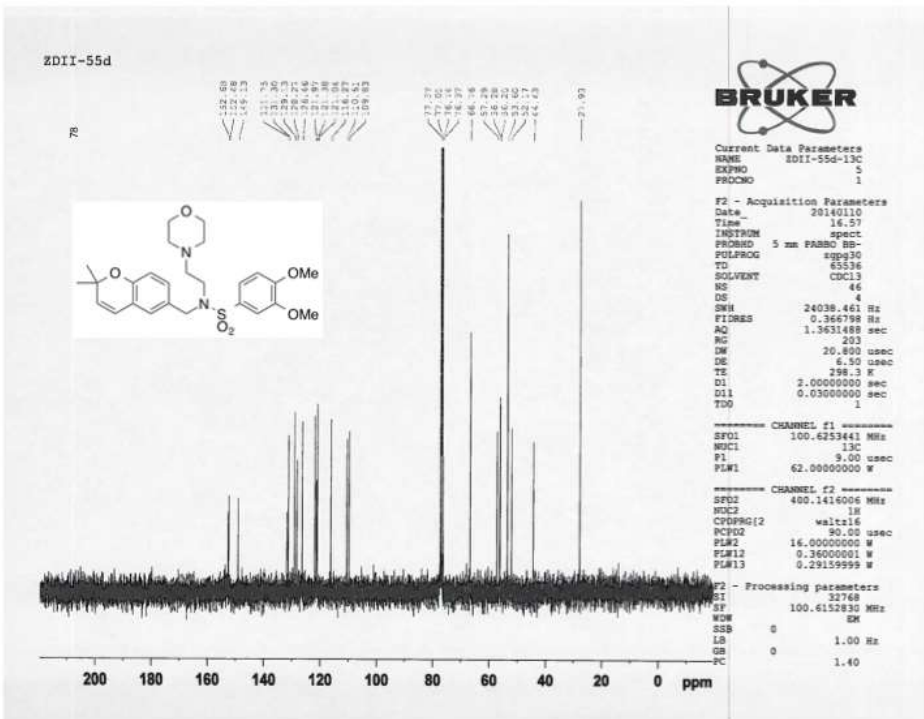
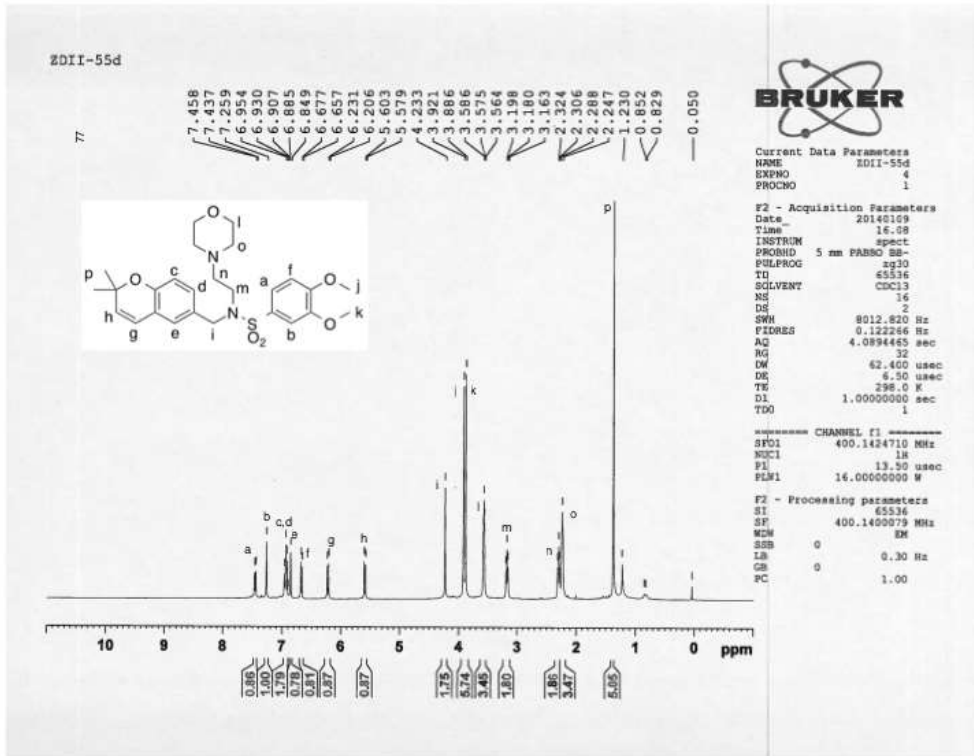
Maximum: 5.0 5.0 50.0

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

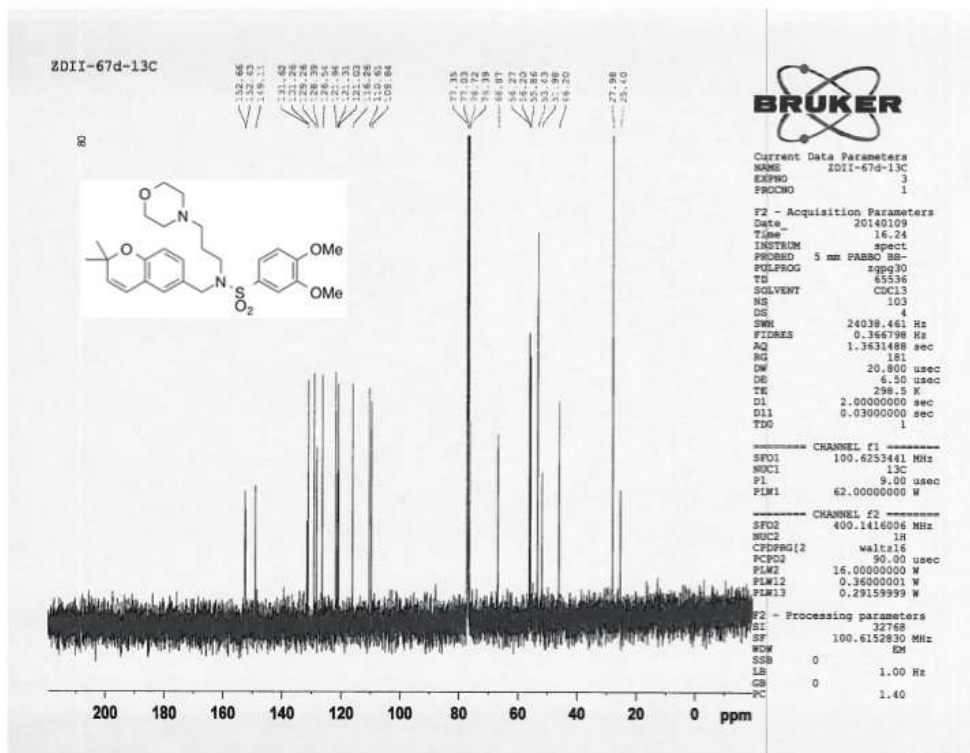
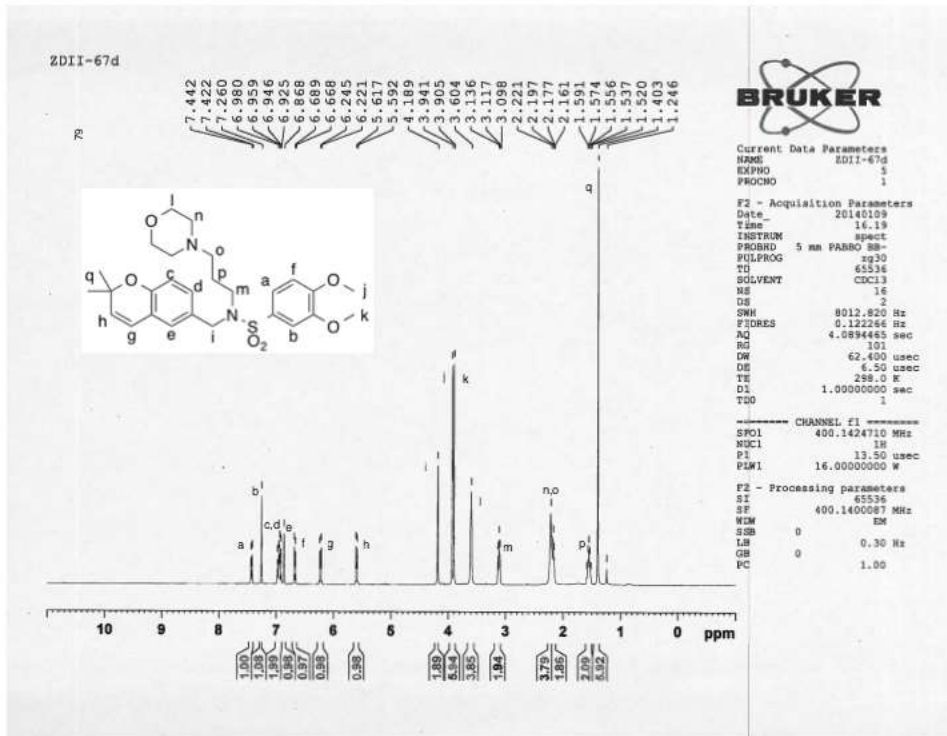




**N-((2,2-Dimethyl-2H-chromen-6-yl)methyl)-3,4-dimethoxy-N-(2-morpholinoethyl)benzenesulfonamide (5a)**

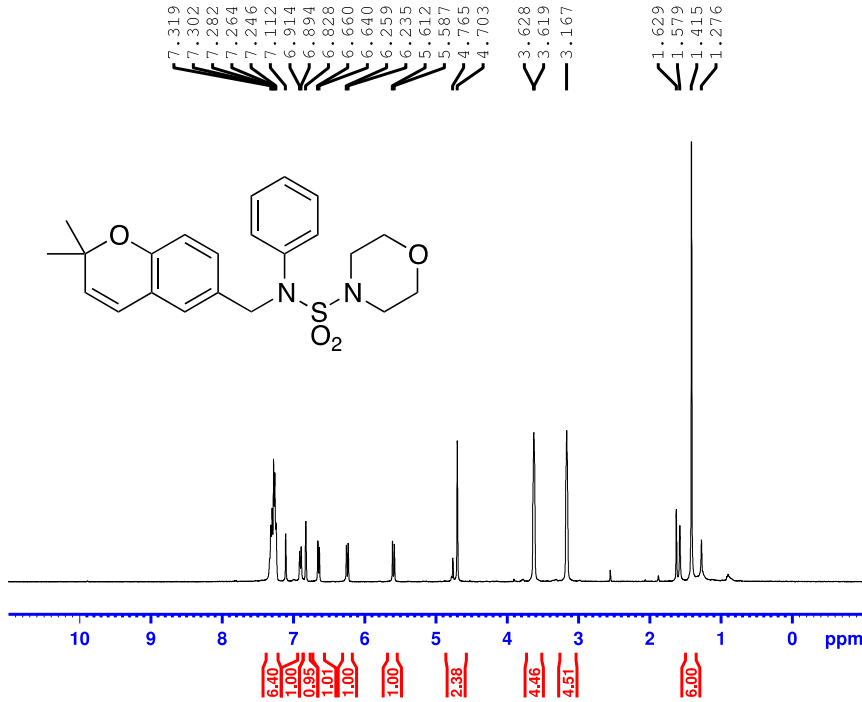


**N-((2,2-Dimethyl-2H-chromen-6-yl)methyl)-3,4-dimethoxy-N-(3-morpholinopropyl)benzenesulfonamide (5b)**



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

SB-V-82d



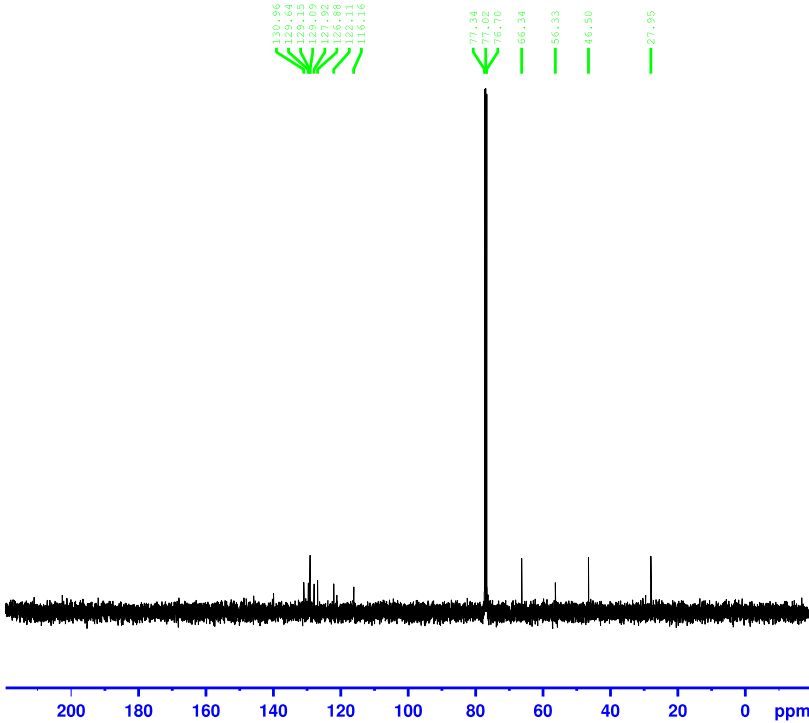
Current Data Parameters  
 NAME SB-V-82d  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20130220  
 Time\_ 13.36  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 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

SB-V-82d



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 CDCl3  
 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

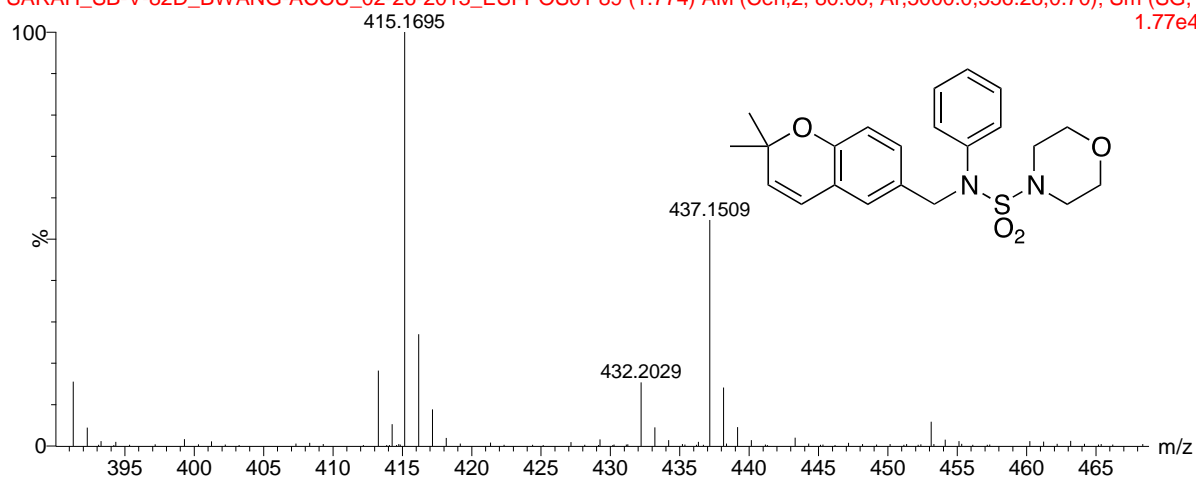
----- CHANNEL f2 -----  
 SFO2 400.1416006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 16.00000000 W  
 PLW12 0.36000001 W  
 PLW13 0.29159999 W

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

MeOH

14:59:03 26-Feb-2013

SARAH\_SB-V-82D\_BWANG-ACCU\_02-26-2013\_ESI-POS01 89 (1.774) AM (Cen,2, 80.00, Ar,5000.0,556.28,0.70); Sm (SG, 1.77e4



### 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:

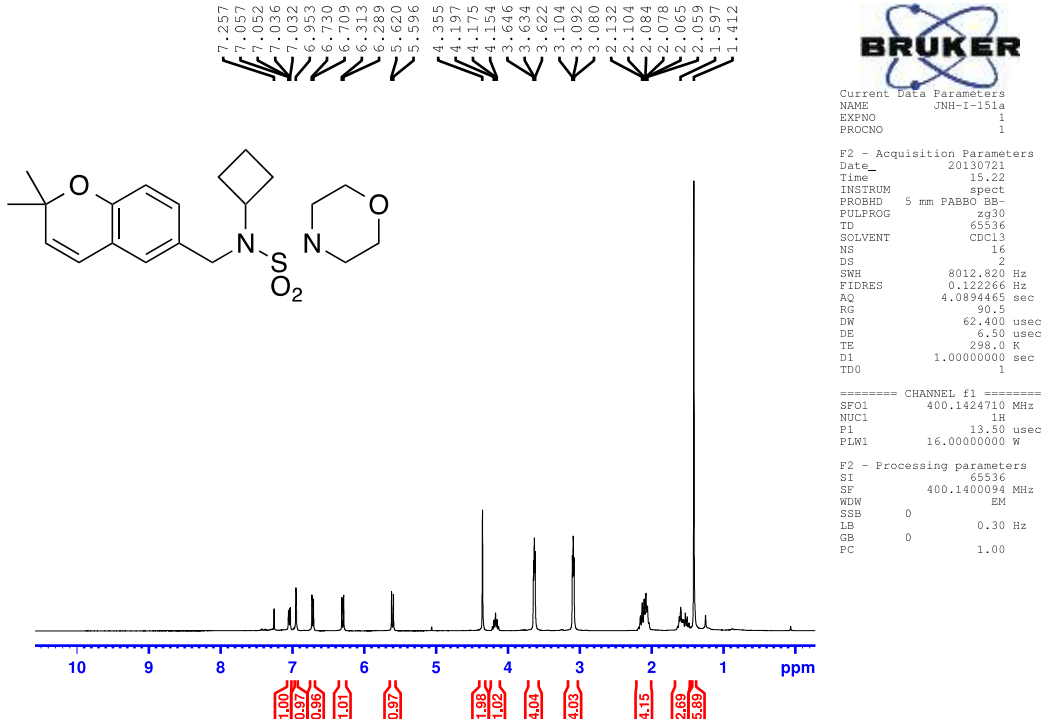
C: 1-150 H: 1-150 N: 1-6 O: 1-30 S: 1-10

Minimum: -1.5

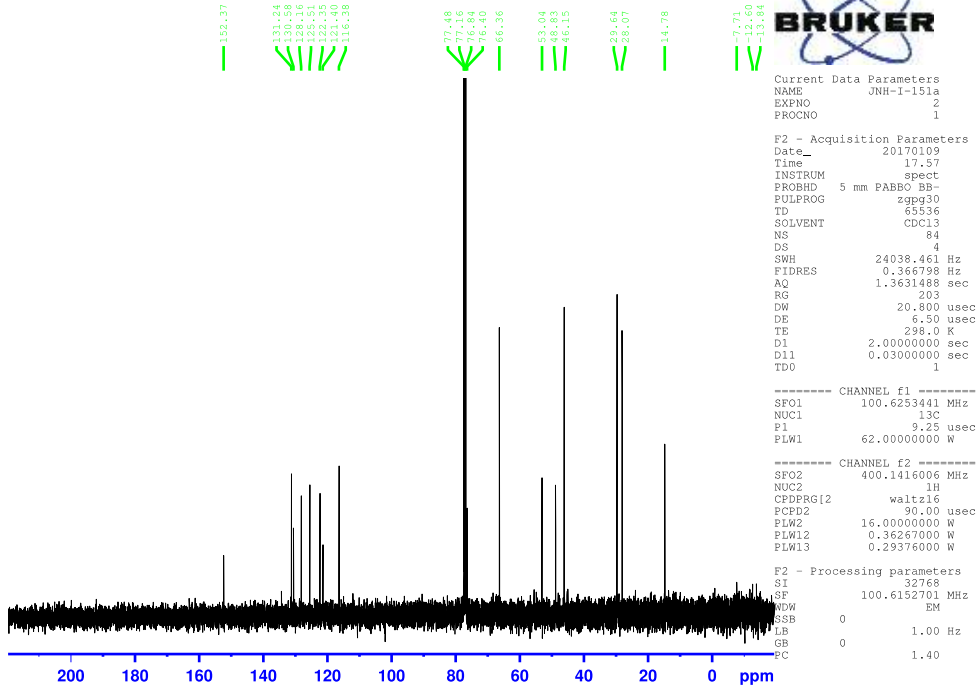
Maximum: 5.0 5.0 50.0

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

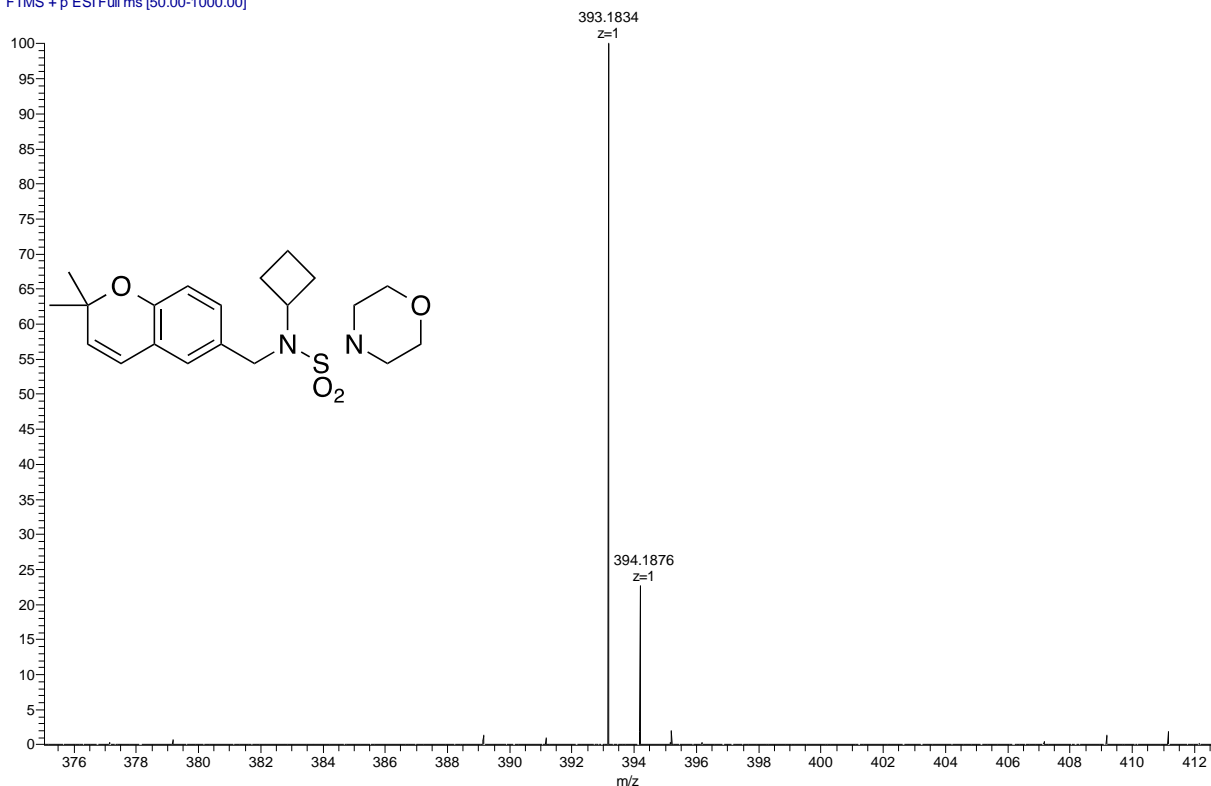
**N-Cyclobutyl-N-((2,2-dimethyl-2H-chromen-6-yl)methyl)morpholine-4-sulfonamide (6b)**



JNH-I-151a 13C



JLISA\_1\_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]



Thermo Xcalibur Qual Browser - JLISA\_1\_151a\_ESIPOS\_BWANG\_041317 #107-119

File Edit View Display Run Actions Tools Windows Help

Elemental composition search on mass 393.1834

m/z= 393.1834-393.1834

m/z	Theor. Mass	Delta (ppm)	RDB equiv.	Composition
393.1834	393.1836	-0.42	17.0	C <sub>26</sub> H <sub>29</sub> O <sub>3</sub> N <sub>3</sub> S
	393.1825	1.24	8.0	C <sub>18</sub> H <sub>17</sub> O <sub>3</sub> N <sub>2</sub> S
	393.1843	-2.17	7.5	C <sub>20</sub> H <sub>25</sub> O <sub>3</sub> N <sub>2</sub> S
	393.1822	3.00	17.5	C <sub>24</sub> H <sub>27</sub> N <sub>3</sub> S
	393.1849	-3.83	16.5	C <sub>26</sub> H <sub>25</sub> O <sub>2</sub>
	393.1816	4.64	3.0	C <sub>17</sub> H <sub>21</sub> O <sub>2</sub> N <sub>2</sub> S
	393.1816	4.66	8.5	C <sub>18</sub> H <sub>25</sub> O <sub>2</sub> N <sub>2</sub> S

General composition: Single mass

Mass: 393.1834

Mass results table:

Rank	Formula	Mass	Delta (ppm)
1	C <sub>26</sub> H <sub>29</sub> O <sub>3</sub> N <sub>3</sub> S	393.1836	-0.411
2	C <sub>18</sub> H <sub>17</sub> O <sub>3</sub> N <sub>2</sub> S	393.1825	1.241
3	C <sub>20</sub> H <sub>25</sub> O <sub>3</sub> N <sub>2</sub> S	393.1843	-2.113
4	C <sub>24</sub> H <sub>27</sub> N <sub>3</sub> S	393.1822	2.988
5	C <sub>26</sub> H <sub>25</sub> O <sub>2</sub>	393.1849	-3.832
6	C <sub>17</sub> H <sub>21</sub> O <sub>2</sub> N <sub>2</sub> S	393.1816	4.643
7	C <sub>18</sub> H <sub>25</sub> O <sub>2</sub> N <sub>2</sub> S	393.1816	4.658

Units: Change 1 (g)

Elemental composition search parameters:

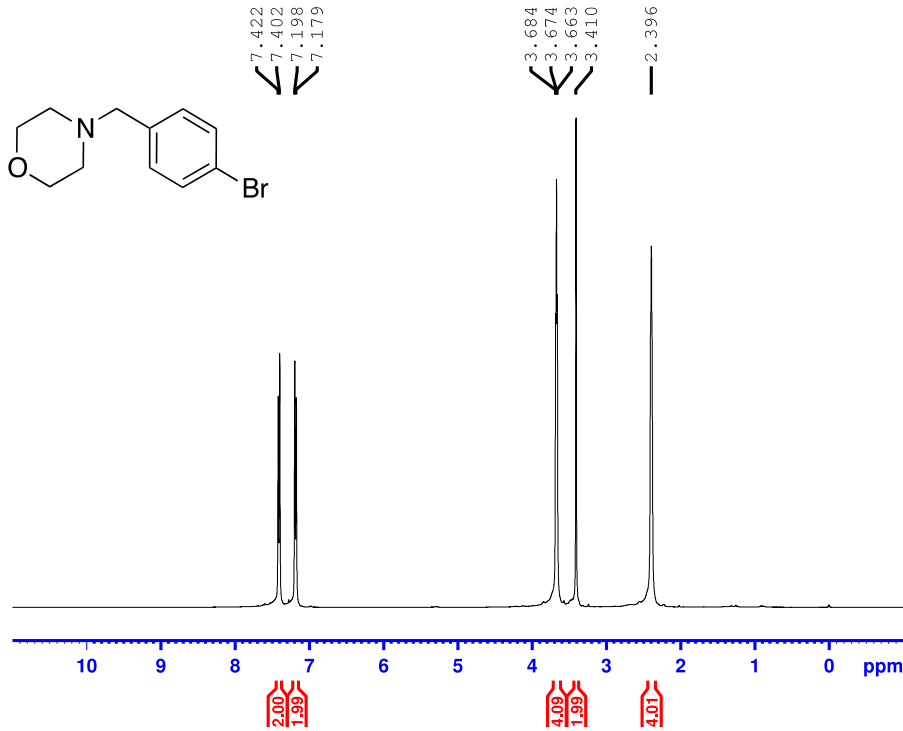
Elemental composition search table:

Element	Min	Max	DB (ppm)	Mass
H	0	10	0.5	14,000
C	0	10	0.5	14,000
N	0	10	0.5	14,000
O	0	10	0.5	14,000
S	0	10	0.5	14,000

ThermoFisher

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

SB-IV-110



```

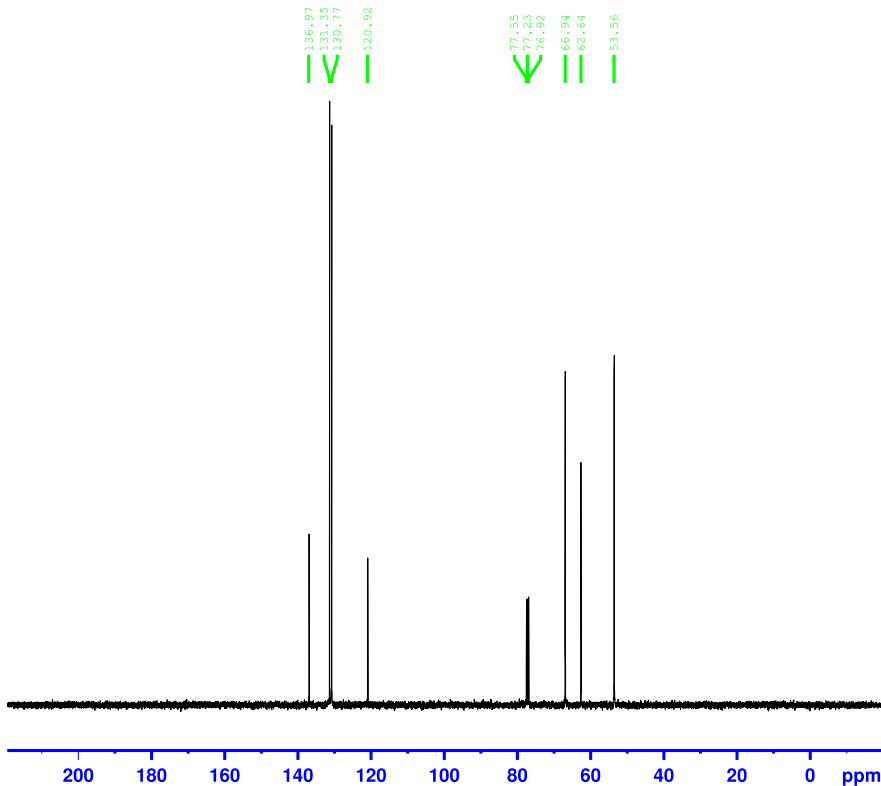
Current Data Parameters
NAME      SB-IV-110
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20120726
Time     13.24
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zg30
TD       65536
SOLVENT  CDC13
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  zpgq30
TD       65536
SOLVENT  CDC13
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

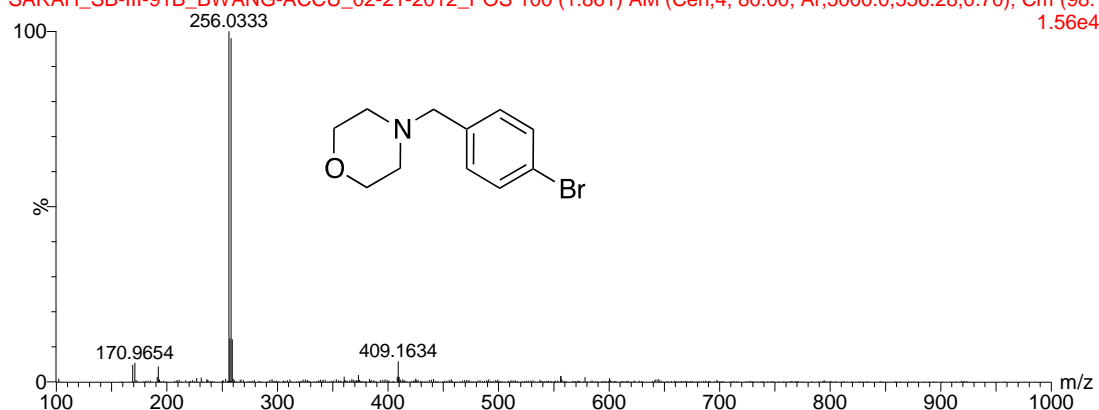
===== CHANNEL f2 =====
SFO2     400.1416006 MHz
NUC2     1H
CPDPRG2  waltz16
PCPD2    90.00 usec
PLW2     16.00000000 W
PLW12    0.36000001 W
PLW13    0.29159999 W

F2 - Processing parameters
SI       32768
SF       100.6152850 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
    
```

100%MeOH+0.1%HCOOH

13:20:16 21-Feb-2012

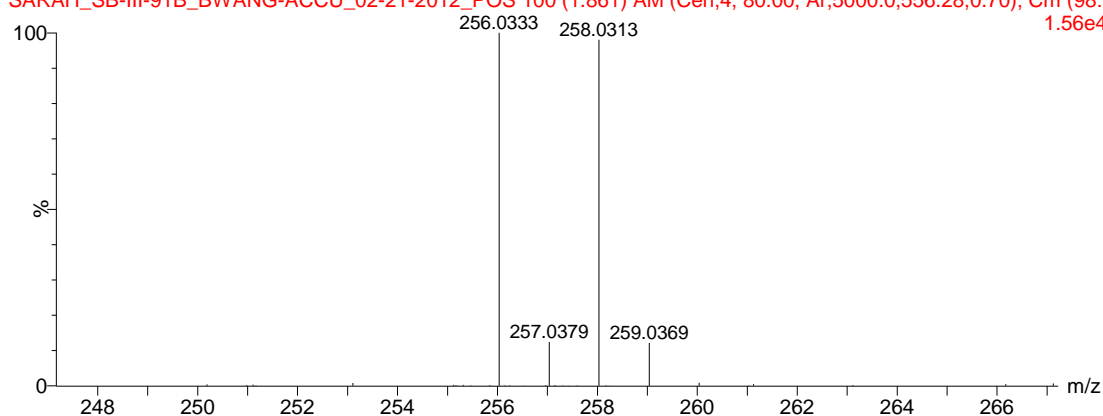
SARAH\_SB-III-91B\_BWANG-ACCU\_02-21-2012\_POS 100 (1.861) AM (Cen,4, 80.00, Ar,5000.0,556.28,0.70); Cm (98:1 1.56e4



100%MeOH+0.1%HCOOH

13:20:16 21-Feb-2012

SARAH\_SB-III-91B\_BWANG-ACCU\_02-21-2012\_POS 100 (1.861) AM (Cen,4, 80.00, Ar,5000.0,556.28,0.70); Cm (98:1 1.56e4



### 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

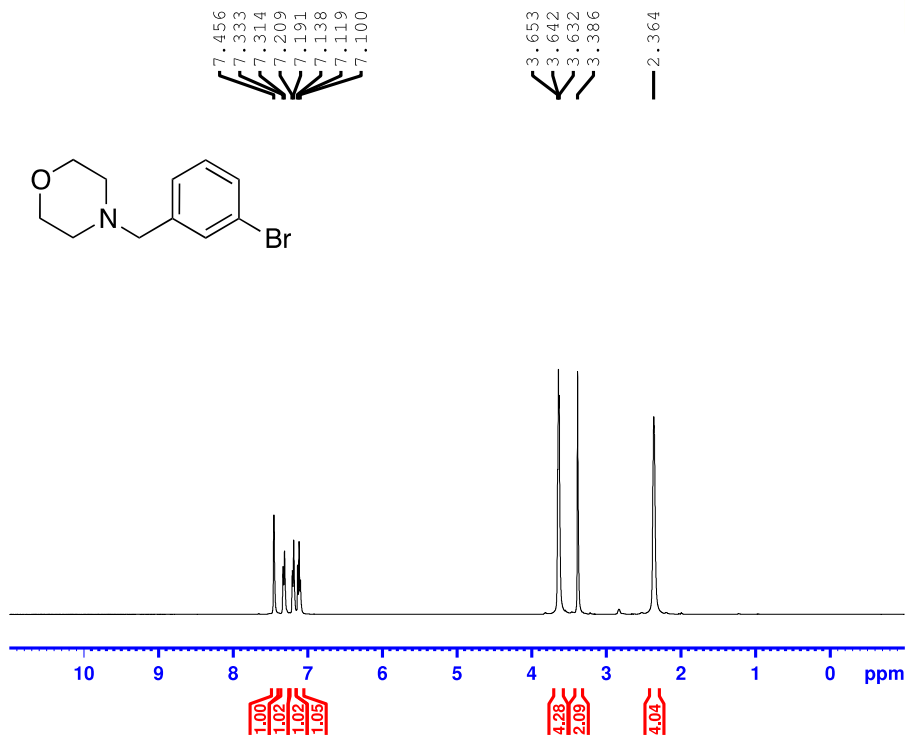
Maximum: 5.0 5.0 50.0

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)

ZD-I-77



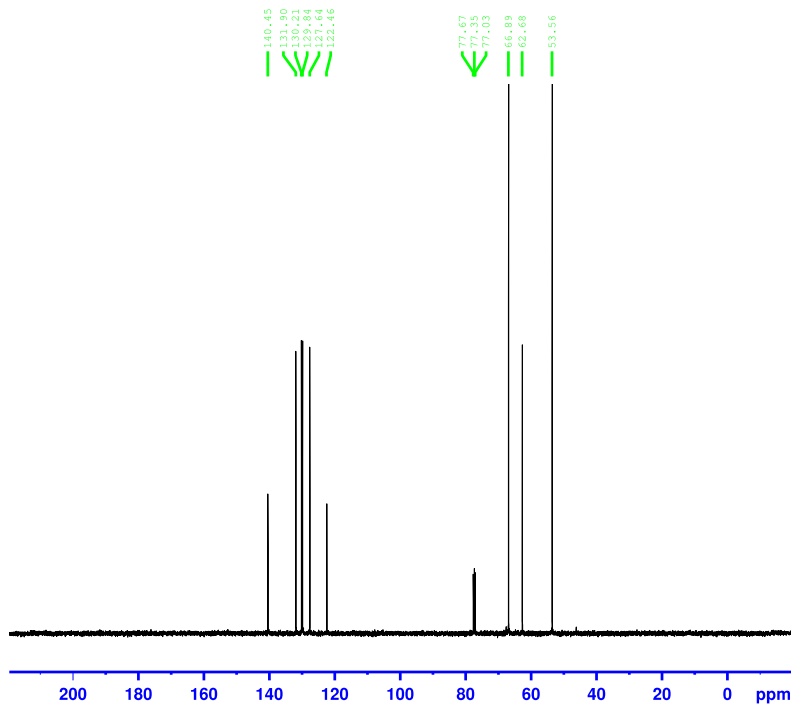
Current Data Parameters  
 NAME ZD-I-77  
 EXPNO 1  
 PROCNO 1

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  
 FC 1.00

ZD-I-77



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

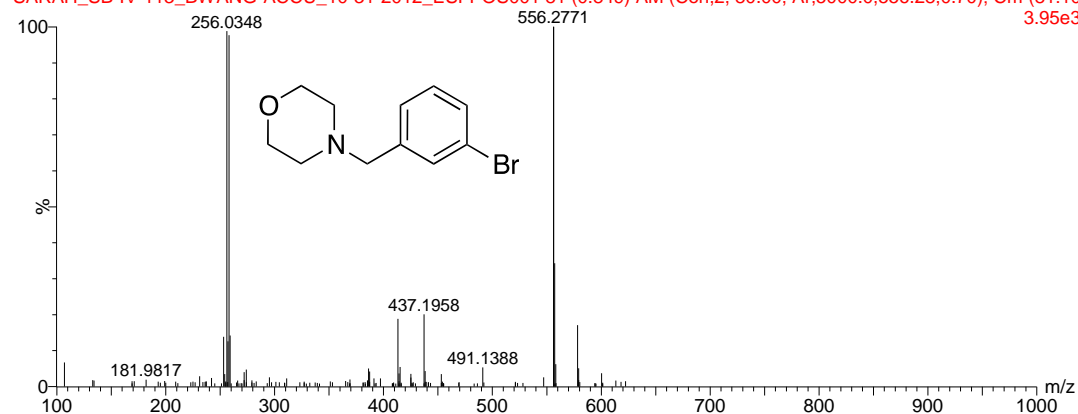
==== CHANNEL f2 =====  
 SFO2 400.1416006 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 16.00000000 W  
 PLW12 0.36000001 W  
 PLW13 0.29159999 W

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

90%ACN+0.1%HCOOH

16:27:04 31-Oct-2012

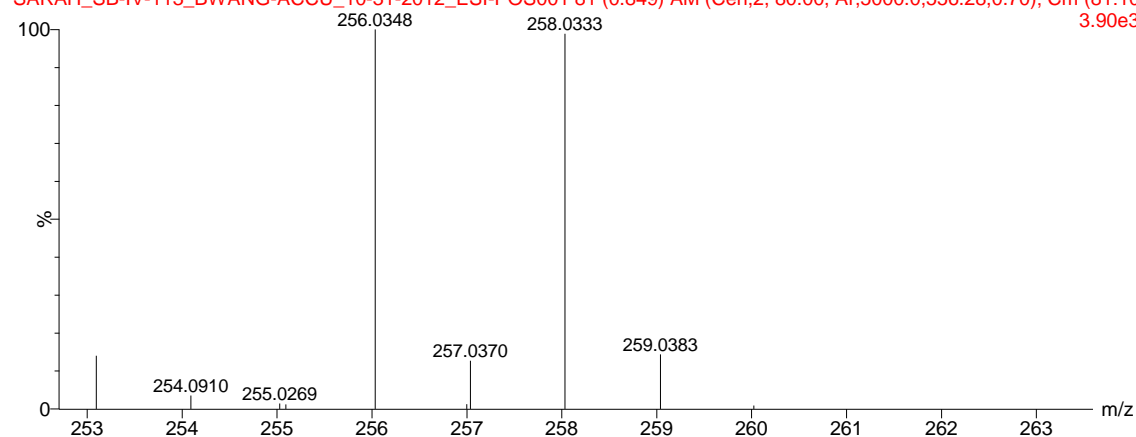
SARAH\_SB-IV-113\_BWANG-ACCU\_10-31-2012\_ESI-POS001 81 (0.849) AM (Cen,2, 80.00, Ar,5000.0,556.28,0.70); Cm (81:10  
3.95e3



90%ACN+0.1%HCOOH

16:27:04 31-Oct-2012

SARAH\_SB-IV-113\_BWANG-ACCU\_10-31-2012\_ESI-POS001 81 (0.849) AM (Cen,2, 80.00, Ar,5000.0,556.28,0.70); Cm (81:10  
3.90e3



### 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

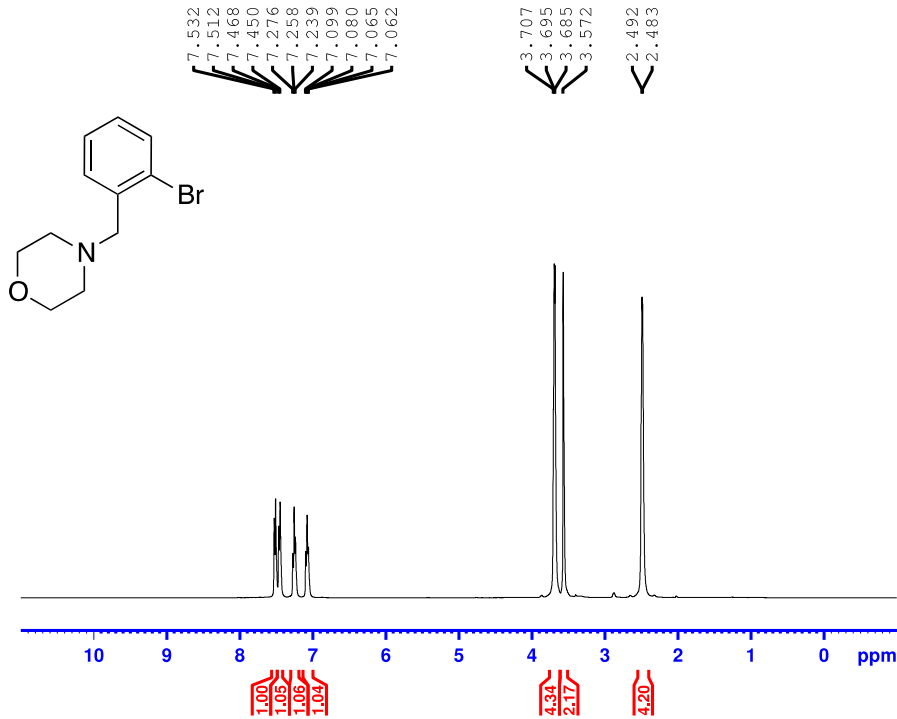
Maximum:

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)

ZD-I-78



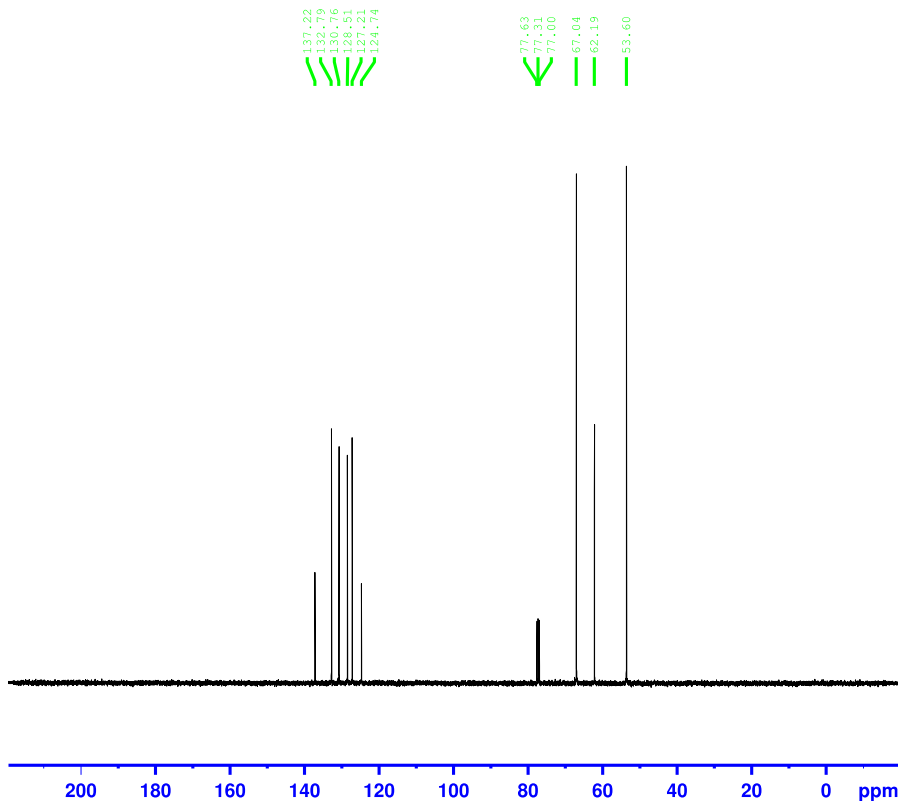
Current Data Parameters  
 NAME ZD-I-78  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20130213  
 Time 9.57  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDC13  
 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

ZD-I-78



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 CDC13  
 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

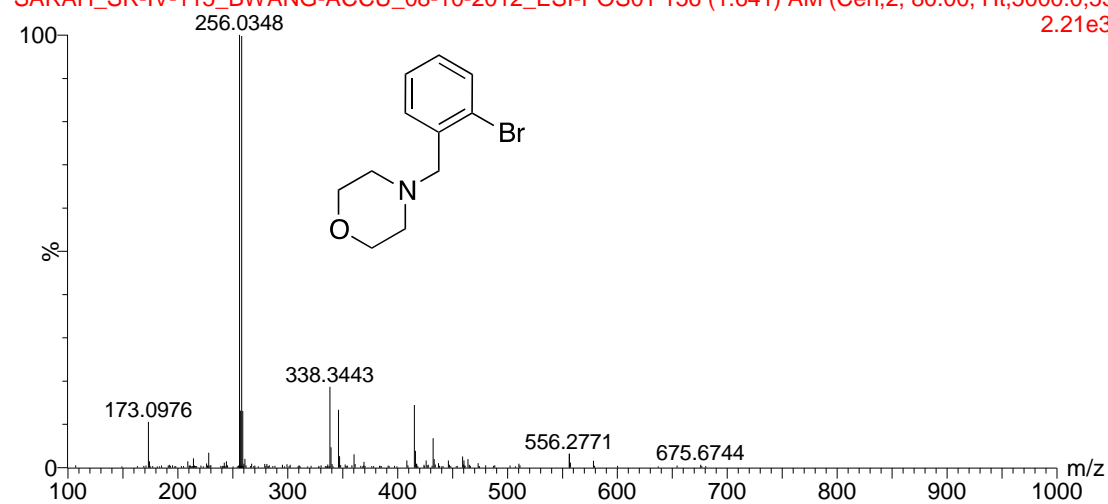
===== CHANNEL f2 =====  
 SFO2 400.1416006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 16.00000000 W  
 PLW12 0.36000001 W  
 PLW13 0.29159999 W

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

100%MeOH

18:26:34 10-Aug-2012

SARAH\_SR-IV-115\_BWANG-ACCU\_08-10-2012\_ESI-POS01 156 (1.641) AM (Cen,2, 80.00, Ht,5000.0,55  
2.21e3



### 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)

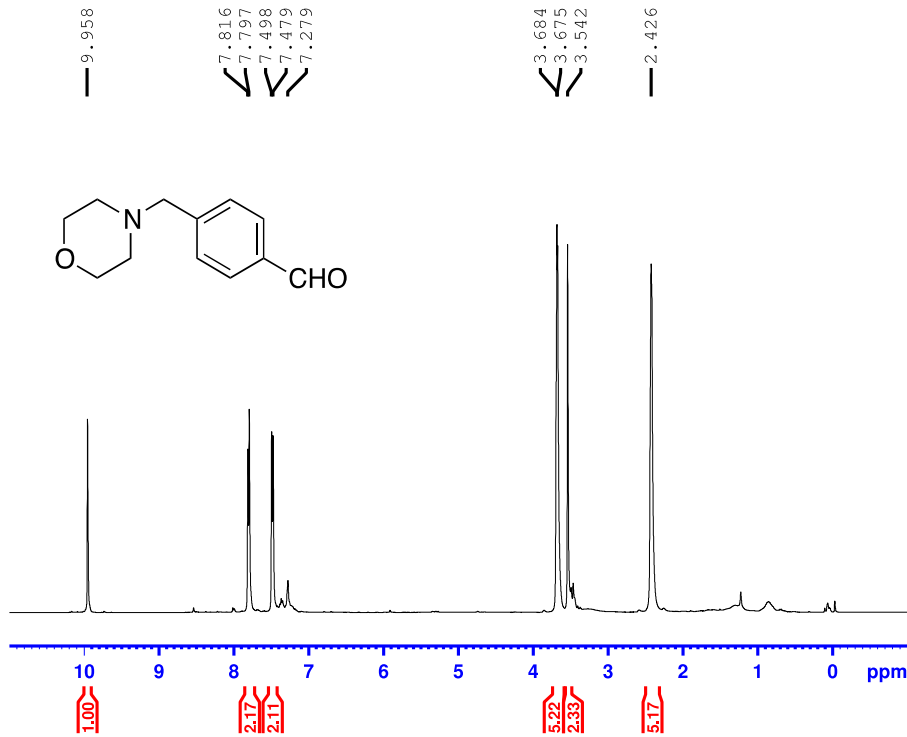
Elements Used:

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



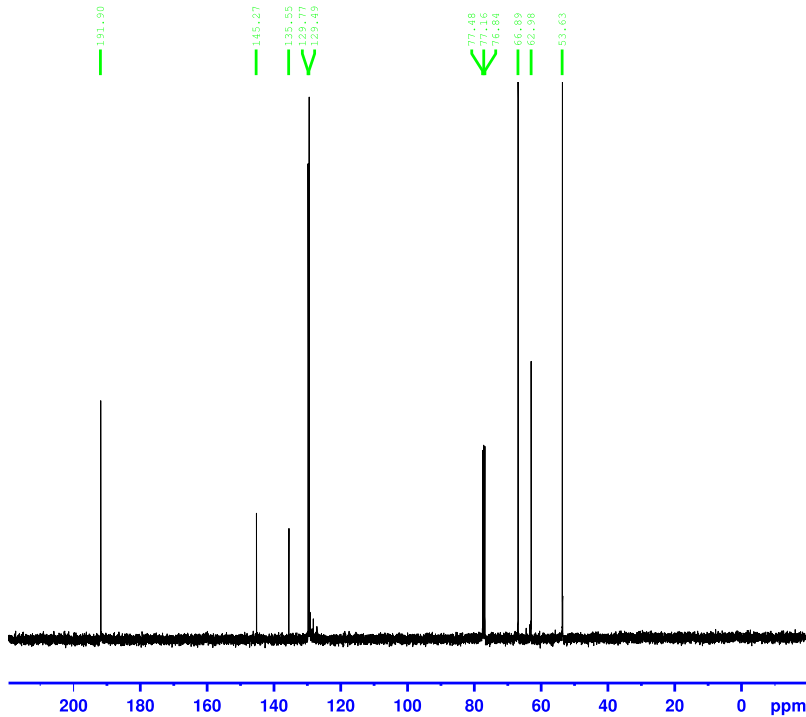
Current Data Parameters  
 NAME SB-IV-30  
 EXPNO 1  
 PROCNO 1

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



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

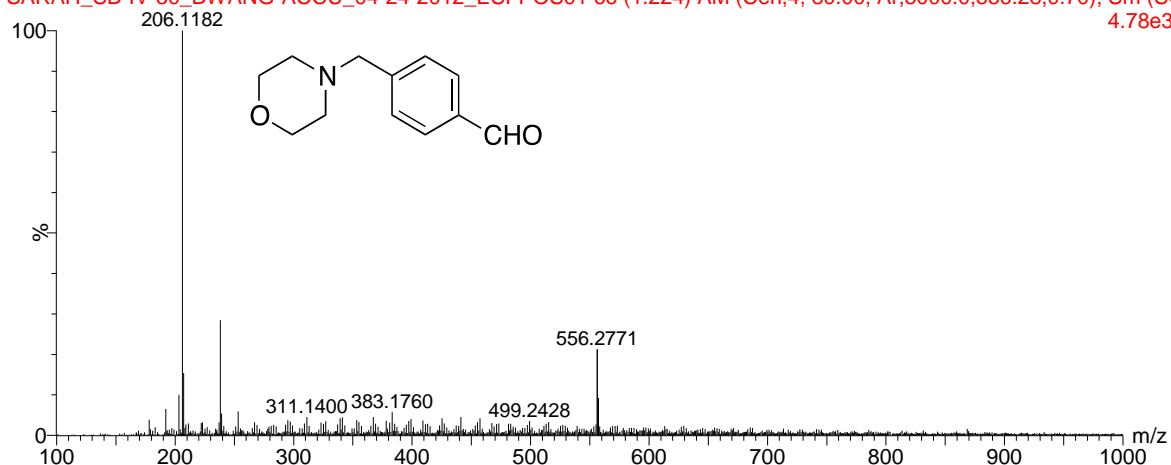
F2 - Acquisition Parameters  
 Date\_ 20120420  
 Time 15.51  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 4  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 203  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.4 K  
 D1 2.00000000 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  
 CPDPRG12 waltz16  
 FPCP2 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

in 100%MeOH+0.1%HCOOH

16:01:58 24-Apr-2012

SARAH\_SB-IV-30\_BWANG-ACCU\_04-24-2012\_ESI-POS01 66 (1.224) AM (Cen,4, 80.00, Ar,5000.0,556.28,0.70); Sm (SC 4.78e3



### 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

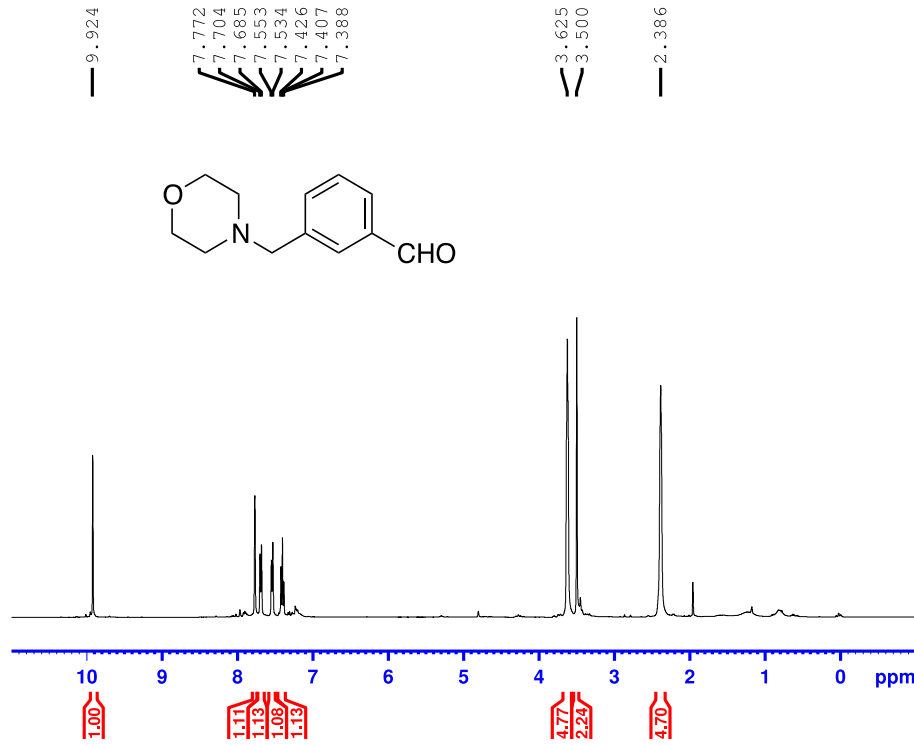
Minimum: -1.5

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



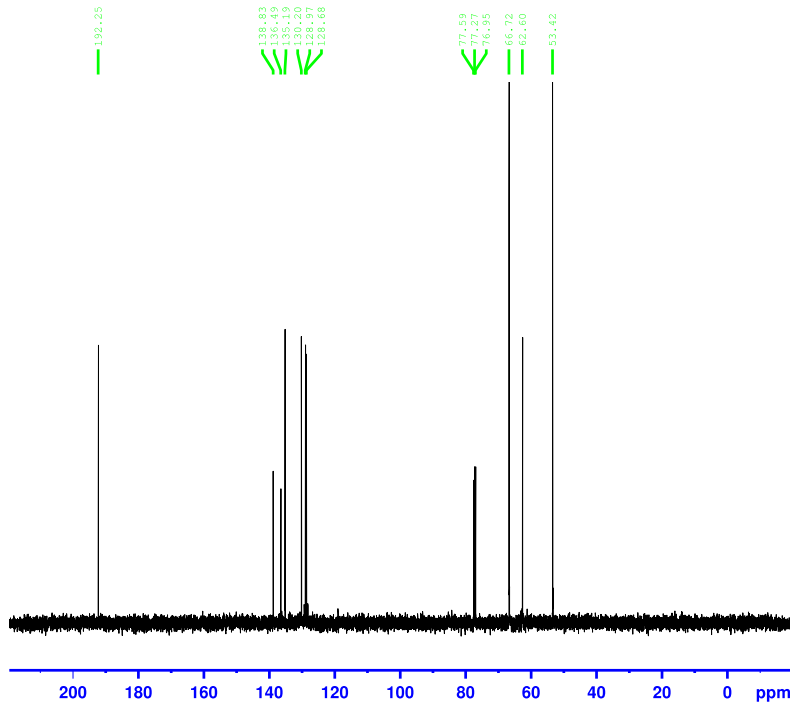
```
Current Data Parameters
NAME      SB-V-80b
EXPNO    1
PROCNO   1

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
TDO      1

===== CHANNEL f1 =====
SF01    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
TDO      1

===== CHANNEL f1 =====
SF01    100.6253441 MHz
NUC1     13C
P1      9.00 usec
PLW1    62.00000000 W

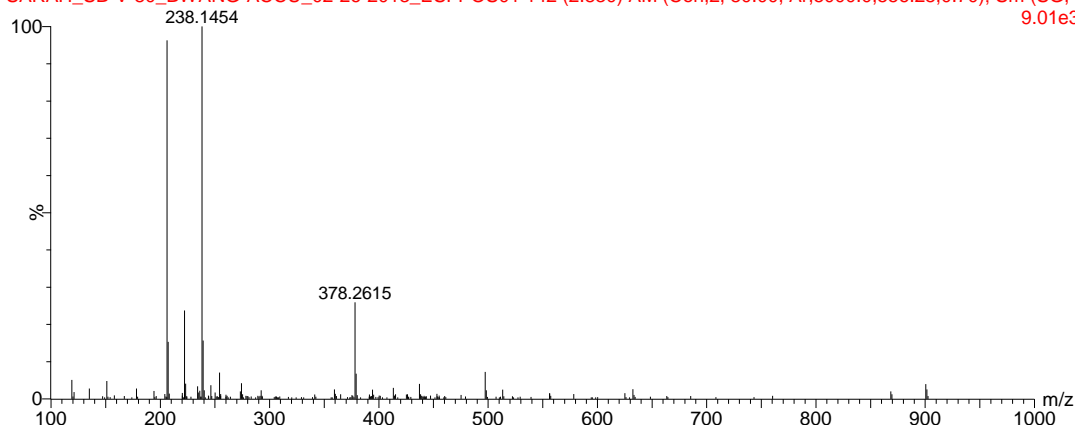
===== CHANNEL f2 =====
SF02    400.1416006 MHz
NUC2     1H
CPDPRG2 waltz16
PCPD2   80.00 usec
PLW2    16.00000000 W
PLW12   0.36000001 W
PLW13   0.29159999 W

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

MeOH

14:10:36 26-Feb-2013

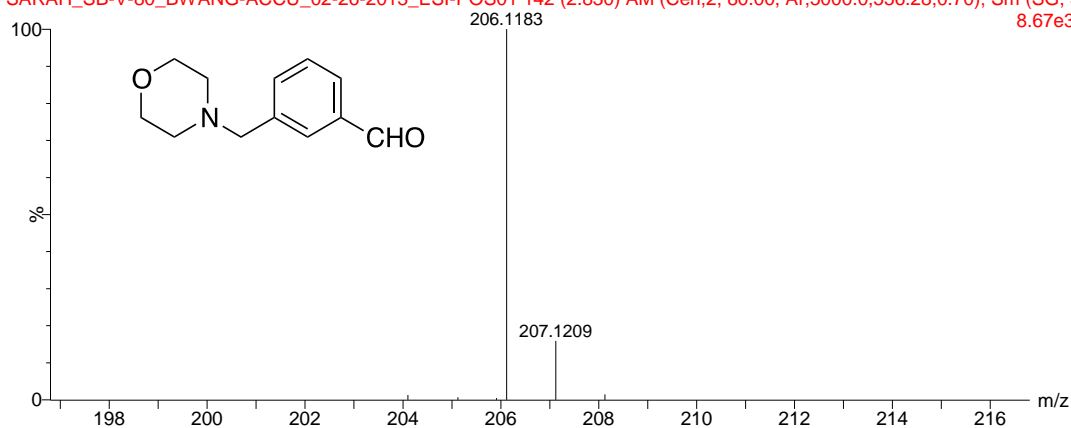
SARAH\_SB-V-80\_BWANG-ACCU\_02-26-2013\_ESI-POS01 142 (2.830) AM (Cen,2, 80.00, Ar,5000.0,556.28,0.70); Sm (SG, 3 9.01e3



MeOH

14:10:36 26-Feb-2013

SARAH\_SB-V-80\_BWANG-ACCU\_02-26-2013\_ESI-POS01 142 (2.830) AM (Cen,2, 80.00, Ar,5000.0,556.28,0.70); Sm (SG, 3 8.67e3



### 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

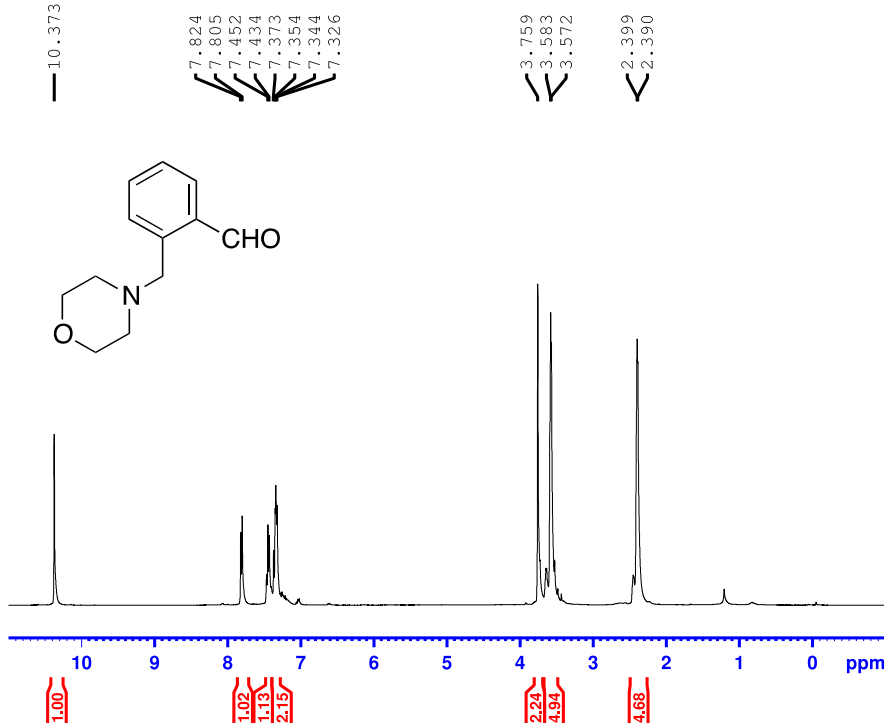
Maximum: 5.0 5.0 50.0

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



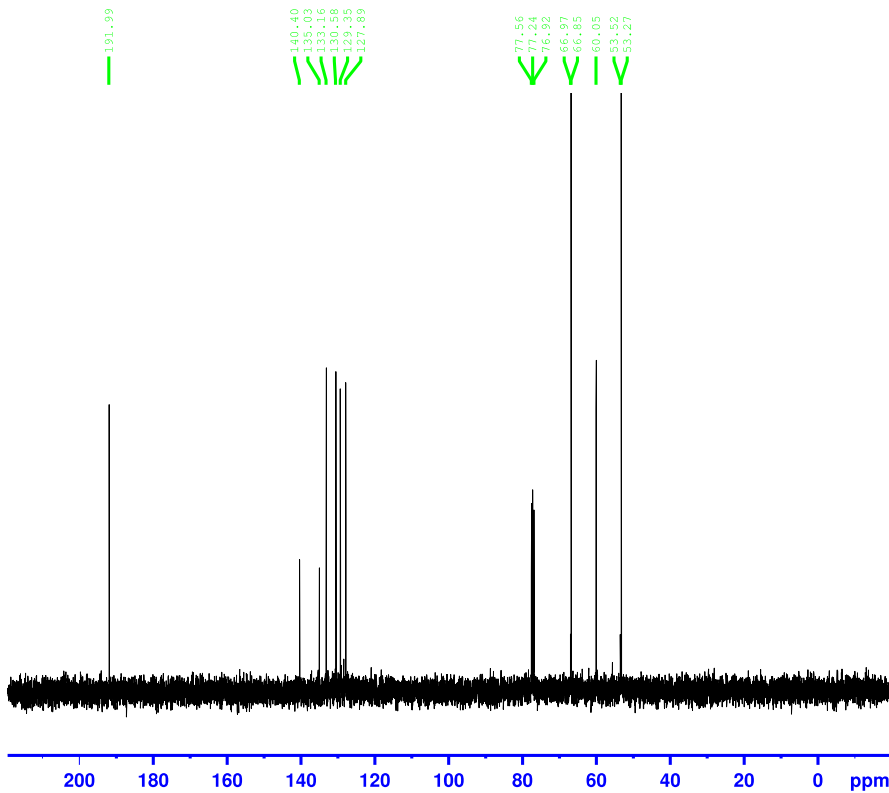
Current Data Parameters  
 NAME SB-V-17c1  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20121120  
 Time 11.38  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDC13  
 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  
 TDO 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 CDC13  
 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  
 TDO 1

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

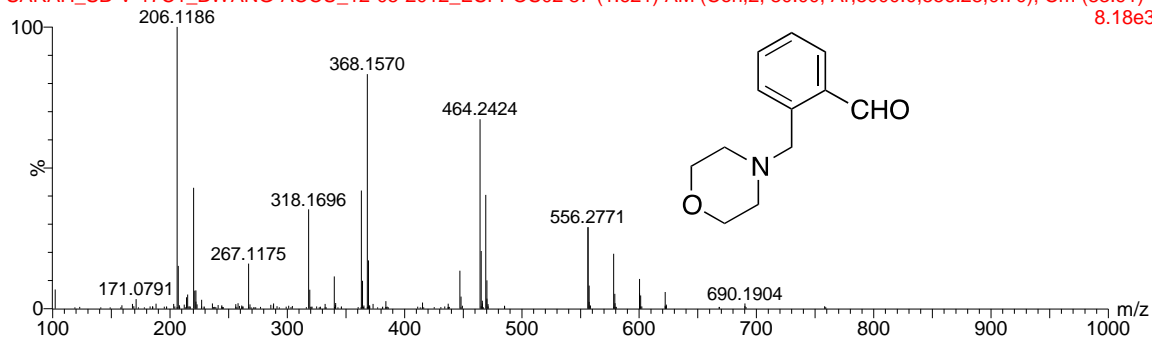
==== CHANNEL f2 =====  
 SFO2 400.1416006 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 P1 90.00 usec  
 PLW2 16.00000000 W  
 PLW12 0.36000001 W  
 PLW13 0.29159999 W

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

90%MeOH+0.1%HCOOH

15:48:53 05-Dec-2012

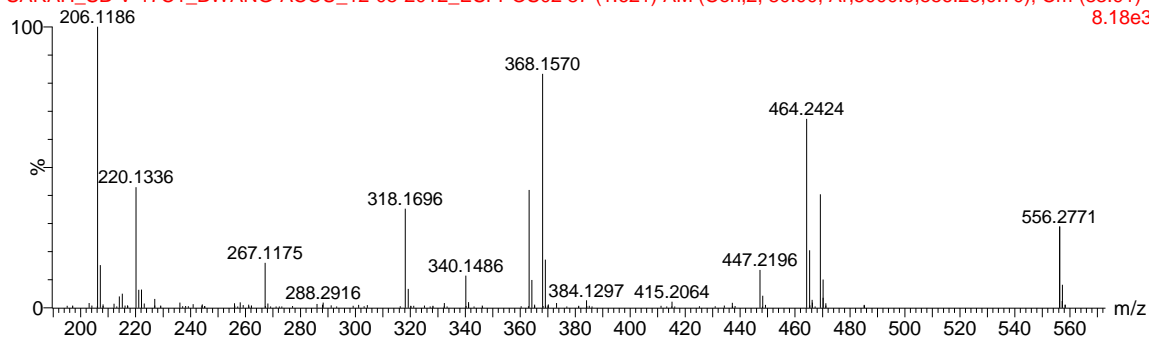
SARAH\_SB-V-17C1\_BWANG-ACCU\_12-05-2012\_ESI-POS02 87 (1.621) AM (Cen,2, 80.00, Ar,5000.0,556.28,0.70); Cm (83:91) 8.18e3



90%MeOH+0.1%HCOOH

15:48:53 05-Dec-2012

SARAH\_SB-V-17C1\_BWANG-ACCU\_12-05-2012\_ESI-POS02 87 (1.621) AM (Cen,2, 80.00, Ar,5000.0,556.28,0.70); Cm (83:91) 8.18e3



### 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

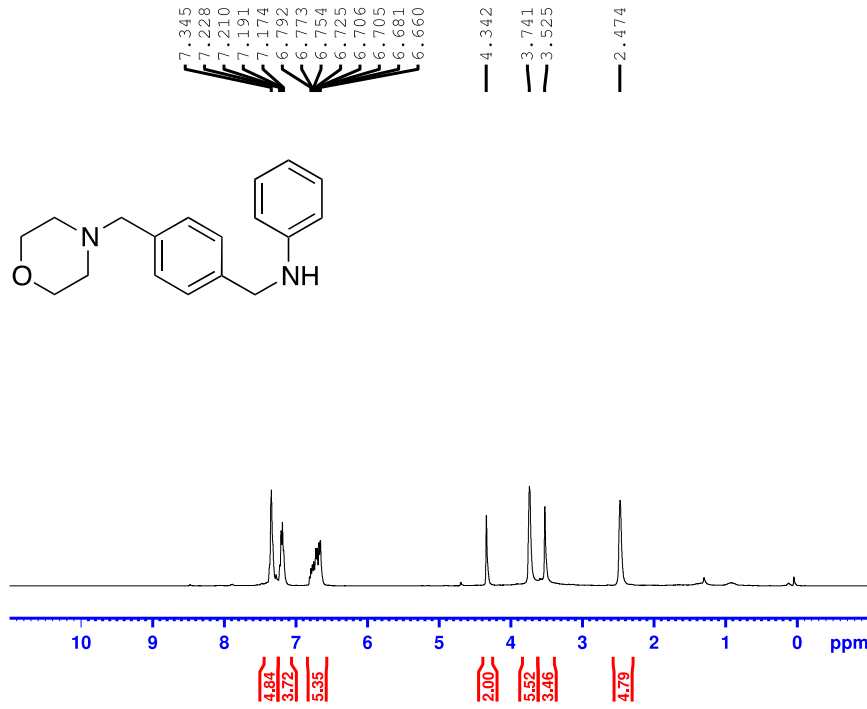
Minimum: -1.5

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



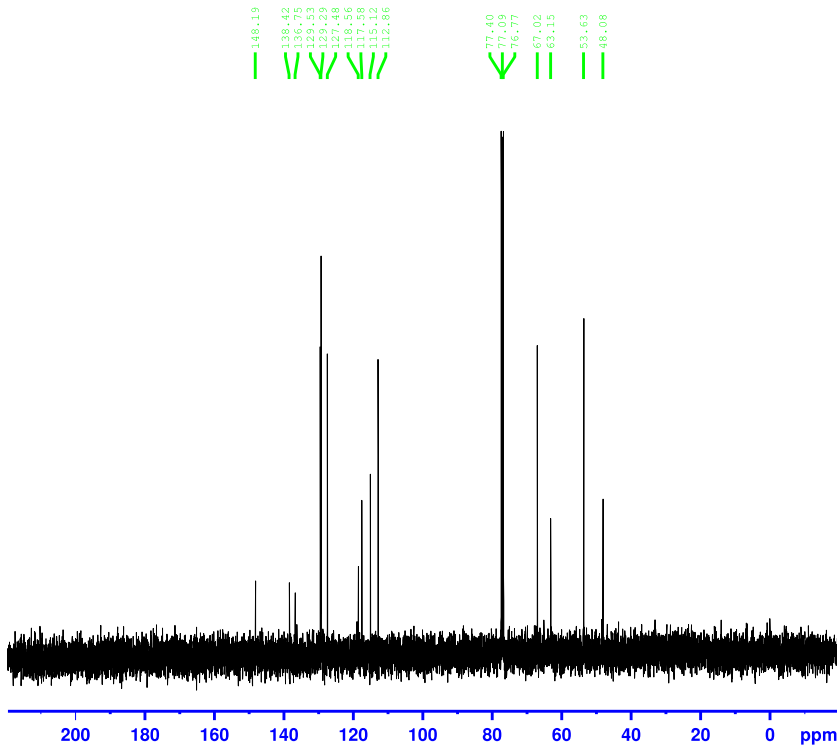
Current Data Parameters  
 NAME SB-IV-37a  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120426  
 Time 11.04  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDC13  
 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



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

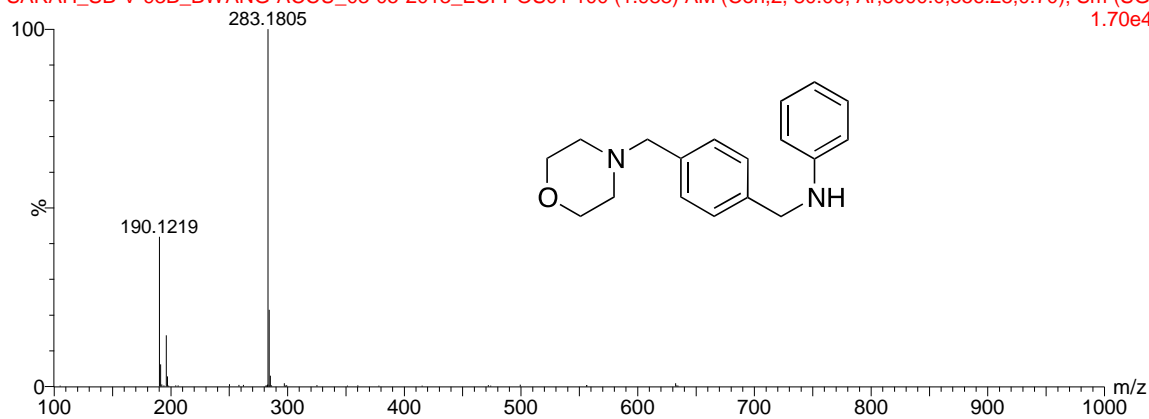
F2 - Acquisition Parameters  
 Date\_ 20120426  
 Time 11.06  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 22  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 203  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.3 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TDO 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

in 90%MeOH

17:58:03 05-Mar-2013

SARAH\_SB-V-93B\_BWANG-ACCU\_03-05-2013\_ESI-POS01 100 (1.988) AM (Cen,2, 80.00, Ar,5000.0,556.28,0.70); Sm (SG, 1.70e4



### 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

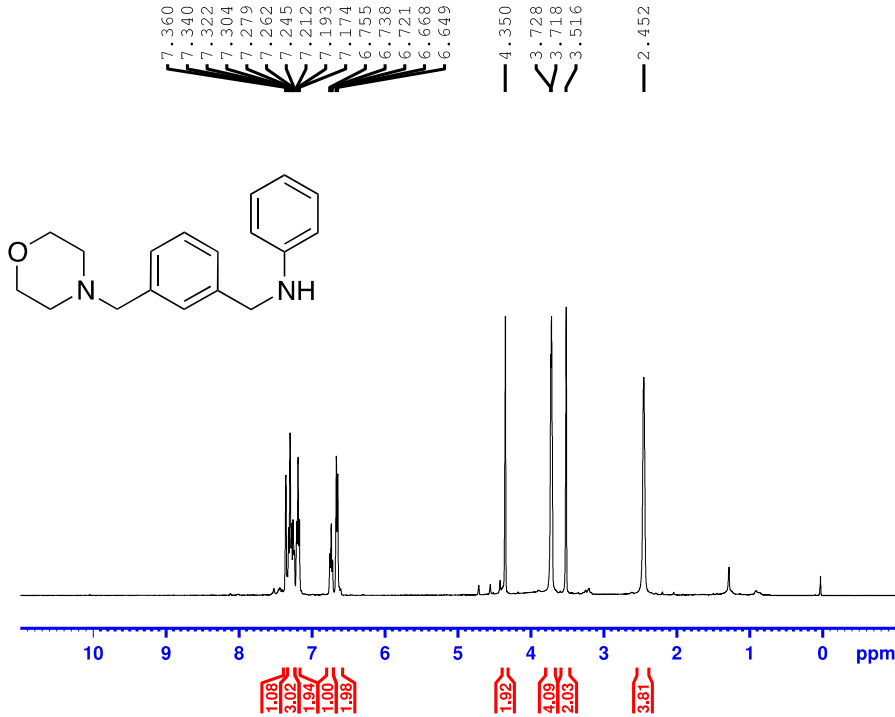
Maximum:

5.0 5.0 50.0

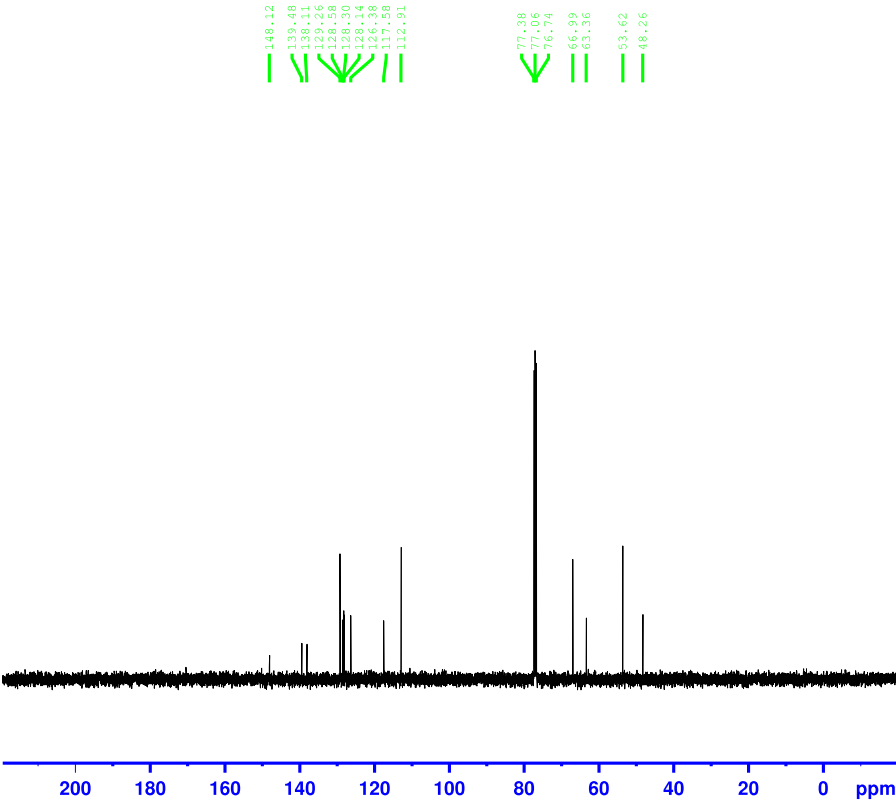
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
283.1805	283.1810	-0.5	-1.8	8.5	12.4	C18 H23 N2 O
	283.1815	-1.0	-3.5	1.5	741.3	C3 H19 N14 O2

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

SB-V-107d



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 4.089465 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



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

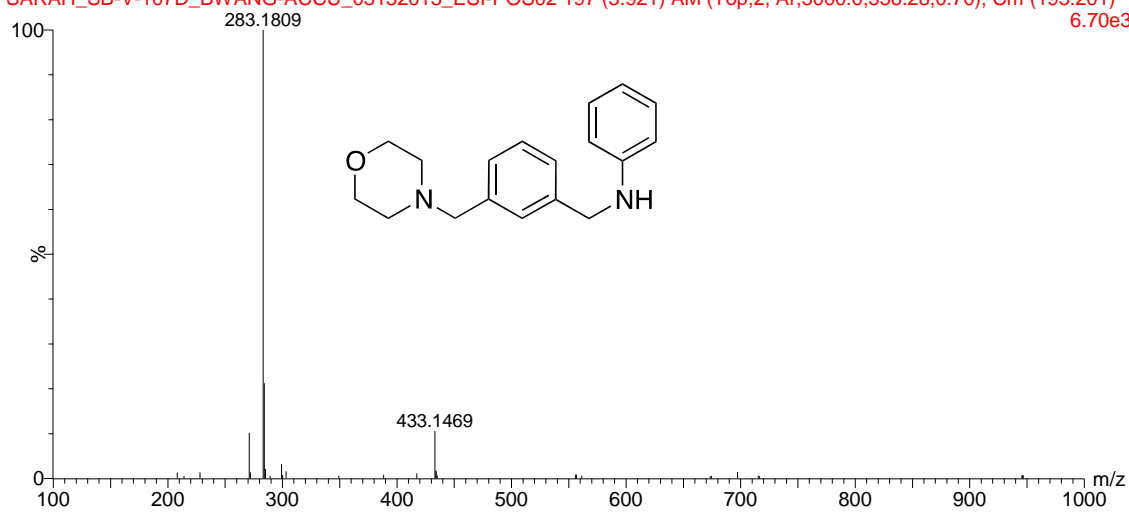
===== CHANNEL f2 =====  
 SFO2 400.1416006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 16.00000000 W  
 PLW12 0.36000001 W  
 PLW13 0.29159999 W

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

80%MeOH

14:18:33 15-Mar-2013

SARAH\_SB-V-107D\_BWANG-ACCU\_03152013\_ESI-POS02 197 (3.921) AM (Top,2, Ar,5000.0,556.28,0.70); Cm (193:201)  
6.70e3



### 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

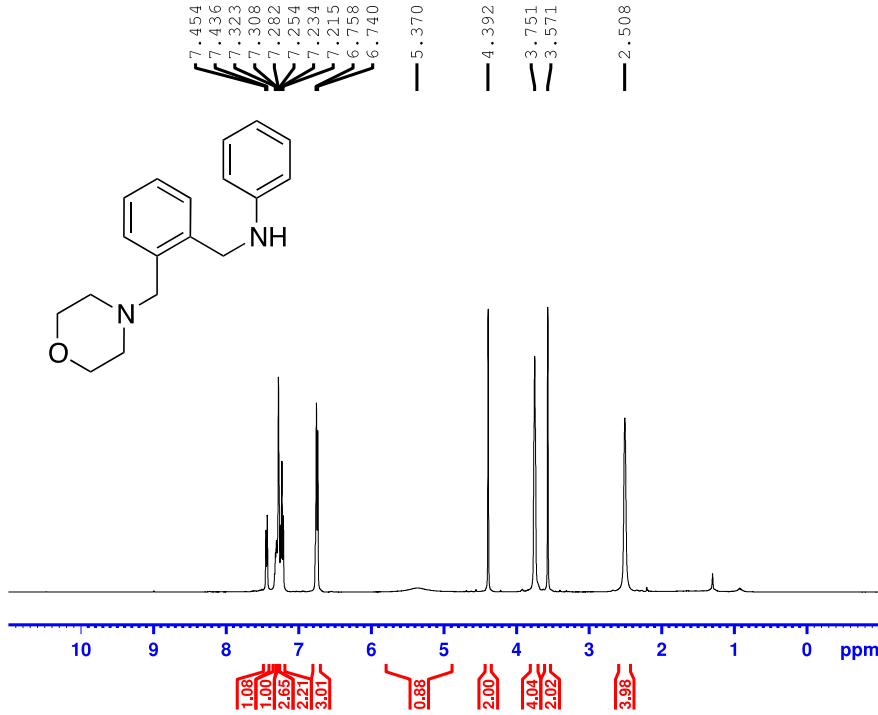
Minimum: -1.5

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)

SB-V-93b-dry



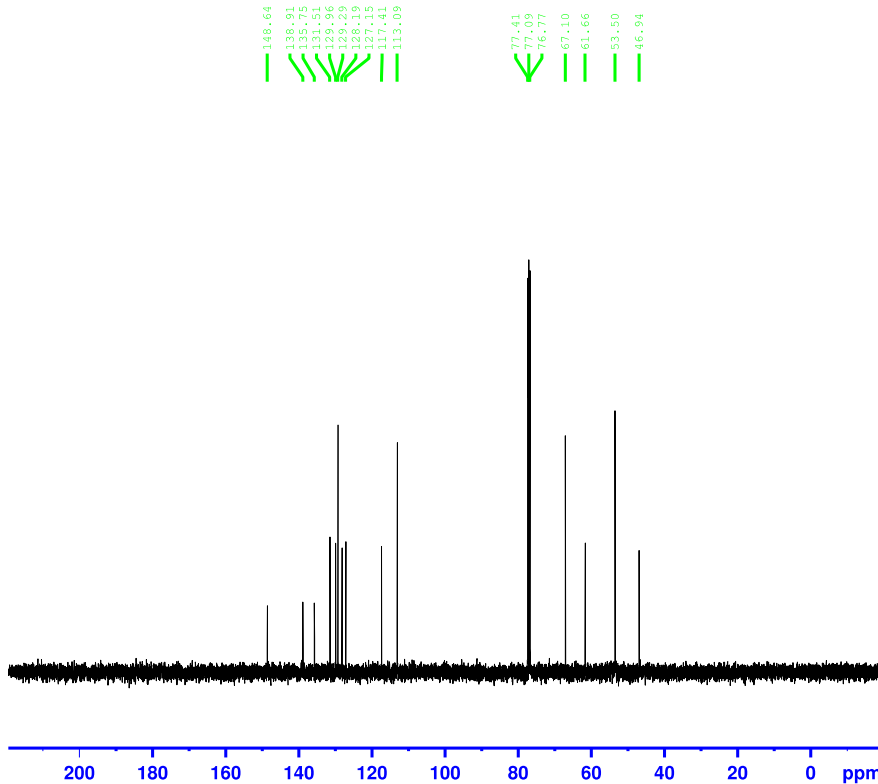
Current Data Parameters  
 NAME SB-V-93b-dry  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20130305  
 Time 16.10  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDC13  
 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  
 TDO 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-93b-dry



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 CDC13  
 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  
 TDO 1

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

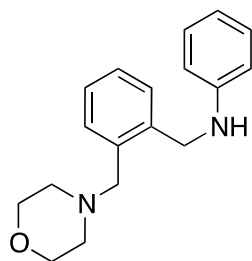
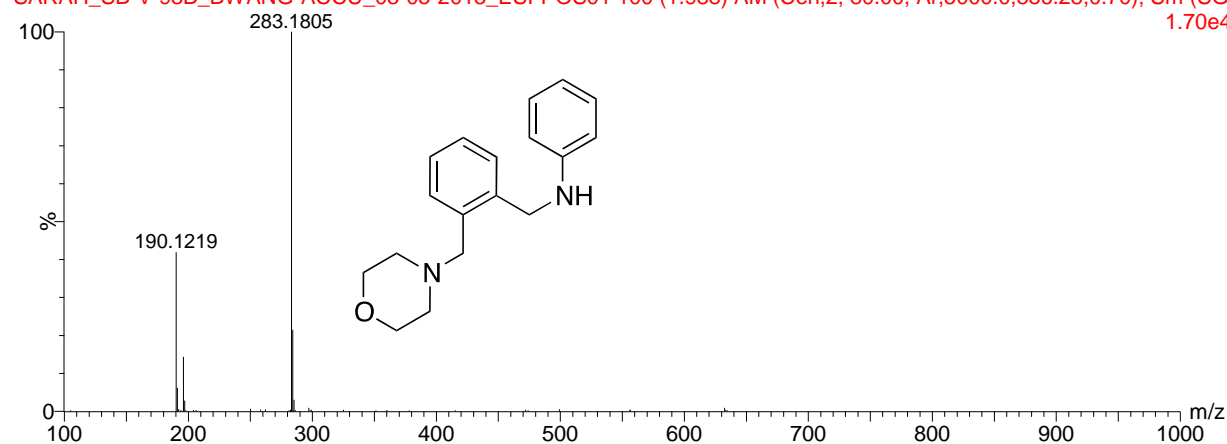
==== CHANNEL f2 =====  
 SFO2 400.1416006 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 16.00000000 W  
 PLW12 0.36000001 W  
 PLW13 0.29159999 W

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

in 90%MeOH

17:58:03 05-Mar-2013

SARAH\_SB-V-93B\_BWANG-ACCU\_03-05-2013\_ESI-POS01 100 (1.988) AM (Cen,2, 80.00, Ar,5000.0,556.28,0.70); Sm (SG, 1.70e4



### 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

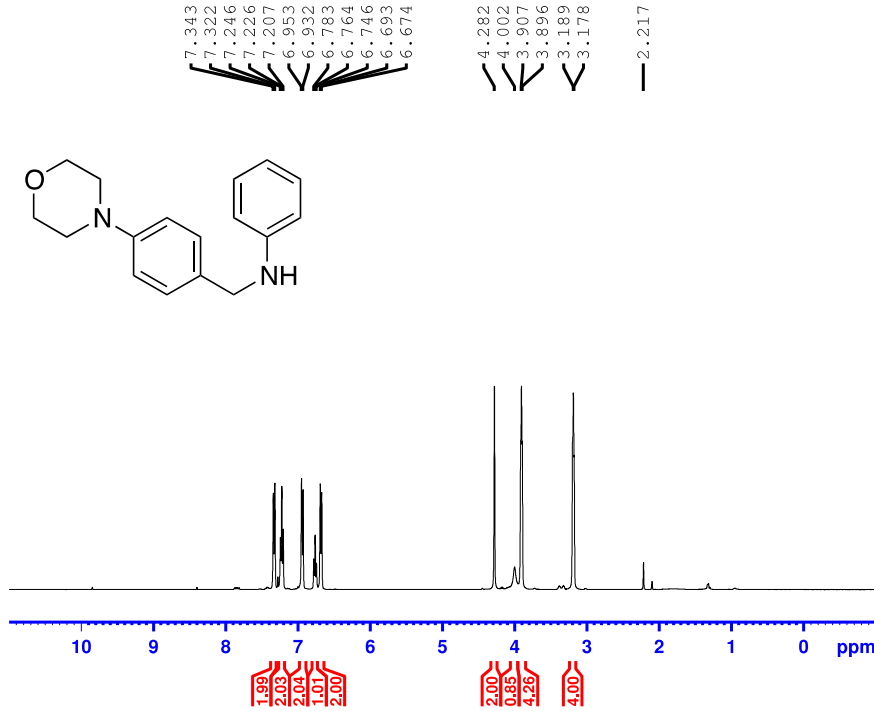
Maximum: 5.0 5.0 50.0

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)

ZD-I-75c



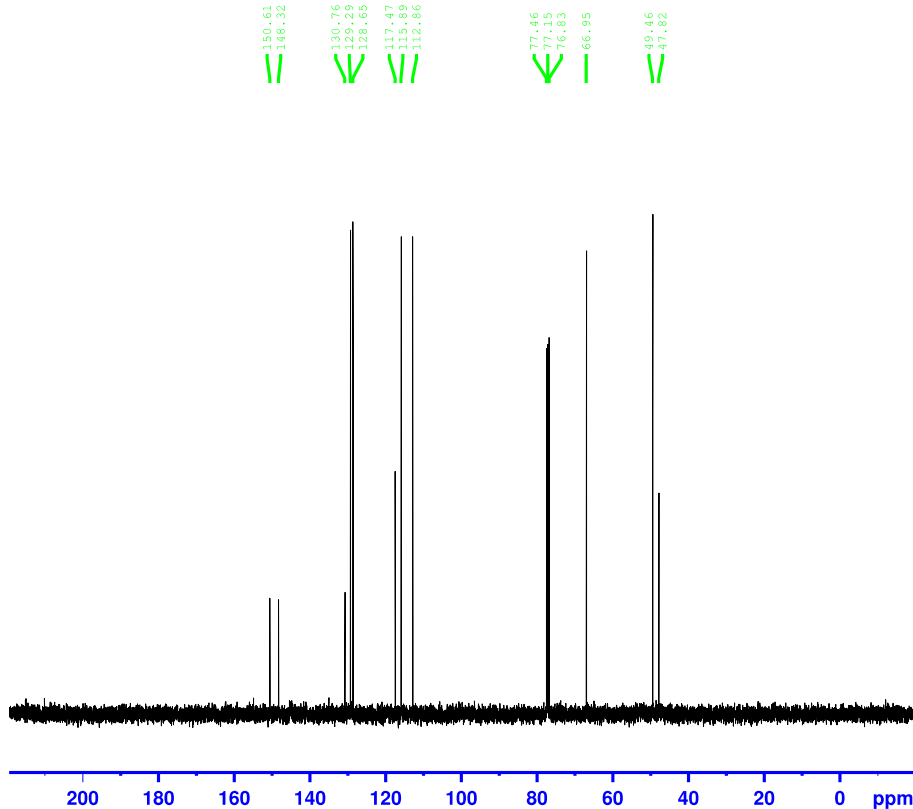
Current Data Parameters  
 NAME ZD-I-75c  
 EXPNO 1  
 PROCNO 1

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  
 SDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

ZD-I-75c



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 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

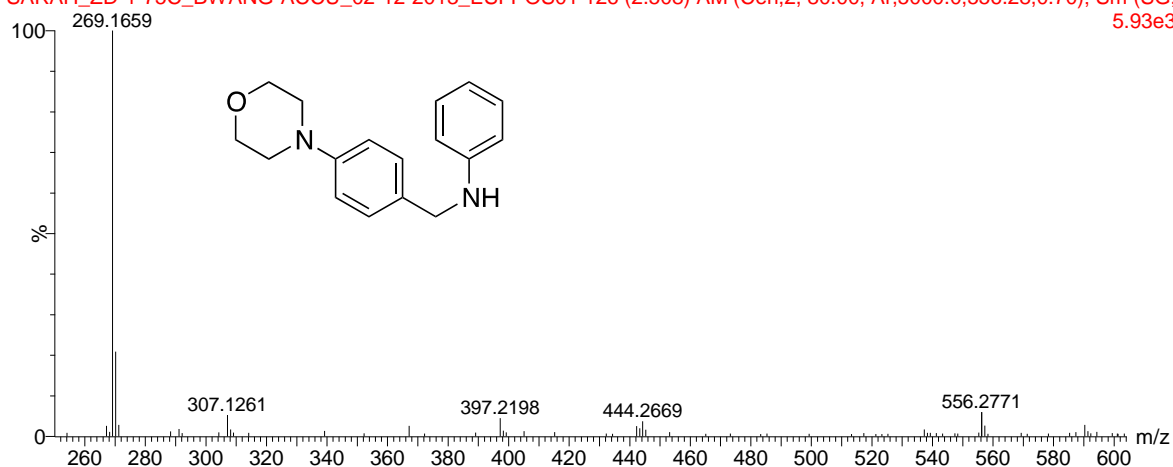
===== CHANNEL f2 =====  
 SFO2 400.1416006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 16.00000000 W  
 PLW12 0.36000001 W  
 PLW13 0.29159999 W

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

diluted in MeOH+0.1%HCOOH

17:08:59 12-Feb-2013

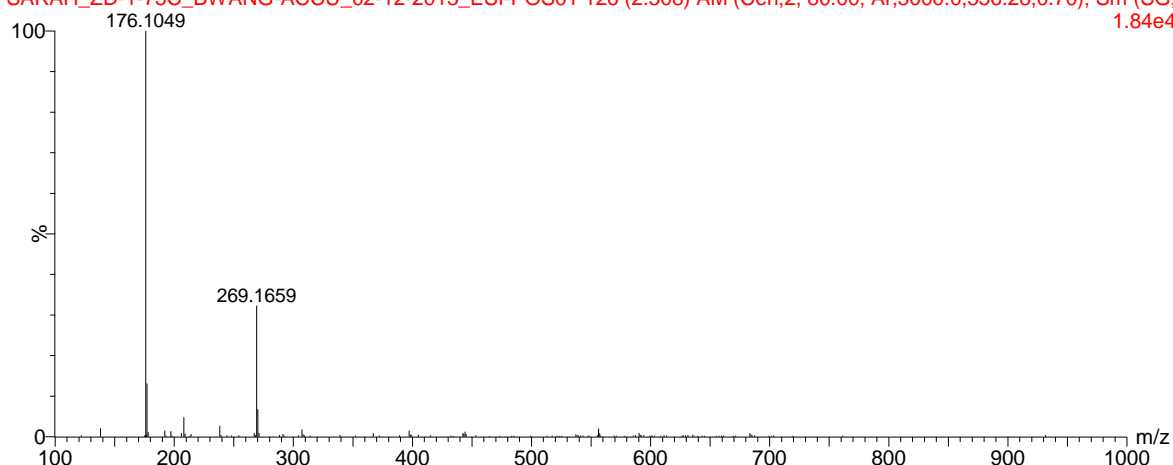
SARAH\_ZD-1-75C\_BWANG-ACCU\_02-12-2013\_ESI-POS01 126 (2.508) AM (Cen,2, 80.00, Ar,5000.0,556.28,0.70); Sm (SG, 5.93e3



diluted in MeOH+0.1%HCOOH

17:08:59 12-Feb-2013

SARAH\_ZD-1-75C\_BWANG-ACCU\_02-12-2013\_ESI-POS01 126 (2.508) AM (Cen,2, 80.00, Ar,5000.0,556.28,0.70); Sm (SG, 1.84e4



### 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

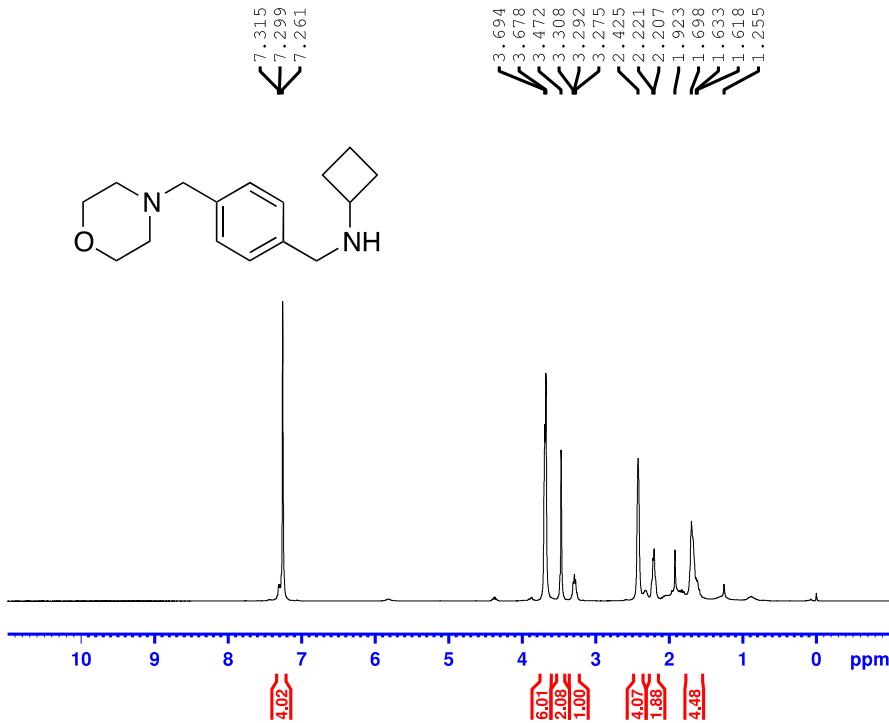
0.5 1.9

8.5 n/a

C17H21N2O

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

SB-IV-39a



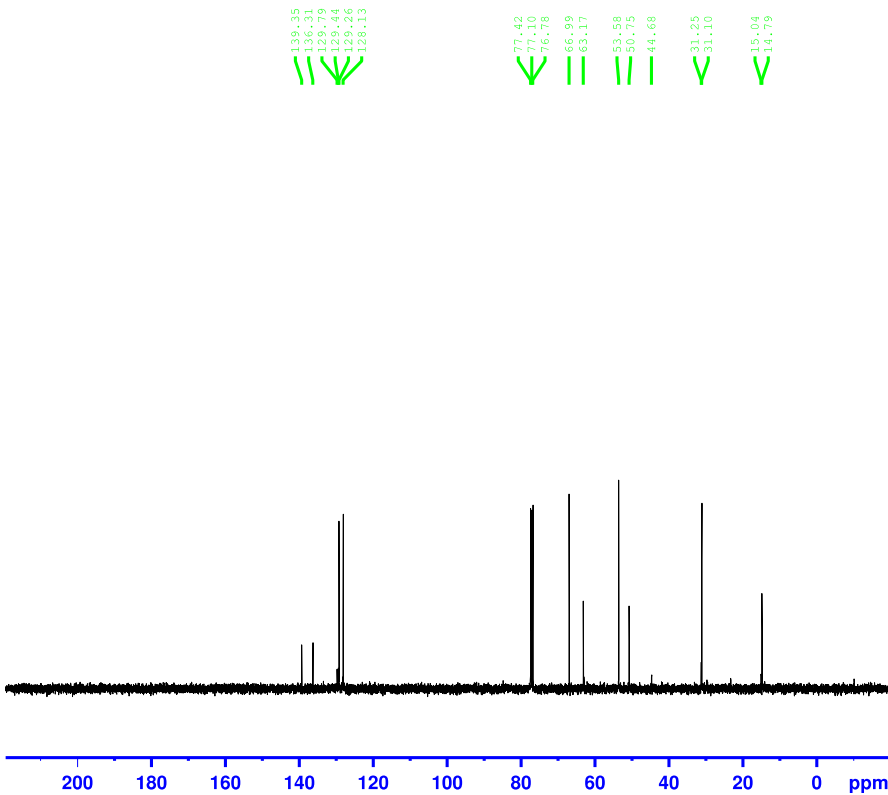
Current Data Parameters  
 NAME SB-IV-39a  
 EXPNO 1  
 PROCNO 1

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 16.0000000 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 62.0000000 W  
 SFO1 100.6253441 MHz

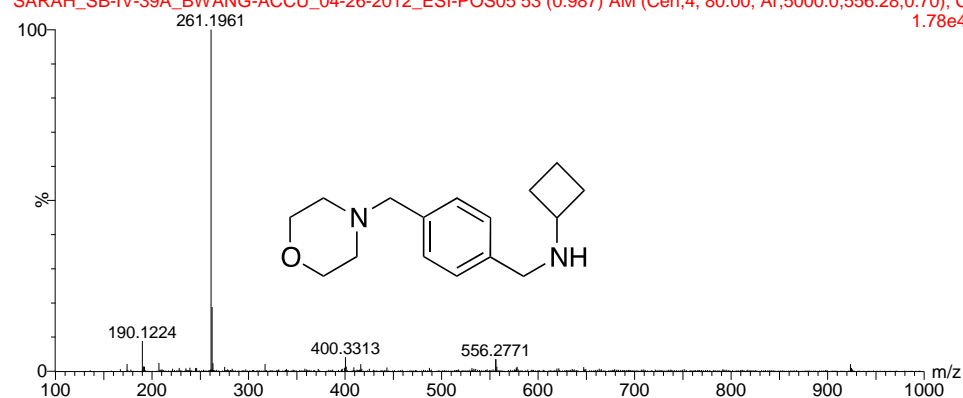
==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PLW2 16.0000000 W  
 PLW12 0.3600000 W  
 PLW13 0.2915999 W  
 SFO2 400.1416006 MHz

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

in 100%MeOH+0.1%HCOOH

17:49:34 26-Apr-2012

SARAH\_SB-IV-39A\_BWANG-ACCU\_04-26-2012\_ESI-POS05 53 (0.987) AM (Cen,4, 80.00, Ar,5000.0,556.28,0.70); C  
1.78e4



### 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

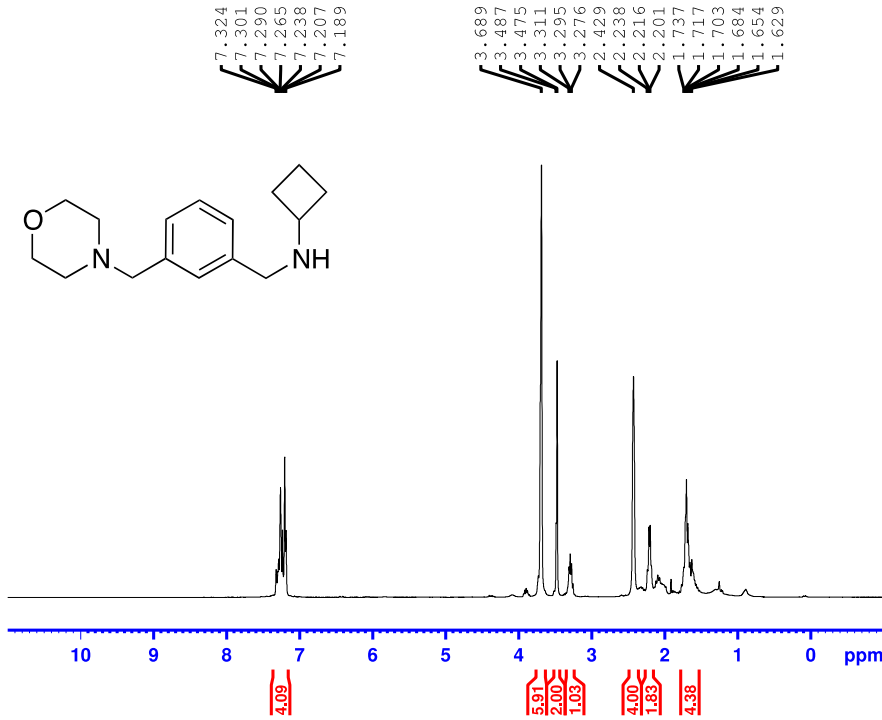
Minimum: -1.5

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)

SB-V-90



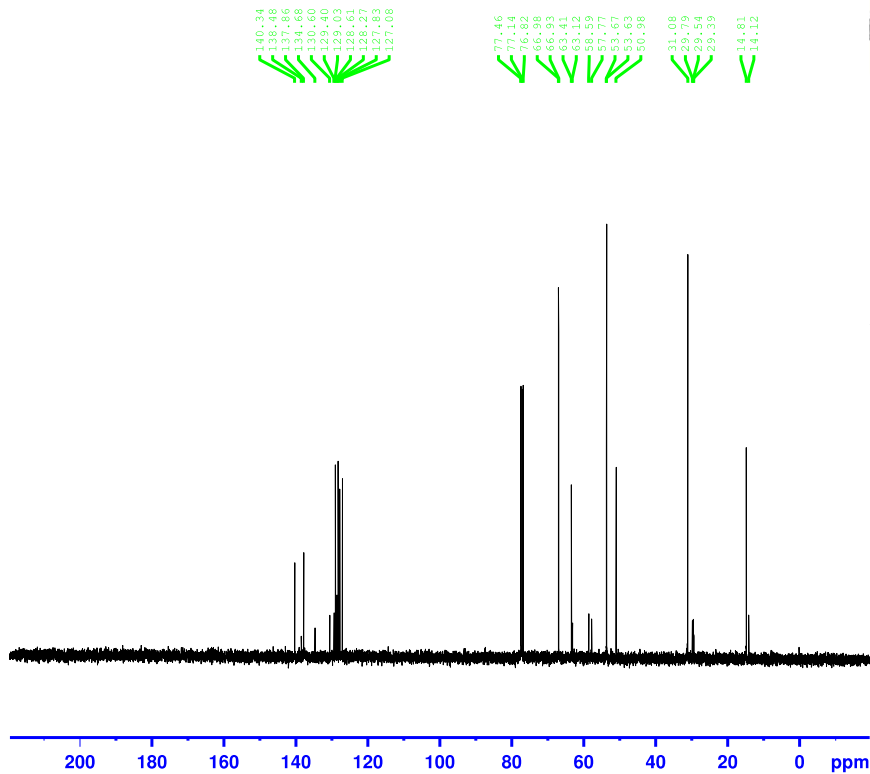
Current Data Parameters  
 NAME SB-V-90  
 EXPNO 1  
 PROCNO 1

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

SB-V-90



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

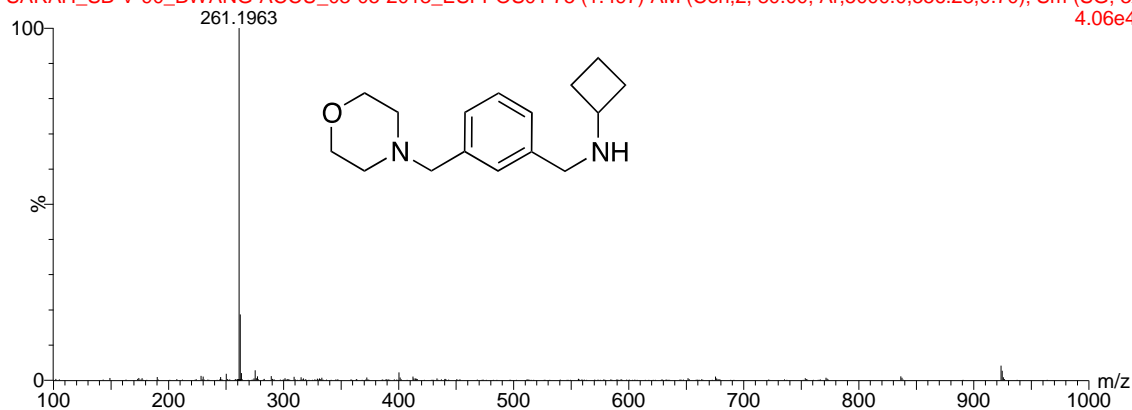
==== CHANNEL f2 =====  
 SFO2 400.1416006 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 FCPD2 90.00 usec  
 PLW2 16.00000000 W  
 PLW12 0.36000001 W  
 PLW13 0.29159999 W

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

in 90%MeOH

17:37:00 05-Mar-2013

SARAH\_SB-V-90\_BWANG-ACCU\_03-05-2013\_ESI-POS01 75 (1.497) AM (Cen,2, 80.00, Ar,5000.0,556.28,0.70); Sm (SG, 3x 4.06e4



### 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

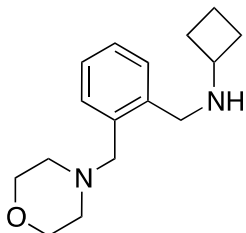
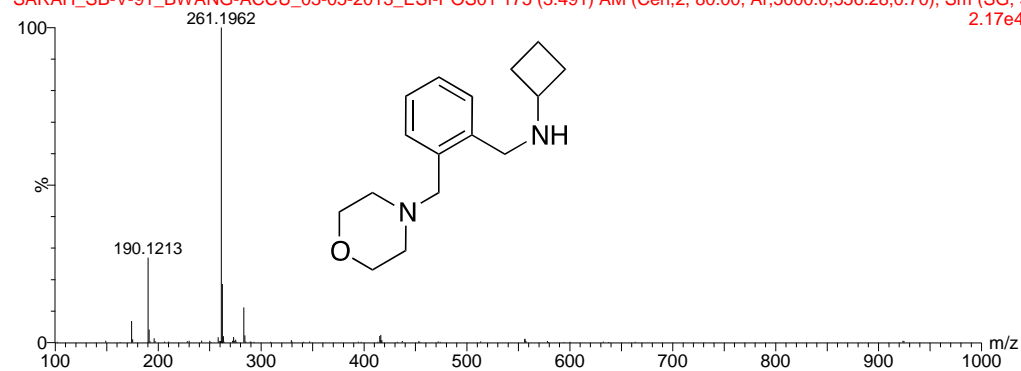
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
261.1963	261.1967	-0.4	-1.5	5.5	2.5	C16 H25 N2 O



in 90%MeOH

18:08:53 05-Mar-2013

SARAH\_SB-V-91\_BWANG-ACCU\_03-05-2013\_ESI-POS01 175 (3.491) AM (Cen,2, 80.00, Ar,5000.0,556.28,0.70); Sm (SG, 3  
2.17e4



### 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	

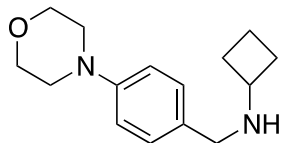
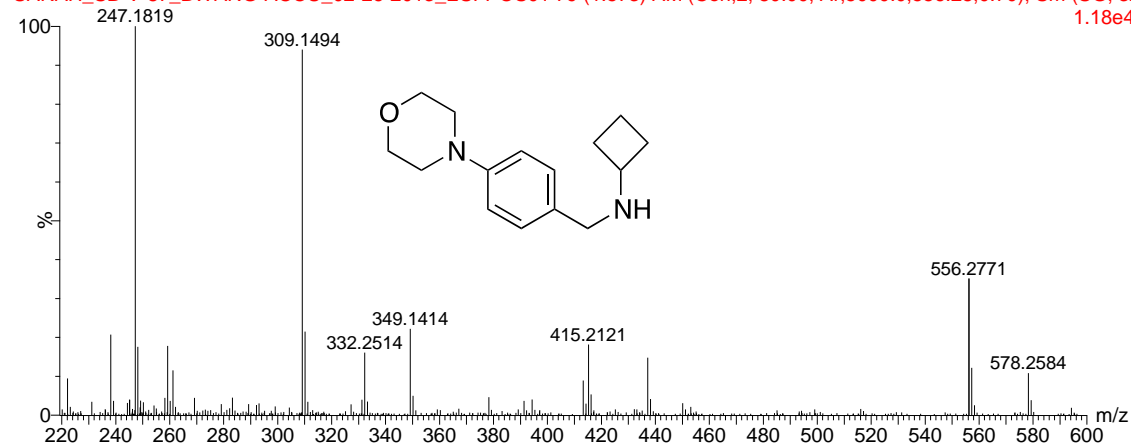


# N-(4-Morpholinobenzyl)cyclobutanamine (11d)

MeOH

14:20:04 26-Feb-2013

SARAH\_SB-V-87\_BWANG-ACCU\_02-26-2013\_ESI-POS01 79 (1.573) AM (Cen,2, 80.00, Ar,5000.0,556.28,0.70); Sm (SG, 3x 1.18e4



## 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

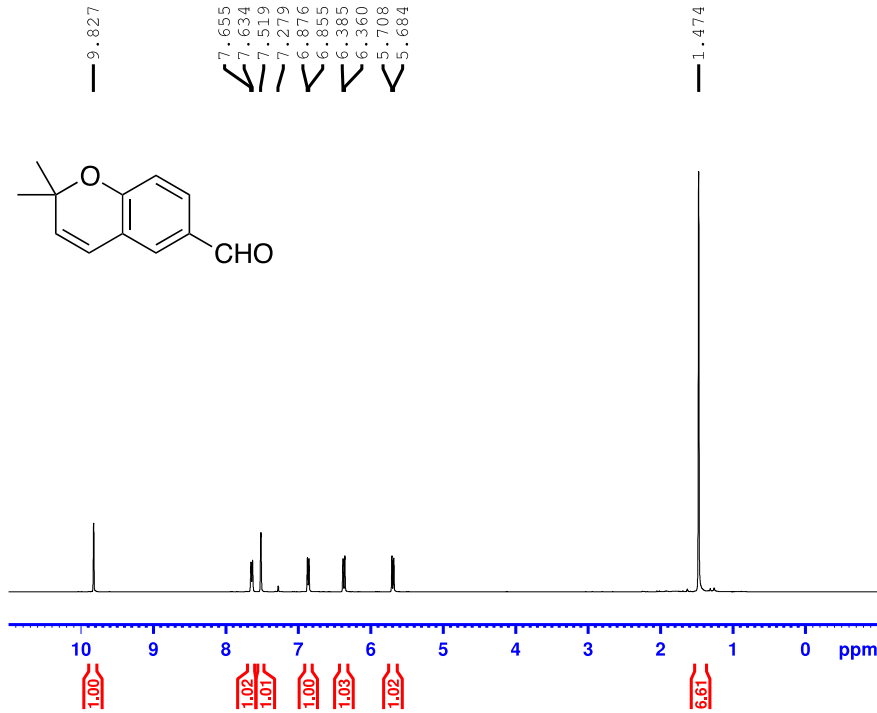
5.0

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-2H-chromene-6-carbaldehyde (12)

JH-I-50ca



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

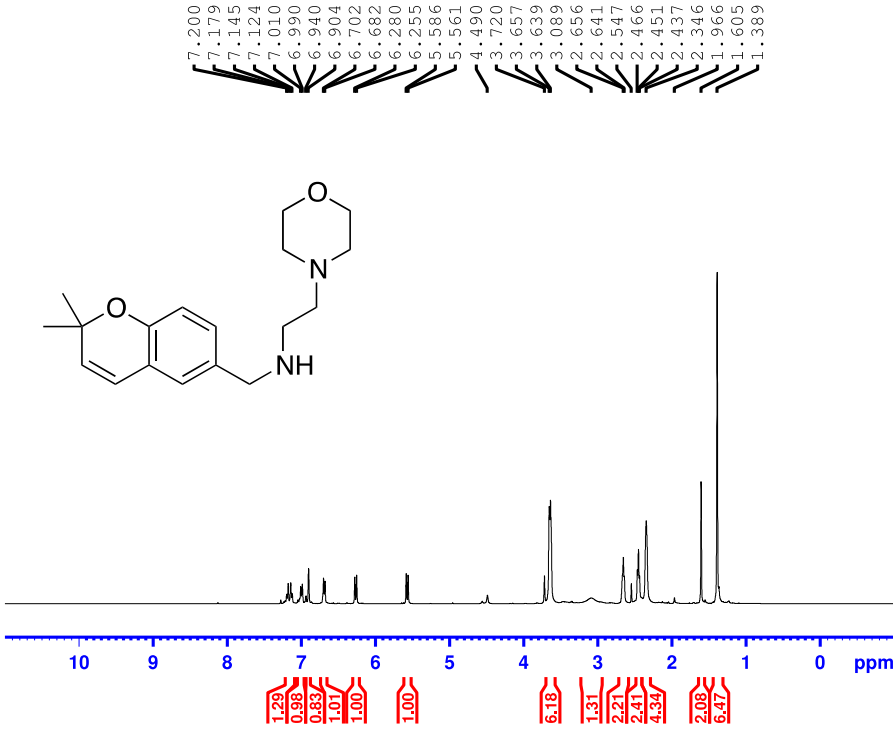
F2 - Acquisition Parameters  
Date\_ 20130118  
Time 9.45  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 50.8  
DW 62.400 usec  
DE 6.50 usec  
TE 293.8 K  
D1 1.00000000 sec  
TD0 1

===== 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-2H-chromen-6-yl)methyl)-2-morpholinoethanamine (13a)

SB-V-84



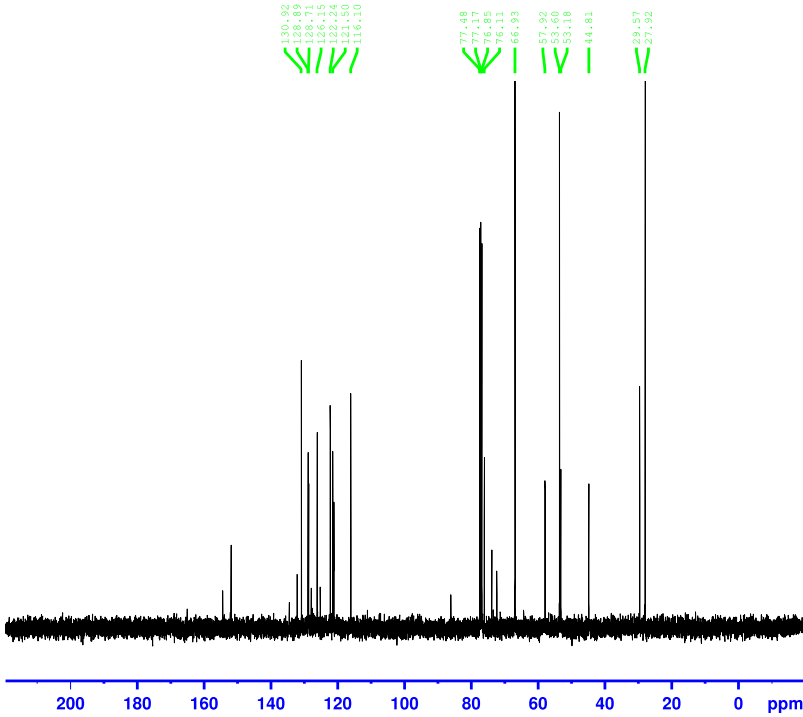
Current Data Parameters  
 NAME SB-V-84  
 EXPNO 1  
 PROCNO 1

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 4.089465 sec  
 RG 18  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 1.0000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 400.1424710 MHz  
 NUC1 1H  
 P1 13.50 usec  
 PLW1 16.0000000 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-84



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 2.0000000 sec  
 D11 0.0300000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 100.6253441 MHz  
 NUC1 13C  
 P1 9.00 usec  
 PLW1 62.0000000 W

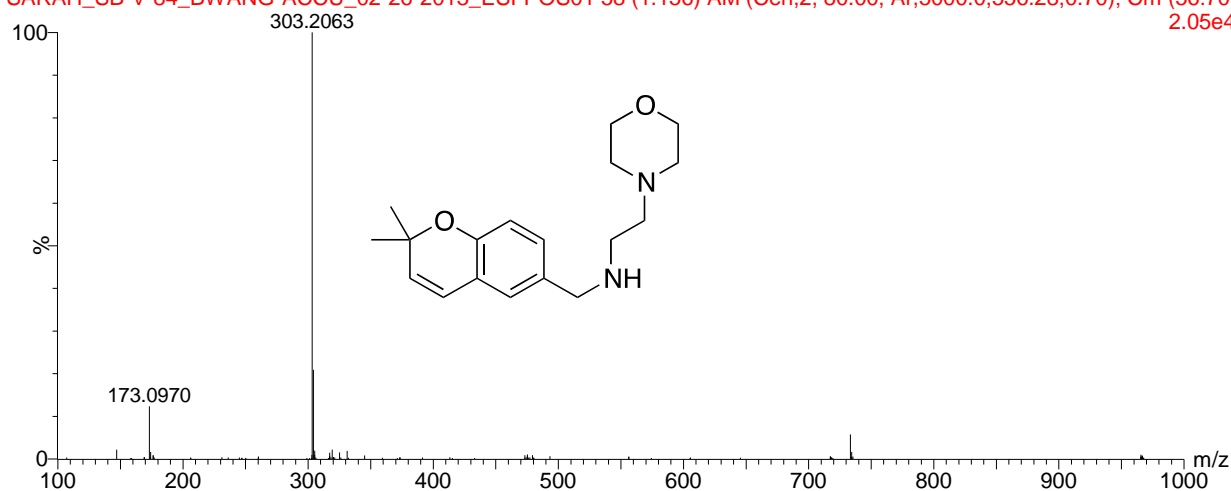
===== CHANNEL f2 =====  
 SFO2 400.1416006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 FCPD2 30.00 usec  
 FLW2 16.0000000 W  
 PLW2 0.3600001 W  
 FLW3 0.29159999 W

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

MeOH

14:26:13 26-Feb-2013

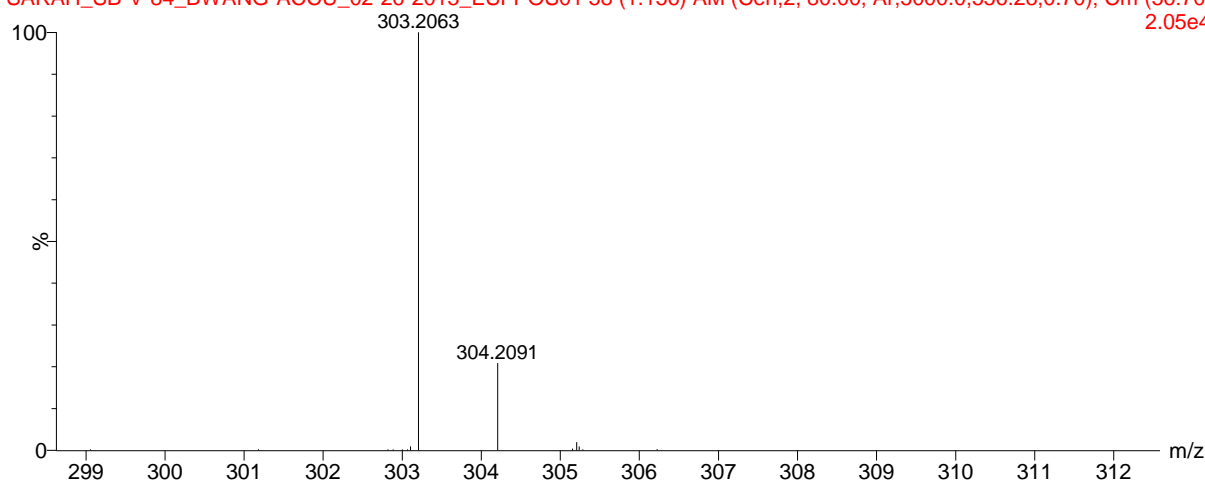
SARAH\_SB-V-84\_BWANG-ACCU\_02-26-2013\_ESI-POS01 58 (1.156) AM (Cen,2, 80.00, Ar,5000.0,556.28,0.70); Cm (56:70) 2.05e4



MeOH

14:26:13 26-Feb-2013

SARAH\_SB-V-84\_BWANG-ACCU\_02-26-2013\_ESI-POS01 58 (1.156) AM (Cen,2, 80.00, Ar,5000.0,556.28,0.70); Cm (56:70) 2.05e4



### 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

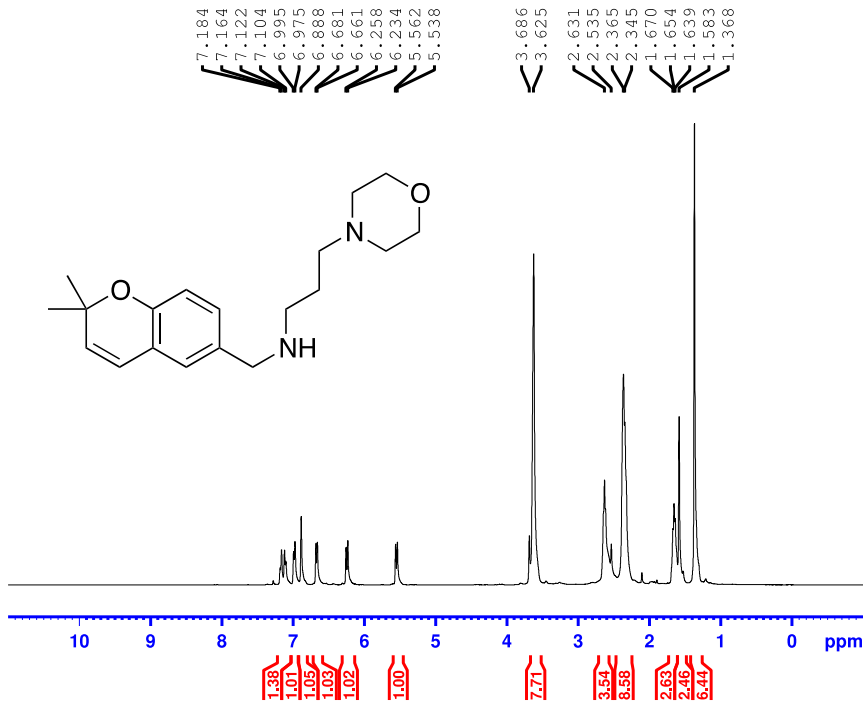
Minimum: -1.5

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-2H-chromen-6-yl)methyl)-3-morpholinopropan-1-amine (13b)

SB-V-85



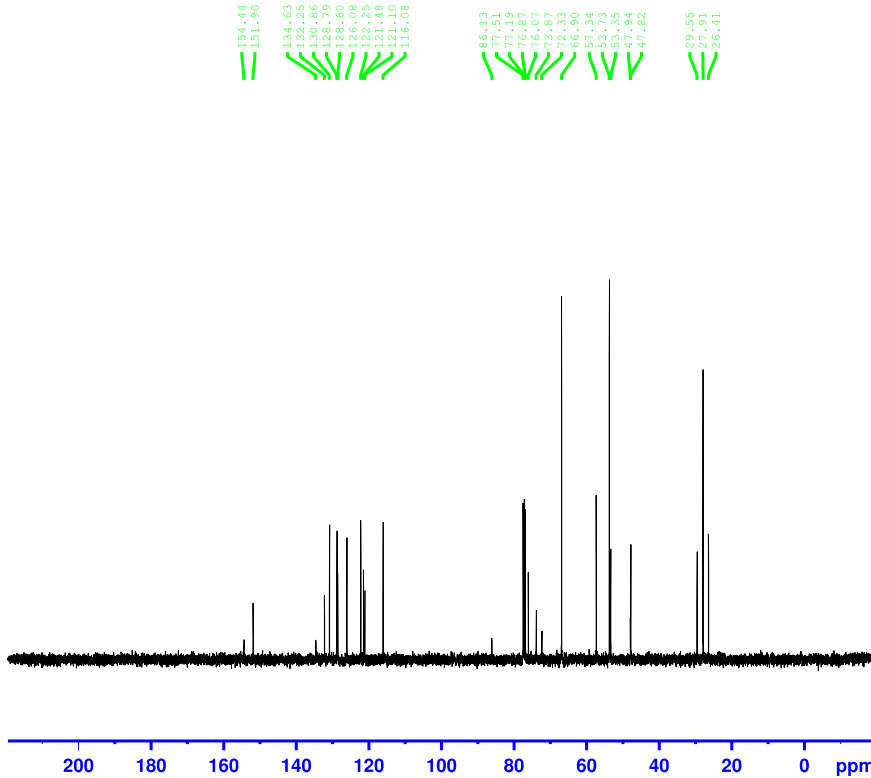
Current Data Parameters  
 NAME SB-V-85  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20130216  
 Time 15.55  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDC13  
 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

SB-V-85



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 CDC13  
 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

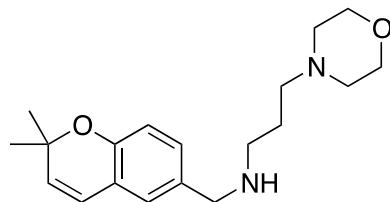
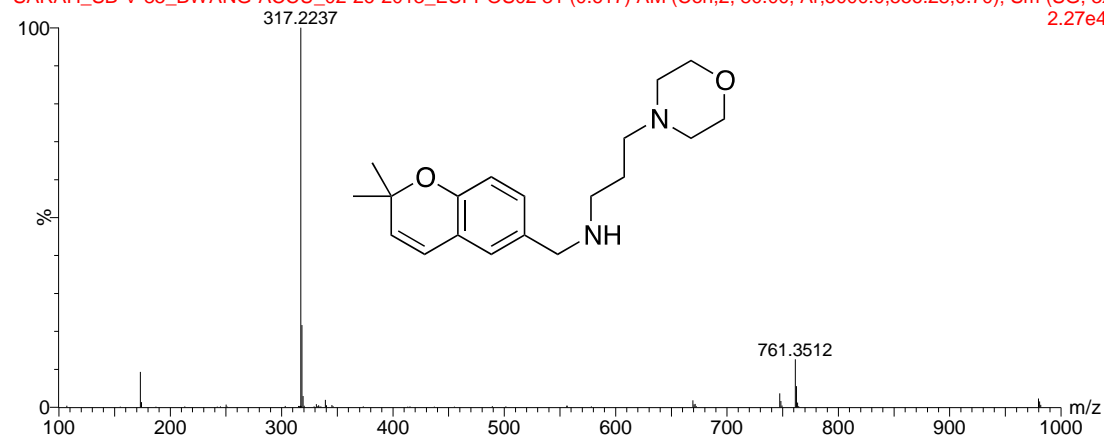
----- CHANNEL f2 -----  
 SFO2 400.1416006 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 16.00000000 W  
 PLW12 0.36000001 W  
 PLW13 0.29159999 W

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

MeOH

14:37:29 26-Feb-2013

SARAH\_SB-V-85\_BWANG-ACCU\_02-26-2013\_ESI-POS02 31 (0.617) AM (Cen,2, 80.00, Ar,5000.0,556.28,0.70); Sm (SG, 3x 2.27e4



### 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

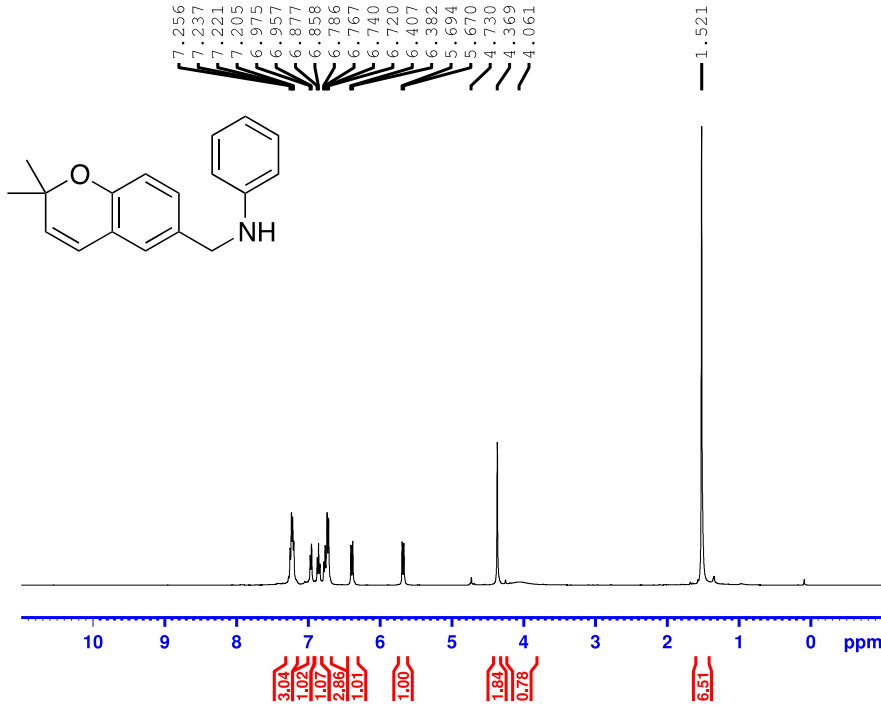
Maximum:

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

SB-IV-53



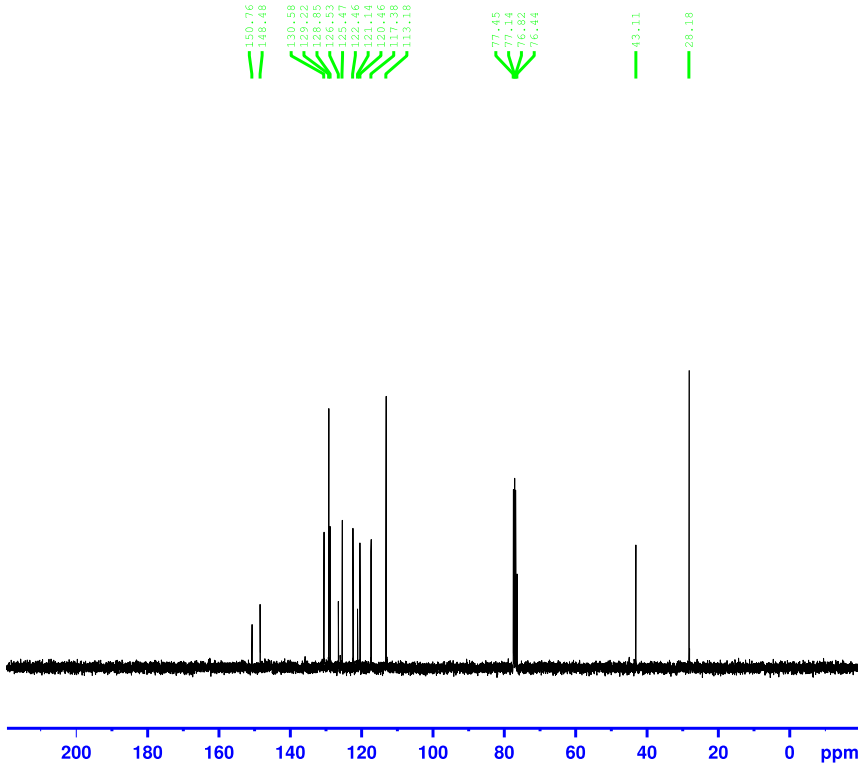
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 NAME SB-IV-53  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
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 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



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 =====  
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 P1 9.00 usec  
 PLW1 62.00000000 W  
 SFO1 100.6253441 MHz

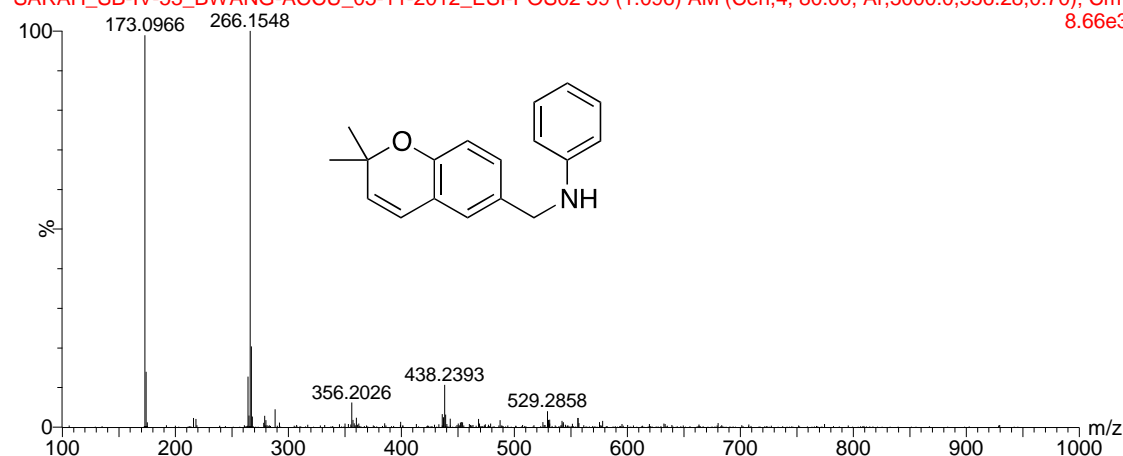
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 PCPD2 90.00 usec  
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 PLW12 0.36000001 W  
 PLW13 0.29159999 W  
 SFO2 400.1416006 MHz

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

100%MeOH+HCOOH

13:24:05 11-May-2012

SARAH\_SB-IV-53\_BWANG-ACCU\_05-11-2012\_ESI-POS02 59 (1.096) AM (Cen,4, 80.00, Ar,5000.0,556.28,0.70); Cm (8.66e3



### 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

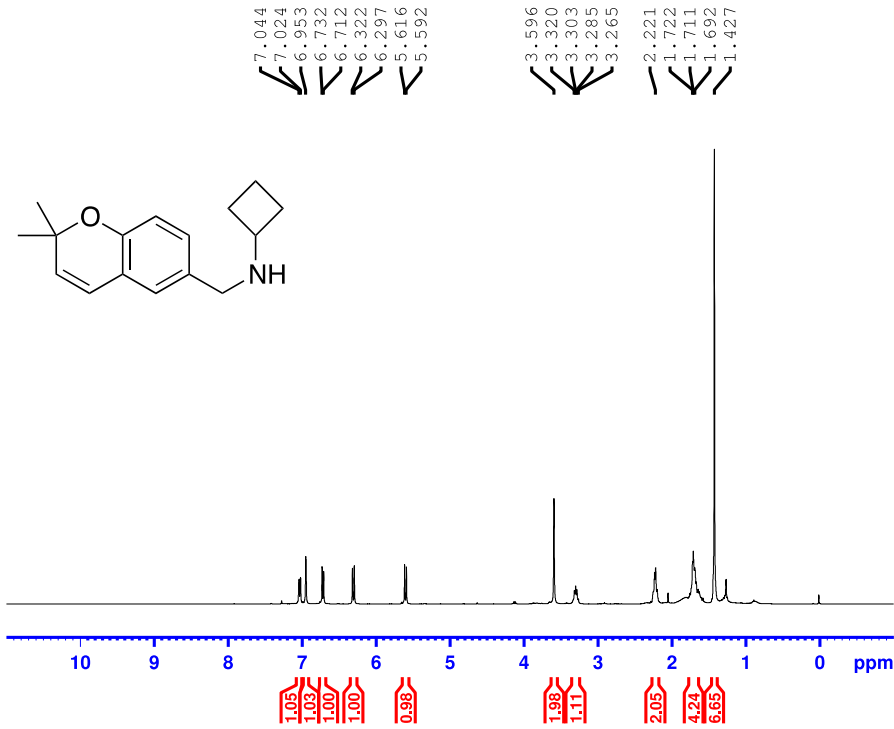
Maximum: 5.0 5.0 50.0

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-2H-chromen-6-yl)methyl)cyclobutanamine (14b)

SB-IV-9a



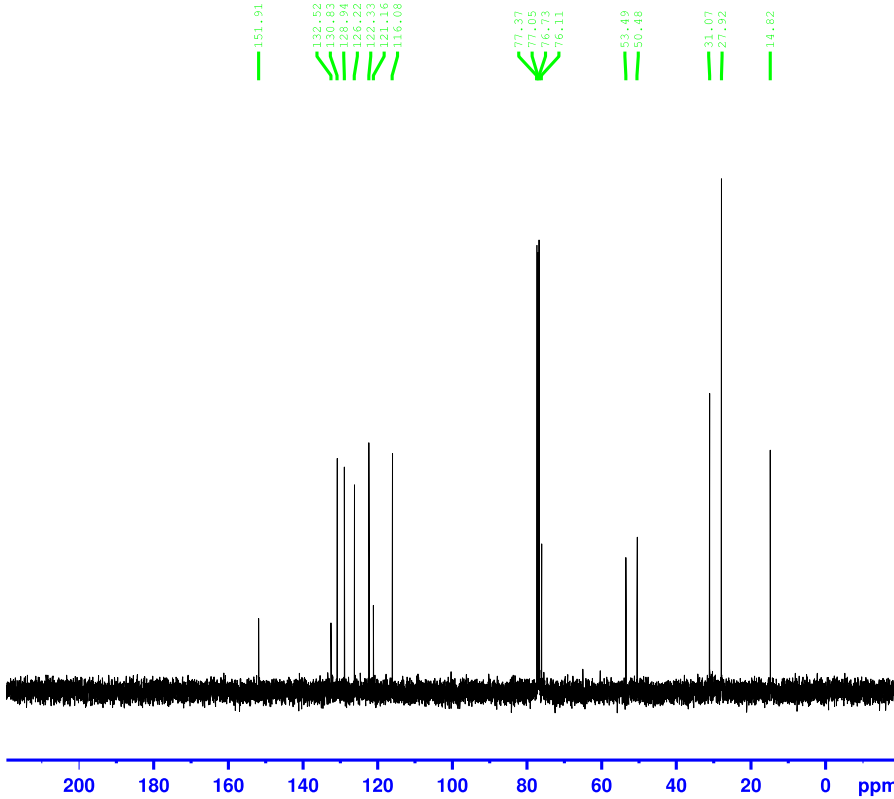
Current Data Parameters  
 NAME SB-IV-9a  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120405  
 Time 16.15  
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 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 =====  
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 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 0.38000001 W  
 PLW13 0.29159999 W  
 SFO2 400.1416006 MHz

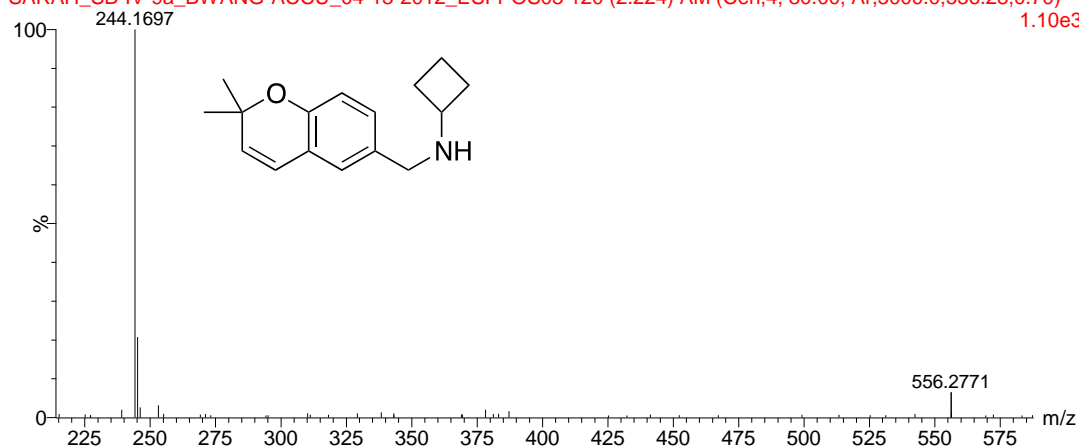
F2 - Processing parameters  
 SI 32768  
 SF 100.6152830 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

100%MeOH+0.1%HCOOH

15:32:23 13-Apr-2012

SARAH\_SB-IV-9a\_BWANG-ACCU\_04-13-2012\_ESI-POS03 120 (2.224) AM (Cen,4, 80.00, Ar,5000.0,556.28,0.70)

1.10e3



### 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

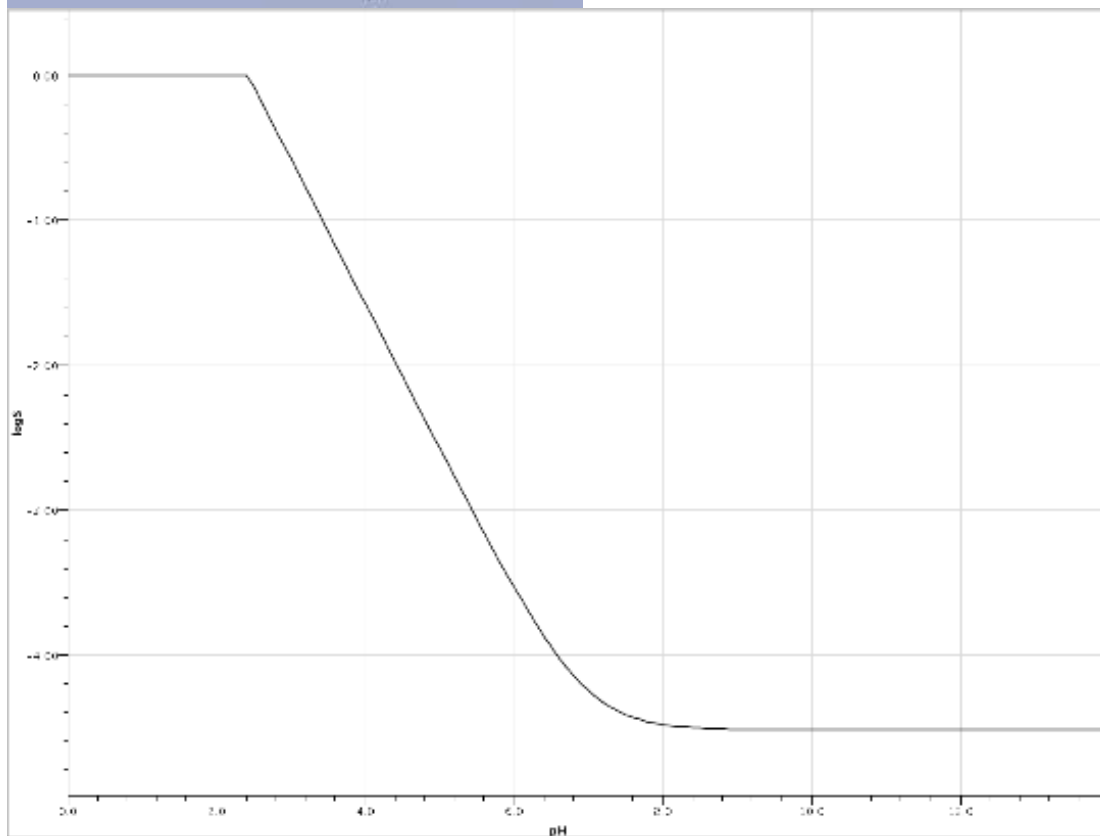
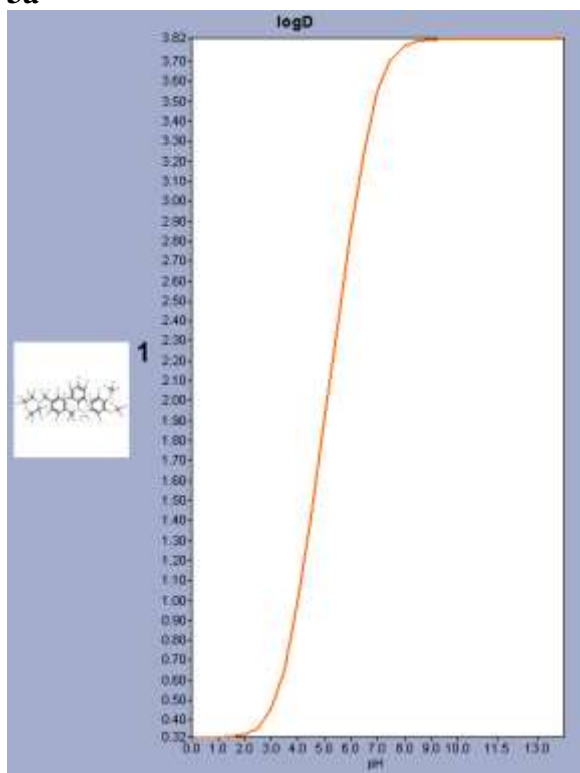
PPM DBE i-FIT Formula

244.1697 244.1701 -0.4

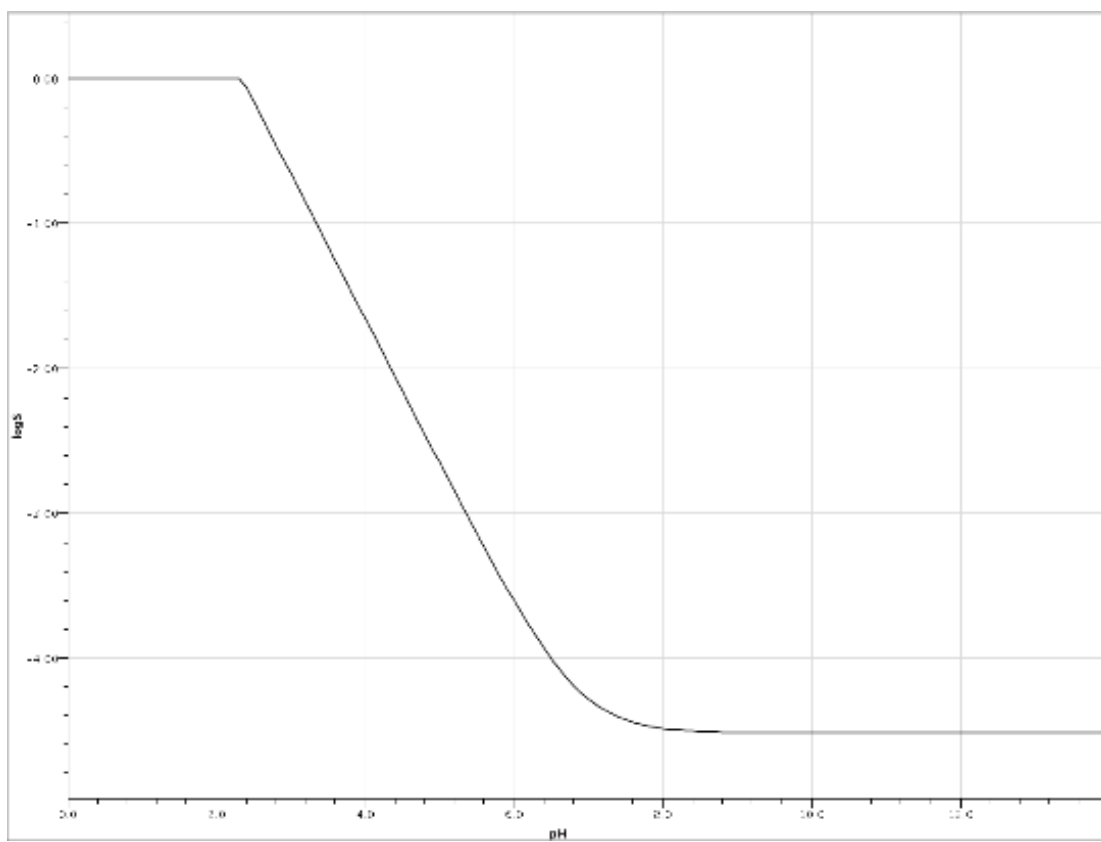
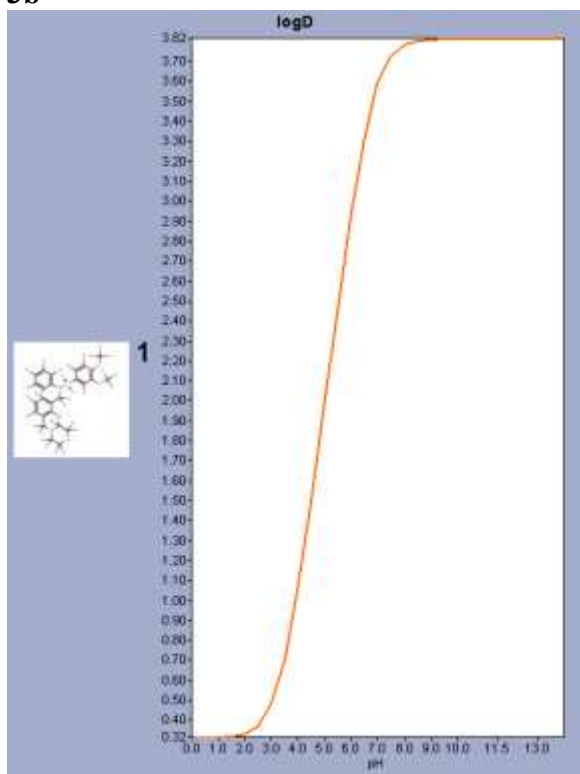
-1.6 6.5 2.7 C16 H22 N O

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

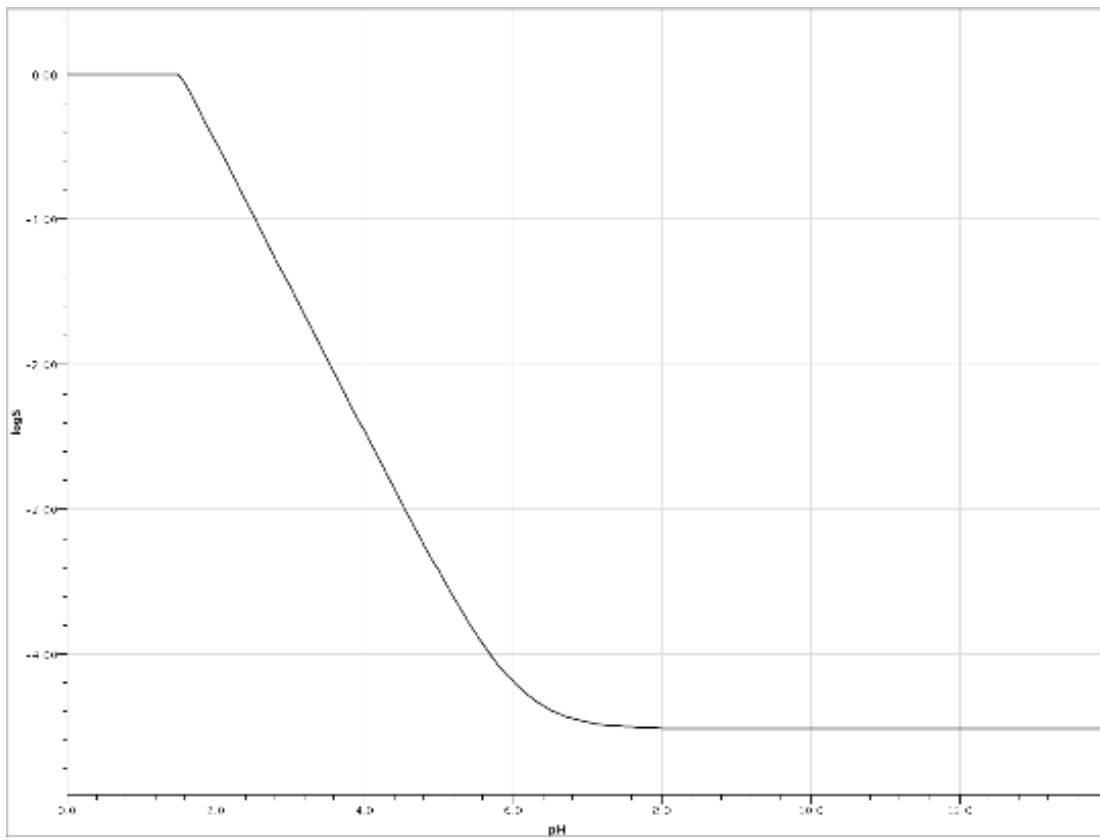
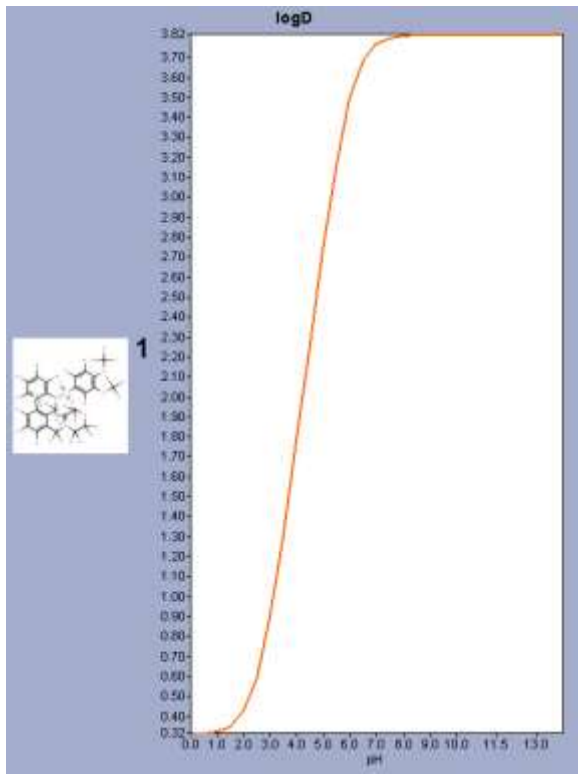
**3a**



3b

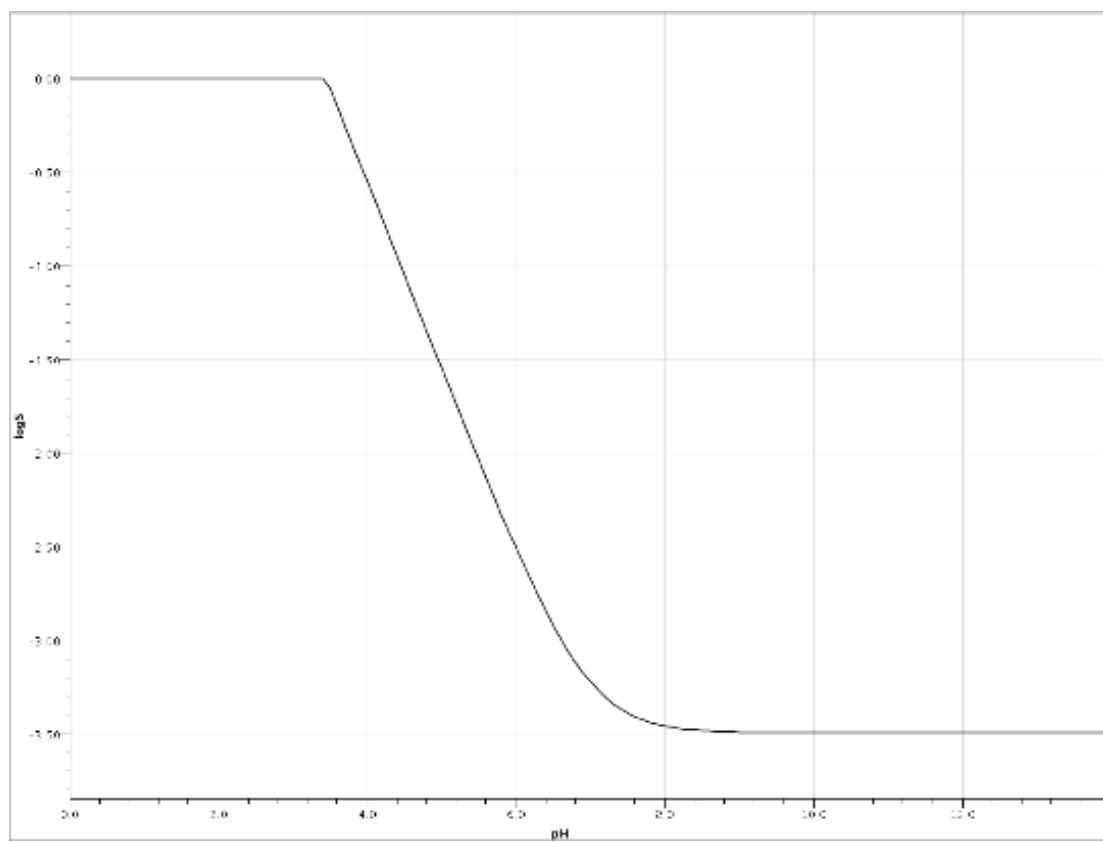
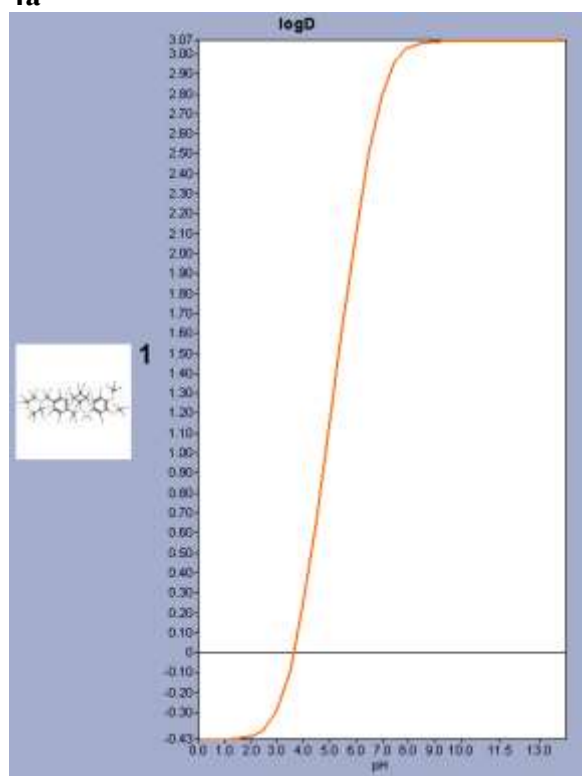


3c

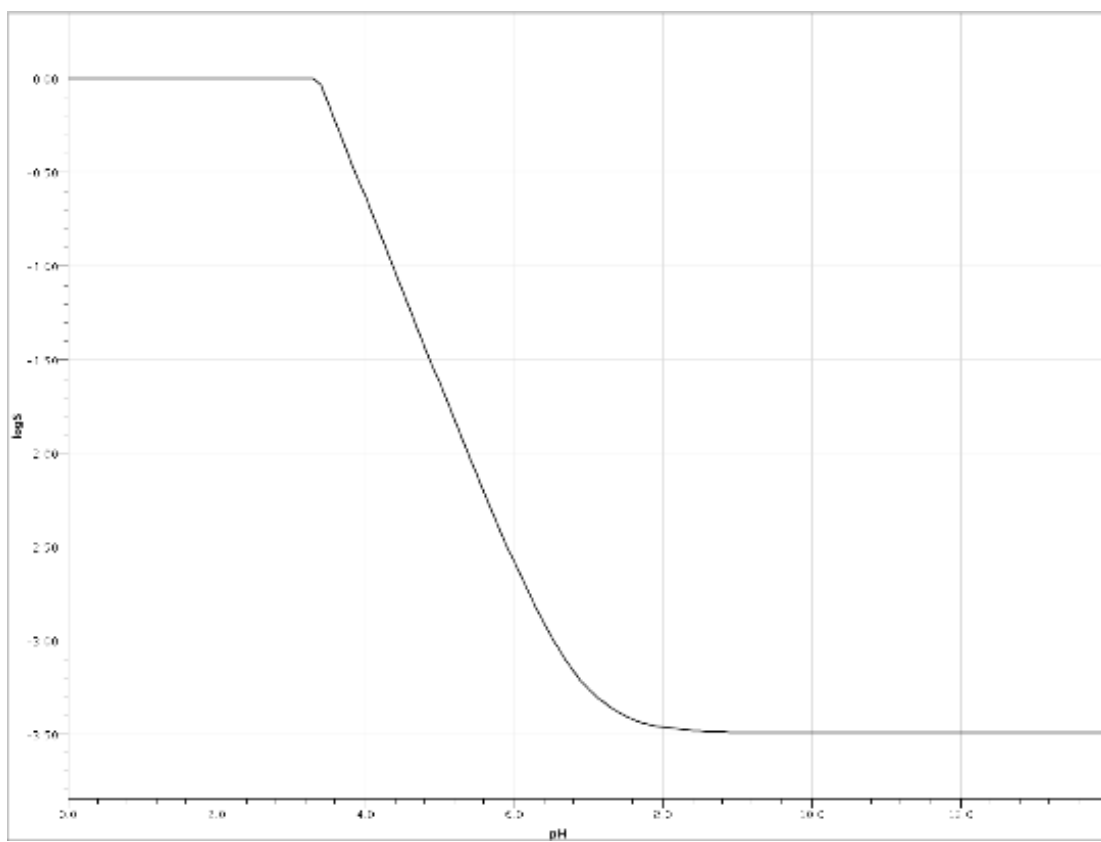
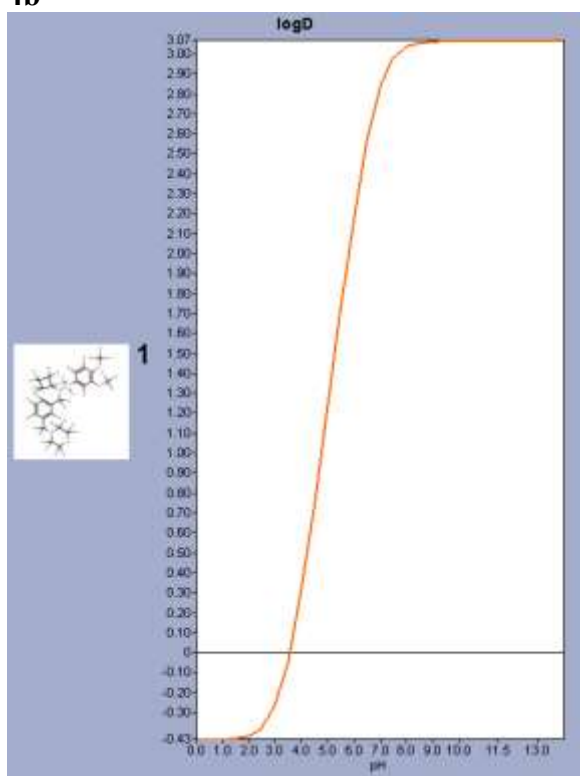




4a

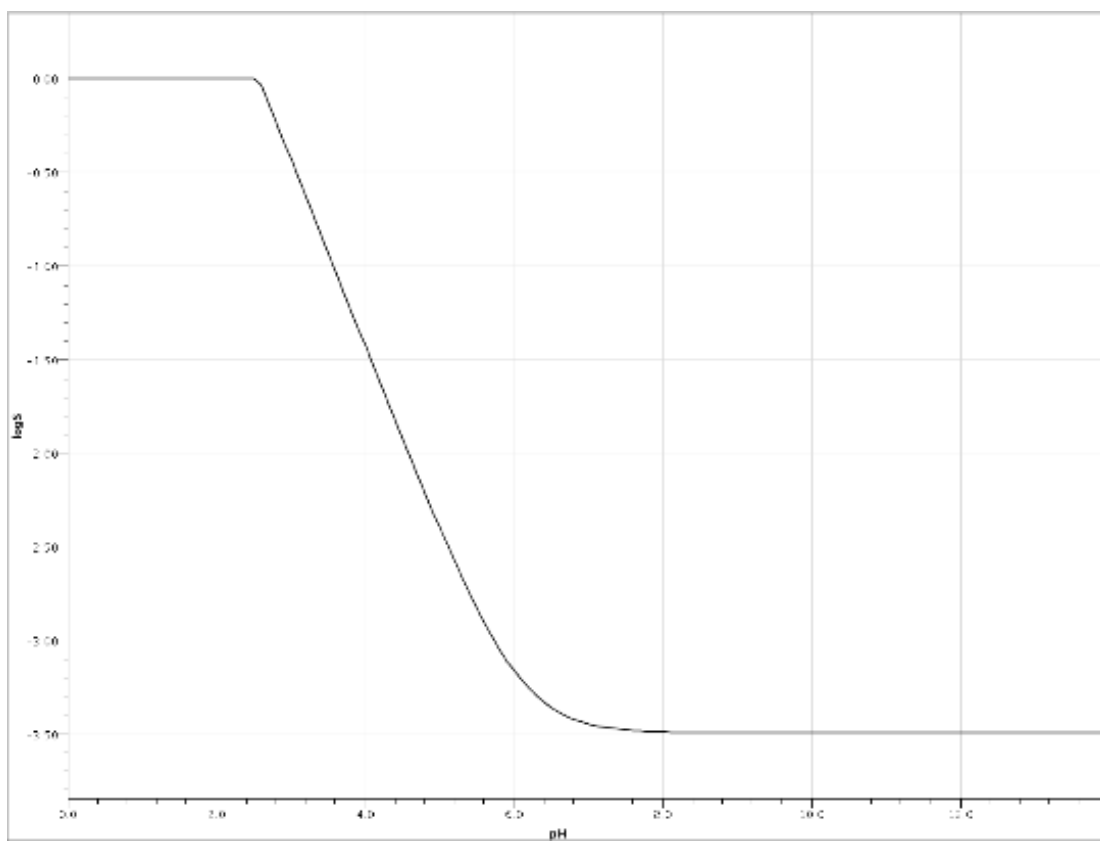
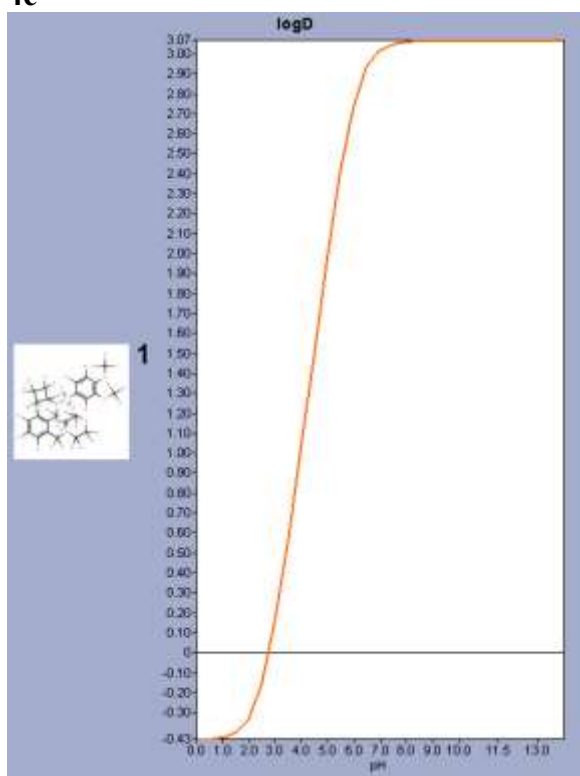


4b

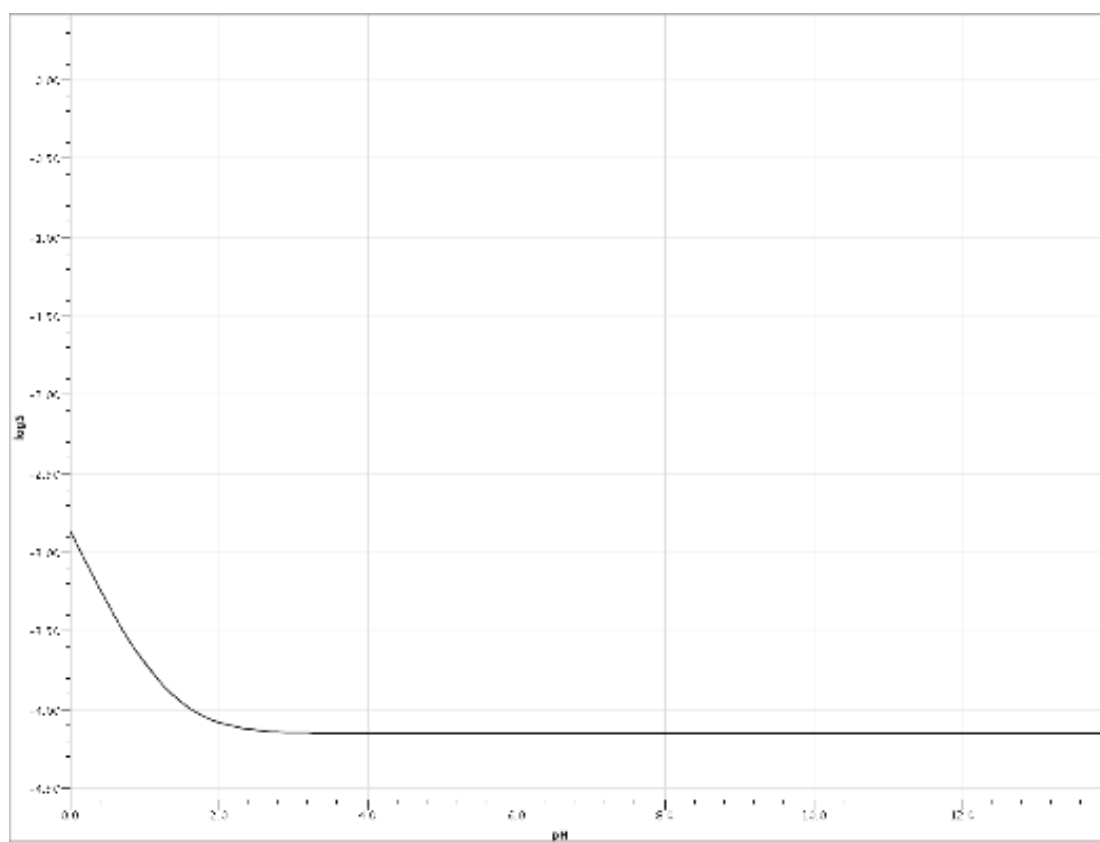
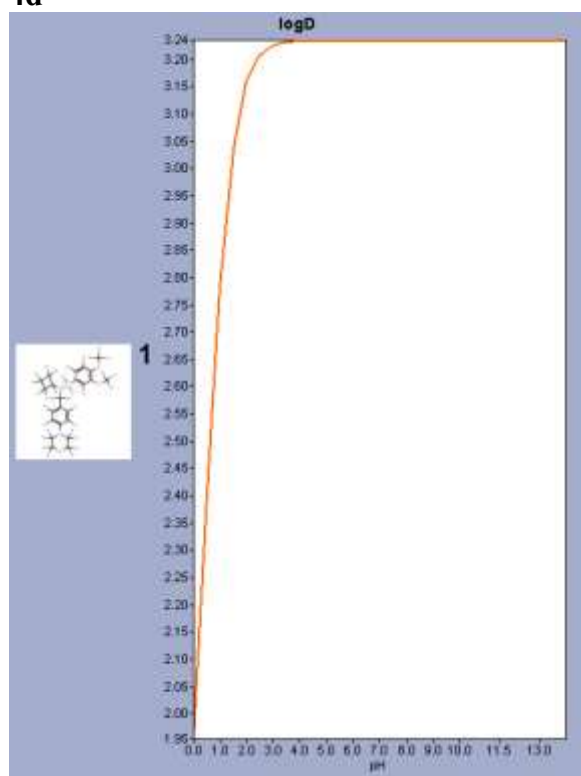




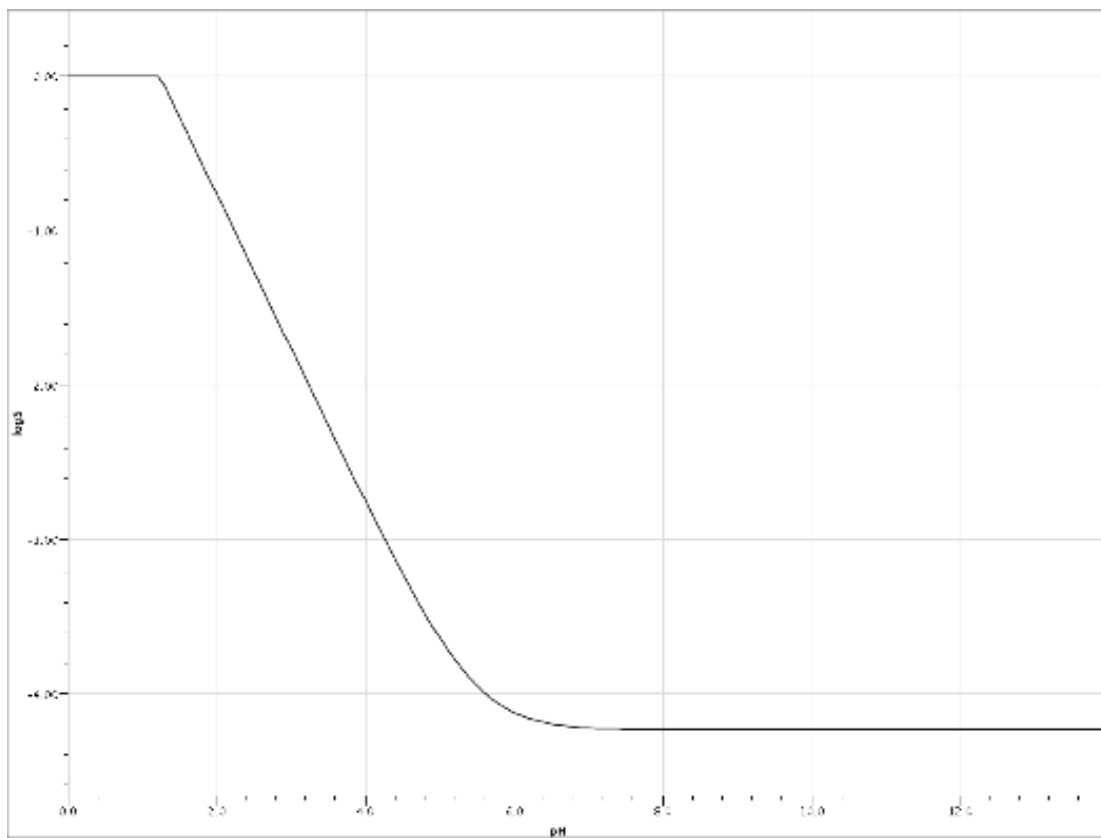
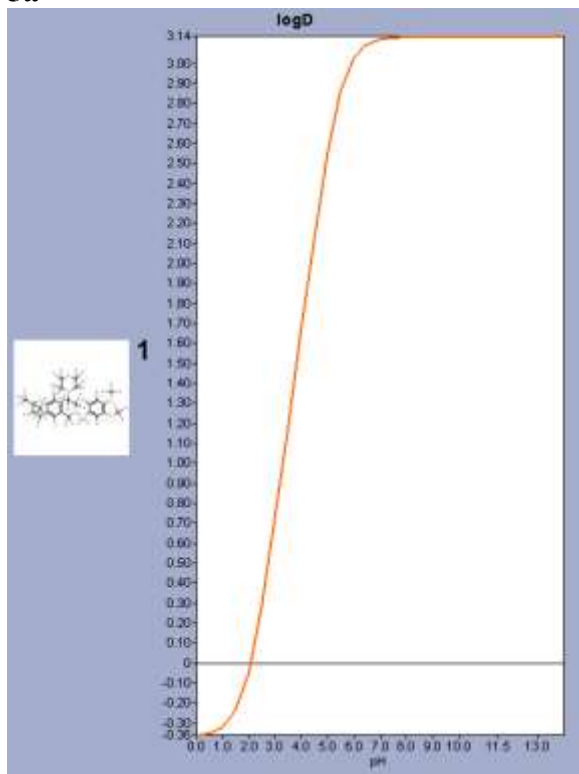
4c



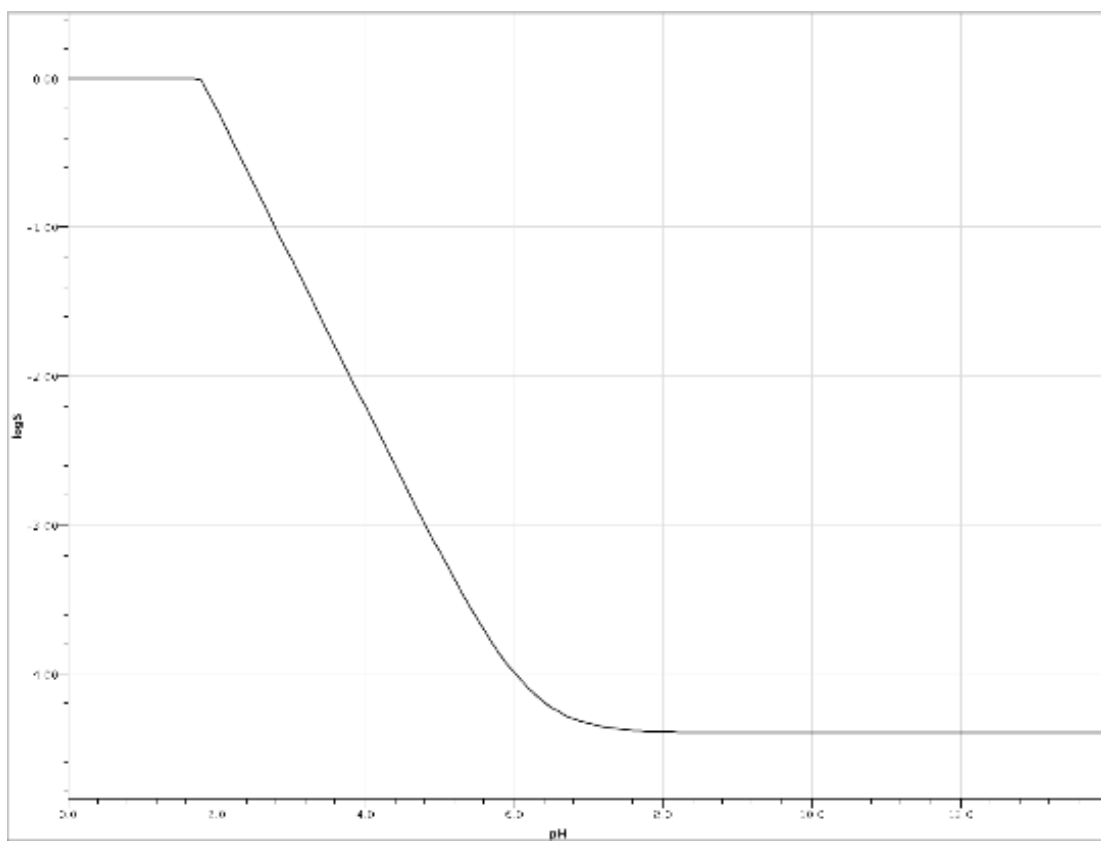
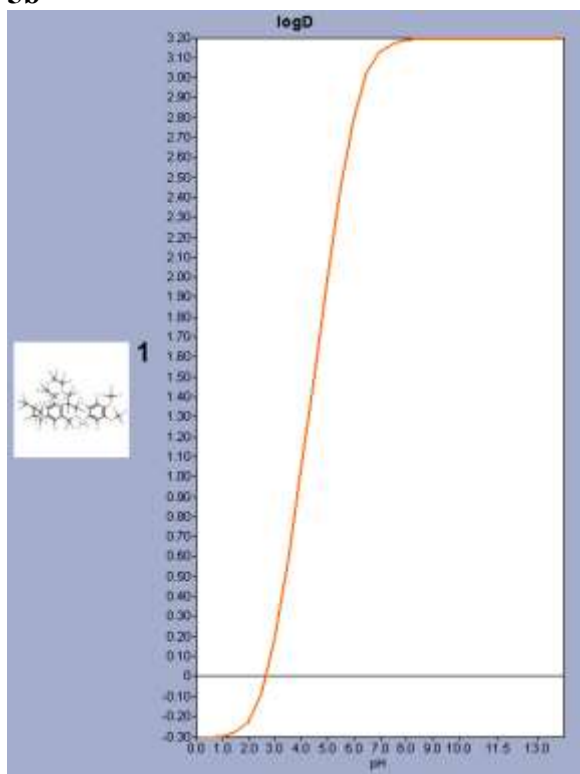
4d



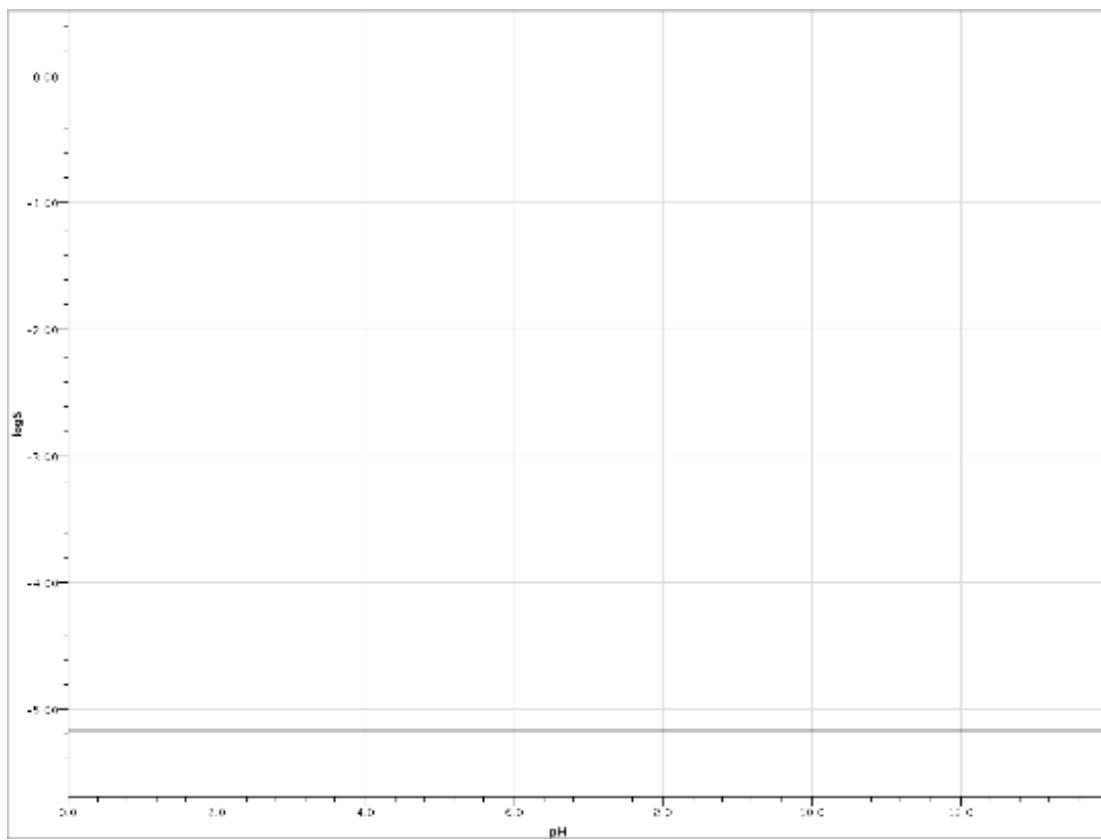
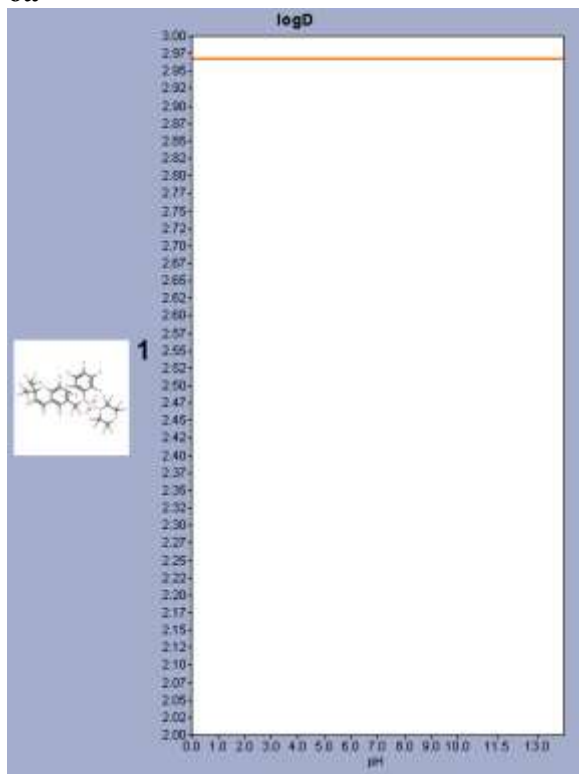
5a



5b



6a



6b

