Electronic Supplementary Material (ESI) for RSC Advances.


# Supporting Information

## An Approach Towards Expanding the Scope of Masked *o*-Benzoquinone dimers to Generate Diverse Compound Libraries

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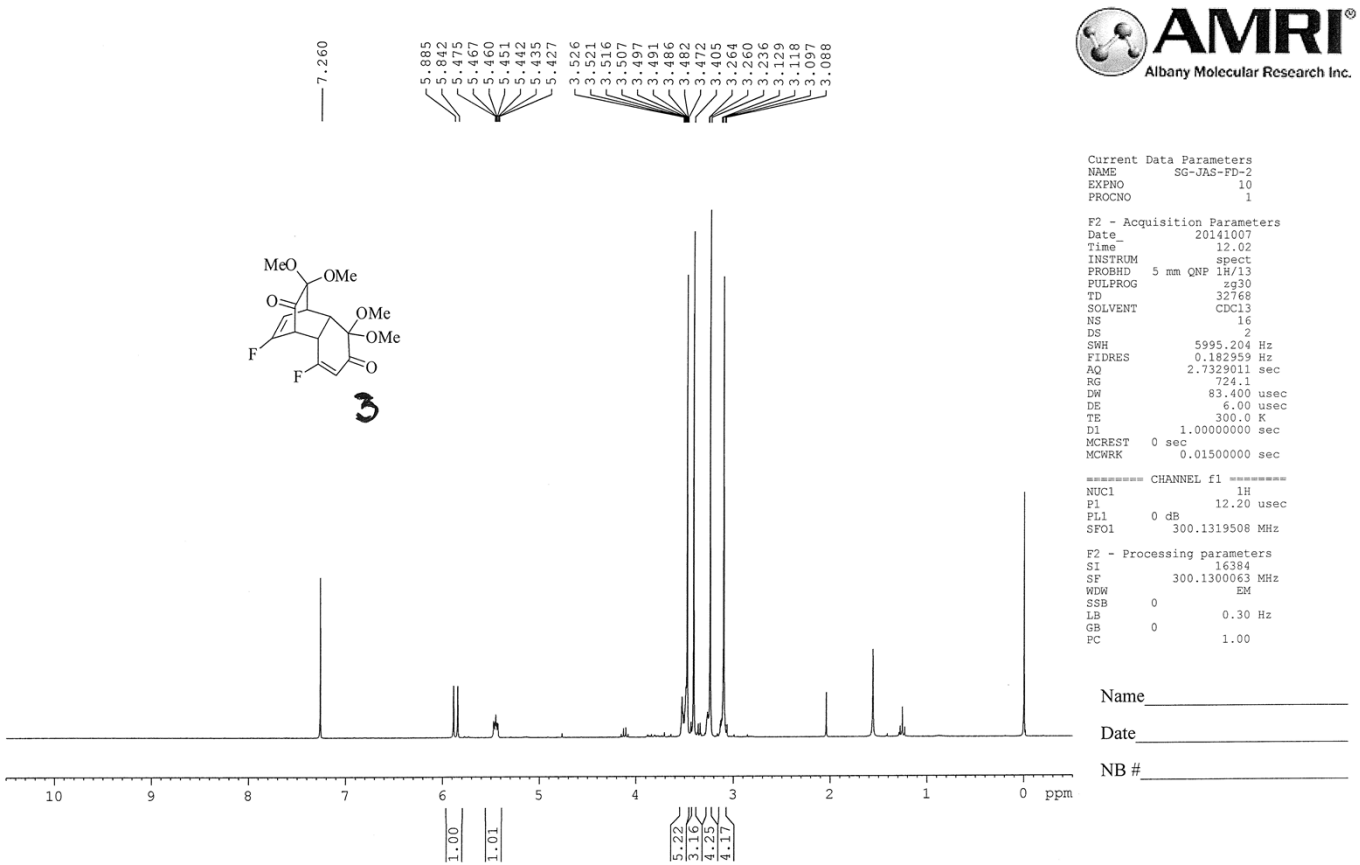


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```
Current Data Parameters
NAME          SG-JAS-FD-2
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_           20141007
Time               12.02
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    2
SWH             5995.204 Hz
FIDRES          0.182959 Hz
AQ              2.7329011 sec
RG                 724.1
DW                83.400 usec
DE                 6.00 usec
TE                300.0 K
D1             1.00000000 sec
MCREST    0 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                 12.20 usec
PL1       0 dB
SFO1         300.1319508 MHz

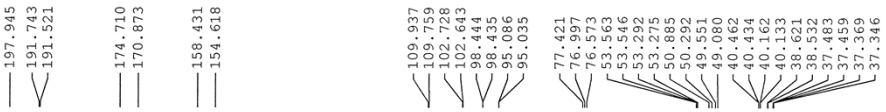
F2 - Processing parameters
SI                 16384
SF          300.1300063 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Name_____

Date_____

NB #_____

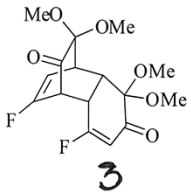
AMRI; SRC
location; 15




Name_____

Date_____

NB #_____

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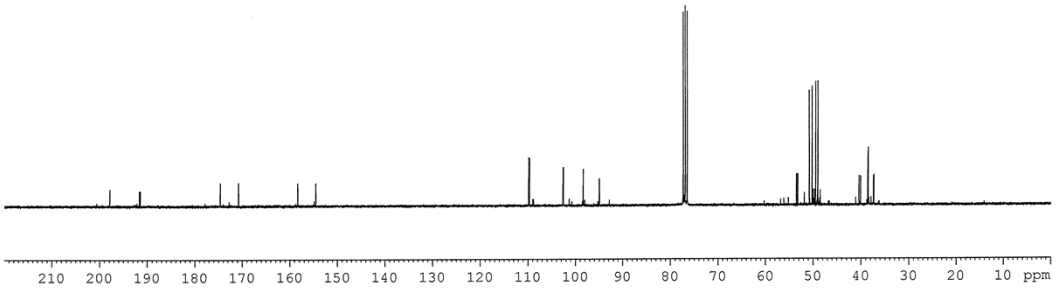


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Current Data Parameters
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EXPNO                  21
PROCNO                  1

F2 - Acquisition Parameters
Date_           20140724
Time                0.04
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 7000
DS                    0
SWH           22675.736 Hz
FIDRES         0.346004 Hz
AQ             1.4451188 sec
RG                1824.6
DW                22.050 usec
DE                 6.00 usec
TE                300.0 K
D1           0.50000000 sec
d11          0.03000000 sec
DELTA        0.40000001 sec
MCREST   0 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                 8.00 usec
PL1               -2.00 dB
SFO1         75.4767751 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             80.00 usec
PL2       0 dB
PL12              16.33 dB
PL13              16.00 dB
SFO2        300.1315007 MHz

F2 - Processing parameters
SI                131072
SF           75.4677504 MHz
WDW                  EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.40
```

# Mass Spectrum SmartFormula Report

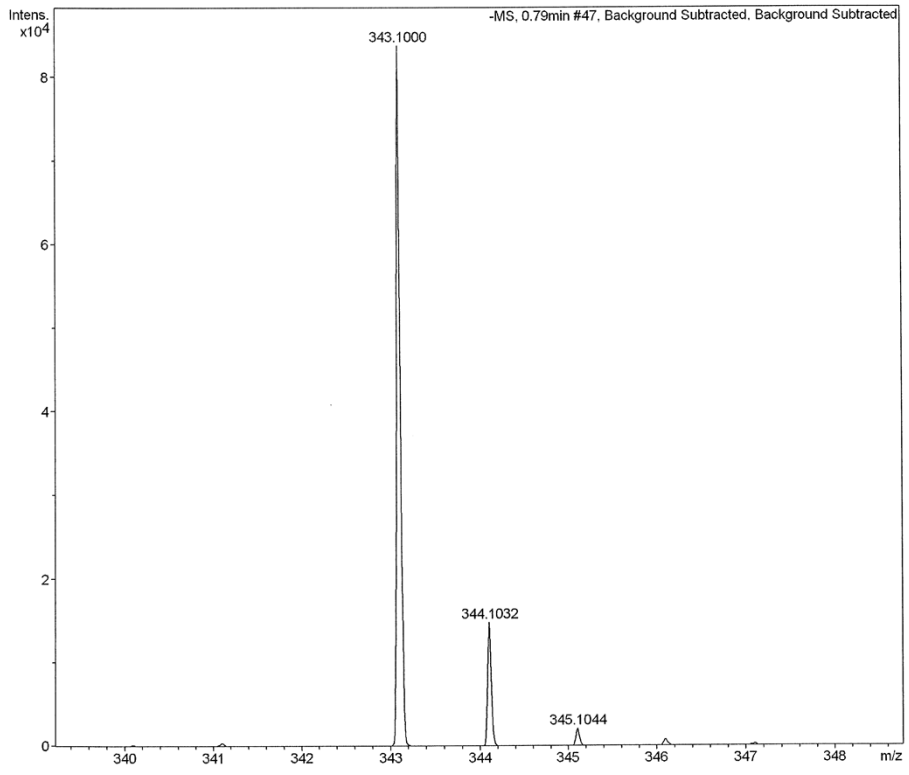
**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Chemistry\Outside\AMRI\5F-Dimer-1.d | Acquisition Date | 1/14/2015 10:31:34 AM |
| Method | YCH_Neg-150-1800.m | Operator | default user |
| Sample Name | 5F-Dimer | Instrument / Ser# | micrOTOF-Q II 10269 |
| Comment | AMRI | | |

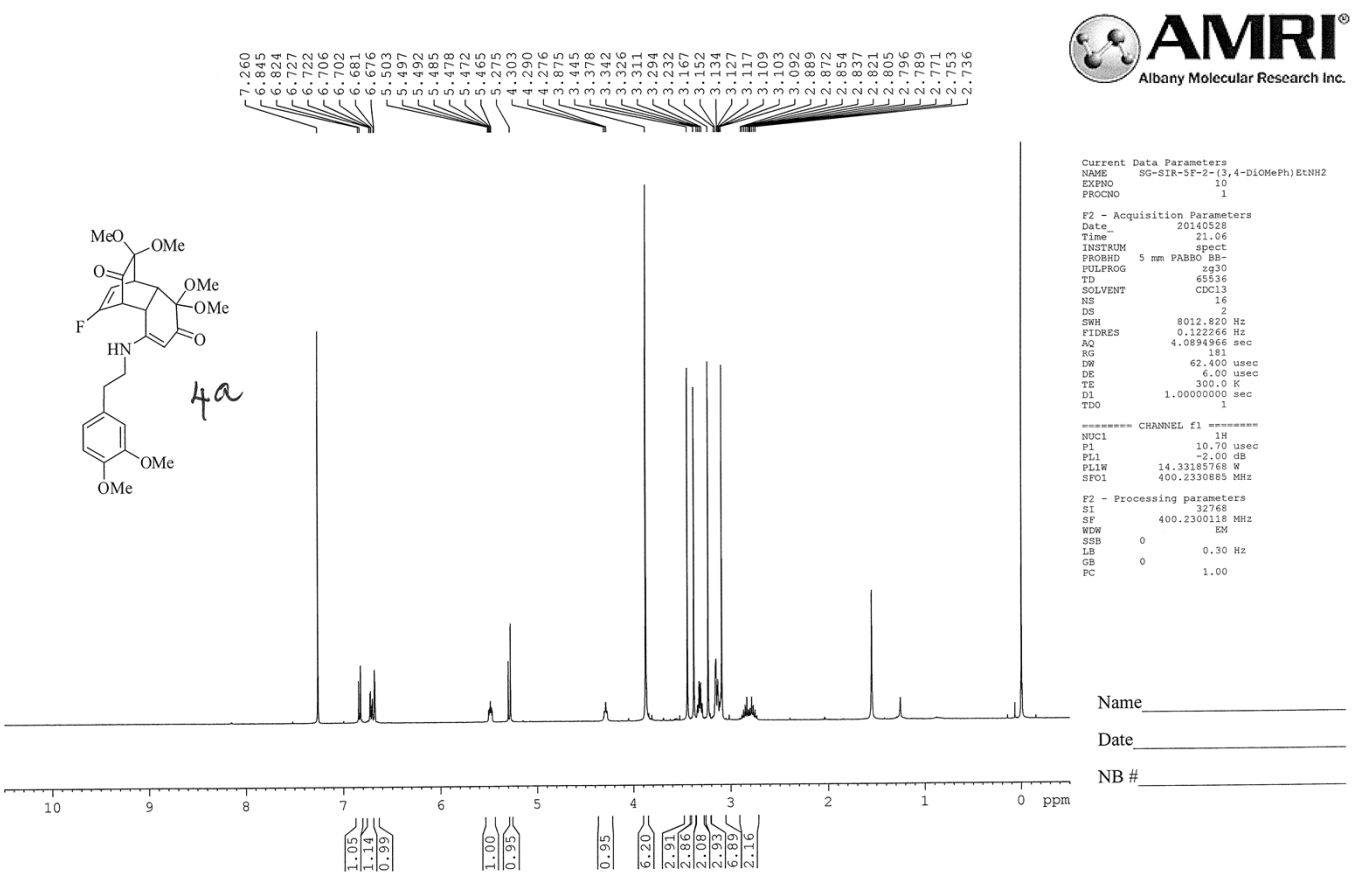
**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Negative | Set Nebulizer | 2.0 Bar |
| Focus | Not active | Set Capillary | 3500 V | Set Dry Heater | 200 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 6.0 l/min |
| Scan End | 1000 m/z | Set Collision Cell RF | 300.0 Vpp | Set Divert Valve | Waste |

| Meas. m/z | # | Formula | m/z | err [ppm] | rdb | e⁻ Conf | N-Rule |
|---|---|---|---|---|---|---|---|
| 343.1000 | 1 | C 16 H 17 F 2 O 6 | 343.0999 | -0.4 | 7.5 | even | ok |




Bruker Compass DataAnalysis 4.0 printed: 1/14/2015 10:39:55 AM Page 1 of 1

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```
Current Data Parameters
NAME      SG-SIR-5F-2-(3,4-DiOMePh)EtNH2
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140528
Time              21.06
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             4.0894966 sec
RG                  181
DW               62.400 usec
DE                6.00 usec
TE                300.0 K
D1             1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.70 usec
PL1               -2.00 dB
PL1W          14.33185768 W
SFO1          400.2330885 MHz

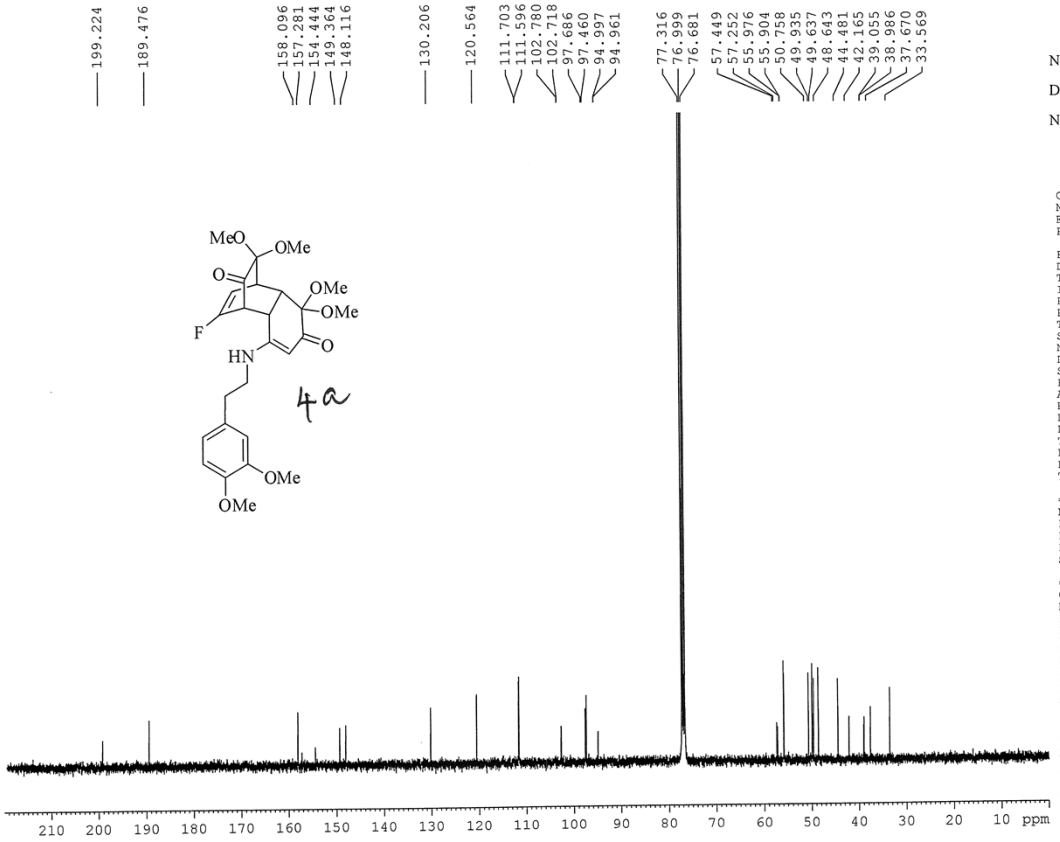
F2 - Processing parameters
SI                 32768
SF            400.2300118 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Name_____

Date_____

NB #_____

AMRI; SRC AV400
location; 18




AMRI

Name_____

Date_____

NB #_____

```
Current Data Parameters
NAME      SG-SIR-5F-2-(3,4-DiOMePh)EtNH2
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140529
Time                2.29
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                10000
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                  114
DW               20.800 usec
DE                6.50 usec
TE                300.0 K
D1            0.50000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 8.60 usec
PL1               -1.00 dB
PL1W        44.58811569 W
SFO1       100.6479769 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2               -2.00 dB
PL12              15.47 dB
PL13              15.72 dB
PL2W        14.33185768 W
PL12W        0.25662708 W
PL13W        0.24227159 W
SFO2       400.2316009 MHz

F2 - Processing parameters
SI                32768
SF         100.6379151 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

# Mass Spectrum SmartFormula Report

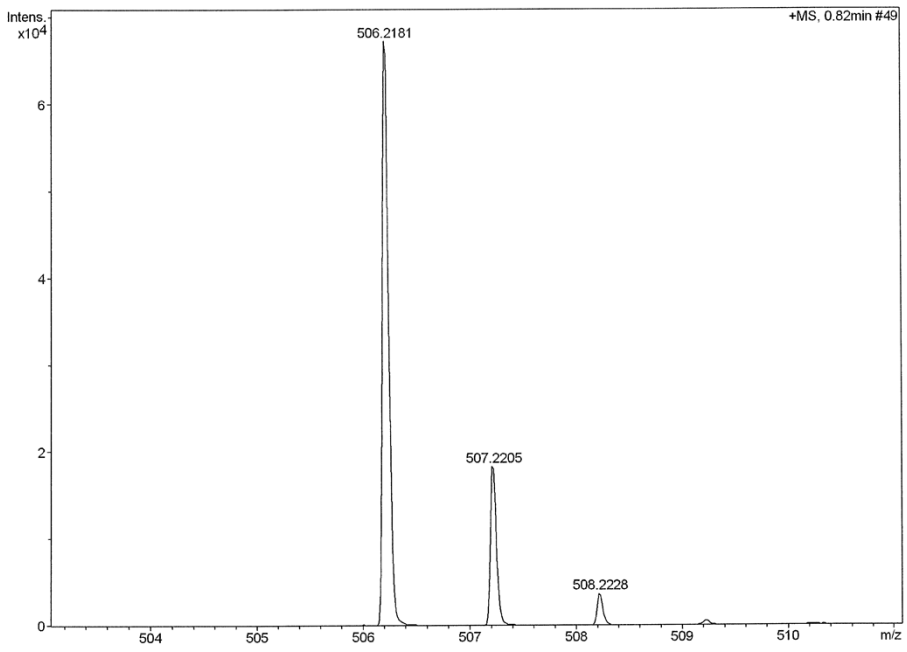
**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Chemistry\Outside\AMRI\20141103\5F-3,4-DiOMe-PhEt-NH2-1.d | Acquisition Date | 11/3/2014 2:55:55 PM |
| Method | YCH_Pos-150-1800.m | Operator | default user |
| Sample Name | 5F-3,4-DiOMe-PhEt-NH2 | Instrument / Ser# | micrOTOF-Q II 10269 |
| Comment | AMRI<br>Santhosh Kumar Chittimalla | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 2.0 Bar |
| Focus | Not active | Set Capillary | 4500 V | Set Dry Heater | 200 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 6.0 l/min |
| Scan End | 1800 m/z | Set Collision Cell RF | 200.0 Vpp | Set Divert Valve | Waste |

| Meas. m/z | # | Formula | m/z | err [ppm] | rdb | $e^-$ Conf | N-Rule |
|---|---|---|---|---|---|---|---|
| 506.2181 | 1 | C 26 H 33 F N O 8 | 506.2185 | 0.7 | 10.5 | even | ok |



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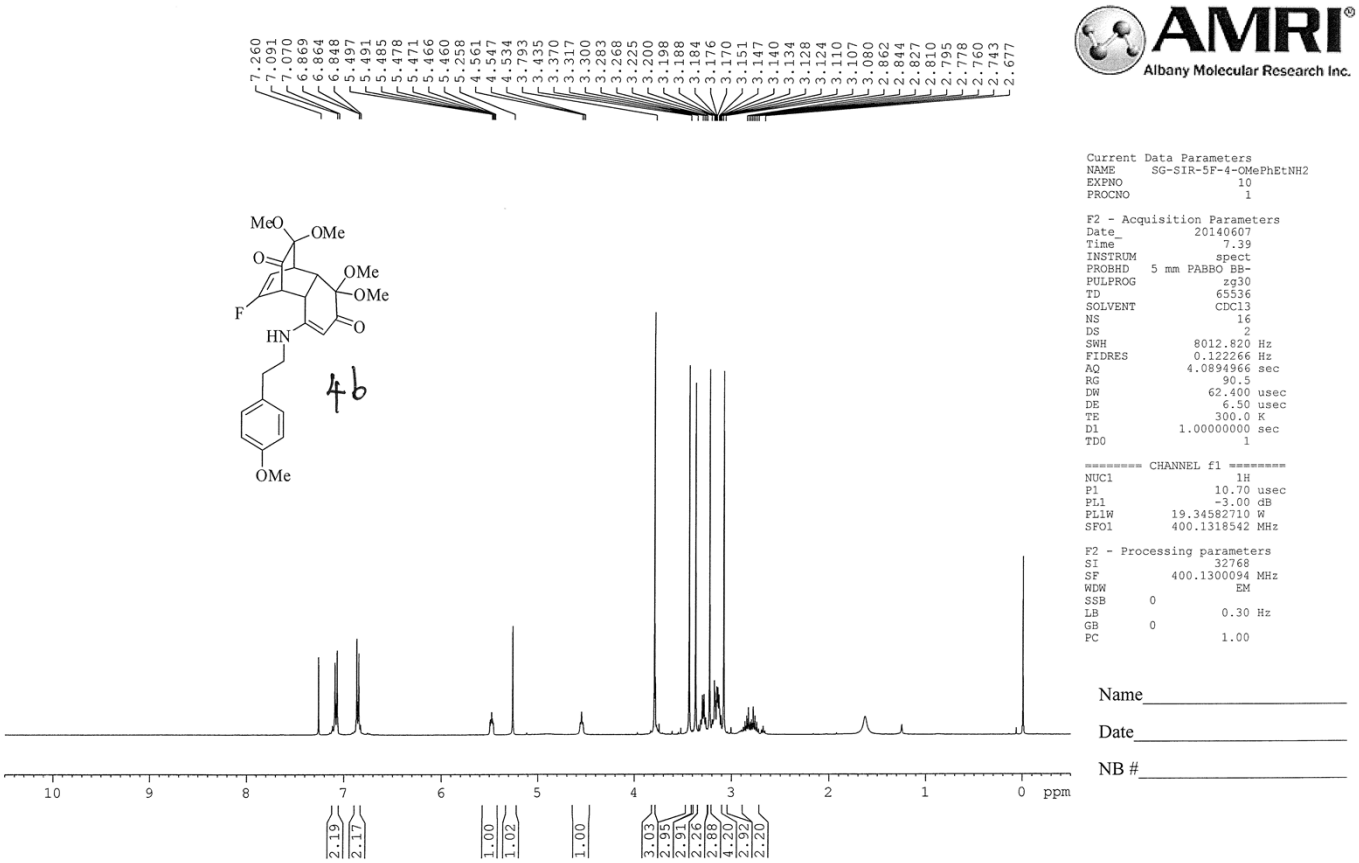


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Current Data Parameters
NAME      SG-SIR-5F-4-OMePhEtNH2
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140607
Time                7.39
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              4.0894966 sec
RG                  90.5
DW                62.400 usec
DE                 6.50 usec
TE                300.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 10.70 usec
PL1                -3.00 dB
PL1W         19.34582710 W
SFO1         400.1318542 MHz

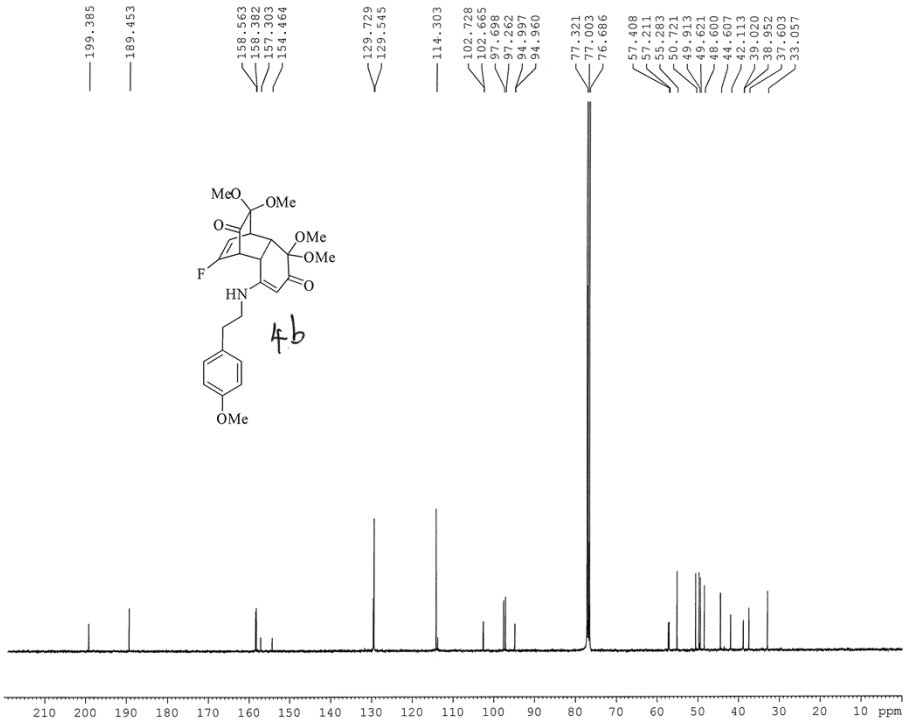
F2 - Processing parameters
SI                 32768
SF           400.1300094 MHz
WDW                   EM
SSB        0
LB                 0.30 Hz
GB         0
PC                 1.00
```

Name_____

Date_____

NB #_____

AMRI SRC
location; 17




AMRI

Name_____

Date_____

NB #_____

```
Current Data Parameters
NAME        SG-SIR-5F-4-OMePhEtNH2
EXPNO                           11
PROCNO                           1

F2 - Acquisition Parameters
Date_                     20140607
Time                         14.22
INSTRUM                      spect
PROBHD     5 mm PABBO BB-
PULPROG                   zgpg30
TD                             65536
SOLVENT                      CDCl3
NS                              7000
DS                                 4
SWH                     23980.814 Hz
FIDRES                      0.365918 Hz
AQ                        1.3664756 sec
RG                          18390.4
DW                           20.850 usec
DE                            6.50 usec
TE                           300.0 K
D1                        2.00000000 sec
D11                       0.03000000 sec
TD0                              1

======== CHANNEL f1 ========
NUC1                           13C
P1                            7.10 usec
PL1                          -4.00 dB
PL1W                   82.02445221 W
SFO1                  100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                   waltz16
NUC2                           1H
PCPD2                        80.00 usec
PL2                          -3.00 dB
PL12                         14.47 dB
PL13                         15.06 dB
PL2W                  19.34582710 W
PL12W                  0.34640750 W
PL13W                  0.30240381 W
SFO2                  400.1316005 MHz

F2 - Processing parameters
SI                             32768
SF                    100.6127710 MHz
WDW                               EM
SSB                0
LB                            1.00 Hz
GB                 0
PC                            1.40
```

# Mass Spectrum SmartFormula Report

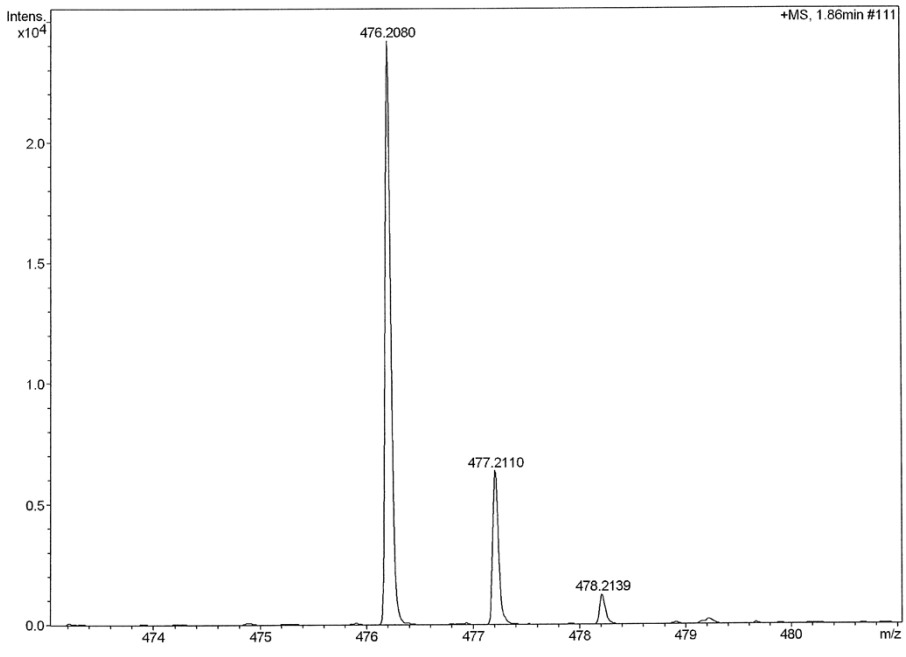
**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Chemistry\Outside\AMRI\20141103\5F-4-OMe-PhEt-NH2-1.d | Acquisition Date | 11/3/2014 11:32:00 AM |
| Method | YCH_Pos-150-1800.m | Operator | default user |
| Sample Name | 5F-4-OMe-PhEt-NH2 | Instrument / Ser# | micrOTOF-Q II 10269 |
| Comment | AMRI<br>Santhosh Kumar Chittimalla | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 2.0 Bar |
| Focus | Not active | Set Capillary | 4500 V | Set Dry Heater | 200 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 6.0 l/min |
| Scan End | 1800 m/z | Set Collision Cell RF | 200.0 Vpp | Set Divert Valve | Source |

| Meas. m/z | # | Formula | Score | m/z | err [mDa] | err [ppm] | mSigma | rdb | e⁻ Conf | N-Rule |
|---|---|---|---|---|---|---|---|---|---|---|
| 476.2080 | 1 | C 25 H 31 F N O 7 | 100.00 | 476.2079 | -0.1 | -0.2 | 7.4 | 10.5 | even | ok |

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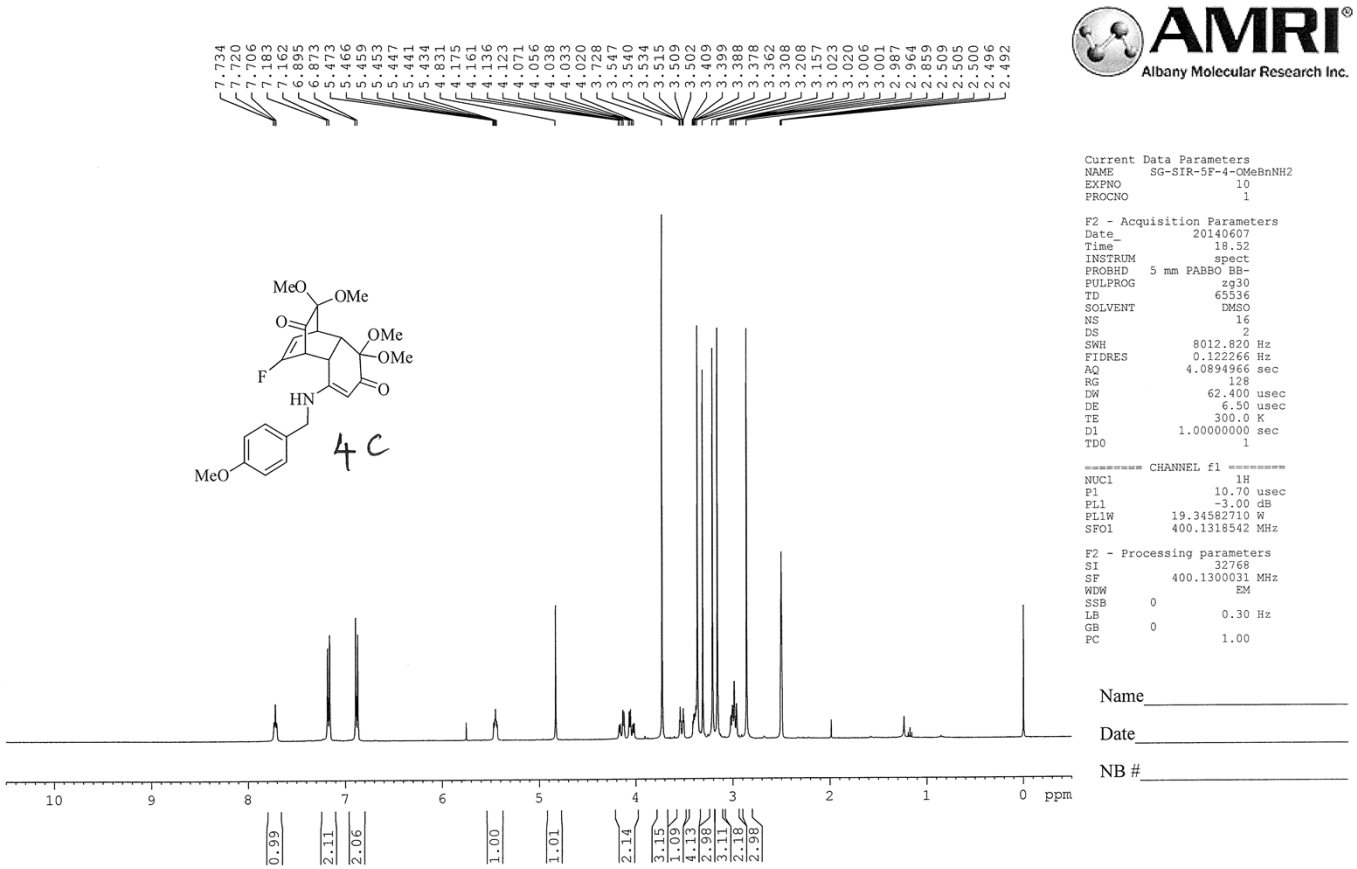


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Current Data Parameters
NAME      SG-SIR-5F-4-OMeBnNH2
EXPNO                       10
PROCNO                       1

F2 - Acquisition Parameters
Date_             20140607
Time_                18.52
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                DMSO
NS                       16
DS                        2
SWH                8012.820 Hz
FIDRES             0.122266 Hz
AQ                 4.0894966 sec
RG                       128
DW                    62.400 usec
DE                     6.50 usec
TE                    300.0 K
D1                 1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                       10.70 usec
PL1                      -3.00 dB
PL1W              19.34582710 W
SFO1              400.1318542 MHz

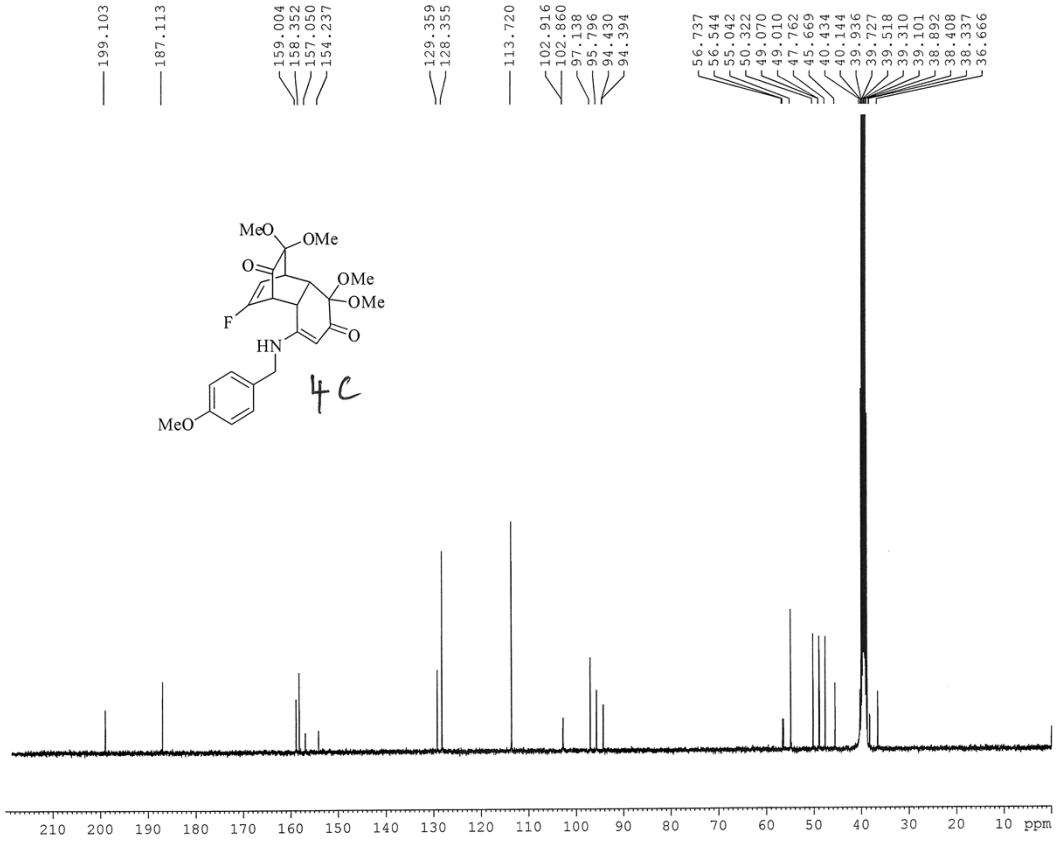
F2 - Processing parameters
SI                       32768
SF                400.1300031 MHz
WDW                         EM
SSB          0
LB                       0.30 Hz
GB           0
PC                       1.00
```

Name_____

Date_____

NB #_____

AMRI SRC
location; 17




Name_____

Date_____

NB #_____

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Current Data Parameters
NAME       SG-SIR-5F-4-OMeBnNH2
EXPNO                        11
PROCNO                        1

F2 - Acquisition Parameters
Date_              20140608
Time                   1.35
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT                DMSO
NS                     7000
DS                        4
SWH               23980.814 Hz
FIDRES             0.365918 Hz
AQ                1.3664756 sec
RG                    13004
DW                   20.850 usec
DE                    6.50 usec
TE                   300.0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                        13C
P1                         7.10 usec
PL1                       -4.00 dB
PL1W              82.02445221 W
SFO1             100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                        1H
PCPD2                     80.00 usec
PL2                       -3.00 dB
PL12                      14.47 dB
PL13                      15.06 dB
PL2W              19.34582710 W
PL12W              0.34640750 W
PL13W              0.30240381 W
SFO2             400.1316005 MHz

F2 - Processing parameters
SI                        32768
SF               100.6128185 MHz
WDW                          EM
SSB          0
LB                        1.00 Hz
GB           0
PC                        1.40
```

# Mass Spectrum SmartFormula Report

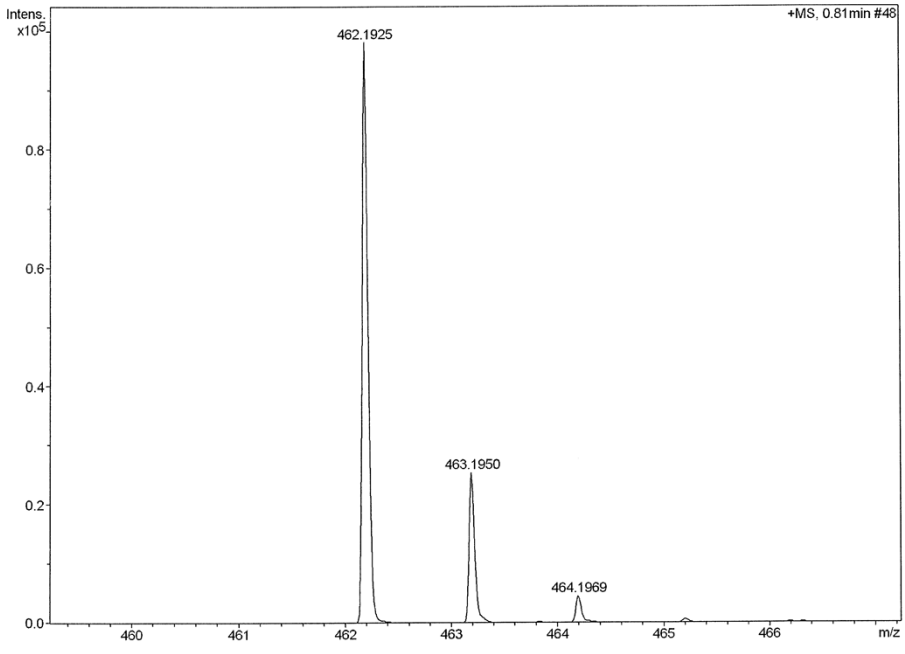
**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Chemistry\Outside\AMRI\20141103\5F-PMB-NH2-1.d | Acquisition Date | 11/3/2014 12:12:32 PM |
| Method | YCH_Pos-150-1800.m | Operator | default user |
| Sample Name | 5F-PMB-NH2 | Instrument / Ser# | micrOTOF-Q II 10269 |
| Comment | AMRI<br>Santhosh Kumar Chittimalla | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 2.0 Bar |
| Focus | Not active | Set Capillary | 4500 V | Set Dry Heater | 200 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 6.0 l/min |
| Scan End | 1800 m/z | Set Collision Cell RF | 200.0 Vpp | Set Divert Valve | Waste |

| Meas. m/z | # | Formula | m/z | err [ppm] | rdb | $e^-$ Conf | N-Rule |
|---|---|---|---|---|---|---|---|
| 462.1925 | 1 | C 24 H 29 F N O 7 | 462.1923 | -0.6 | 10.5 | even | ok |



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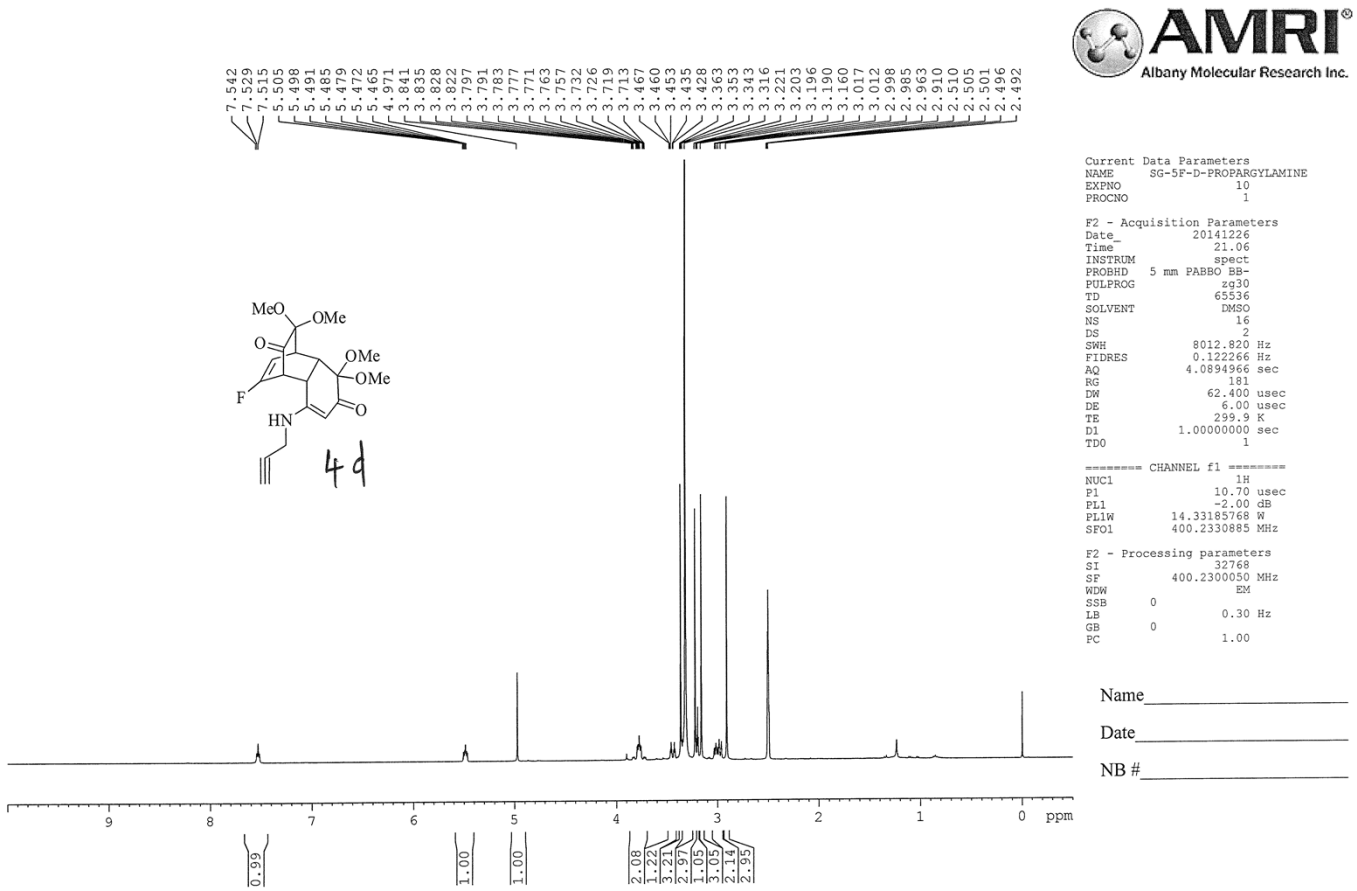


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```
Current Data Parameters
NAME      SG-5F-D-PROPARGYLAMINE
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20141226
Time              21.06
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD               65536
SOLVENT           DMSO
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ             4.0894966 sec
RG                  181
DW               62.400 usec
DE                6.00 usec
TE               299.9 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                10.70 usec
PL1               -2.00 dB
PL1W        14.33185768 W
SFO1        400.2330885 MHz

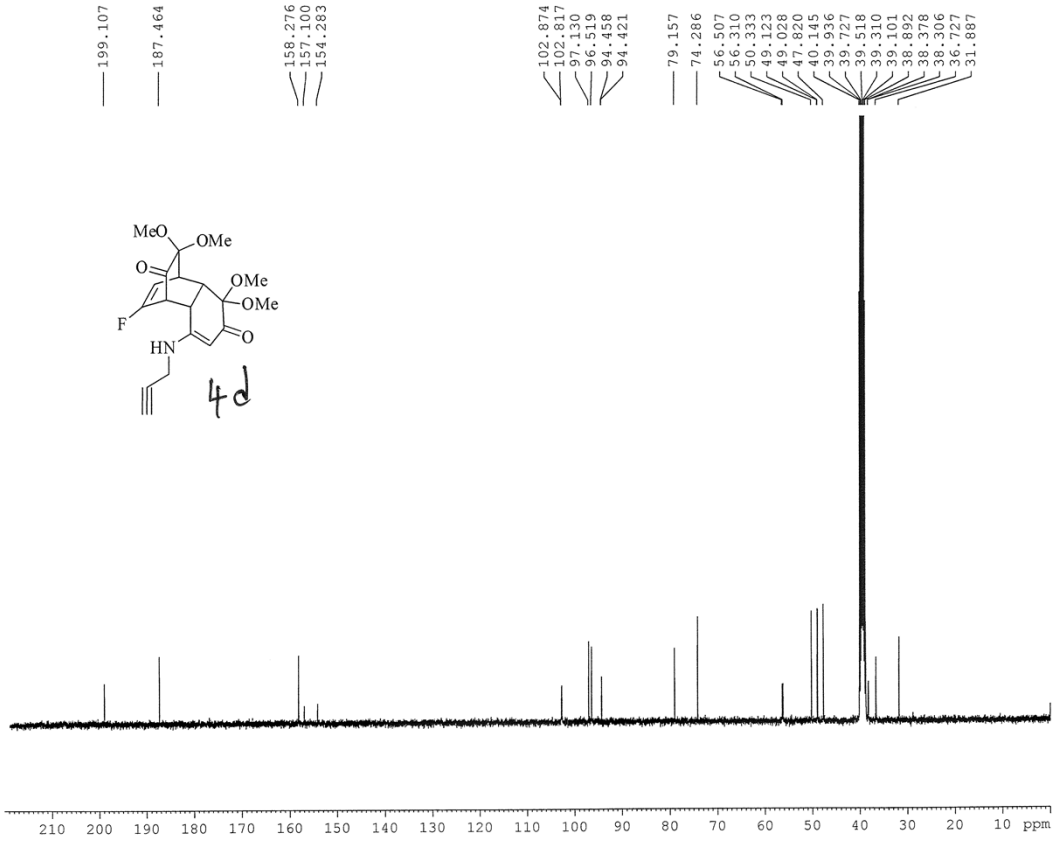
F2 - Processing parameters
SI                32768
SF          400.2300050 MHz
WDW               EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

Name_____

Date_____

NB #_____

AMRI; SRC AV400
location; 18




Name_____

Date_____

NB #_____

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Current Data Parameters
NAME      SG-5F-D-PROPARGYLAMINE
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20141227
Time                1.24
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                65536
SOLVENT             DMSO
NS                   8000
DS                      4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                    101
DW                20.800 usec
DE                 6.50 usec
TE                300.0 K
D1            0.50000000 sec
D11           0.03000000 sec
TD0                    1

========== CHANNEL f1 ========
NUC1                  13C
P1                   8.60 usec
PL1                 -1.00 dB
PL1W         44.58811569 W
SFO1        100.6479769 MHz

========== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2                80.00 usec
PL2                  -2.00 dB
PL12                 15.47 dB
PL13                 15.72 dB
PL2W         14.33185768 W
PL12W         0.25662708 W
PL13W         0.24227159 W
SFO2        400.2316009 MHz

F2 - Processing parameters
SI                   32768
SF          100.6379636 MHz
WDW                     EM
SSB      0
LB                   1.00 Hz
GB       0
PC                   1.40
```

# Mass Spectrum SmartFormula Report

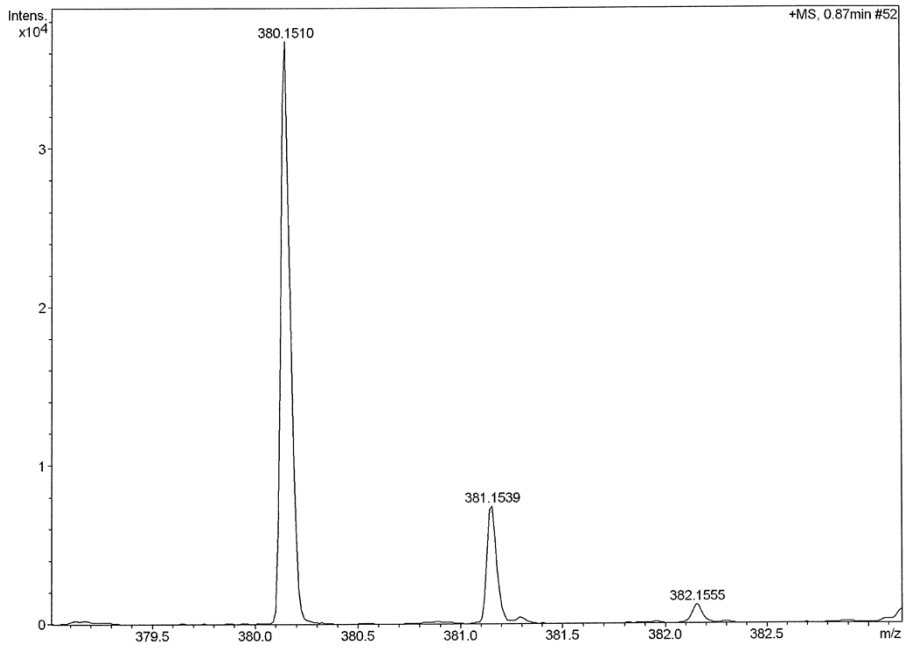
**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Chemistry\Outside\AMRI\20141218\5F-Prg-Amine-1.d | Acquisition Date | 12/18/2014 4:23:49 PM |
| Method | YCH_Pos-150-1800.m | Operator | default user |
| Sample Name | 5F-Prg-Amine | Instrument / Ser# | micrOTOF-Q II 10269 |
| Comment | AMRI<br>Santhosh Kumar Chittimalla | | |

**Acquisition Parameter**

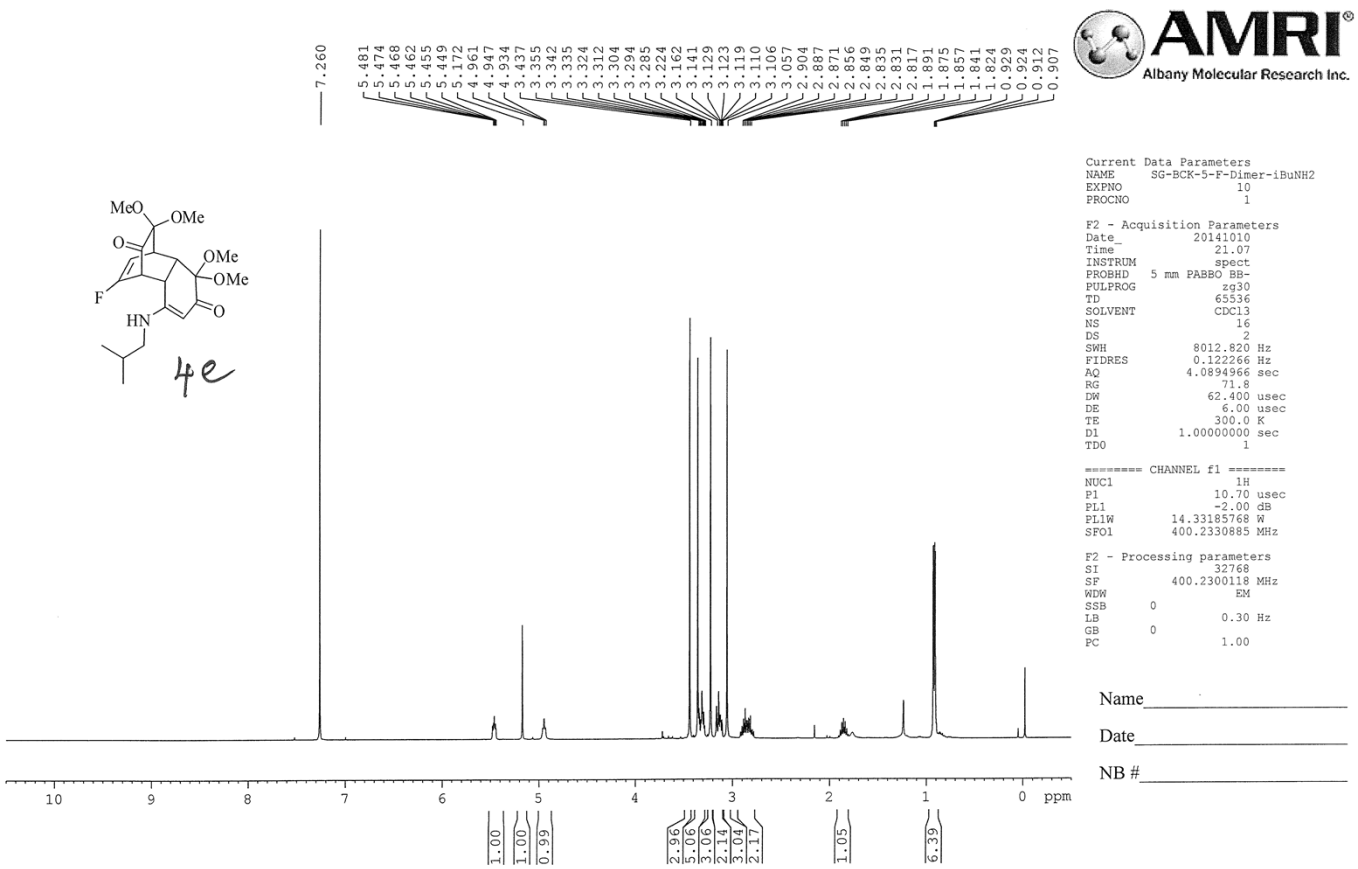
| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 2.0 Bar |
| Focus | Not active | Set Capillary | 4500 V | Set Dry Heater | 200 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 6.0 l/min |
| Scan End | 1800 m/z | Set Collision Cell RF | 200.0 Vpp | Set Divert Valve | Waste |

| Meas. m/z | # | Formula | m/z | err [ppm] | rdb | e¯ Conf | N-Rule |
|---|---|---|---|---|---|---|---|
| 380.1510 | 1 | C 19 H 23 F N O 6 | 380.1504 | -1.5 | 8.5 | even | ok |






Submitted to *RSC Advances*


7.260
5.481
5.474
5.468
5.462
5.455
5.449
5.172
4.961
4.947
4.934
4.437
3.355
3.342
3.335
3.324
3.312
3.304
3.294
3.285
3.224
3.162
3.141
3.129
3.123
3.119
3.110
3.106
3.057
2.904
2.887
2.871
2.856
2.849
2.835
2.831
2.817
1.891
1.875
1.857
1.841
1.824
0.929
0.924
0.912
0.907
MeO
OMe
O
OMe
OMe
F
HN
O
4e
Current Data Parameters
NAME SG-BCK-5-F-Dimer-iBuNH2
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141010
Time 21.07
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 4.0894966 sec
RG 71.8
DW 62.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.70 usec
PL1 -2.00 dB
PL1W 14.33185768 W
SFO1 400.2330885 MHz
F2 - Processing parameters
SI 32768
SF 400.2300118 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.00
0.99
2.96
3.06
3.06
2.14
3.04
2.17
1.05
6.39

Name_____

Date_____

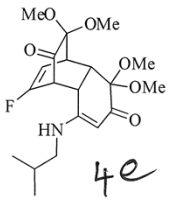
NB #_____

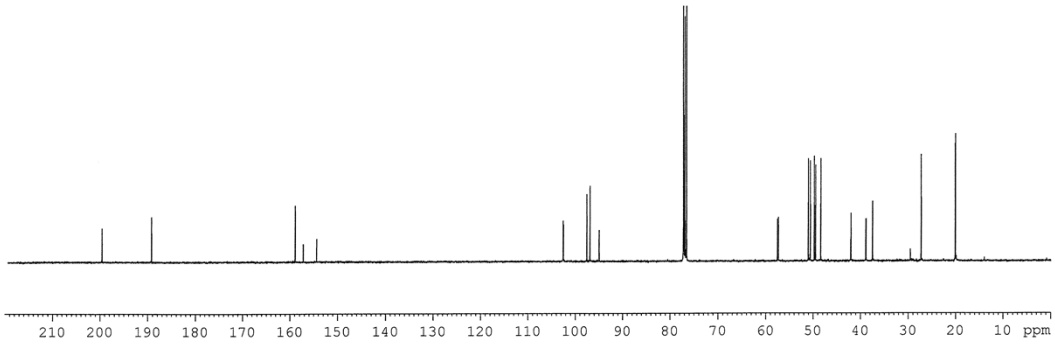
AMRI; SRC AV400
location; 18


Name_____

Date_____

NB #_____




```
Current Data Parameters
NAME      SG-BCK-5-F-Dimer-iBuNH2
EXPNO                          11
PROCNO                          1

F2 - Acquisition Parameters
Date_                    20141010
Time                        23.17
INSTRUM                     spect
PROBHD   5 mm PABBO BB-
PULPROG                   zgpg30
TD                         65536
SOLVENT                    CDCl3
NS                          4000
DS                             4
SWH                    24038.461 Hz
FIDRES                  0.366798 Hz
AQ                      1.3631988 sec
RG                            101
DW                         20.800 usec
DE                          6.50 usec
TE                         300.0 K
D1                     0.50000000 sec
D11                    0.03000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                         13C
P1                          8.60 usec
PL1                        -1.00 dB
PL1W                44.58811569 W
SFO1               100.6479769 MHz

======== CHANNEL f2 ========
CPDPRG2                  waltz16
NUC2                         1H
PCPD2                      80.00 usec
PL2                        -2.00 dB
PL12                       15.47 dB
PL13                       15.72 dB
PL2W                14.33185768 W
PL12W                0.25662708 W
PL13W                0.24227159 W
SFO2               400.2316009 MHz

F2 - Processing parameters
SI                           32768
SF                 100.6379176 MHz
WDW                             EM
SSB                0
LB                           1.00 Hz
GB                 0
PC                           1.40
```

# Mass Spectrum SmartFormula Report

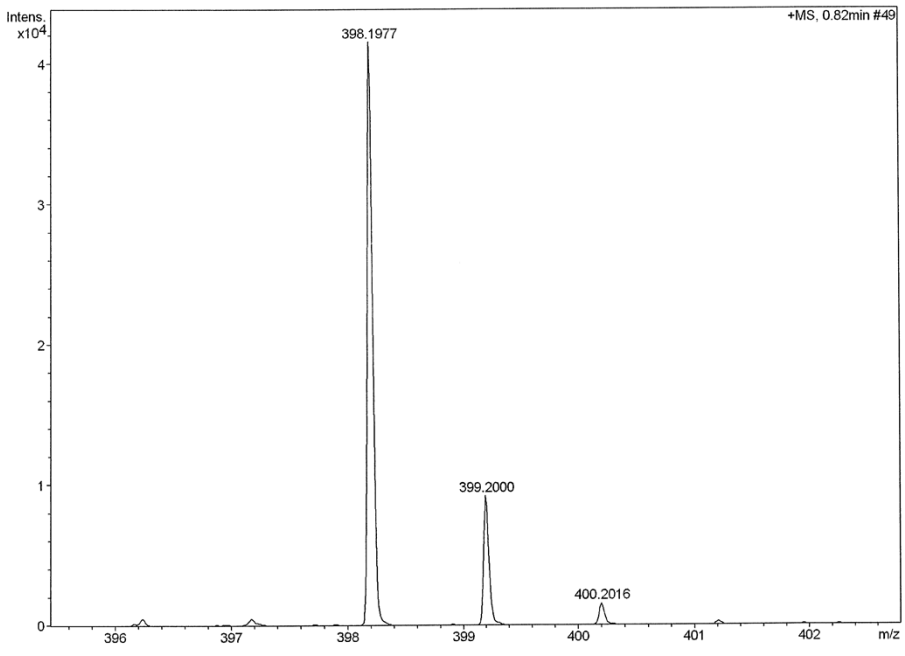
**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Chemistry\Outside\AMRI\20141103\5F-IBu-NH2-1.d | Acquisition Date | 11/3/2014 11:59:44 AM |
| Method | YCH_Pos-150-1800.m | Operator | default user |
| Sample Name | 5F-IBu-NH2 | Instrument / Ser# | micrOTOF-Q II 10269 |
| Comment | AMRI | | |
| | Santhosh Kumar Chittimalla | | |

**Acquisition Parameter**

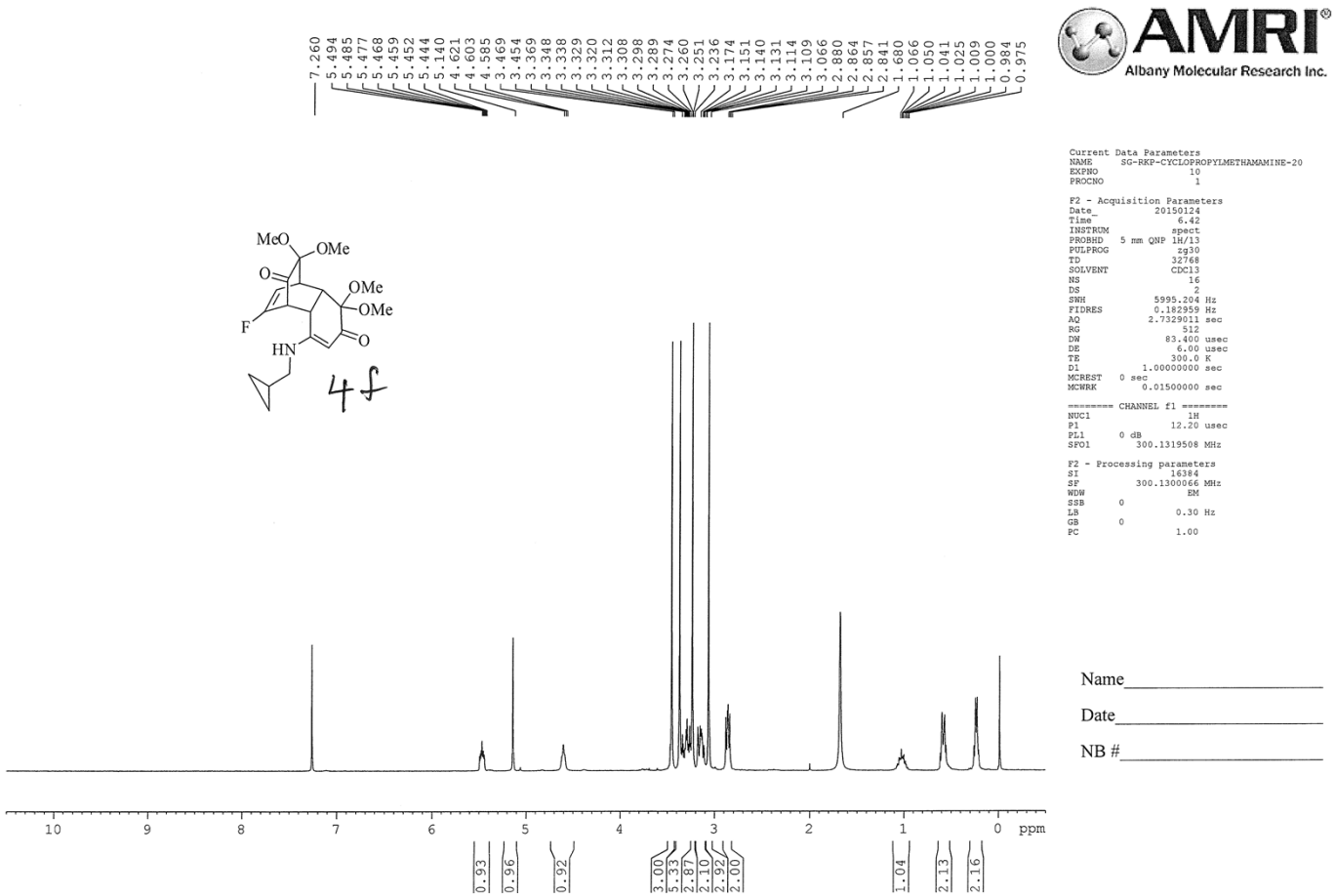
| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 2.0 Bar |
| Focus | Not active | Set Capillary | 4500 V | Set Dry Heater | 200 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 6.0 l/min |
| Scan End | 1800 m/z | Set Collision Cell RF | 200.0 Vpp | Set Divert Valve | Waste |

| Meas. m/z | # | Formula | m/z | err [ppm] | rdb | $e^-$ Conf | N-Rule |
|---|---|---|---|---|---|---|---|
| 398.1977 | 1 | C 20 H 29 F N O 6 | 398.1973 | -0.8 | 6.5 | even | ok |






Submitted to *RSC Advances*

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```
Current Data Parameters
NAME       SG-RKP-CYCLOPROPYLMETHAMAMINE-20
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150124
Time                6.42
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             5995.204 Hz
FIDRES          0.182959 Hz
AQ              2.7329011 sec
RG                   512
DW                83.400 usec
DE                 6.00 usec
TE                 300.0 K
D1              1.00000000 sec
MCREST    0 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                 12.20 usec
PL1        0 dB
SFO1          300.1319508 MHz

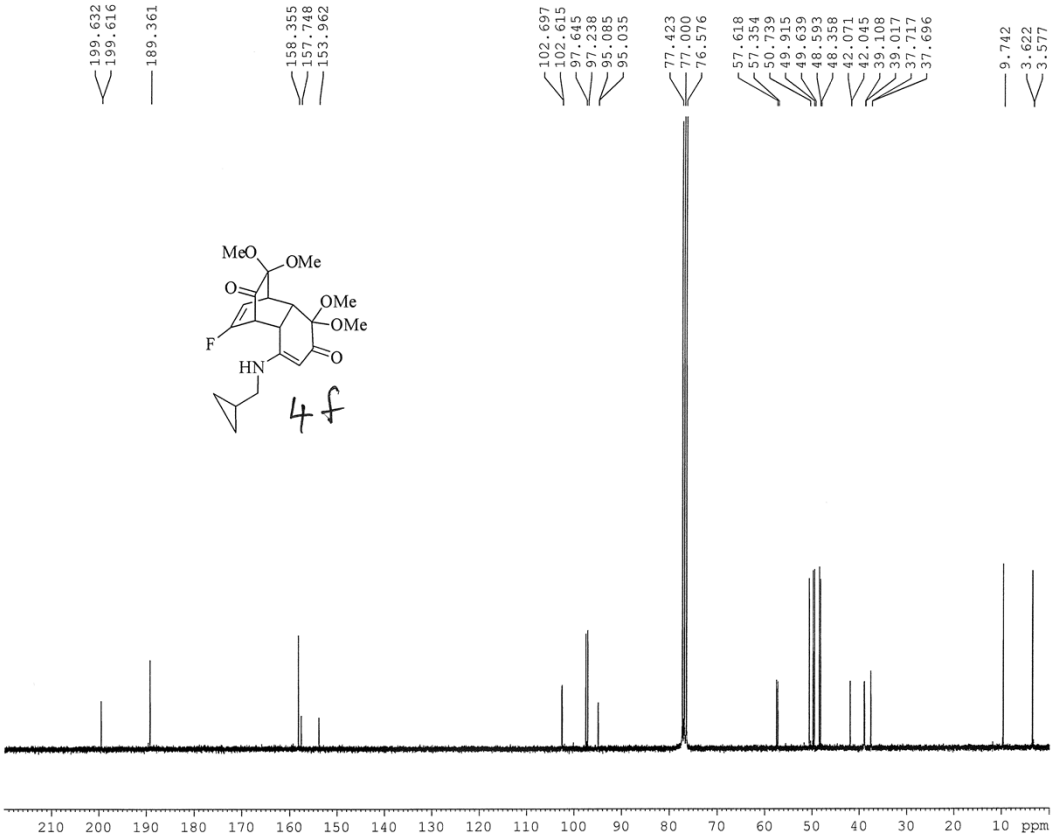
F2 - Processing parameters
SI                 16384
SF            300.1300066 MHz
WDW                   EM
SSB        0
LB                 0.30 Hz
GB         0
PC                 1.00
```

Name_____

Date_____

NB #_____

AMRI; SRC
location; 15




Name_____

Date_____

NB #_____

```
Current Data Parameters
NAME          SG-RKP-CYCLOPROPYLMETHAMAMINE-20
EXPNO                   11
PROCNO                   1

F2 - Acquisition Parameters
Date_              20150124
Time                 15.39
INSTRUM              spect
PROBHD   5 mm QNP 1H/13
PULPROG           zgpg30
TD                 65536
SOLVENT              CDCl3
NS                   16000
DS                       0
SWH              22675.736 Hz
FIDRES           0.346004 Hz
AQ               1.4451188 sec
RG                  1824.6
DW                  22.050 usec
DE                   6.00 usec
TE                  300.0 K
D1              0.50000000 sec
d11             0.03000000 sec
DELTA           0.40000001 sec
MCREST    0 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                   13C
P1                   8.00 usec
PL1                 -2.00 dB
SFO1           75.4767751 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2        0 dB
PL12                16.33 dB
PL13                16.00 dB
SFO2          300.1315007 MHz

F2 - Processing parameters
SI                     131072
SF             75.4677502 MHz
WDW                       EM
SSB        0
LB                    0.30 Hz
GB         0
PC                    1.40
```

# Mass Spectrum SmartFormula Report

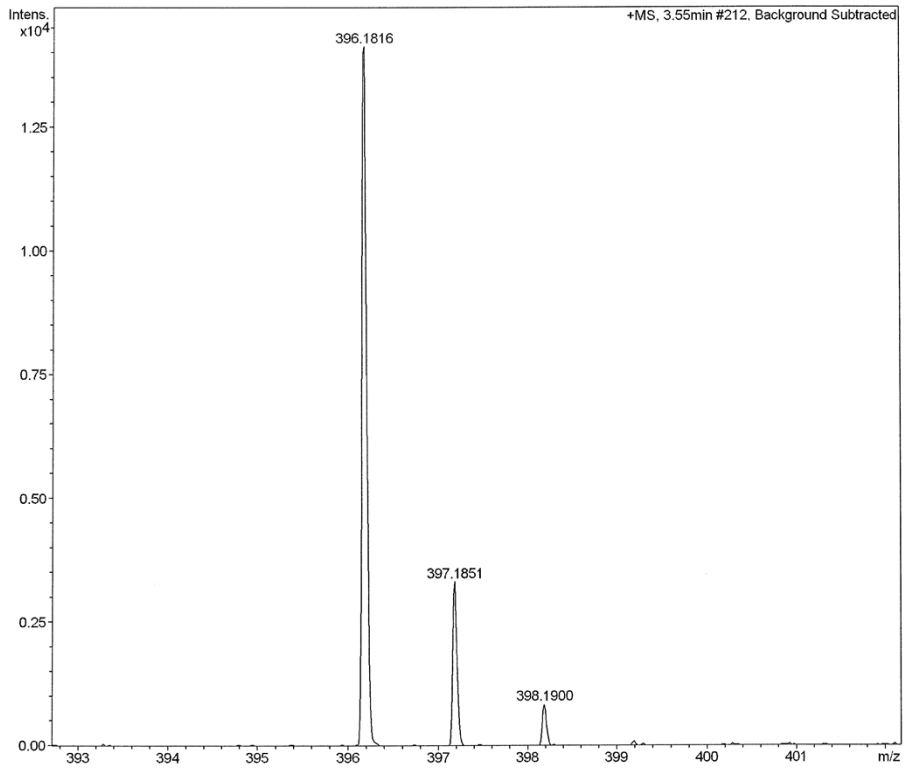
**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Chemistry\Outside\AMRI\20150107\5F-Cyp-Me-Amine.d | Acquisition Date | 1/7/2015 2:56:25 PM |
| Method | YCH_Pos-150-1800.m | Operator | default user |
| Sample Name | 5F-Cyp-Me-Amine | Instrument / Ser# | micrOTOF-Q II 10269 |
| Comment | AMRI | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 2.0 Bar |
| Focus | Not active | Set Capillary | 4500 V | Set Dry Heater | 200 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 6.0 l/min |
| Scan End | 1000 m/z | Set Collision Cell RF | 200.0 Vpp | Set Divert Valve | Waste |

| Meas. m/z | # | Formula | m/z | err [ppm] | rdb | e⁻ Conf | N-Rule |
|---|---|---|---|---|---|---|---|
| 396.1816 | 1 | C 20 H 27 F N O 6 | 396.1817 | 0.2 | 7.5 | even | ok |



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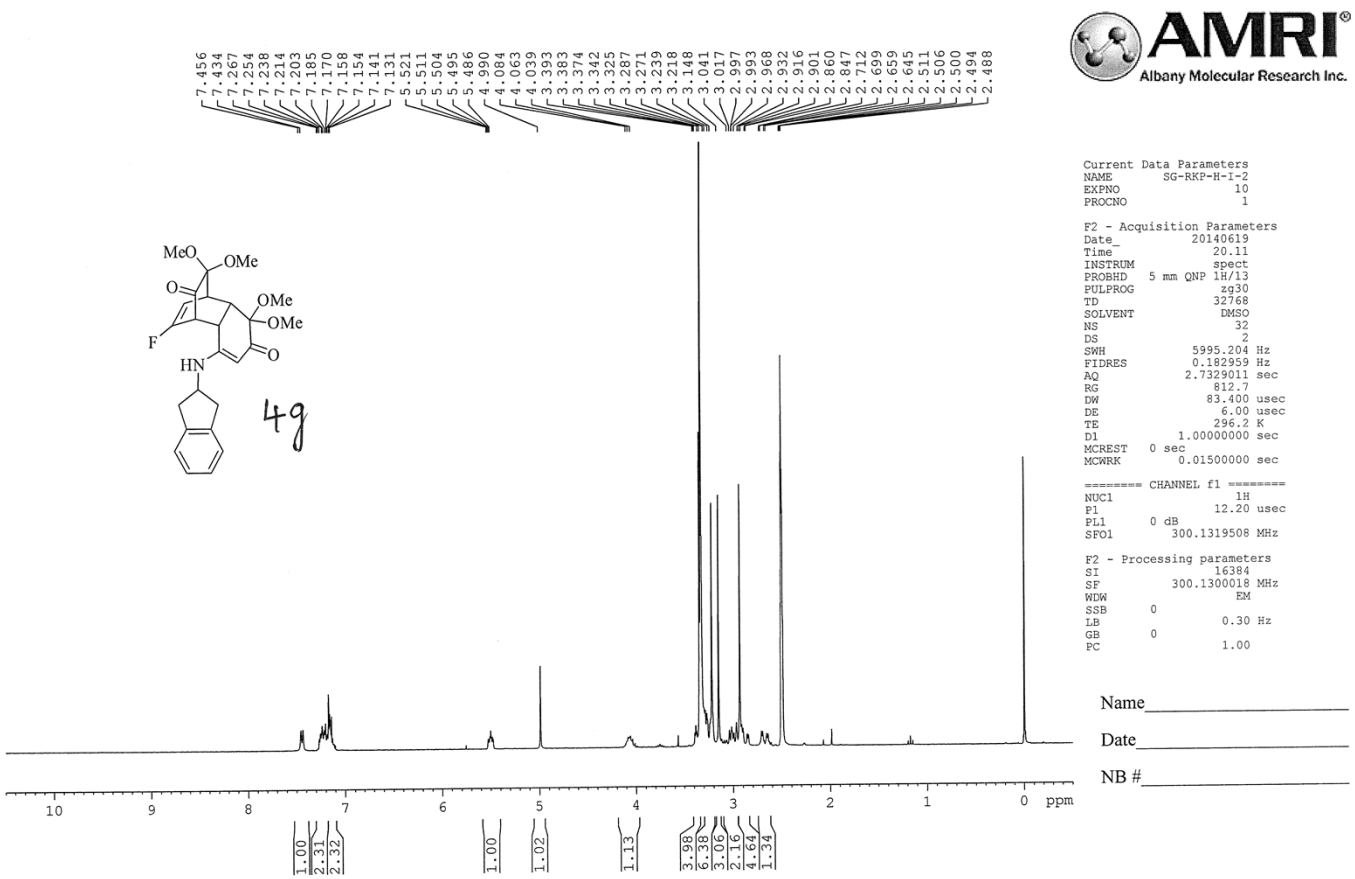


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```
Current Data Parameters
NAME        SG-RKP-H-I-2
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140619
Time               20.11
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                    32
DS                     2
SWH             5995.204 Hz
FIDRES          0.182959 Hz
AQ              2.7329011 sec
RG                 812.7
DW                83.400 usec
DE                 6.00 usec
TE                296.2 K
D1             1.00000000 sec
MCREST    0 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                 12.20 usec
PL1       0 dB
SFO1         300.1319508 MHz

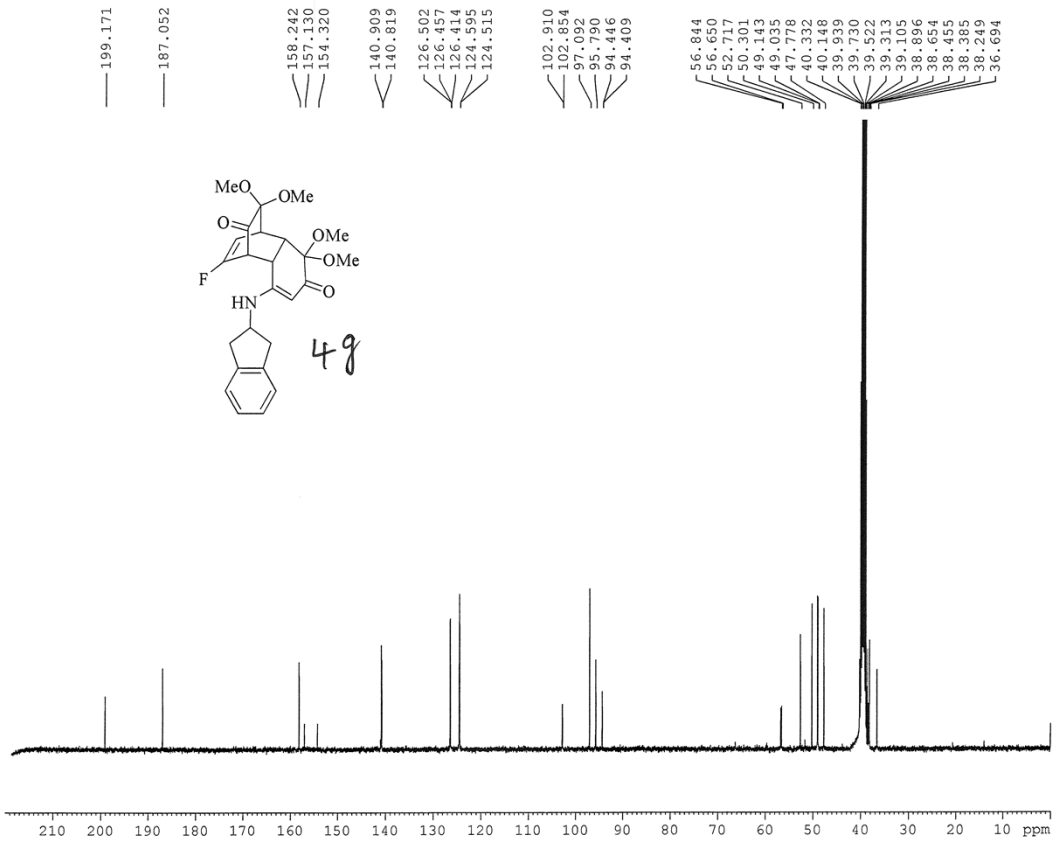
F2 - Processing parameters
SI                 16384
SF           300.1300018 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Name_____

Date_____

NB #_____

AMRI SRC
location; 17




Name_____

Date_____

NB #_____

```
Current Data Parameters
NAME      SG-RKP-2-AMINOINDAN
EXPNO                      11
PROCNO                      1

F2 - Acquisition Parameters
Date_              20150117
Time_                  1.53
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg30
TD                  65536
SOLVENT               DMSO
NS                    6000
DS                       4
SWH             23980.814 Hz
FIDRES          0.365918 Hz
AQ              1.3664756 sec
RG                 7298.2
DW                20.850 usec
DE                 6.50 usec
TE                300.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                   7.10 usec
PL1                 -4.00 dB
PL1W          82.02445221 W
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                  -3.00 dB
PL12                 14.47 dB
PL13                 15.06 dB
PL2W          19.34582710 W
PL12W          0.34640750 W
PL13W          0.30240381 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF           100.6128177 MHz
WDW                     EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

# Mass Spectrum SmartFormula Report

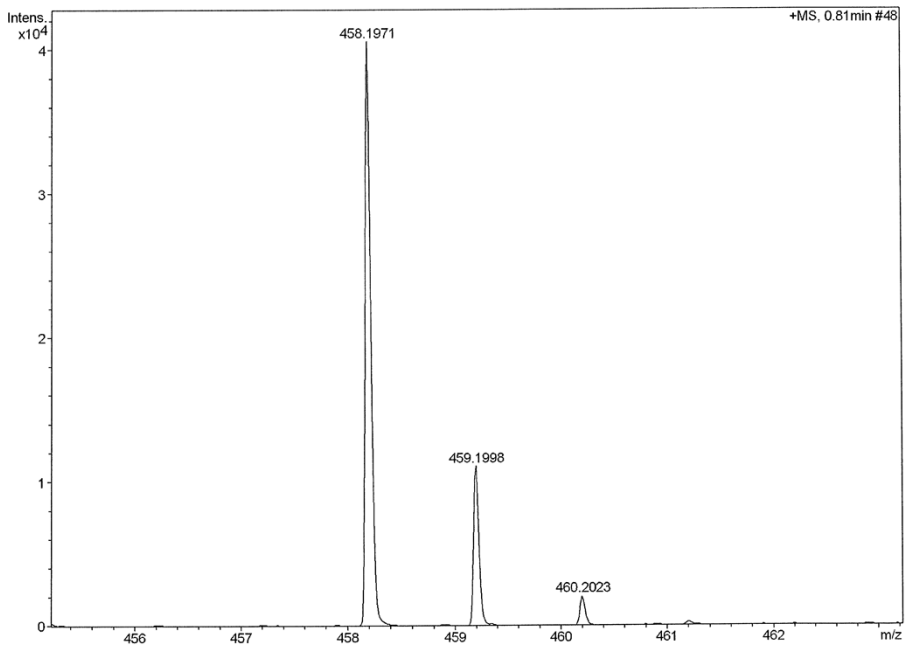
**Analysis Info**

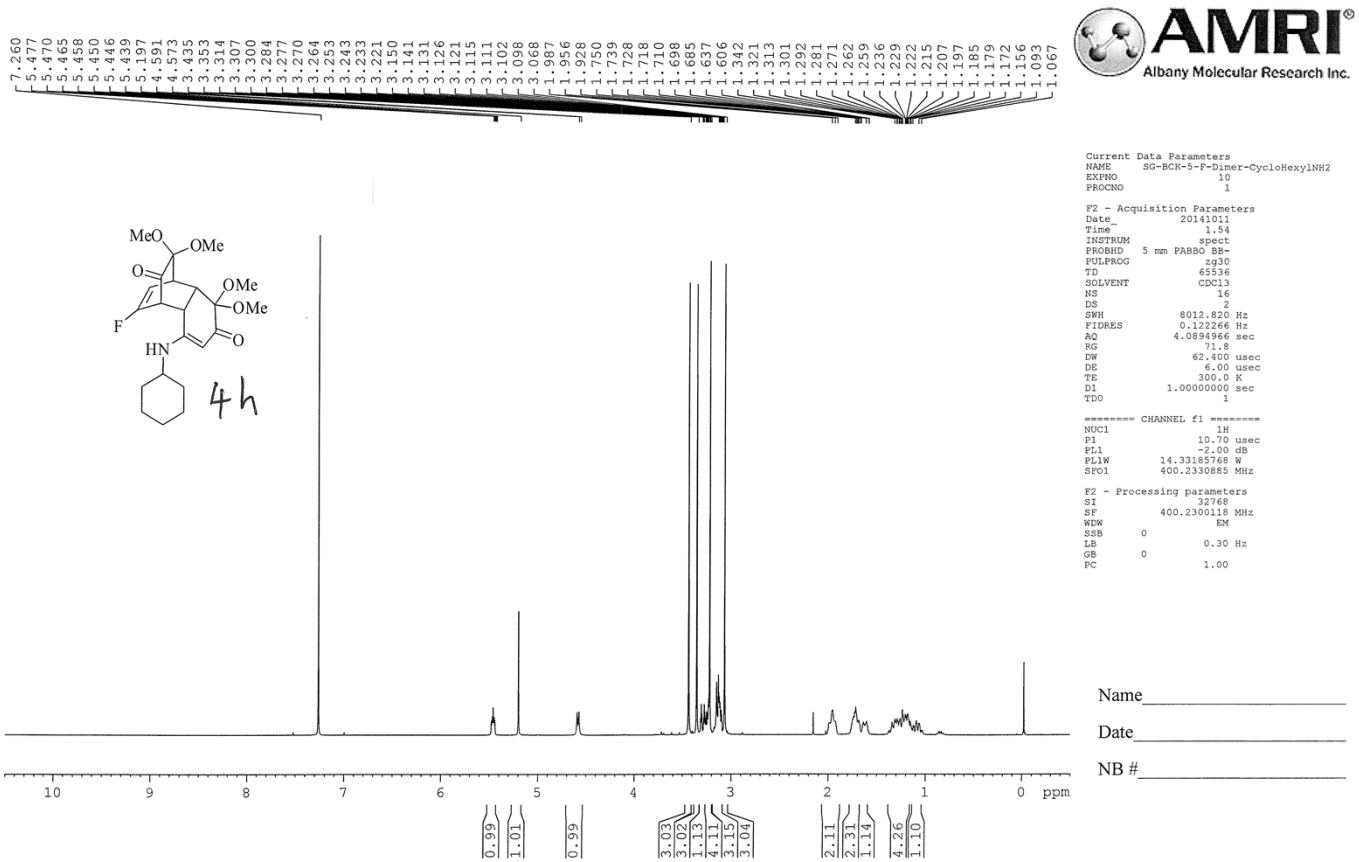
| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Chemistry\Outside\AMRI\20141103\5F-Am-Indane-1.d | Acquisition Date | 11/3/2014 3:09:03 PM |
| Method | YCH_Pos-150-1800.m | Operator | default user |
| Sample Name | 5F-Am-Indane | Instrument / Ser# | micrOTOF-Q II 10269 |
| Comment | AMRI<br>Santhosh Kumar Chittimalla | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 2.0 Bar |
| Focus | Not active | Set Capillary | 4500 V | Set Dry Heater | 200 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 6.0 l/min |
| Scan End | 1800 m/z | Set Collision Cell RF | 200.0 Vpp | Set Divert Valve | Waste |

| Meas. m/z | # | Formula | m/z | err [ppm] | rdb | e⁻ Conf | N-Rule |
|---|---|---|---|---|---|---|---|
| 458.1971 | 1 | C 25 H 29 F N O 6 | 458.1973 | 0.6 | 11.5 | even | ok |



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```
Current Data Parameters
NAME      SG-BCK-5-F-Dimer-CycloHexylNH2
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20141011
Time                1.54
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               4.0894966 sec
RG                  71.8
DW                 62.400 usec
DE                  6.00 usec
TE                300.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 10.70 usec
PL1                -2.00 dB
PL1W         14.33185768 W
SFO1         400.2330885 MHz

F2 - Processing parameters
SI                 32768
SF           400.2300118 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Name_____

Date_____

NB #_____

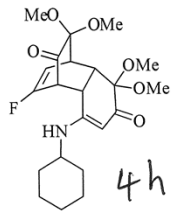
AMRI; SRC AV400
location; 18

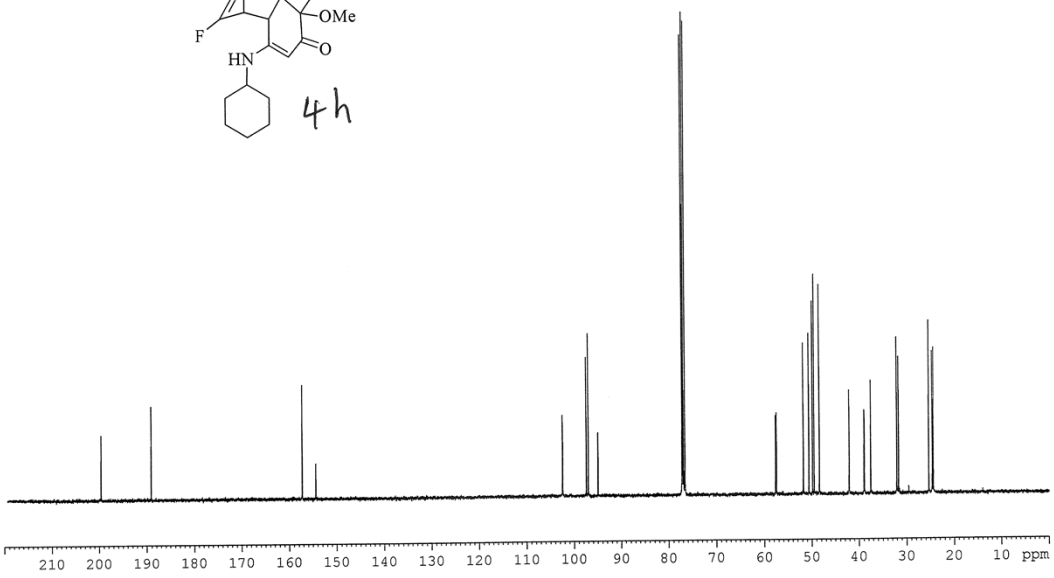
199.678
189.173
157.376
157.331
154.492
102.572
102.511
97.521
97.111
95.064
95.028
77.316
76.999
76.681
57.729
57.531
51.881
50.696
49.933
49.585
48.483
42.178
42.166
39.030
38.963
37.620
32.136
31.760
25.419
24.701
24.431

Name_____

Date_____

NB #_____




```
Current Data Parameters
NAME      SG-BCK-5-F-Dimer-CycloHexylNH2
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20141011
Time                4.05
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 4000
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                  101
DW                20.800 usec
DE                 6.50 usec
TE                300.0 K
D1             0.50000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                   8.60 usec
PL1                 -1.00 dB
PL1W          44.58811569 W
SFO1         100.6479769 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2               80.00 usec
PL2                 -2.00 dB
PL12                15.47 dB
PL13                15.72 dB
PL2W          14.33185768 W
PL12W          0.25662708 W
PL13W          0.24227159 W
SFO2         400.2316009 MHz

F2 - Processing parameters
SI                 32768
SF           100.6379180 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

# Mass Spectrum SmartFormula Report

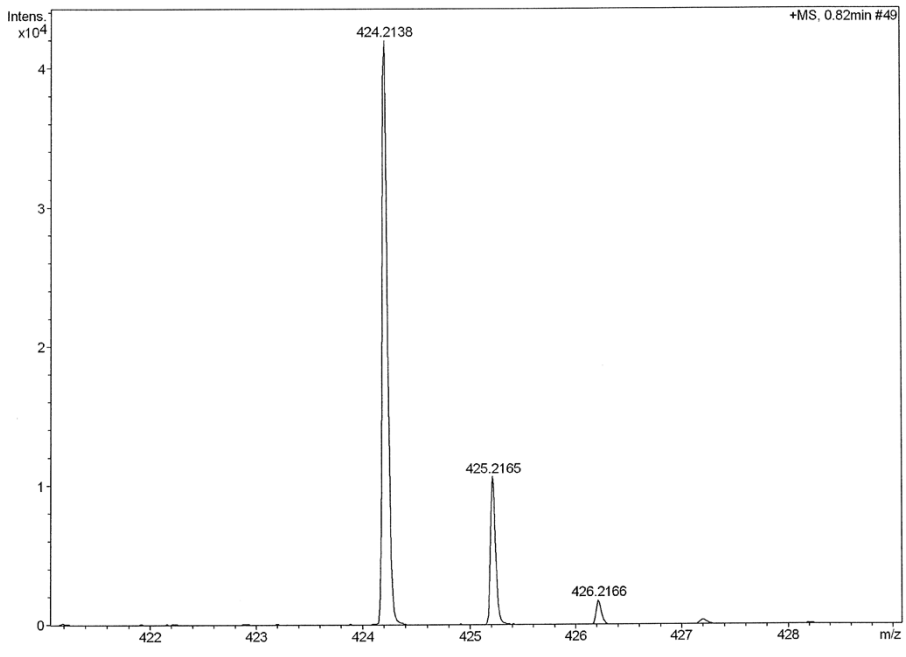
**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Chemistry\Outside\AMRI\20141103\5F-CycHex-NH2-1.d | Acquisition Date | 11/3/2014 11:39:56 AM |
| Method | YCH_Pos-150-1800.m | Operator | default user |
| Sample Name | 5F-CycHex-NH2 | Instrument / Ser# | micrOTOF-Q II 10269 |
| Comment | AMRI<br>Santhosh Kumar Chittimalla | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 2.0 Bar |
| Focus | Not active | Set Capillary | 4500 V | Set Dry Heater | 200 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 6.0 l/min |
| Scan End | 1800 m/z | Set Collision Cell RF | 200.0 Vpp | Set Divert Valve | Waste |

| Meas. m/z | # | Formula | m/z | err [ppm] | rdb | $e^-$ Conf | N-Rule |
|---|---|---|---|---|---|---|---|
| 424.2138 | 1 | C 22 H 31 F N O 6 | 424.2130 | -1.9 | 7.5 | even | ok |



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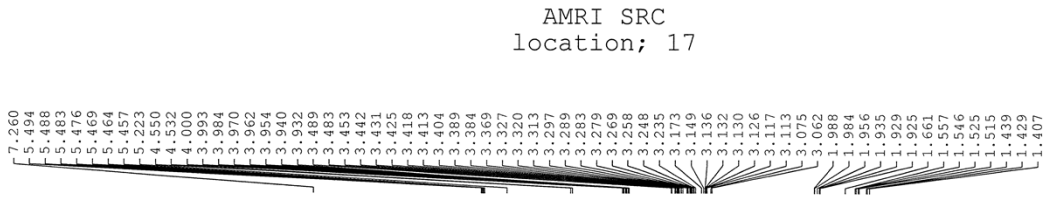
AMRI SRC
location; 17



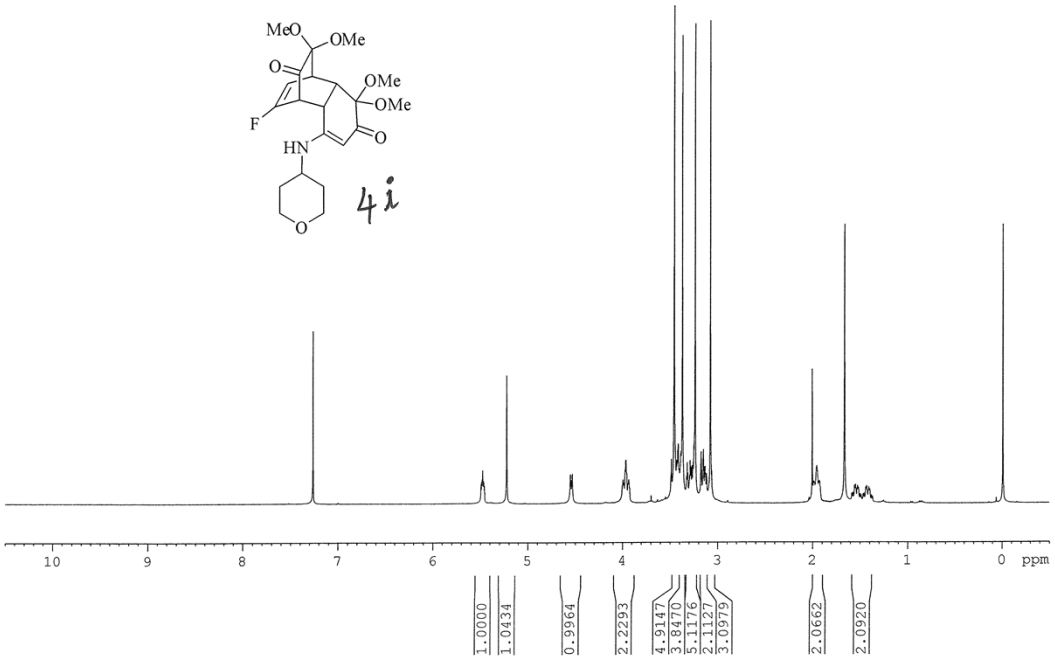

Name_____

Date_____

NB #_____




4i



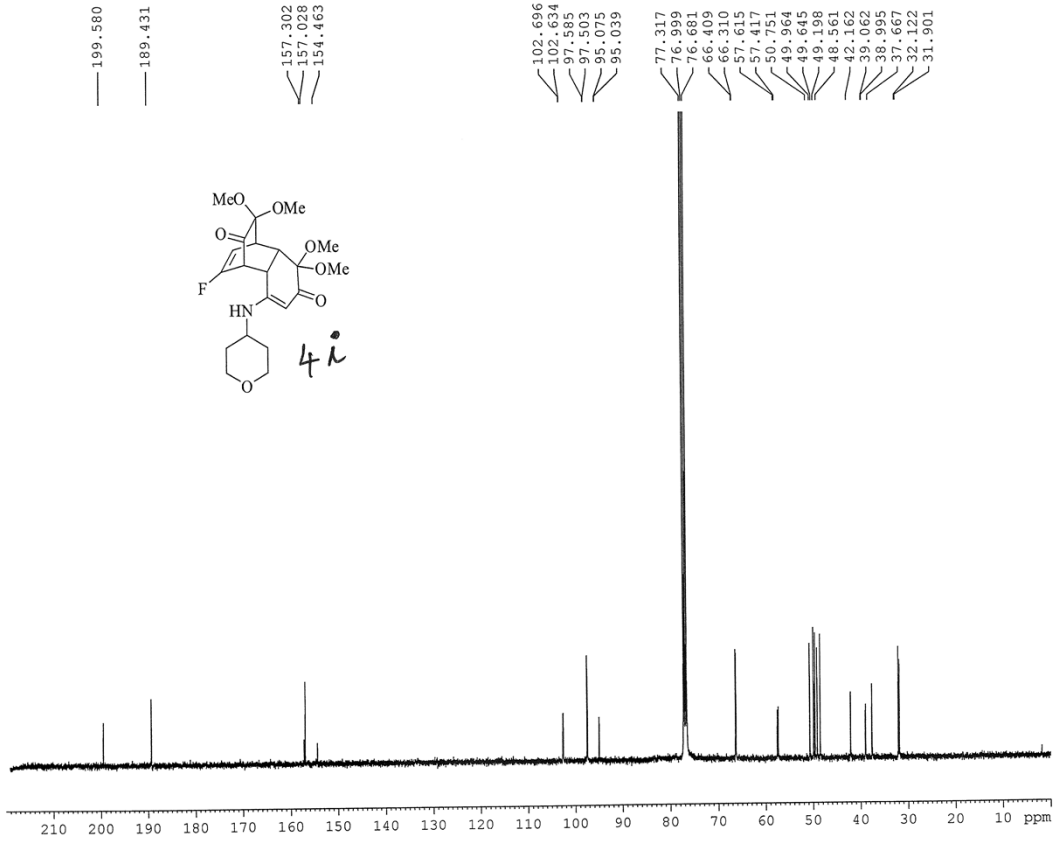

```
Current Data Parameters
NAME        SG-RKP-H-3-I
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140621
Time                2.50
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              4.0894966 sec
RG                  90.5
DW                62.400 usec
DE                 6.50 usec
TE                300.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.70 usec
PL1               -3.00 dB
PL1W         19.34582710 W
SFO1         400.1318542 MHz

F2 - Processing parameters
SI                 32768
SF           400.1300094 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

AMRI SRC
location; 17




Name_____

Date_____

NB #_____

```
Current Data Parameters
NAME          SG-RKP-H-3-I
EXPNO                   11
PROCNO                   1

F2 - Acquisition Parameters
Date_           20140621
Time                8.35
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 6000
DS                    4
SWH           23980.814 Hz
FIDRES        0.365918 Hz
AQ            1.3664756 sec
RG                16384
DW               20.850 usec
DE                6.50 usec
TE               300.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                  7.10 usec
PL1                -4.00 dB
PL1W        82.02445221 W
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              80.00 usec
PL2                -3.00 dB
PL12               14.47 dB
PL13               15.06 dB
PL2W        19.34582710 W
PL12W        0.34640750 W
PL13W        0.30240381 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                  32768
SF         100.6127711 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

# Mass Spectrum SmartFormula Report

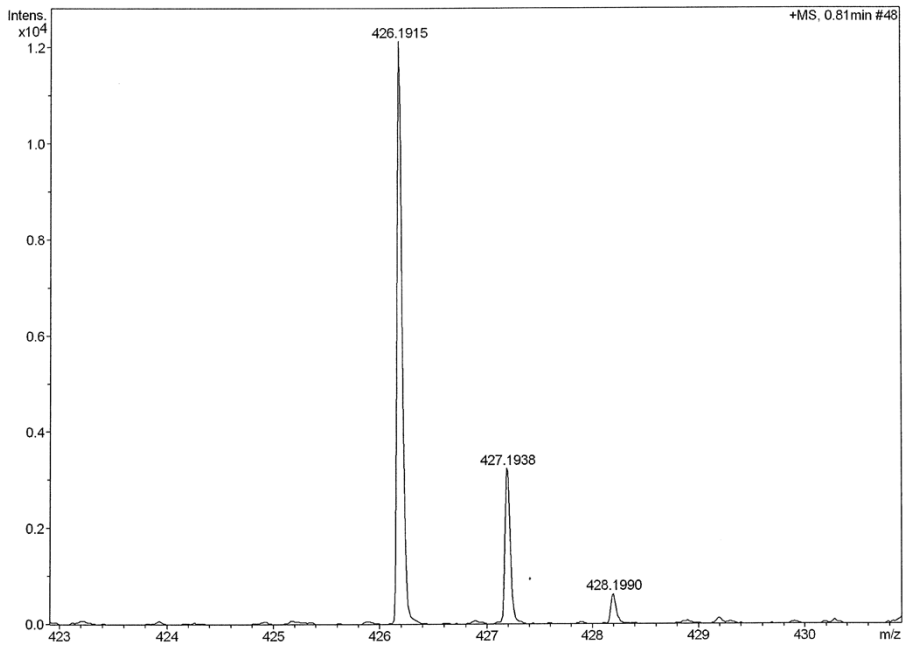
**Analysis Info**

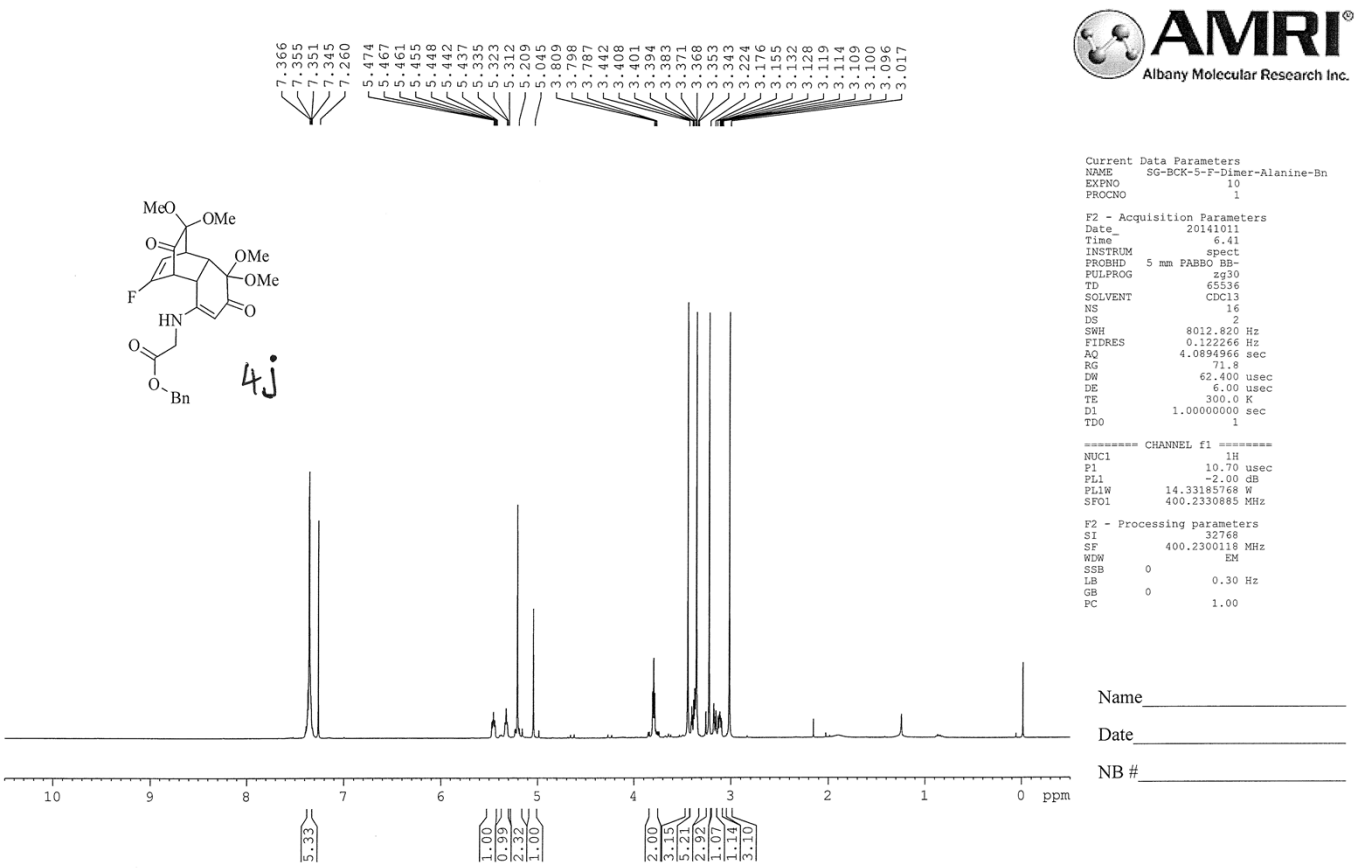
| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Chemistry\Outside\AMRI\20141103\5F-4Am-Pyrane-1.d | Acquisition Date | 11/3/2014 3:02:22 PM |
| Method | YCH_Pos-150-1800.m | Operator | default user |
| Sample Name | 5F-4Am-Pyrane | Instrument / Ser# | micrOTOF-Q II 10269 |
| Comment | AMRI<br>Santhosh Kumar Chittimalla | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 2.0 Bar |
| Focus | Not active | Set Capillary | 4500 V | Set Dry Heater | 200 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 6.0 l/min |
| Scan End | 1800 m/z | Set Collision Cell RF | 200.0 Vpp | Set Divert Valve | Waste |

| Meas. m/z | # | Formula | m/z | err [ppm] | rdb | e¯ Conf | N-Rule |
|---|---|---|---|---|---|---|---|
| 426.1915 | 1 | C 21 H 29 F N O 7 | 426.1923 | 1.8 | 7.5 | even | ok |



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```
Current Data Parameters
NAME       SG-BCK-5-F-Dimer-Alanine-Bn
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20141011
Time                6.41
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               4.0894966 sec
RG                    71.8
DW                 62.400 usec
DE                  6.00 usec
TE                 300.0 K
D1              1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 10.70 usec
PL1                -2.00 dB
PL1W          14.33185768 W
SFO1          400.2330885 MHz

F2 - Processing parameters
SI                 32768
SF            400.2300118 MHz
WDW                   EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

Name_____

Date_____

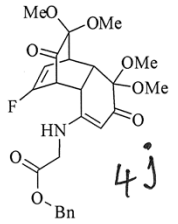
NB #_____

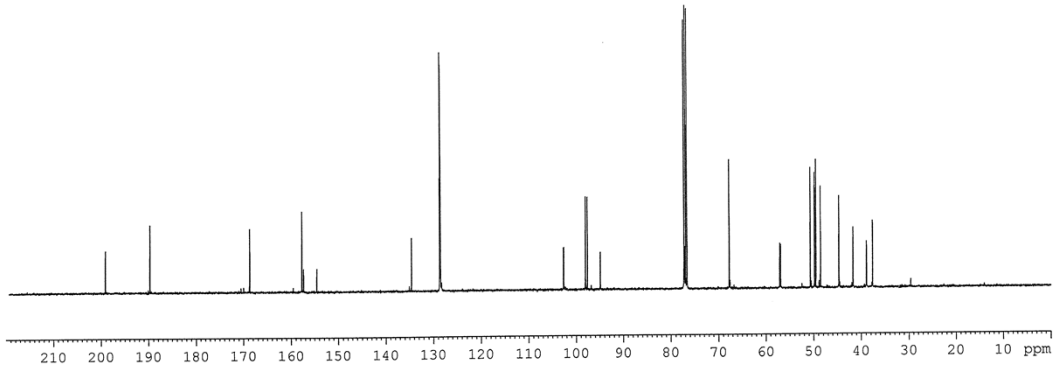
AMRI; SRC AV400
location; 18


Name_____

Date_____

NB #_____




```
Current Data Parameters
NAME       SG-BCK-5-F-Dimer-Glycine-Bn
EXPNO                  11
PROCNO                  1

F2 - Acquisition Parameters
Date_            20141011
Time                8.51
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 4000
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                  101
DW               20.800 usec
DE                6.50 usec
TE                300.0 K
D1            0.50000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                 8.60 usec
PL1               -1.00 dB
PL1W        44.58811569 W
SFO1       100.6479769 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2            80.00 usec
PL2              -2.00 dB
PL12             15.47 dB
PL13             15.72 dB
PL2W        14.33185768 W
PL12W        0.25662708 W
PL13W        0.24227159 W
SFO2       400.2316009 MHz

F2 - Processing parameters
SI                 32768
SF          100.6379194 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

# Mass Spectrum SmartFormula Report

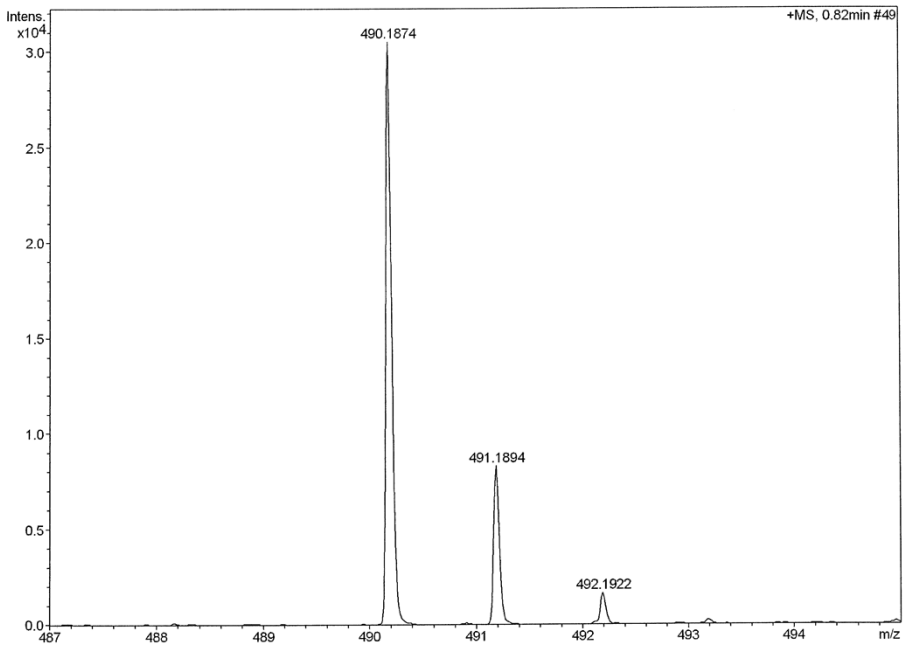
**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Chemistry\Outside\AMRI\20141103\5F-Gly-OBn-1.d | Acquisition Date | 11/3/2014 11:53:29 AM |
| Method | YCH_Pos-150-1800.m | Operator | default user |
| Sample Name | 5F-Gly-OBn | Instrument / Ser# | micrOTOF-Q II 10269 |
| Comment | AMRI<br>Santhosh Kumar Chittimalla | | |

**Acquisition Parameter**

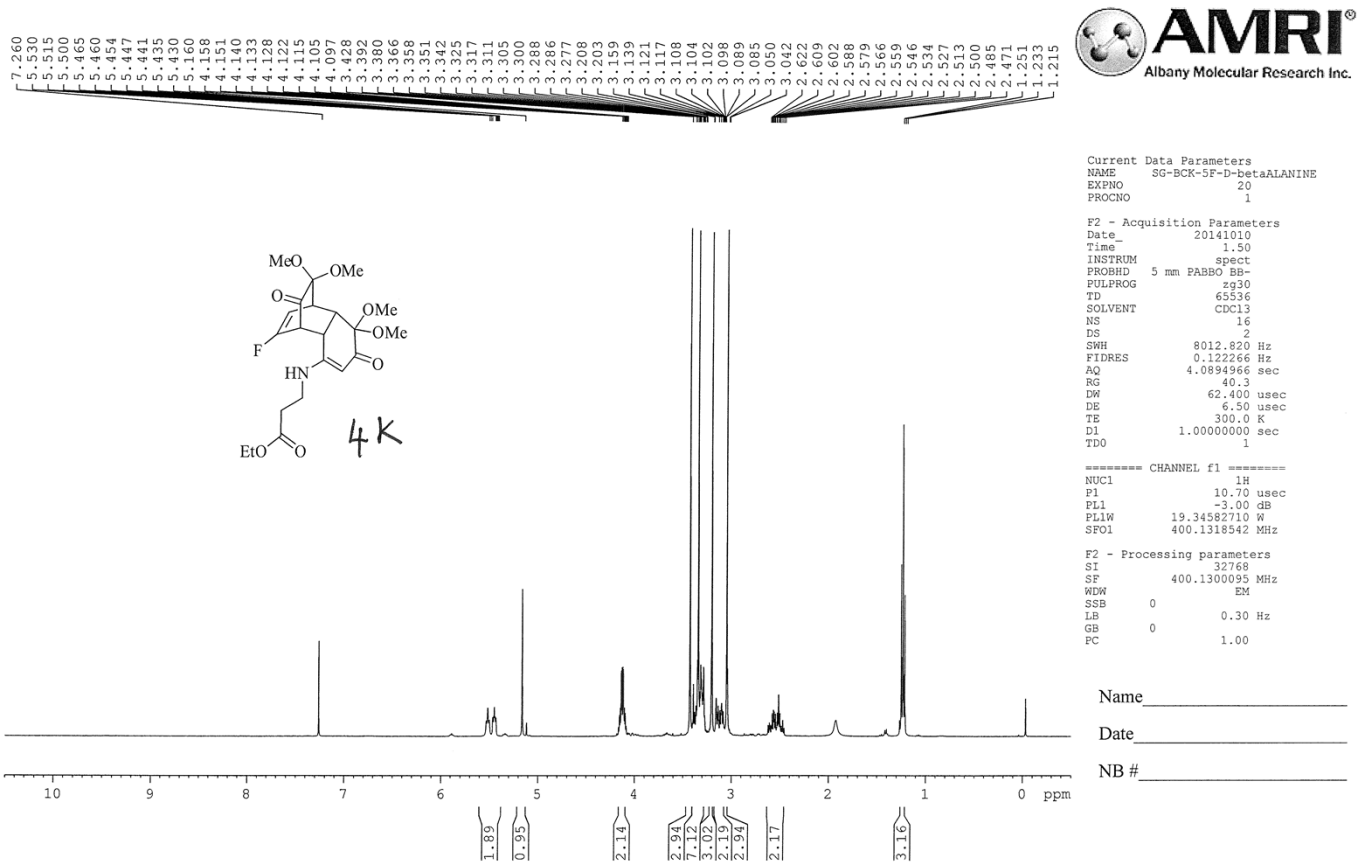
| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 2.0 Bar |
| Focus | Not active | Set Capillary | 4500 V | Set Dry Heater | 200 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 6.0 l/min |
| Scan End | 1800 m/z | Set Collision Cell RF | 200.0 Vpp | Set Divert Valve | Waste |

| Meas. m/z | # | Formula | m/z | err [ppm] | rdb | $e^-$ Conf | N-Rule |
|---|---|---|---|---|---|---|---|
| 490.1874 | 1 | C 25 H 29 F N O 8 | 490.1872 | -0.4 | 11.5 | even | ok |






Submitted to *RSC Advances*

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```
Current Data Parameters
NAME      SG-BCK-5F-D-betaALANINE
EXPNO                  20
PROCNO                  1

F2 - Acquisition Parameters
Date_           20141010
Time                1.50
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              4.0894966 sec
RG                  40.3
DW                 62.400 usec
DE                  6.50 usec
TE                 300.0 K
D1              1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 10.70 usec
PL1                -3.00 dB
PL1W         19.34582710 W
SFO1         400.1318542 MHz

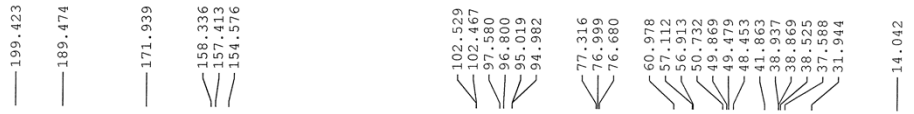
F2 - Processing parameters
SI                 32768
SF          400.1300095 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

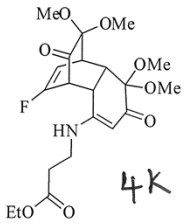
Name_____

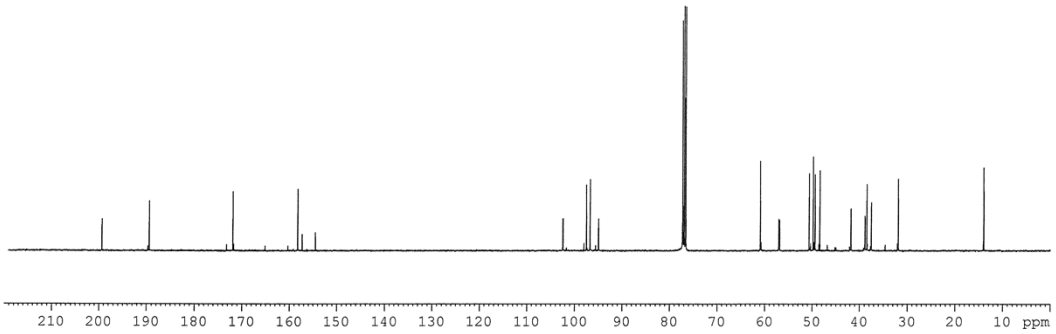
Date_____

NB #_____

AMRI SRC
location; 17




Name_____

Date_____

NB #_____

```
Current Data Parameters
NAME      SG-BCK-5F-D-betaALANINE
EXPNO                  21
PROCNO                  1

F2 - Acquisition Parameters
Date_           20141010
Time                5.12
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT            CDC13
NS                  3500
DS                     4
SWH           23980.814 Hz
FIDRES            0.365918 Hz
AQ             1.3664756 sec
RG                14596.5
DW                20.850 usec
DE                 6.50 usec
TE                300.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                  7.10 usec
PL1                -4.00 dB
PL1W        82.02445221 W
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -3.00 dB
PL12               14.47 dB
PL13               15.06 dB
PL2W        19.34582710 W
PL12W        0.34640750 W
PL13W        0.30240381 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127740 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

# Mass Spectrum SmartFormula Report

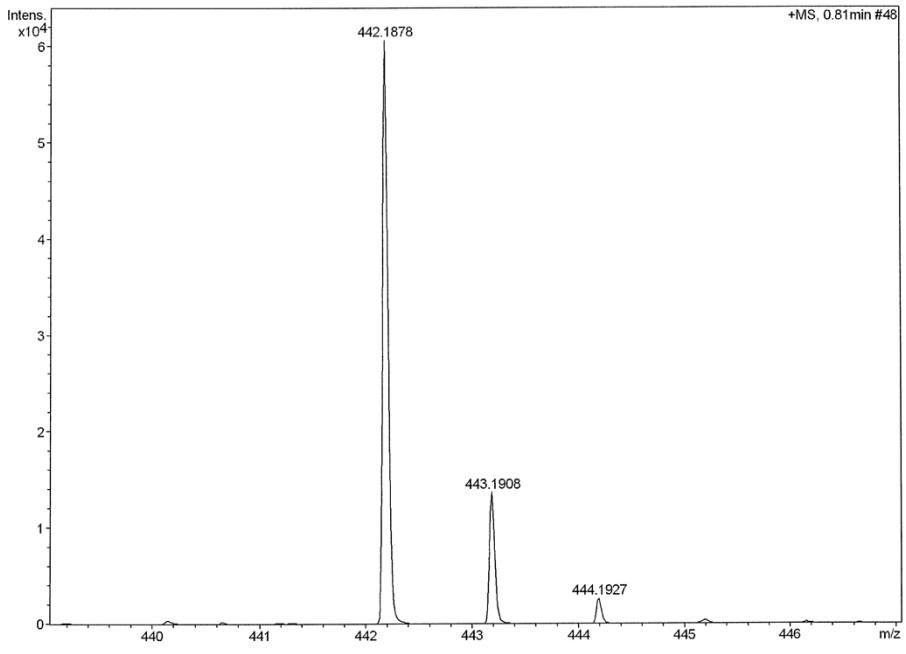
**Analysis Info**

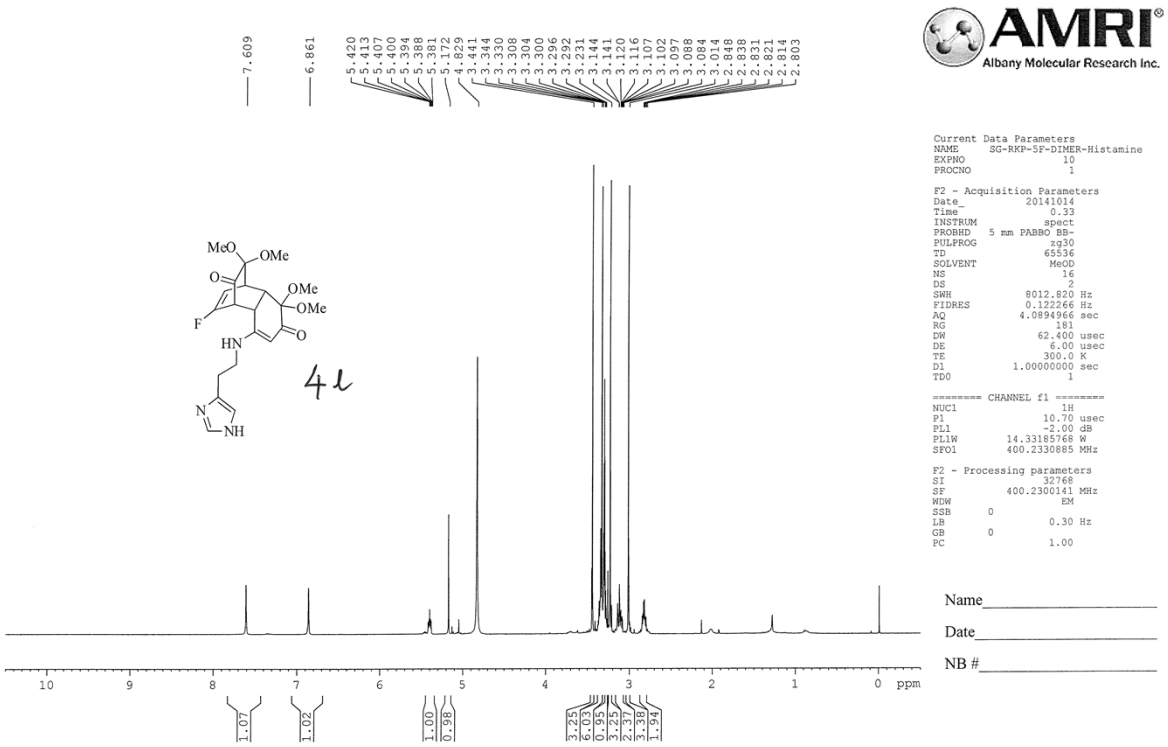
| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Chemistry\Outside\AMRI\20141103\5F-Beta-Alanine-1.d | Acquisition Date | 11/3/2014 12:33:52 PM |
| Method | YCH_Pos-150-1800.m | Operator | default user |
| Sample Name | 5F-Beta-Alanine | Instrument / Ser# | micrOTOF-Q II 10269 |
| Comment | AMRI<br>Santhosh Kumar Chittimalla | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 2.0 Bar |
| Focus | Not active | Set Capillary | 4500 V | Set Dry Heater | 200 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 6.0 l/min |
| Scan End | 1800 m/z | Set Collision Cell RF | 200.0 Vpp | Set Divert Valve | Waste |

| Meas. m/z | # | Formula | m/z | err [ppm] | rdb | e¯ Conf | N-Rule |
|---|---|---|---|---|---|---|---|
| 442.1878 | 1 | C 21 H 29 F N O 8 | 442.1872 | -1.5 | 7.5 | even | ok |



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```
Current Data Parameters
NAME       SG-RKP-5F-DIMER-Histamine
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20141014
Time                0.33
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT            MeOD
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ             4.0894966 sec
RG                  181
DW                62.400 usec
DE                 6.00 usec
TE                300.0 K
D1             1.00000000 sec
TD0                    1

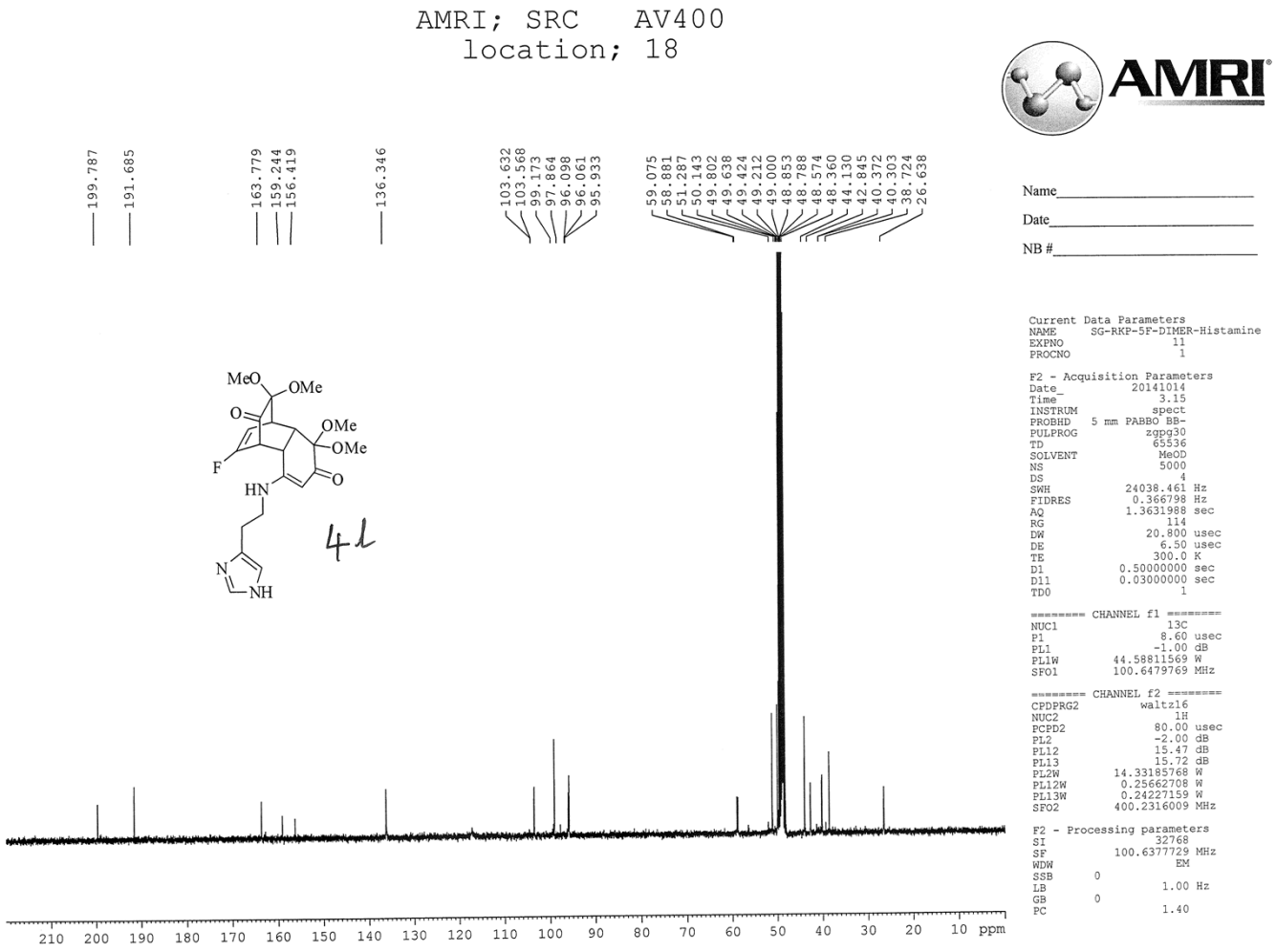
======== CHANNEL f1 ========
NUC1                1H
P1                10.70 usec
PL1               -2.00 dB
PLlW        14.33185768 W
SFO1        400.2330885 MHz

F2 - Processing parameters
SI                 32768
SF          400.2300141 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Name_____

Date_____

NB #_____




AMRI

Name_____

Date_____

NB #_____

```
Current Data Parameters
NAME       SG-RKP-5F-DIMER-Histamine
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20141014
Time                3.15
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT            MeOD
NS                 5000
DS                    4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                  114
DW               20.800 usec
DE                6.50 usec
TE                300.0 K
D1           0.50000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                 8.60 usec
PL1               -1.00 dB
PL1W        44.58811569 W
SFO1       100.6479769 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            80.00 usec
PL2              -2.00 dB
PL12             15.47 dB
PL13             15.72 dB
PL2W        14.33185768 W
PL12W        0.25662708 W
PL13W        0.24227159 W
SFO2       400.2316009 MHz

F2 - Processing parameters
SI                32768
SF         100.6377729 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

# Mass Spectrum SmartFormula Report

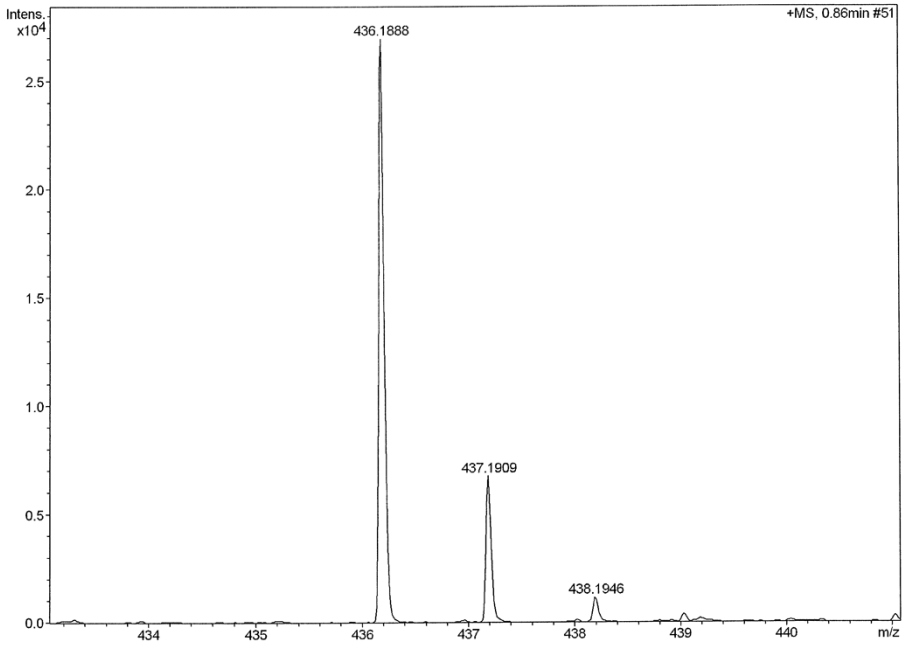
**Analysis Info**

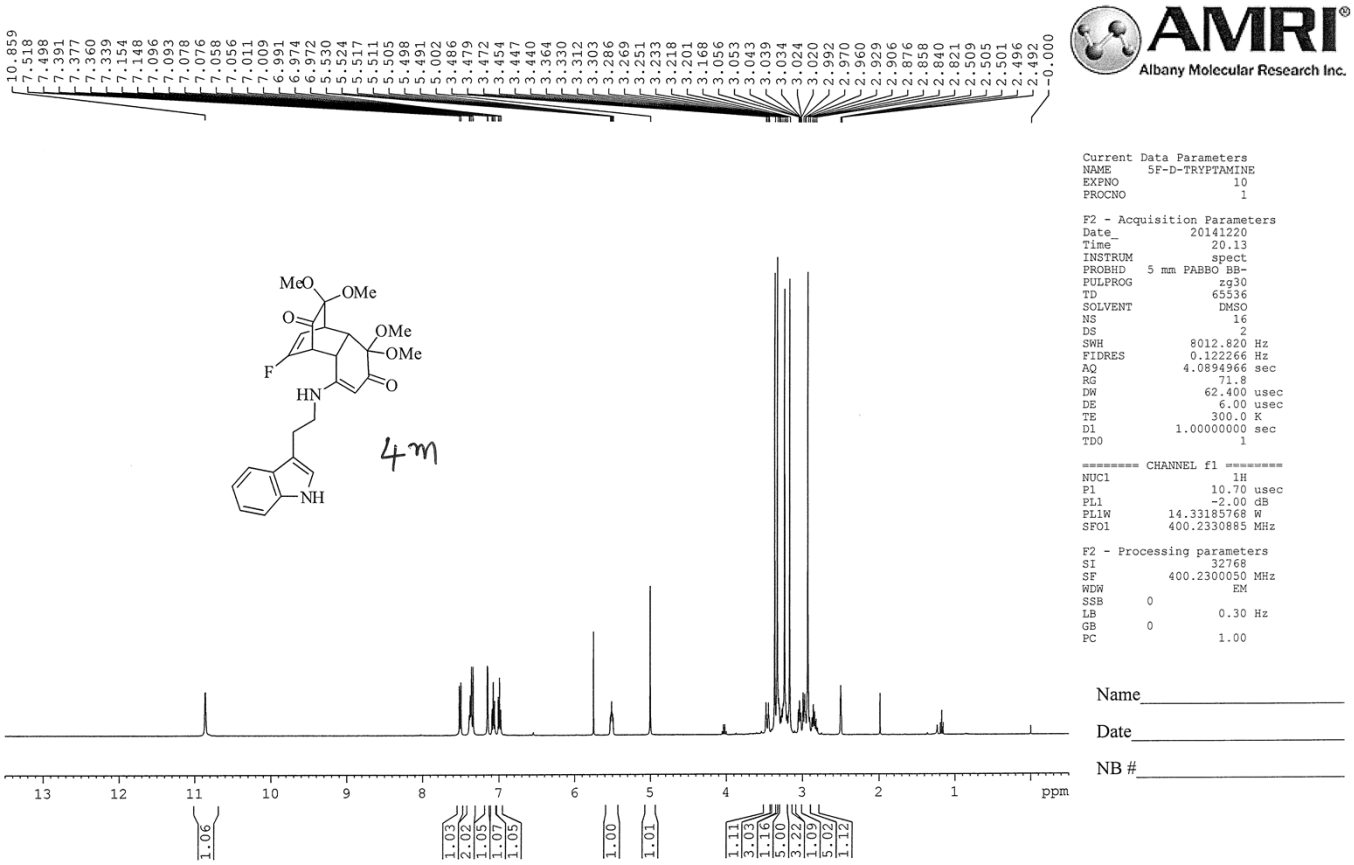
| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Chemistry\Outside\AMRI\20141103\5F-Histamin-1.d | Acquisition Date | 11/3/2014 11:46:13 AM |
| Method | YCH_Pos-150-1800.m | Operator | default user |
| Sample Name | 5F-Histamin | Instrument / Ser# | micrOTOF-Q II 10269 |
| Comment | AMRI<br>Santhosh Kumar Chittimalla | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 2.0 Bar |
| Focus | Not active | Set Capillary | 4500 V | Set Dry Heater | 200 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 6.0 l/min |
| Scan End | 1800 m/z | Set Collision Cell RF | 200.0 Vpp | Set Divert Valve | Waste |

| Meas. m/z | # | Formula | m/z | err [ppm] | rdb | e¯ Conf | N-Rule |
|---|---|---|---|---|---|---|---|
| 436.1888 | 1 | C 21 H 27 F N 3 O 6 | 436.1878 | -2.2 | 9.5 | even | ok |



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```
Current Data Parameters
NAME      5F-D-TRYPTAMINE
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_            20141220
Time                20.13
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894966 sec
RG                  71.8
DW                 62.400 usec
DE                  6.00 usec
TE                 300.0 K
D1              1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                   1H
P1                 10.70 usec
PL1                -2.00 dB
PL1W         14.33185768 W
SFO1         400.2330885 MHz

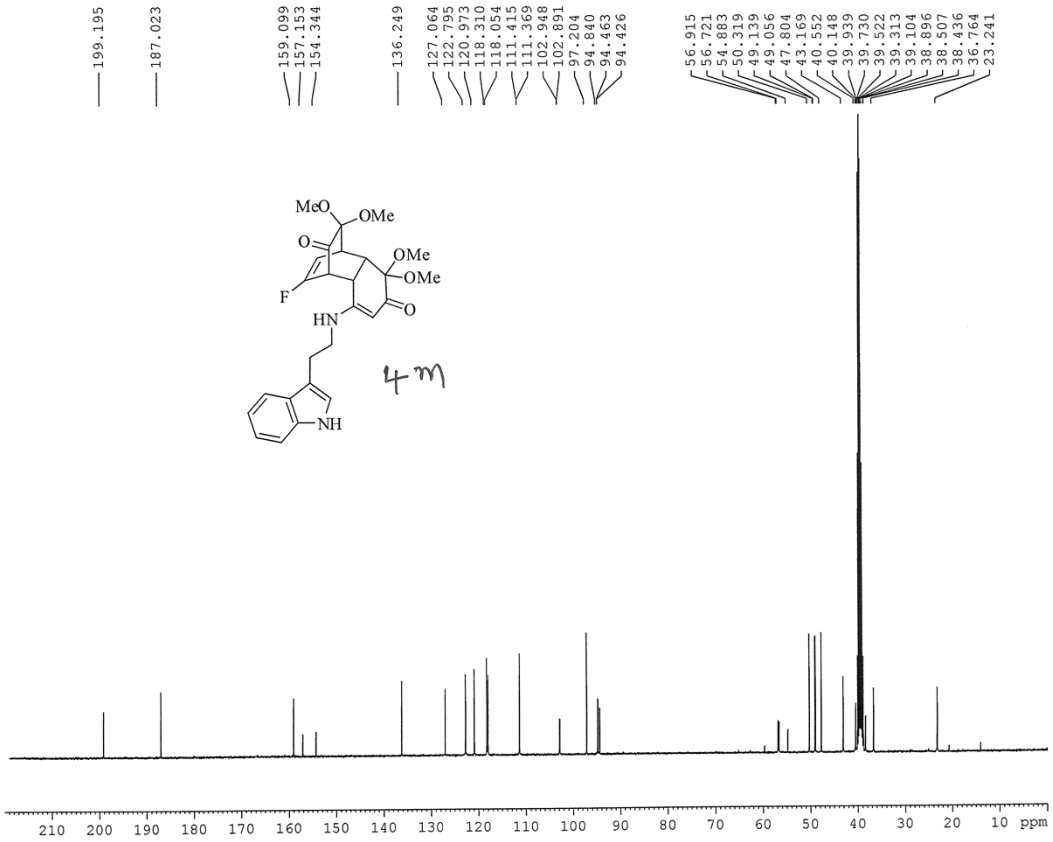
F2 - Processing parameters
SI                 32768
SF           400.2300050 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Name_____

Date_____

NB #_____

AMRI; SRC AV400
location; 18




Name_____

Date_____

NB #_____

```
Current Data Parameters
NAME      5F-D-TRYPTAMINE
EXPNO                  11
PROCNO                  1

F2 - Acquisition Parameters
Date_           20141221
Time                0.32
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                  8000
DS                     4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                   101
DW                20.800 usec
DE                 6.50 usec
TE                300.0 K
D1             0.50000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                   8.60 usec
PL1                 -1.00 dB
PL1W          44.58811569 W
SFO1         100.6479769 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                 -2.00 dB
PL12                15.47 dB
PL13                15.72 dB
PL2W          14.33185768 W
PL12W          0.25662708 W
PL13W          0.24227159 W
SFO2         400.2316009 MHz

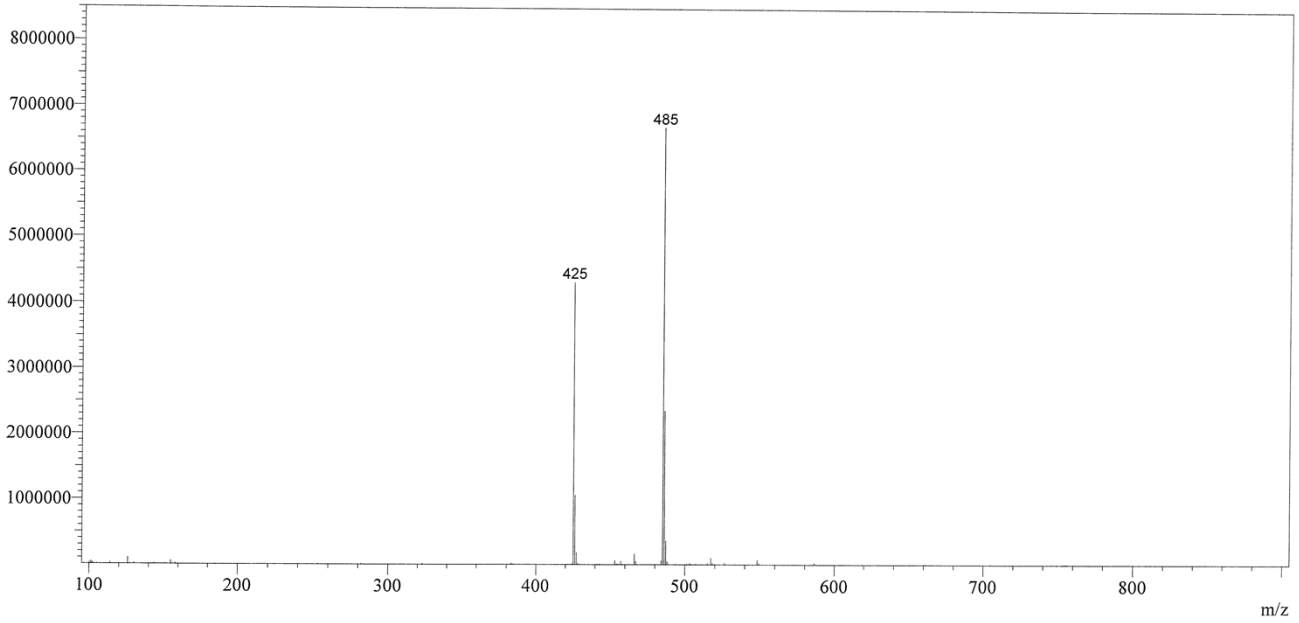
F2 - Processing parameters
SI                    32768
SF           100.6379622 MHz
WDW                      EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

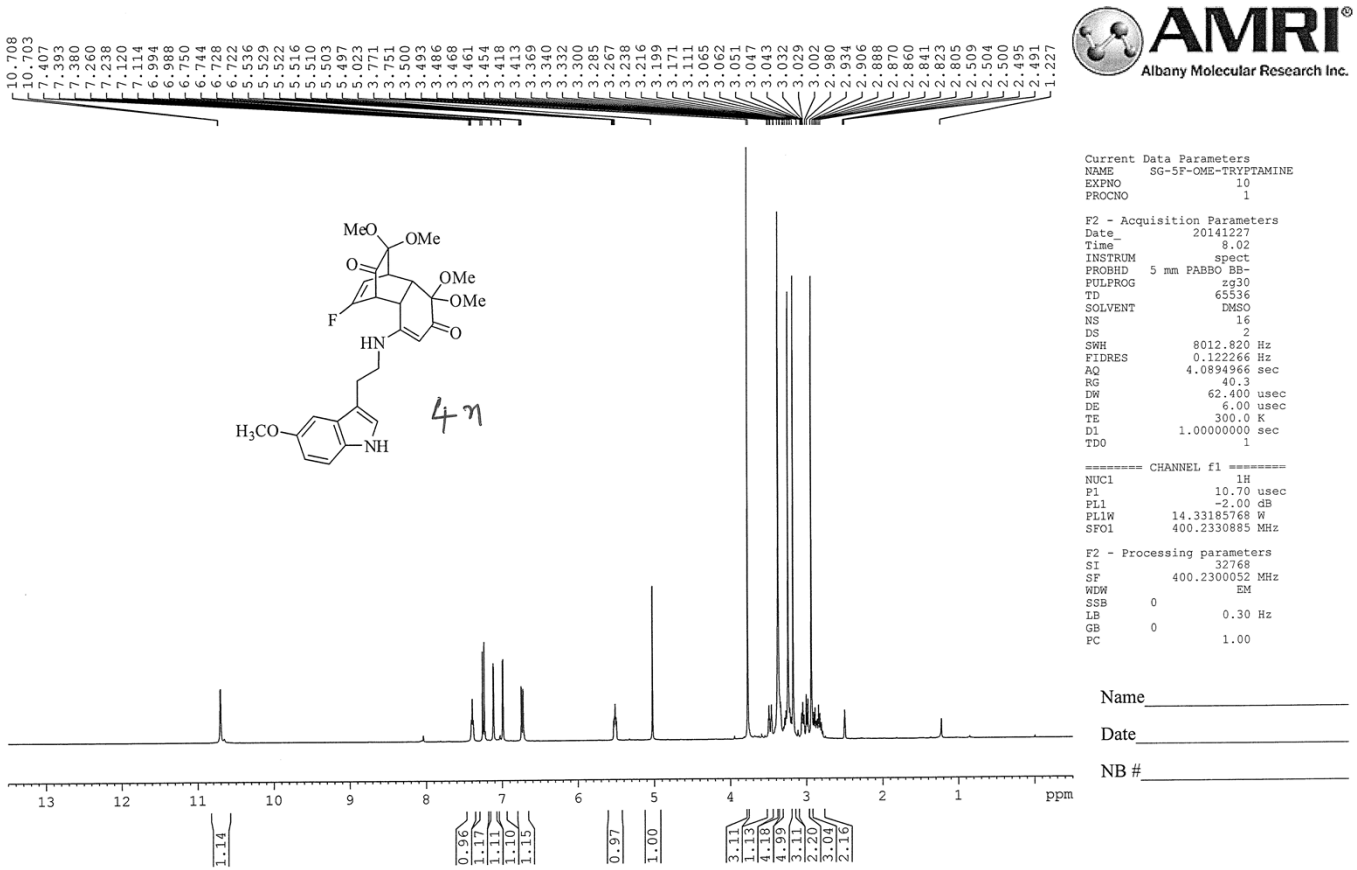
# AMRI Direct MS Analysis Report

| | |
|---|---|
| Acquired by | : System Administrator |
| Sample Name | : SG-RKP-5F-TRYPTAMINE |
| Data File | : SG-RKP-5F-TRYPTAMINE.lcd |
| Method File | : ESI-LCMS Method3.lcm |
| Month-Day Acquired | : 2/4/2015 |

Mass Spectrum

Peak # : 1, Retention Time : 2.867 min
Base Peak m/z : 485, Base Peak Intensity : 66882376688237
Polarity :Positive, Event : 1 - 1



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```
Current Data Parameters
NAME      SG-5F-OME-TRYPTAMINE
EXPNO                       10
PROCNO                       1

F2 - Acquisition Parameters
Date_              20141227
Time                   8.02
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                        16
DS                         2
SWH                8012.820 Hz
FIDRES             0.122266 Hz
AQ                 4.0894966 sec
RG                      40.3
DW                    62.400 usec
DE                     6.00 usec
TE                    300.0 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     10.70 usec
PL1                    -2.00 dB
PL1W           14.33185768 W
SFO1           400.2330885 MHz

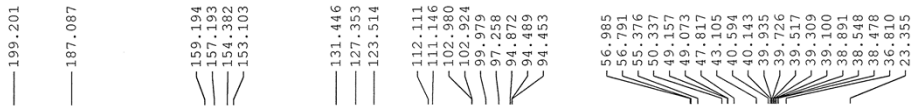
F2 - Processing parameters
SI                     32768
SF             400.2300052 MHz
WDW                       EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

Name_____

Date_____

NB #_____

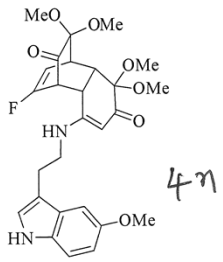
AMRI; SRC AV400
location; 18

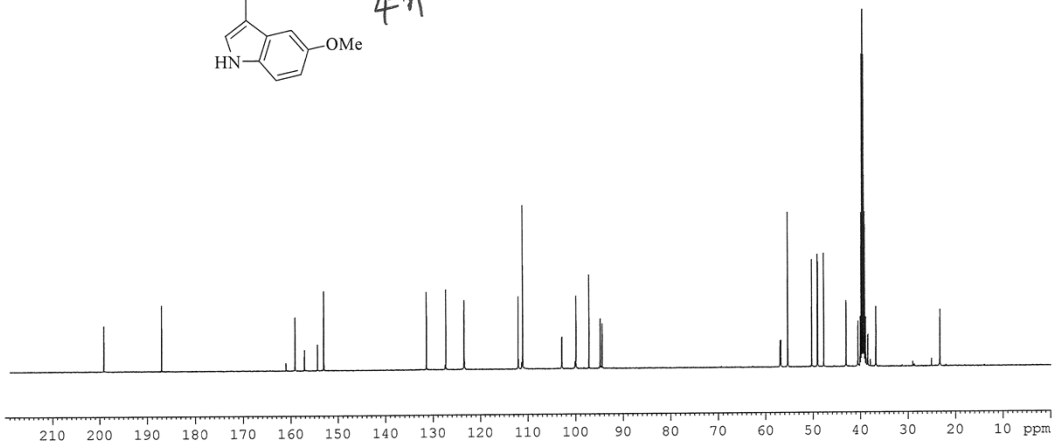



Name_____

Date_____

NB #_____




```
Current Data Parameters
NAME      SG-5F-OME-TRYPTAMINE
EXPNO                   11
PROCNO                   1

F2 - Acquisition Parameters
Date_           20141227
Time              12.21
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT             DMSO
NS                  8000
DS                     4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                   101
DW               20.800 usec
DE                6.50 usec
TE                300.0 K
D1           0.50000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                   8.60 usec
PL1                 -1.00 dB
PL1W        44.58811569 W
SFO1       100.6479769 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2               80.00 usec
PL2                 -2.00 dB
PL12                15.47 dB
PL13                15.72 dB
PL2W        14.33185768 W
PL12W        0.25662708 W
PL13W        0.24227159 W
SFO2       400.2316009 MHz

F2 - Processing parameters
SI                 32768
SF          100.6379595 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

# Mass Spectrum SmartFormula Report

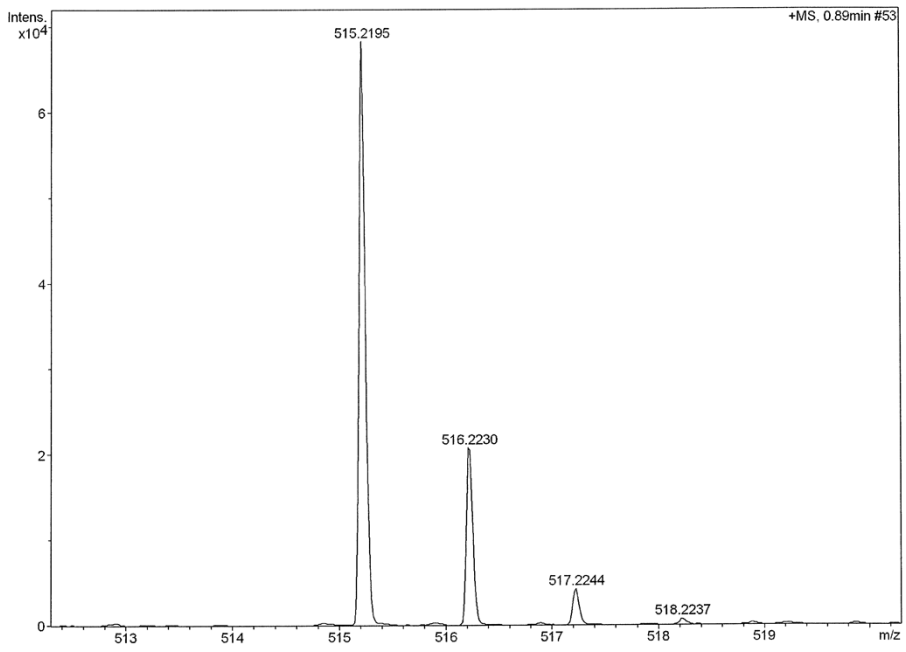
**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Chemistry\Outside\AMRI\20141218\5F-OMe-Tryp-1.d | Acquisition Date | 12/18/2014 4:44:46 PM |
| Method | YCH_Pos-150-1800.m | Operator | default user |
| Sample Name | 5F-OMe-Tryp | Instrument / Ser# | micrOTOF-Q II 10269 |
| Comment | AMRI<br>Santhosh Kumar Chittimalla | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 2.0 Bar |
| Focus | Not active | Set Capillary | 4500 V | Set Dry Heater | 200 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 6.0 l/min |
| Scan End | 1800 m/z | Set Collision Cell RF | 200.0 Vpp | Set Divert Valve | Waste |

| Meas. m/z | # | Formula | m/z | err [ppm] | rdb | e⁻ Conf | N-Rule |
|---|---|---|---|---|---|---|---|
| 515.2195 | 1 | C 27 H 32 F N 2 O 7 | 515.2188 | -1.4 | 12.5 | even | ok |

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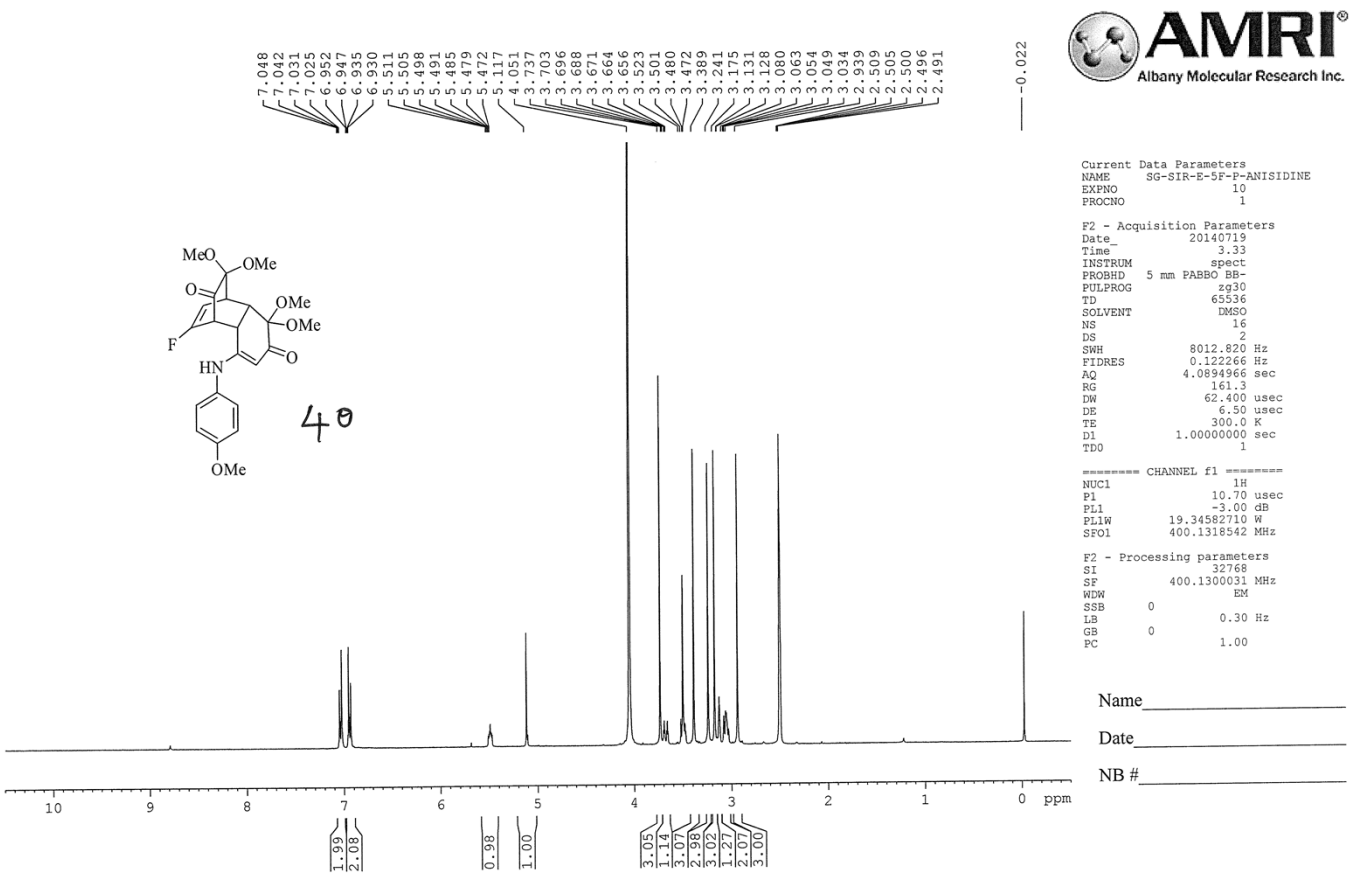


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```
Current Data Parameters
NAME      SG-SIR-E-5F-P-ANISIDINE
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140719
Time                3.33
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894966 sec
RG                  161.3
DW                 62.400 usec
DE                  6.50 usec
TE                 300.0 K
D1              1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                   1H
P1                 10.70 usec
PL1                -3.00 dB
PL1W         19.34582710 W
SFO1         400.1318542 MHz

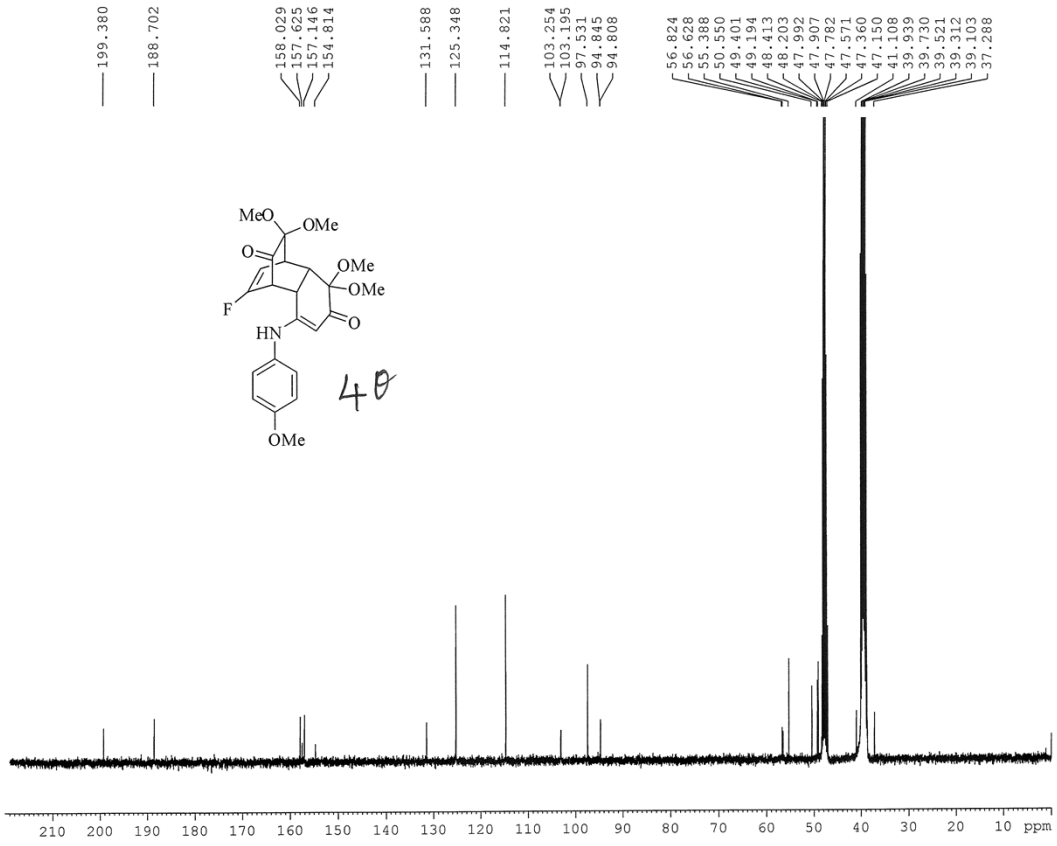
F2 - Processing parameters
SI                 32768
SF           400.1300031 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Name_____

Date_____

NB #_____

AMRI SRC
location; 17




Name_____

Date_____

NB #_____

```
Current Data Parameters
NAME      SG-SIR-E-5F-P-ANISIDINE
EXPNO                  11
PROCNO                  1

F2 - Acquisition Parameters
Date_            20140719
Time                10.16
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT             DMSO
NS                   7000
DS                      4
SWH            23980.814 Hz
FIDRES          0.365918 Hz
AQ             1.3664756 sec
RG               18390.4
DW                20.850 usec
DE                 6.50 usec
TE                300.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                   7.10 usec
PL1                 -4.00 dB
PL1W         82.02445221 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2               80.00 usec
PL2                 -3.00 dB
PL12                14.47 dB
PL13                15.06 dB
PL2W         19.34582710 W
PL12W         0.34640750 W
PL13W         0.30240381 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                  32768
SF          100.6127805 MHz
WDW                    EM
SSB          0
LB                   1.00 Hz
GB           0
PC                   1.40
```

# Mass Spectrum SmartFormula Report

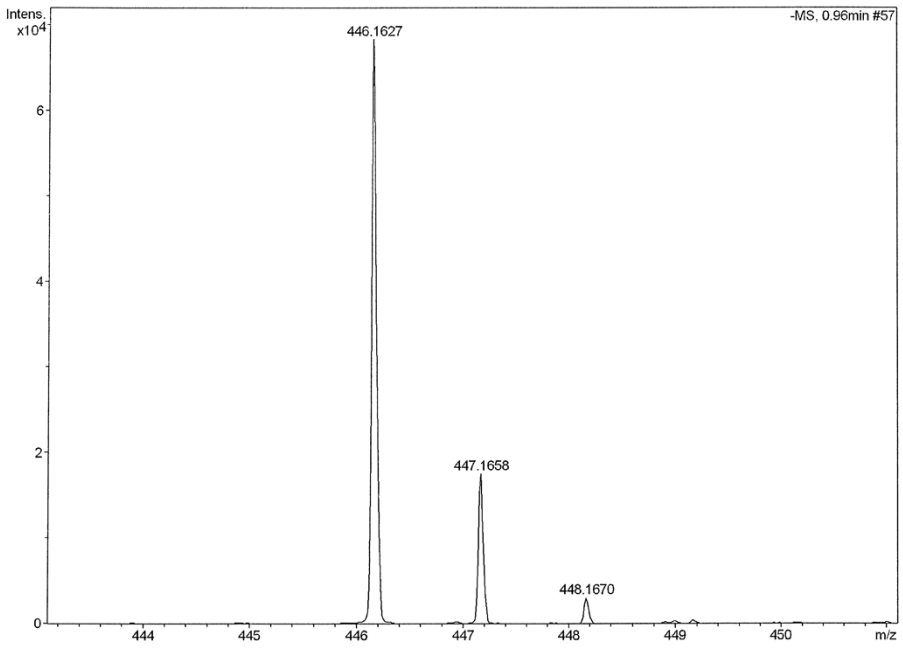
**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Chemistry\Outside\AMRI\20141103\5F-Anisidine-1n.d | Acquisition Date | 11/3/2014 11:04:33 AM |
| Method | YCH_Pos-150-1800.m | Operator | default user |
| Sample Name | 5F-Anisidine | Instrument / Ser# | micrOTOF-Q II 10269 |
| Comment | AMRI<br>Santhosh Kumar Chittimalla | | |

**Acquisition Parameter**

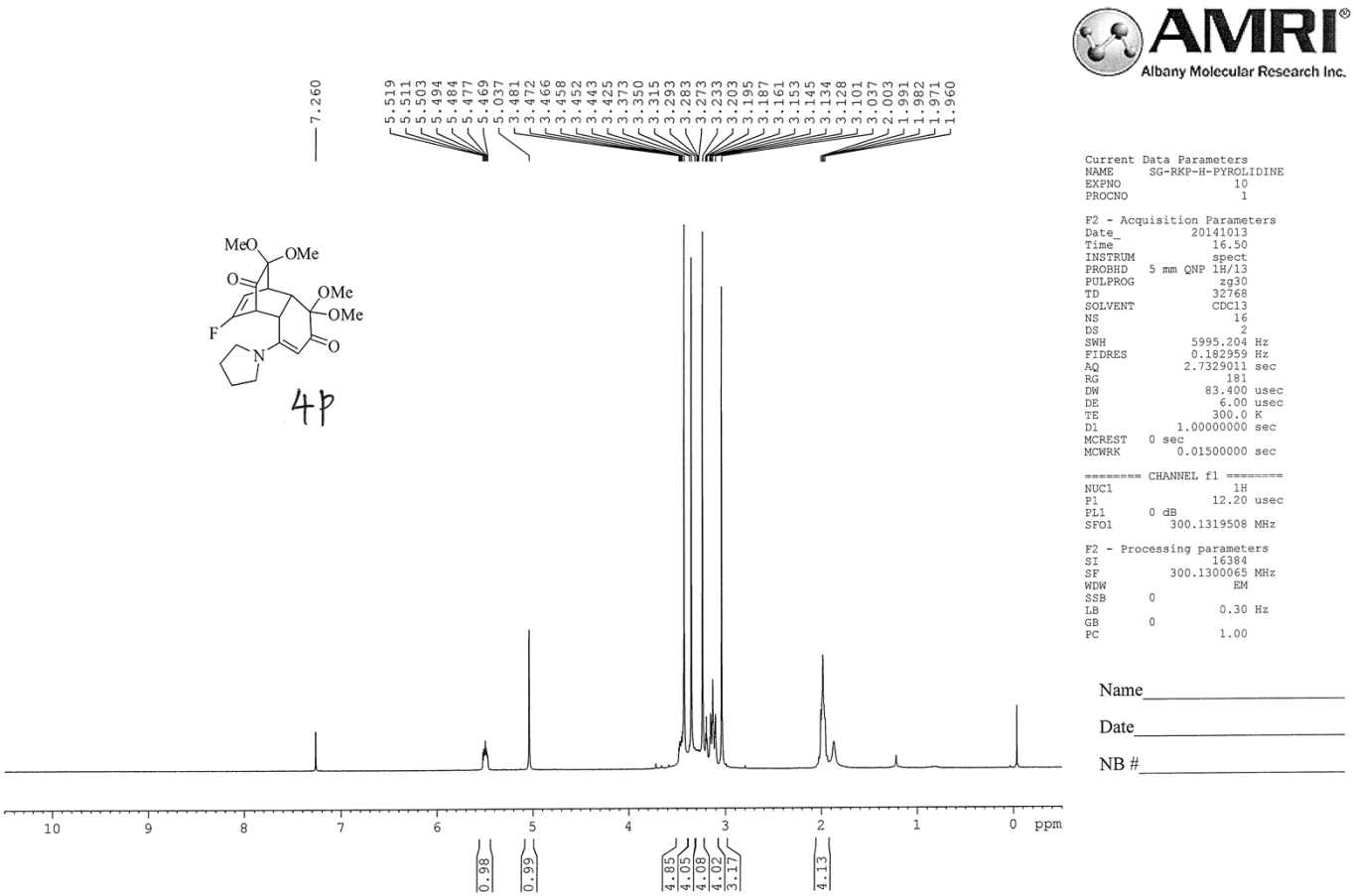
| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Negative | Set Nebulizer | 2.0 Bar |
| Focus | Not active | Set Capillary | 3500 V | Set Dry Heater | 200 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 6.0 l/min |
| Scan End | 1800 m/z | Set Collision Cell RF | 200.0 Vpp | Set Divert Valve | Waste |

| Meas. m/z | # | Formula | m/z | err [ppm] | rdb | e¯ Conf | N-Rule |
|---|---|---|---|---|---|---|---|
| 446.1627 | 1 | C 23 H 25 F N O 7 | 446.1621 | -1.5 | 11.5 | even | ok |






Submitted to *RSC Advances*

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```
Current Data Parameters
NAME      SG-RKP-H-PYROLIDINE
EXPNO                      10
PROCNO                      1

F2 - Acquisition Parameters
Date_              20141013
Time                  16.50
INSTRUM               spect
PROBHD   5 mm QNP 1H/13
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                5995.204 Hz
FIDRES            0.182959 Hz
AQ                2.7329011 sec
RG                      181
DW                   83.400 usec
DE                    6.00 usec
TE                   300.0 K
D1                1.00000000 sec
MCREST    0 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                    12.20 usec
PL1       0 dB
SFO1           300.1319508 MHz

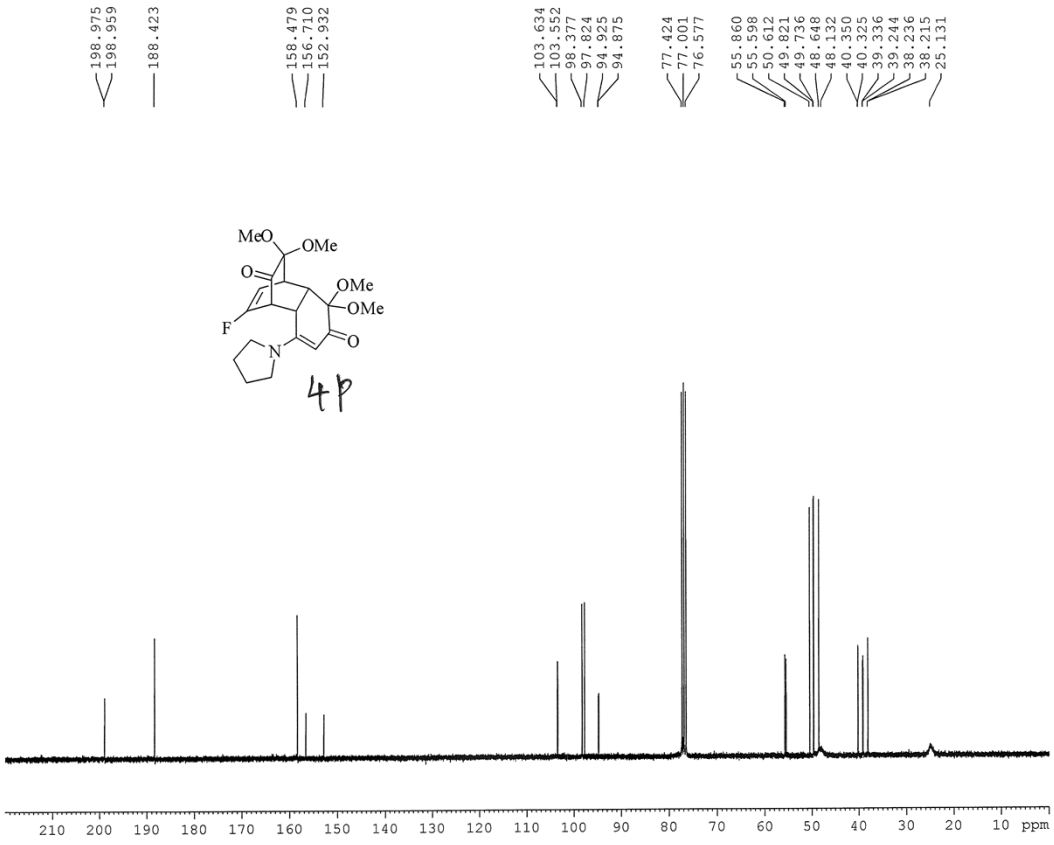
F2 - Processing parameters
SI                       16384
SF              300.1300065 MHz
WDW                        EM
SSB       0
LB                     0.30 Hz
GB        0
PC                     1.00
```

Name_____

Date_____

NB #_____

AMRI; SRC
location; 15




Name_____

Date_____

NB #_____

```
Current Data Parameters
NAME      SG-RKP-5F-PYROLIDINE
EXPNO                   11
PROCNO                   1

F2 - Acquisition Parameters
Date_           20141122
Time                12.57
INSTRUM             spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 6000
DS                    0
SWH           22675.736 Hz
FIDRES         0.346004 Hz
AQ            1.4451188 sec
RG                 4096
DW               22.050 usec
DE                6.00 usec
TE                300.0 K
D1           0.50000000 sec
d11          0.03000000 sec
DELTA        0.40000001 sec
MCREST   0 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                 8.00 usec
PL1               -2.00 dB
SFO1         75.4767751 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2              80.00 usec
PL2       0 dB
PL12              16.33 dB
PL13              16.00 dB
SFO2        300.1315007 MHz

F2 - Processing parameters
SI                131072
SF           75.4677519 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.40
```

# Mass Spectrum SmartFormula Report

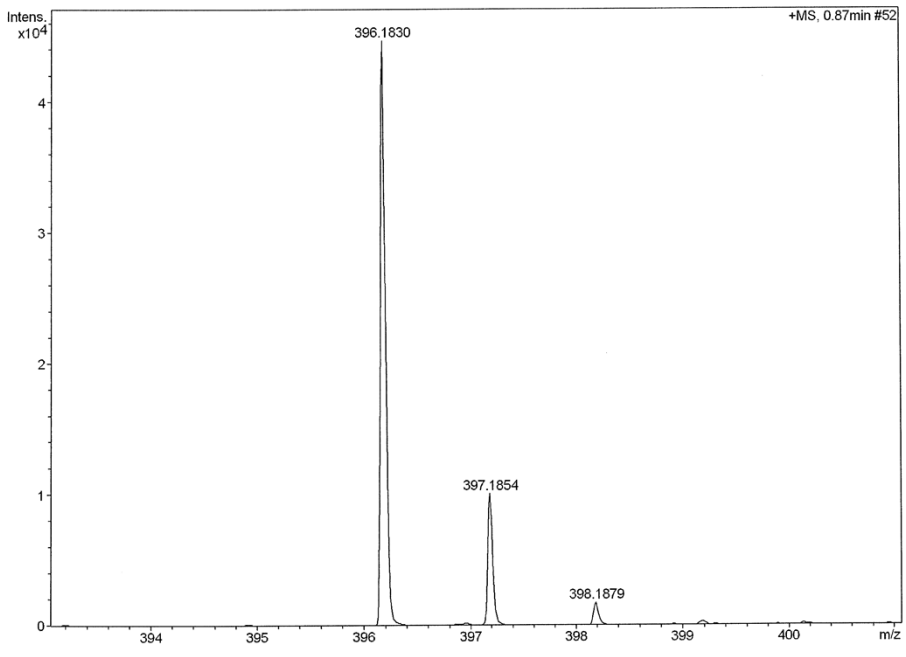
**Analysis Info**

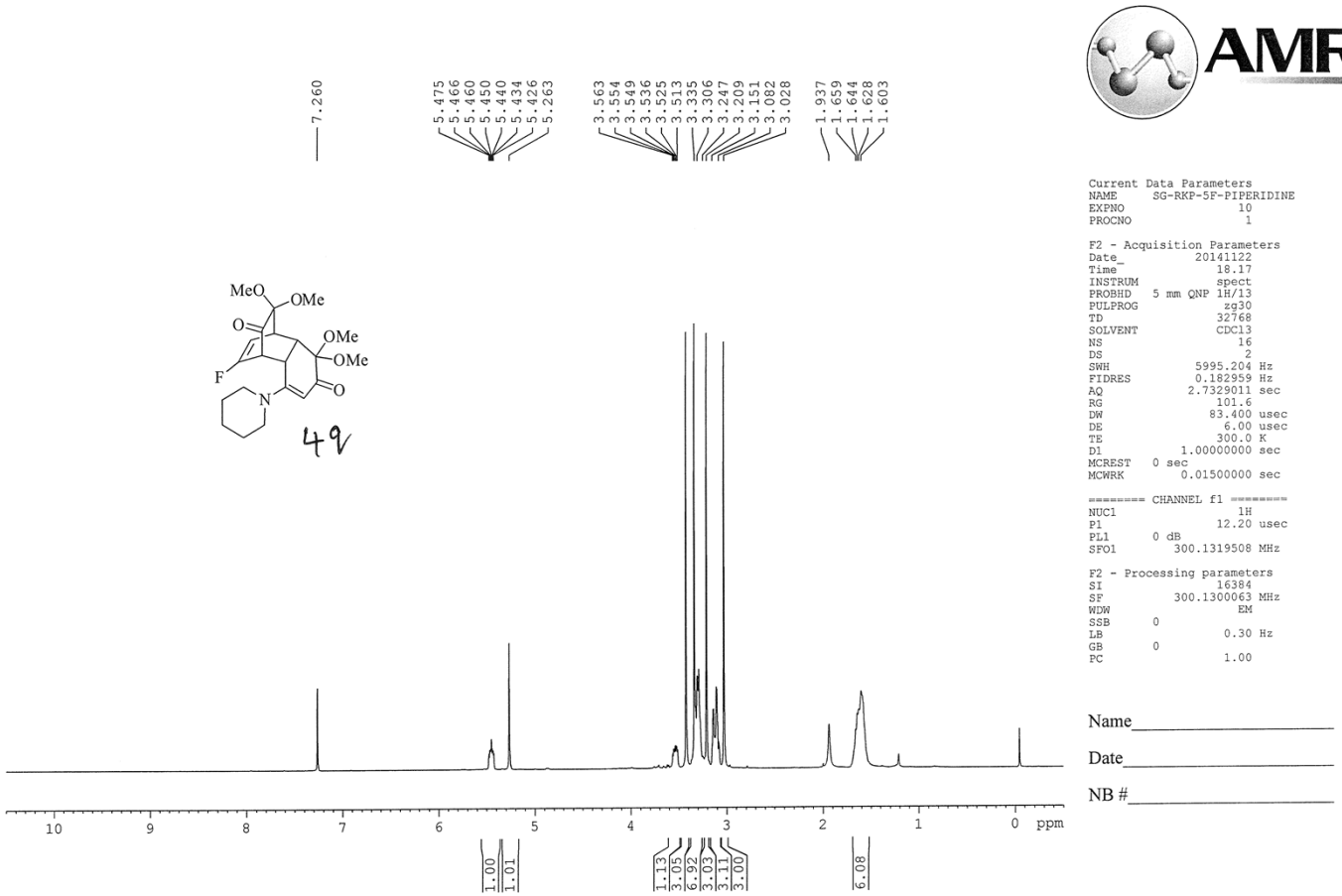
| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Chemistry\Outside\AMRI\20141103\5F-Pyrrolidine-1.d | Acquisition Date | 11/3/2014 12:18:47 PM |
| Method | YCH_Pos-150-1800.m | Operator | default user |
| Sample Name | 5F-Pyrrolidine | Instrument / Ser# | micrOTOF-Q II 10269 |
| Comment | AMRI<br>Santhosh Kumar Chittimalla | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 2.0 Bar |
| Focus | Not active | Set Capillary | 4500 V | Set Dry Heater | 200 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 6.0 l/min |
| Scan End | 1800 m/z | Set Collision Cell RF | 200.0 Vpp | Set Divert Valve | Waste |

| Meas. m/z | # | Formula | m/z | err [ppm] | rdb | e⁻ Conf | N-Rule |
|---|---|---|---|---|---|---|---|
| 396.1830 | 1 | C 20 H 27 F N O 6 | 396.1817 | -3.2 | 7.5 | even | ok |






AMRI

```
Current Data Parameters
NAME      SG-RKP-5F-PIPERIDINE
EXPNO                       10
PROCNO                       1

F2 - Acquisition Parameters
Date_              20141122
Time                  18.17
INSTRUM               spect
PROBHD    5 mm QNP 1H/13
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                5995.204 Hz
FIDRES             0.182959 Hz
AQ                2.7329011 sec
RG                    101.6
DW                   83.400 usec
DE                    6.00 usec
TE                   300.0 K
D1              1.00000000 sec
MCREST    0 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                    12.20 usec
PL1          0 dB
SFO1           300.1319508 MHz

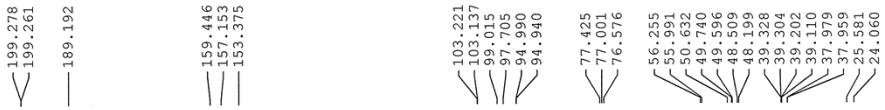
F2 - Processing parameters
SI                    16384
SF              300.1300063 MHz
WDW                      EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

Name_____

Date_____

NB #_____

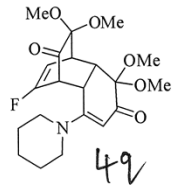
AMRI; SRC
location; 15

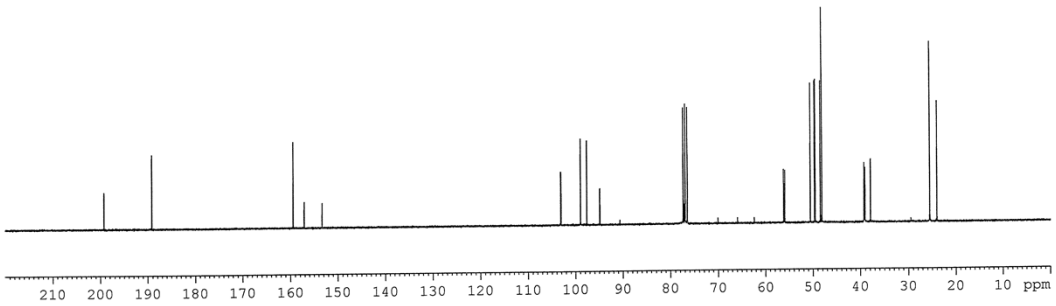



Name_____

Date_____

NB #_____




```
Current Data Parameters
NAME      SG-RKP-5F-PIPERIDINE
EXPNO                   11
PROCNO                   1

F2 - Acquisition Parameters
Date_             20141122
Time                21.38
INSTRUM             spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 6000
DS                    0
SWH           22675.736 Hz
FIDRES         0.346004 Hz
AQ             1.4451188 sec
RG                13004
DW               22.050 usec
DE                6.00 usec
TE               300.0 K
D1            0.50000000 sec
d11           0.03000000 sec
DELTA         0.40000001 sec
MCREST   0 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                8.00 usec
PL1               -2.00 dB
SFO1         75.4767751 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2            80.00 usec
PL2       0 dB
PL12             16.33 dB
PL13             16.00 dB
SFO2        300.1315007 MHz

F2 - Processing parameters
SI                131072
SF           75.4677542 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.40
```

# Mass Spectrum SmartFormula Report

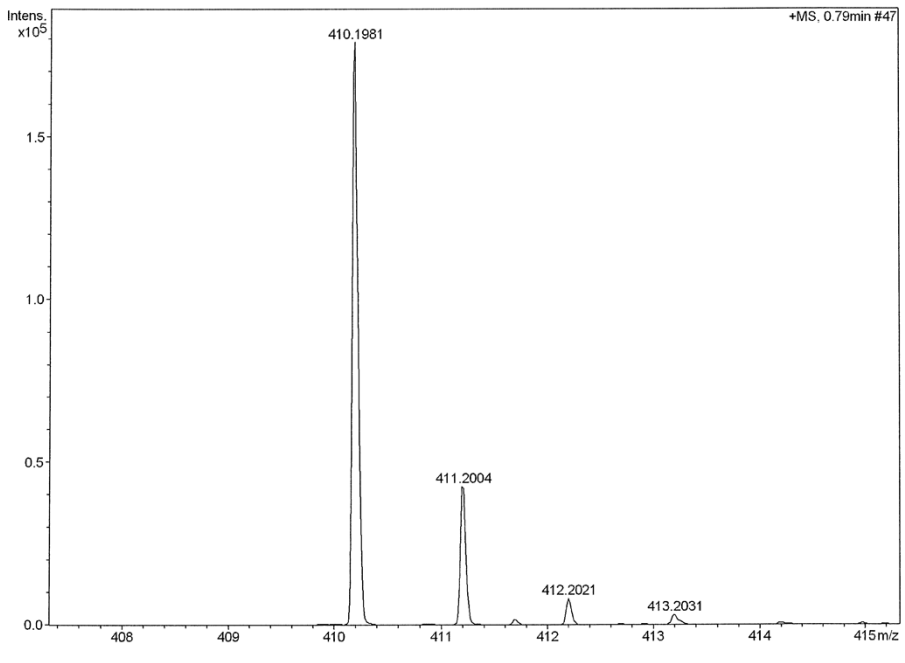
**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Chemistry\Outside\AMRI\20141218\5F-Piperidine-1.d | Acquisition Date | 12/18/2014 5:04:57 PM |
| Method | YCH_Pos-150-1800.m | Operator | default user |
| Sample Name | 5F-Piperidine | Instrument / Ser# | micrOTOF-Q II 10269 |
| Comment | AMRI<br>Santhosh Kumar Chittimalla | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 2.0 Bar |
| Focus | Not active | Set Capillary | 4500 V | Set Dry Heater | 200 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 6.0 l/min |
| Scan End | 1800 m/z | Set Collision Cell RF | 200.0 Vpp | Set Divert Valve | Waste |

| Meas. m/z | # | Formula | m/z | err [ppm] | rdb | e¯ Conf | N-Rule |
|---|---|---|---|---|---|---|---|
| 410.1981 | 1 | C 21 H 29 F N O 6 | 410.1973 | -1.9 | 7.5 | even | ok |

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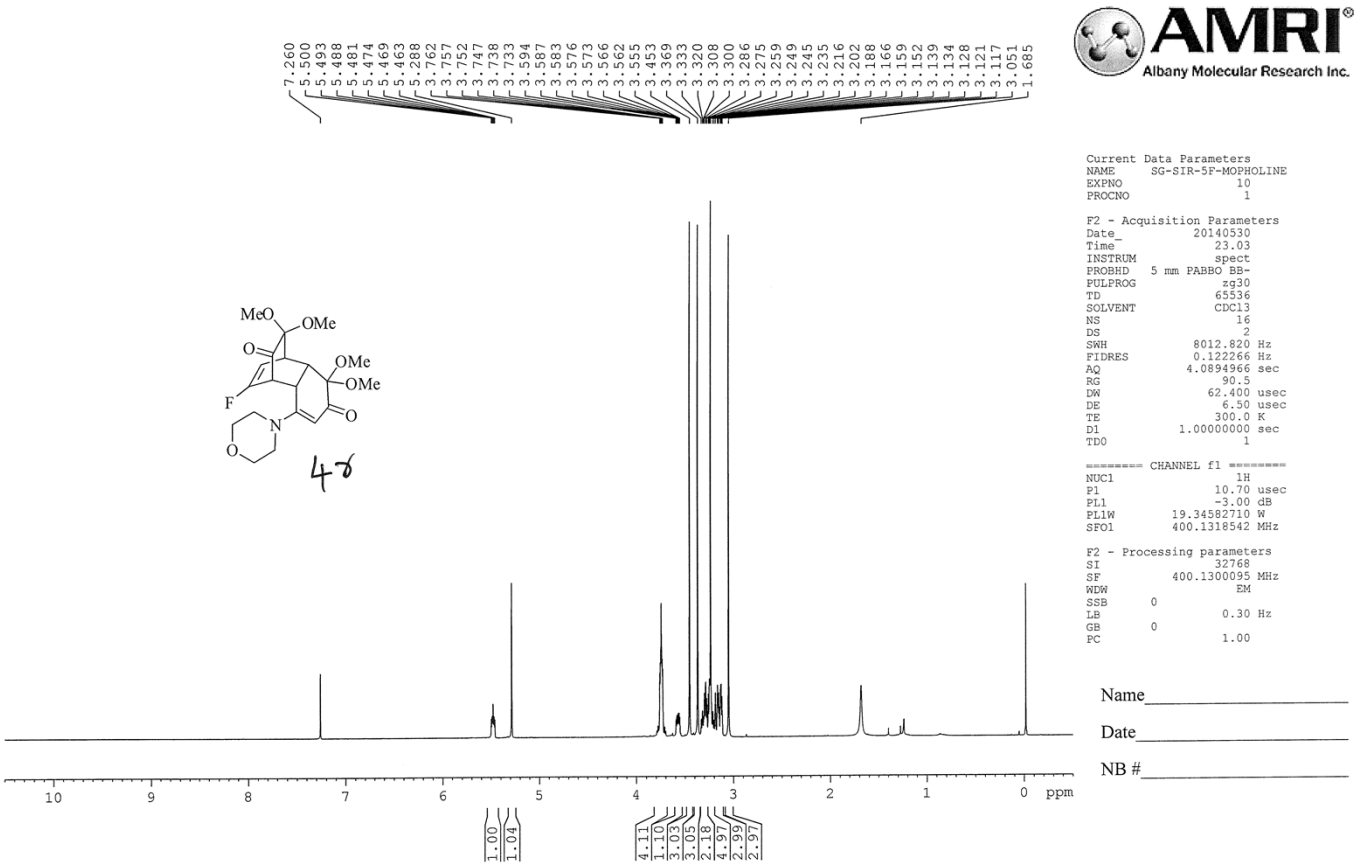


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```
Current Data Parameters
NAME      SG-SIR-5F-MOPHOLINE
EXPNO                      10
PROCNO                      1

F2 - Acquisition Parameters
Date_              20140530
Time                  23.03
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                 4.0894966 sec
RG                      90.5
DW                    62.400 usec
DE                     6.50 usec
TE                    300.0 K
D1                 1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      10.70 usec
PL1                     -3.00 dB
PL1W            19.34582710 W
SFO1            400.1318542 MHz

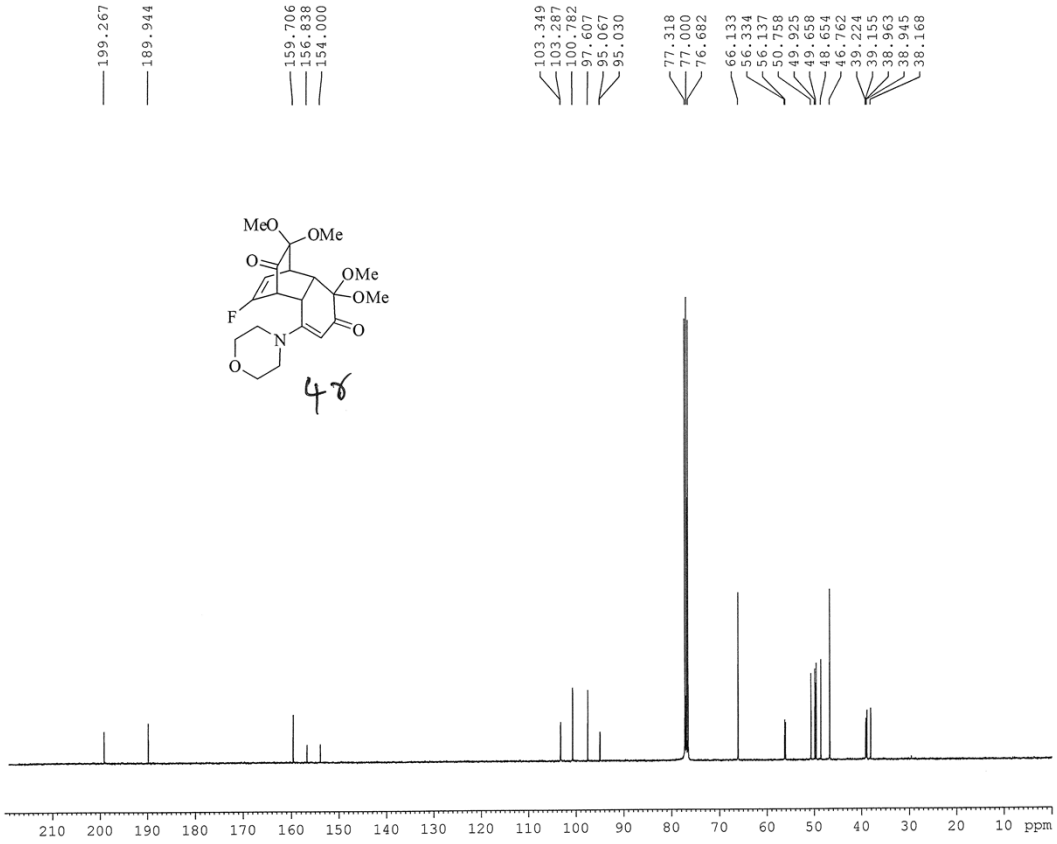
F2 - Processing parameters
SI                      32768
SF              400.1300095 MHz
WDW                        EM
SSB         0
LB                      0.30 Hz
GB          0
PC                      1.00
```

Name_____

Date_____

NB #_____

AMRI SRC
location; 17




AMRI

Name_____

Date_____

NB #_____

```
Current Data Parameters
NAME      SG-SIR-5F-MOPHOLINE
EXPNO                      11
PROCNO                      1

F2 - Acquisition Parameters
Date_              20140531
Time                   5.46
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   7000
DS                      4
SWH             23980.814 Hz
FIDRES              0.365918 Hz
AQ                1.3664756 sec
RG                    13004
DW                   20.850 usec
DE                    6.50 usec
TE                   300.0 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      13C
P1                       7.10 usec
PL1                     -4.00 dB
PL1W          82.02445221 W
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                   80.00 usec
PL2                     -3.00 dB
PL12                    14.47 dB
PL13                    15.06 dB
PL2W          19.34582710 W
PL12W          0.34640750 W
PL13W          0.30240381 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                       32768
SF           100.6127719 MHz
WDW                         EM
SSB          0
LB                       1.00 Hz
GB           0
PC                       1.40
```

# Mass Spectrum SmartFormula Report

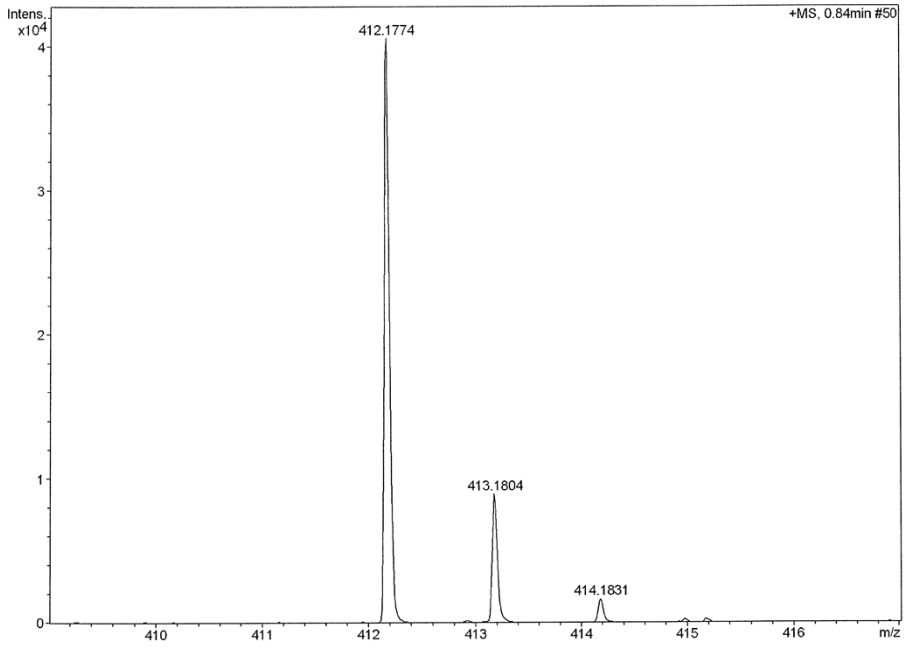
**Analysis Info**

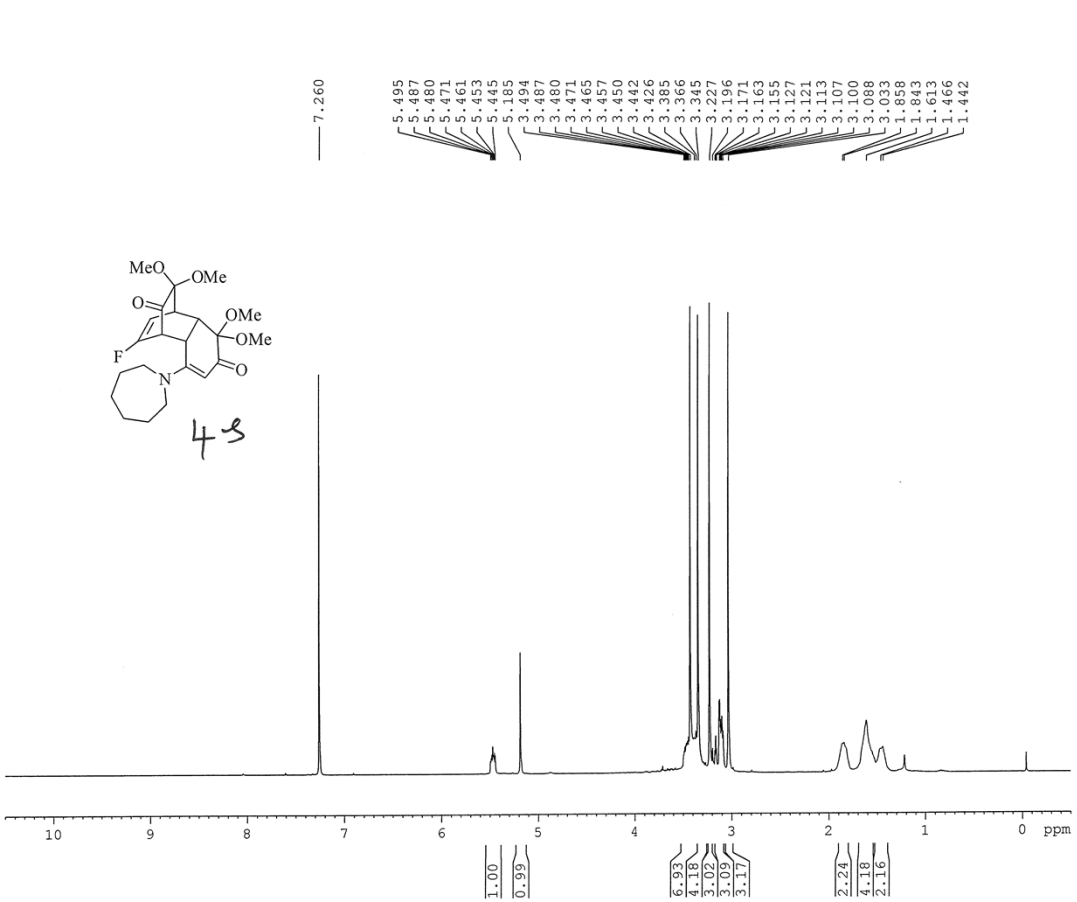
| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Chemistry\Outside\AMRI\20141103\5F-Morpholine-1.d | Acquisition Date | 11/3/2014 12:06:04 PM |
| Method | YCH_Pos-150-1800.m | Operator | default user |
| Sample Name | 5F-Morpholine | Instrument / Ser# | micrOTOF-Q II 10269 |
| Comment | AMRI<br>Santhosh Kumar Chittimalla | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 2.0 Bar |
| Focus | Not active | Set Capillary | 4500 V | Set Dry Heater | 200 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 6.0 l/min |
| Scan End | 1800 m/z | Set Collision Cell RF | 200.0 Vpp | Set Divert Valve | Waste |

| Meas. m/z | # | Formula | m/z | err [ppm] | rdb | e⁻ Conf | N-Rule |
|---|---|---|---|---|---|---|---|
| 412.1774 | 1 | C 20 H 27 F N O 7 | 412.1766 | -2.0 | 7.5 | even | ok |






AMRI

```
Current Data Parameters
NAME      SG-BCK-G-5F-Azepane
EXPNO                      10
PROCNO                      1

F2 - Acquisition Parameters
Date_              20141121
Time                  20.09
INSTRUM               spect
PROBHD   5 mm QNP 1H/13
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                      16
DS                       2
SWH                5995.204 Hz
FIDRES            0.182959 Hz
AQ                2.7329011 sec
RG                    101.6
DW                   83.400 usec
DE                    6.00 usec
TE                   300.0 K
D1                1.00000000 sec
MCREST    0 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 =========
NUC1                      1H
P1                   12.20 usec
PL1       0 dB
SFO1           300.1319508 MHz

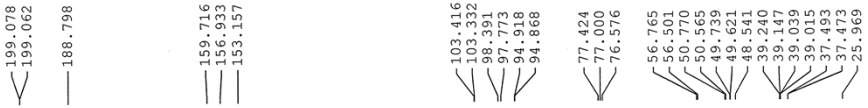
F2 - Processing parameters
SI                       16384
SF             300.1300066 MHz
WDW                        EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

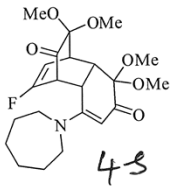
Name_____

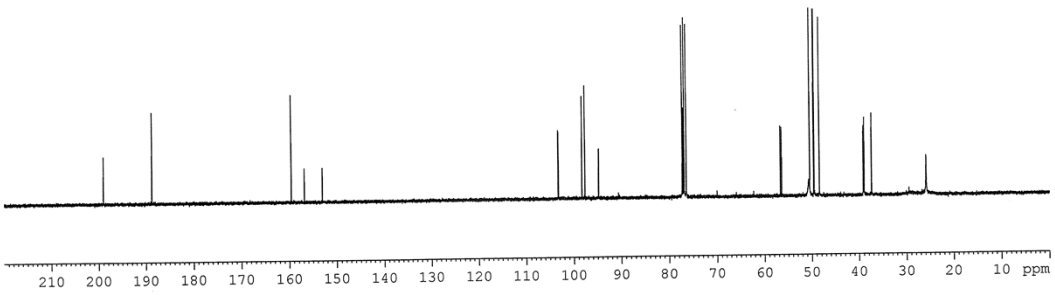
Date_____

NB #_____

AMRI; SRC
location; 15




Name_____

Date_____

NB #_____

```
Current Data Parameters
NAME      SG-BCK-G-5F-Azepane
EXPNO                      11
PROCNO                      1

F2 - Acquisition Parameters
Date_              20141121
Time                  22.24
INSTRUM               spect
PROBHD   5 mm QNP 1H/13
PULPROG             zppg30
TD                   65536
SOLVENT              CDCl3
NS                    4000
DS                       0
SWH              22675.736 Hz
FIDRES           0.346004 Hz
AQ               1.4451188 sec
RG                  5792.6
DW                  22.050 usec
DE                   6.00 usec
TE                  300.0 K
D1              0.50000000 sec
d11             0.03000000 sec
DELTA           0.40000001 sec
MCREST   0 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                   13C
P1                    8.00 usec
PL1                  -2.00 dB
SFO1           75.4767751 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                   1H
PCPD2                80.00 usec
PL2       0 dB
PL12                 16.33 dB
PL13                 16.00 dB
SFO2          300.1315007 MHz

F2 - Processing parameters
SI                   131072
SF             75.4677534 MHz
WDW                     EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.40
```

# Mass Spectrum SmartFormula Report

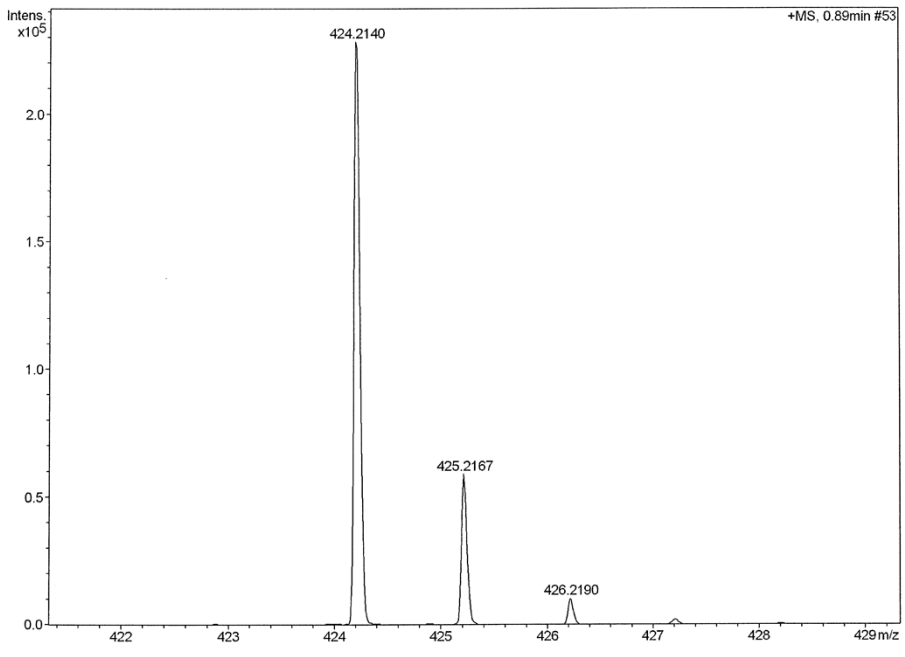
**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Chemistry\Outside\AMRI\20141218\5F-Azep-2.d | Acquisition Date | 12/18/2014 4:38:03 PM |
| Method | YCH_Pos-150-1800.m | Operator | default user |
| Sample Name | 5F-Azep | Instrument / Ser# | micrOTOF-Q II 10269 |
| Comment | AMRI<br>Santhosh Kumar Chittimalla | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 2.0 Bar |
| Focus | Not active | Set Capillary | 4500 V | Set Dry Heater | 200 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 6.0 l/min |
| Scan End | 1800 m/z | Set Collision Cell RF | 200.0 Vpp | Set Divert Valve | Waste |

| Meas. m/z | # | Formula | m/z | err [ppm] | rdb | e¯ Conf | N-Rule |
|---|---|---|---|---|---|---|---|
| 424.2140 | 1 | C 22 H 31 F N O 6 | 424.2130 | -2.3 | 7.5 | even | ok |



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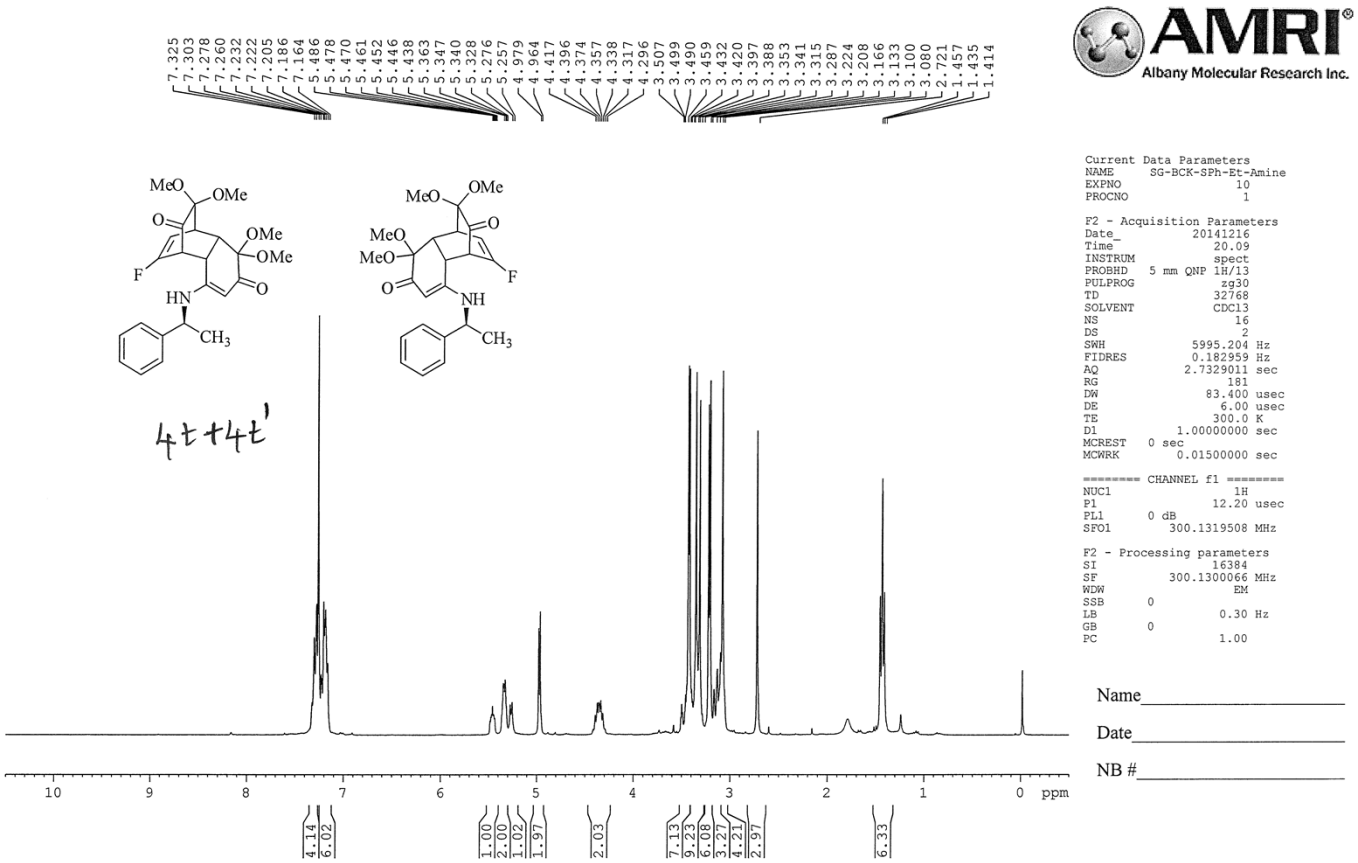


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```
Current Data Parameters
NAME      SG-BCK-SPh-Et-Amine
EXPNO                      10
PROCNO                      1

F2 - Acquisition Parameters
Date_            20141216
Time                 20.09
INSTRUM              spect
PROBHD    5 mm QNP 1H/13
PULPROG              zg30
TD                  32768
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               5995.204 Hz
FIDRES            0.182959 Hz
AQ                2.7329011 sec
RG                     181
DW                  83.400 usec
DE                   6.00 usec
TE                   300.0 K
D1                1.00000000 sec
MCREST    0 sec
MCWRK         0.01500000 sec

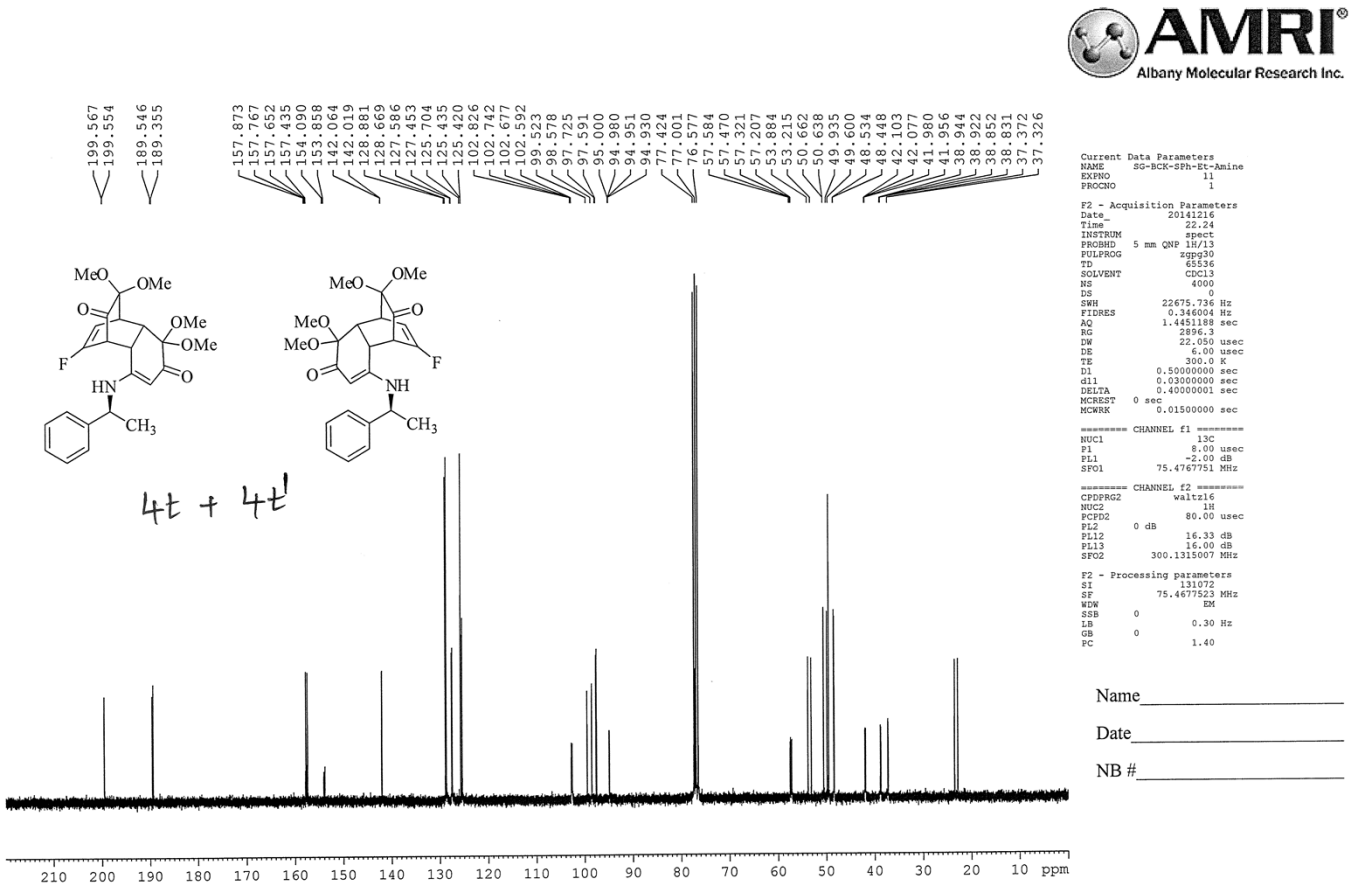
======== CHANNEL f1 ========
NUC1                     1H
P1                   12.20 usec
PL1       0 dB
SFO1          300.1319508 MHz

F2 - Processing parameters
SI                       16384
SF            300.1300066 MHz
WDW                      EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

Name_____

Date_____

NB #_____

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Albany Molecular Research Inc.

```
Current Data Parameters
NAME      SG-BCK-SPh-Et-Amine
EXPNO                      11
PROCNO                      1

F2 - Acquisition Parameters
Date_              20141216
Time                  22.24
INSTRUM                spect
PROBHD    5 mm QNP 1H/13
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    4000
DS                       0
SWH              22675.736 Hz
FIDRES               0.346004 Hz
AQ                1.4451188 sec
RG                   2896.3
DW                   22.050 usec
DE                    6.00 usec
TE                   300.0 K
D1                0.50000000 sec
d11               0.03000000 sec
DELTA             0.40000001 sec
MCREST    0 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                    13C
P1                     8.00 usec
PL1                   -2.00 dB
SFO1             75.4767751 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                    1H
PCPD2                 80.00 usec
PL2       0 dB
PL12                  16.33 dB
PL13                  16.00 dB
SFO2            300.1315007 MHz

F2 - Processing parameters
SI                     131072
SF               75.4677523 MHz
WDW                       EM
SSB       0
LB                     0.30 Hz
GB        0
PC                     1.40
```

Name_____

Date_____

NB #_____

# Mass Spectrum SmartFormula Report

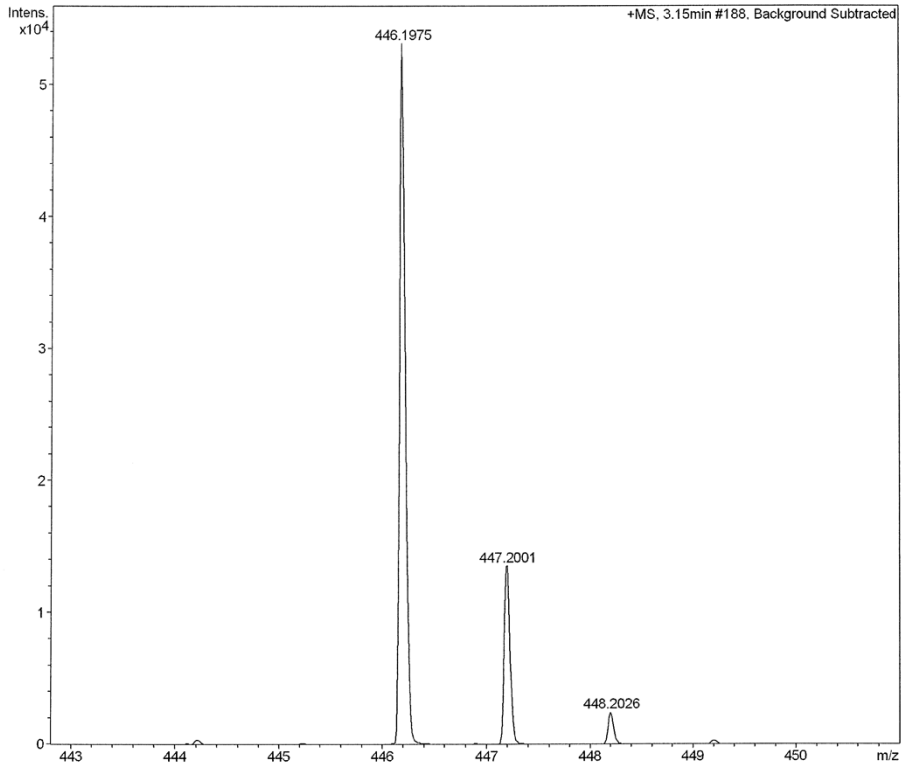
**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Chemistry\Outside\AMRI\20150107\5F-Ph-Et-NH2.d | Acquisition Date | 1/7/2015 3:08:50 PM |
| Method | YCH_Pos-150-1800.m | Operator | default user |
| Sample Name | 5F-Ph-Et-NH2 | Instrument / Ser# | micrOTOF-Q II 10269 |
| Comment | AMRI | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 2.0 Bar |
| Focus | Not active | Set Capillary | 4500 V | Set Dry Heater | 200 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 6.0 l/min |
| Scan End | 1000 m/z | Set Collision Cell RF | 200.0 Vpp | Set Divert Valve | Waste |

| Meas. m/z | # | Formula | m/z | err [ppm] | rdb | e⁻ Conf | N-Rule |
|---|---|---|---|---|---|---|---|
| 446.1975 | 1 | C 24 H 29 F N O 6 | 446.1973 | -0.3 | 10.5 | even | ok |

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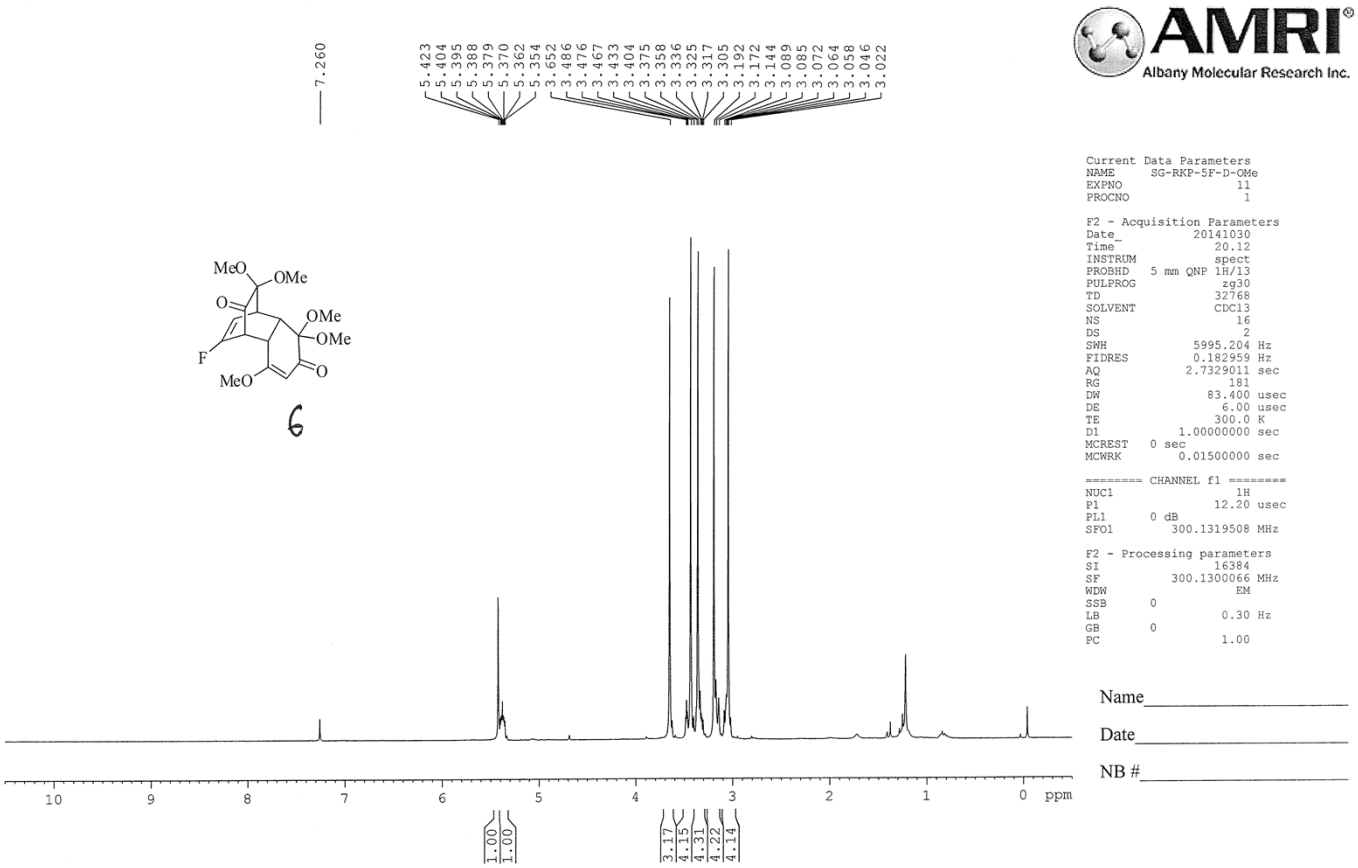


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```
Current Data Parameters
NAME        SG-RKP-5F-D-OMe
EXPNO                    11
PROCNO                    1

F2 - Acquisition Parameters
Date_              20141030
Time                  20.12
INSTRUM               spect
PROBHD   5 mm QNP 1H/13
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                5995.204 Hz
FIDRES            0.182959 Hz
AQ                2.7329011 sec
RG                      181
DW                   83.400 usec
DE                    6.00 usec
TE                   300.0 K
D1                1.00000000 sec
MCREST    0 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                     1H
P1                    12.20 usec
PL1       0 dB
SFO1           300.1319508 MHz

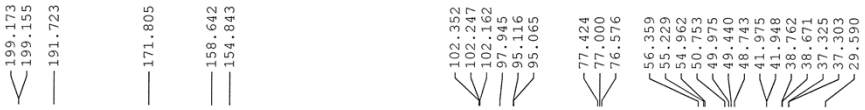
F2 - Processing parameters
SI                       16384
SF             300.1300066 MHz
WDW                      EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

Name_____

Date_____

NB #_____

AMRI; SRC
location; 15

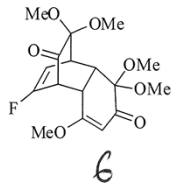



AMRI

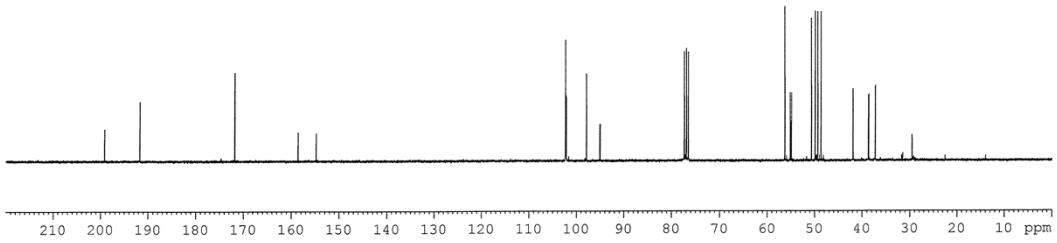
Name_____

Date_____

NB #_____




6




```
Current Data Parameters
NAME      SG-RKP-5F-D-OMe
EXPNO                  21
PROCNO                  1

F2 - Acquisition Parameters
Date_            20141030
Time                21.53
INSTRUM             spect
PROBHD   5 mm QNP 1H/13
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  3000
DS                     0
SWH           22675.736 Hz
FIDRES         0.346004 Hz
AQ            1.4451188 sec
RG               2298.8
DW              22.050 usec
DE               6.00 usec
TE              300.0 K
D1           0.50000000 sec
d11          0.03000000 sec
DELTA        0.40000001 sec
MCREST   0 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                  8.00 usec
PL1                -2.00 dB
SFO1         75.4767751 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              80.00 usec
PL2       0 dB
PL12               16.33 dB
PL13               16.00 dB
SFO2        300.1315007 MHz

F2 - Processing parameters
SI                 131072
SF           75.4677529 MHz
WDW                  EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.40
```

# Mass Spectrum SmartFormula Report

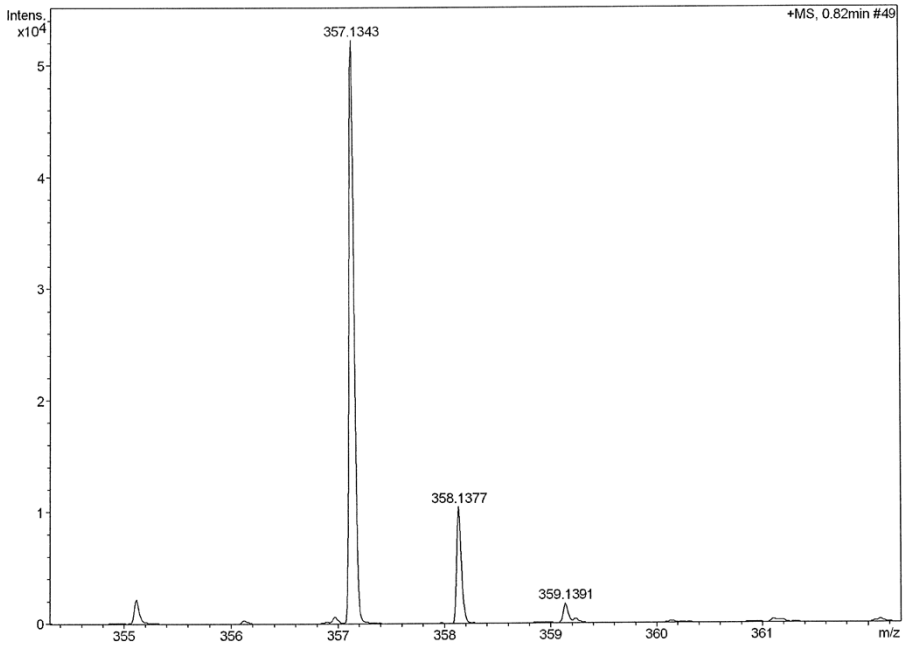
**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Chemistry\Outside\AMRI\20141218\5F-OMe-1.d | Acquisition Date | 12/18/2014 4:51:27 PM |
| Method | YCH_Pos-150-1800.m | Operator | default user |
| Sample Name | 5F-OMe | Instrument / Ser# | micrOTOF-Q II 10269 |
| Comment | AMRI<br>Santhosh Kumar Chittimalla | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 2.0 Bar |
| Focus | Not active | Set Capillary | 4500 V | Set Dry Heater | 200 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 6.0 l/min |
| Scan End | 1800 m/z | Set Collision Cell RF | 200.0 Vpp | Set Divert Valve | Waste |

| Meas. m/z | # | Formula | m/z | err [ppm] | rdb | e⁻ Conf | N-Rule |
|---|---|---|---|---|---|---|---|
| 357.1343 | 1 | C 17 H 22 F O 7 | 357.1344 | 0.3 | 6.5 | even | ok |



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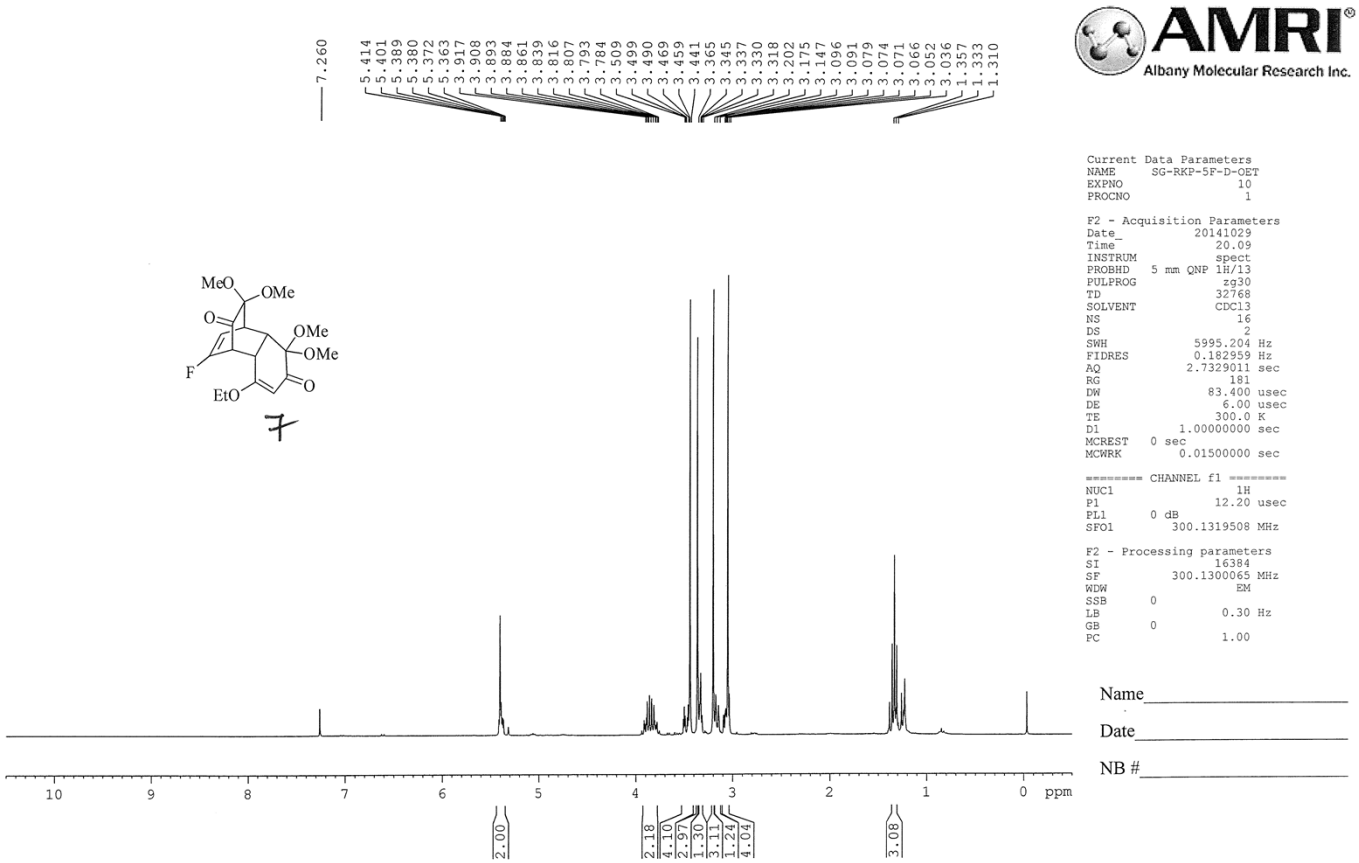


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```
Current Data Parameters
NAME       SG-RKP-5F-D-OET
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_           20141029
Time               20.09
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             5995.204 Hz
FIDRES          0.182959 Hz
AQ              2.7329011 sec
RG                   181
DW                83.400 usec
DE                 6.00 usec
TE                300.0 K
D1             1.00000000 sec
MCREST    0 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                 12.20 usec
PL1       0 dB
SFO1         300.1319508 MHz

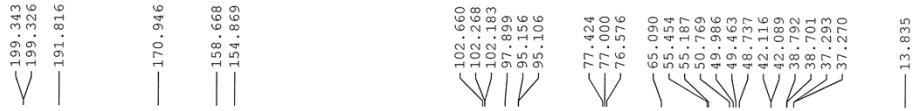
F2 - Processing parameters
SI                 16384
SF           300.1300065 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Name_____

Date_____

NB #_____

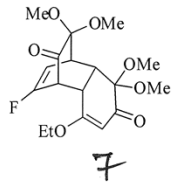
AMRI; SRC
location; 15



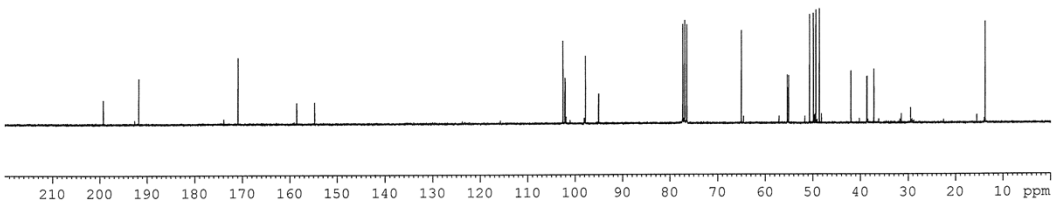

Name_____

Date_____

NB #_____




7




```
Current Data Parameters
NAME      SG-RKP-5F-D-OET
EXPNO                  11
PROCNO                  1

F2 - Acquisition Parameters
Date_           20141029
Time              21.50
INSTRUM           spect
PROBHD   5 mm QNP 1H/13
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                3000
DS                   0
SWH          22675.736 Hz
FIDRES        0.346004 Hz
AQ            1.4451188 sec
RG               2580.3
DW               22.050 usec
DE                6.00 usec
TE                300.0 K
D1           0.50000000 sec
d11          0.03000000 sec
DELTA        0.40000001 sec
MCREST   0 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                 8.00 usec
PL1               -2.00 dB
SFO1         75.4767751 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2              80.00 usec
PL2       0 dB
PL12              16.33 dB
PL13              16.00 dB
SFO2        300.1315007 MHz

F2 - Processing parameters
SI                131072
SF           75.4677521 MHz
WDW                 EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.40
```

# Mass Spectrum SmartFormula Report

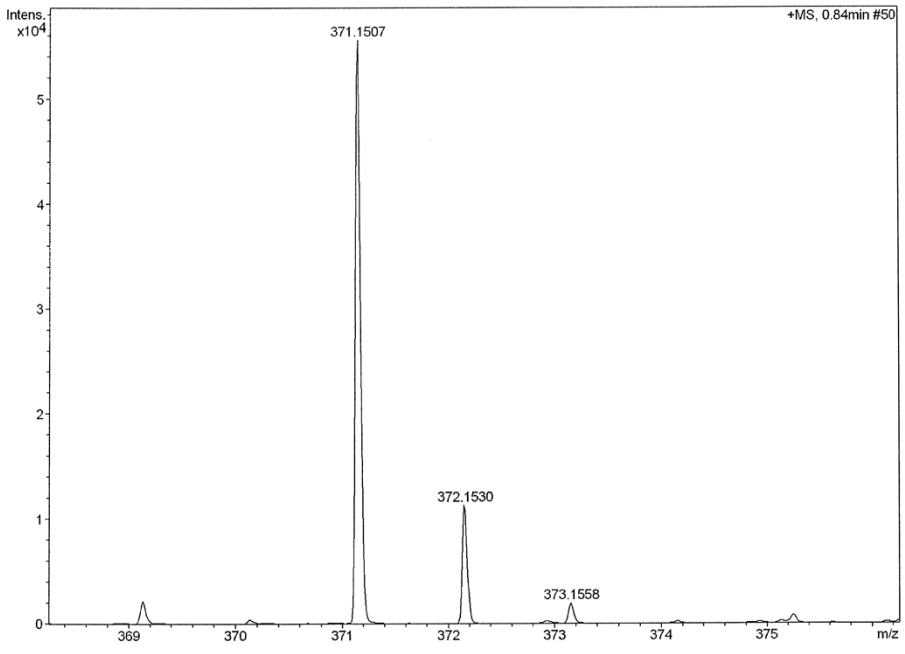
**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Chemistry\Outside\AMRI\20141218\5F-OEt-1.d | Acquisition Date | 12/18/2014 4:58:38 PM |
| Method | YCH_Pos-150-1800.m | Operator | default user |
| Sample Name | 5F-OEt | Instrument / Ser# | micrOTOF-Q II 10269 |
| Comment | AMRI<br>Santhosh Kumar Chittimalla | | |

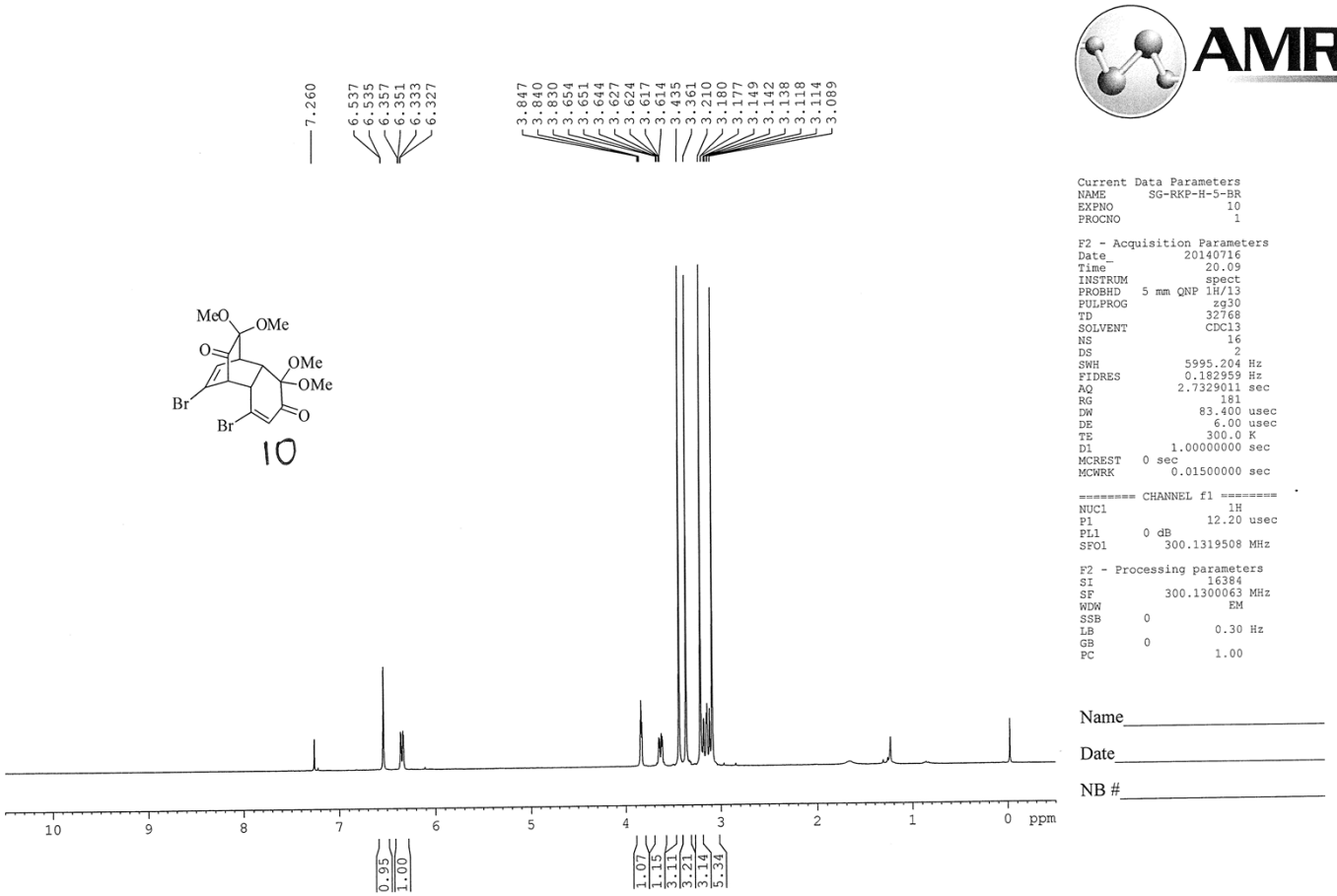
**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 2.0 Bar |
| Focus | Not active | Set Capillary | 4500 V | Set Dry Heater | 200 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 6.0 l/min |
| Scan End | 1800 m/z | Set Collision Cell RF | 200.0 Vpp | Set Divert Valve | Waste |

| Meas. m/z | # | Formula | m/z | err [ppm] | rdb | e¯ Conf | N-Rule |
|---|---|---|---|---|---|---|---|
| 371.1507 | 1 | C 18 H 24 F O 7 | 371.1501 | -1.7 | 6.5 | even | ok |




Bruker Compass DataAnalysis 4.0 printed: 12/18/2014 5:01:32 PM Page 1 of 1




AMRI

```
Current Data Parameters
NAME       SG-RKP-H-5-BR
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140716
Time               20.09
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     2
SWH              5995.204 Hz
FIDRES           0.182959 Hz
AQ               2.7329011 sec
RG                   181
DW                83.400 usec
DE                 6.00 usec
TE                 300.0 K
D1              1.00000000 sec
MCREST    0 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                 12.20 usec
PL1       0 dB
SFO1          300.1319508 MHz

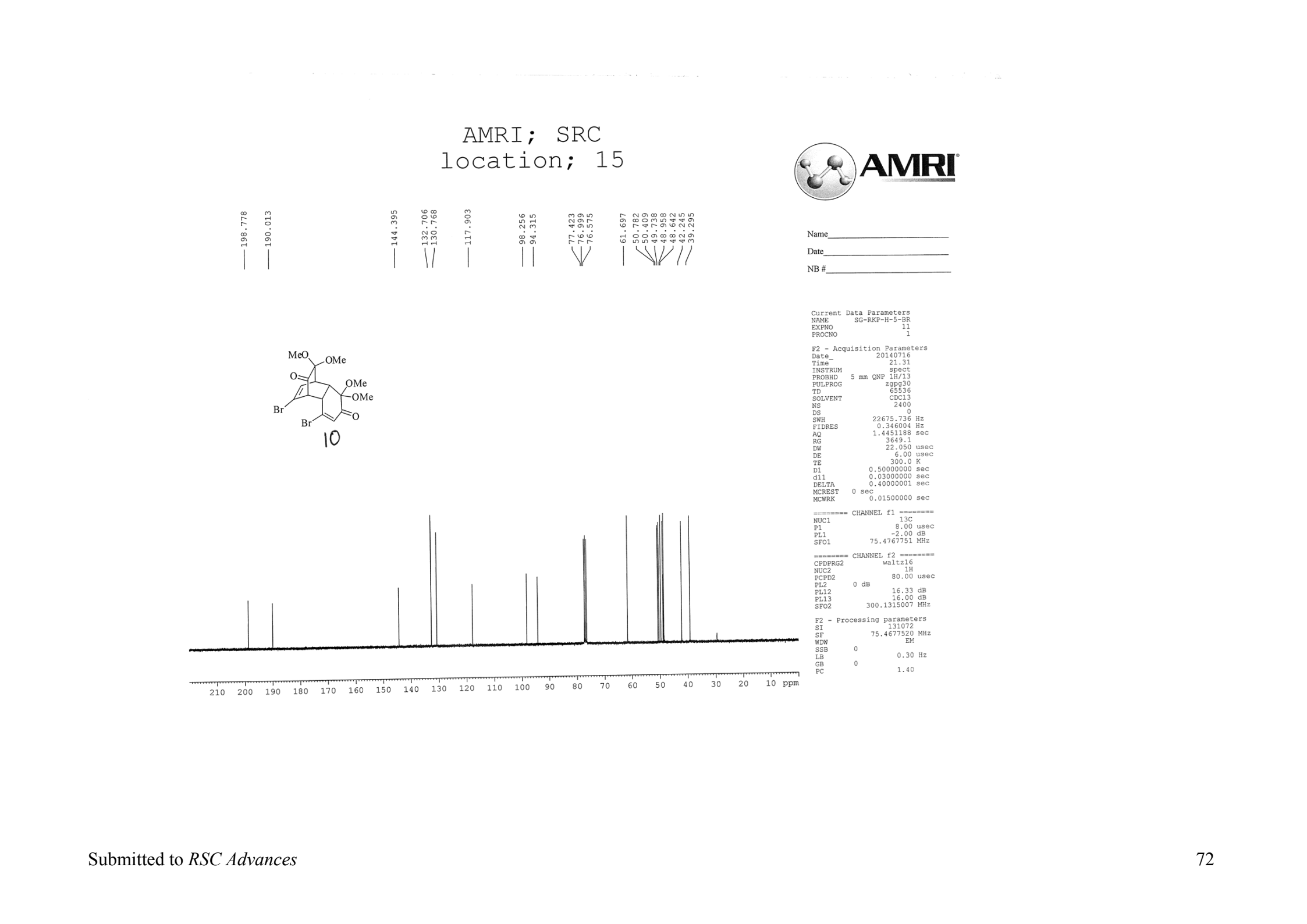
F2 - Processing parameters
SI                 16384
SF           300.1300063 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Name_____

Date_____

NB #_____

AMRI; SRC
location; 15




Name_____

Date_____

NB #_____

```
Current Data Parameters
NAME       SG-RKP-H-5-BR
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140716
Time              21.31
INSTRUM           spect
PROBHD   5 mm QNP 1H/13
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                2400
DS                   0
SWH          22675.736 Hz
FIDRES        0.346004 Hz
AQ           1.4451188 sec
RG              3649.1
DW             22.050 usec
DE              6.00 usec
TE             300.0 K
D1          0.50000000 sec
d11         0.03000000 sec
DELTA       0.40000001 sec
MCREST   0 sec
MCWRK       0.01500000 sec

======== CHANNEL f1 ========
NUC1               13C
P1              8.00 usec
PL1            -2.00 dB
SFO1       75.4767751 MHz

======== CHANNEL f2 ========
CPDPRG2        waltz16
NUC2               1H
PCPD2          80.00 usec
PL2      0 dB
PL12           16.33 dB
PL13           16.00 dB
SFO2      300.1315007 MHz

F2 - Processing parameters
SI               131072
SF         75.4677520 MHz
WDW                EM
SSB      0
LB              0.30 Hz
GB       0
PC              1.40
```

# Mass Spectrum SmartFormula Report

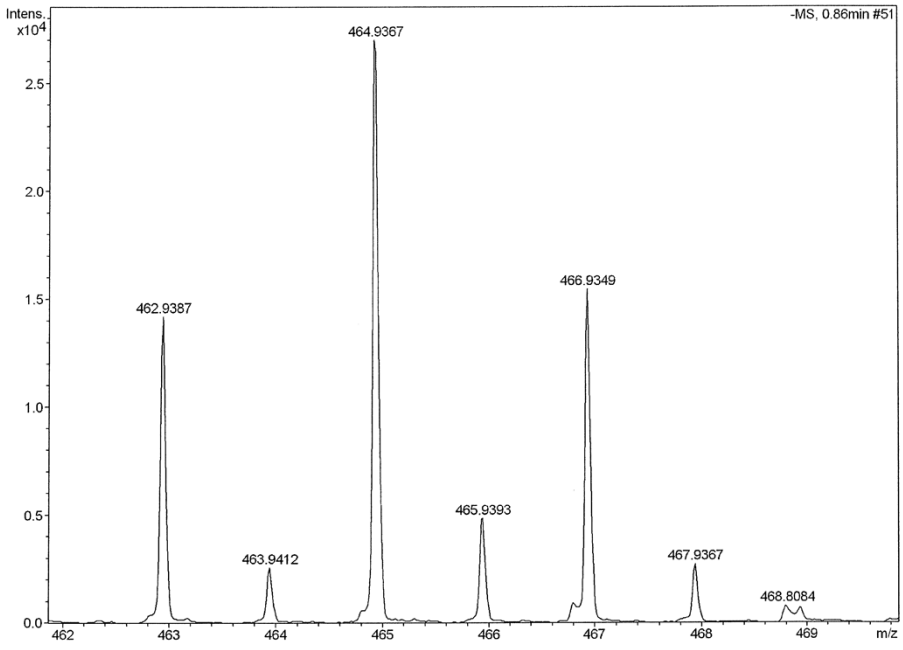
**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Chemistry\Outside\AMRI\20141218\5Br-Dimer-2n.d | Acquisition Date | 12/18/2014 2:52:36 PM |
| Method | YCH_Pos-150-1800.m | Operator | default user |
| Sample Name | 5Br-Dimer | Instrument / Ser# | micrOTOF-Q II 10269 |
| Comment | AMRI<br>Santhosh Kumar Chittimalla | | |

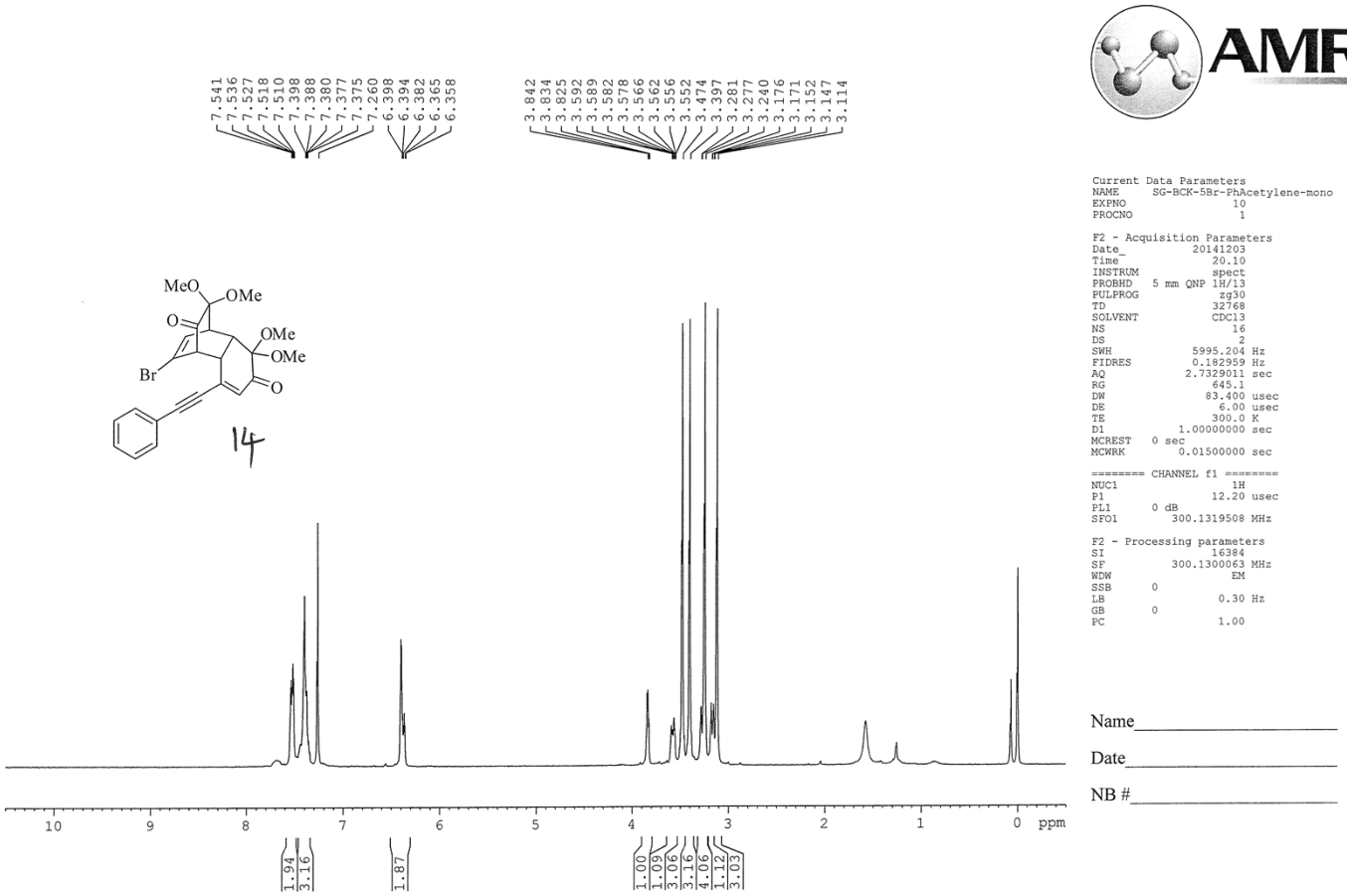
**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Negative | Set Nebulizer | 2.0 Bar |
| Focus | Not active | Set Capillary | 3500 V | Set Dry Heater | 200 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 6.0 l/min |
| Scan End | 1800 m/z | Set Collision Cell RF | 200.0 Vpp | Set Divert Valve | Waste |

| Meas. m/z | # | Formula | m/z | err [ppm] | rdb | $e^-$ Conf | N-Rule |
|---|---|---|---|---|---|---|---|
| 462.9387 | 1 | C 16 H 17 Br 2 O 6 | 462.9397 | 2.2 | 7.5 | even | ok |




Bruker Compass DataAnalysis 4.0 printed: 12/18/2014 2:55:17 PM Page 1 of 1




AMRI

```
Current Data Parameters
NAME      SG-BCK-5Br-PhAcetylene-mono
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20141203
Time                20.10
INSTRUM             spect
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     2
SWH              5995.204 Hz
FIDRES           0.182959 Hz
AQ               2.7329011 sec
RG                 645.1
DW                83.400 usec
DE                 6.00 usec
TE                 300.0 K
D1            1.00000000 sec
MCREST    0 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                 12.20 usec
PL1       0 dB
SFO1          300.1319508 MHz

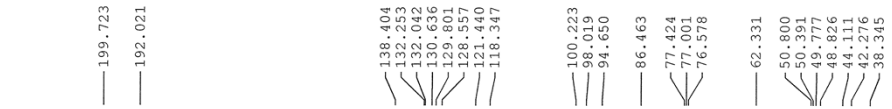
F2 - Processing parameters
SI                 16384
SF           300.1300063 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Name_____

Date_____

NB #_____

AMRI; SRC
location; 15

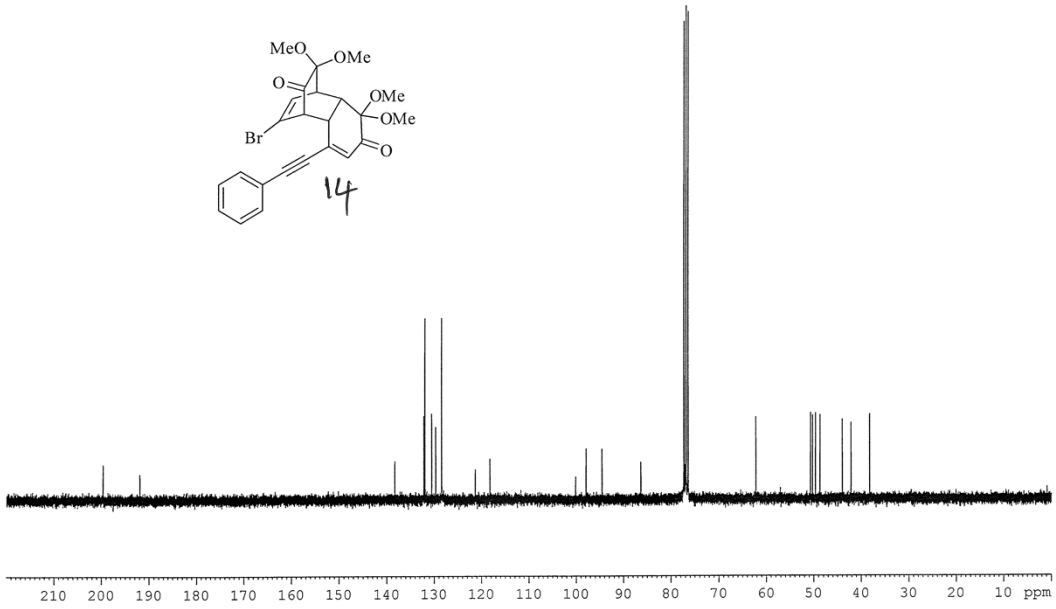



Name_____

Date_____

NB #_____




```
Current Data Parameters
NAME      SG-BCK-5Br-PhAcetylene-mono
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20141203
Time               22.25
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 4000
DS                    0
SWH           22675.736 Hz
FIDRES         0.346004 Hz
AQ            1.4451188 sec
RG               1448.2
DW              22.050 usec
DE               6.00 usec
TE              301.3 K
D1            0.50000000 sec
d11           0.03000000 sec
DELTA         0.40000001 sec
MCREST   0 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                 8.00 usec
PL1               -2.00 dB
SFO1         75.4767751 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2       0 dB
PL12              16.33 dB
PL13              16.00 dB
SFO2        300.1315007 MHz

F2 - Processing parameters
SI               131072
SF           75.4677495 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.40
```

# Mass Spectrum SmartFormula Report

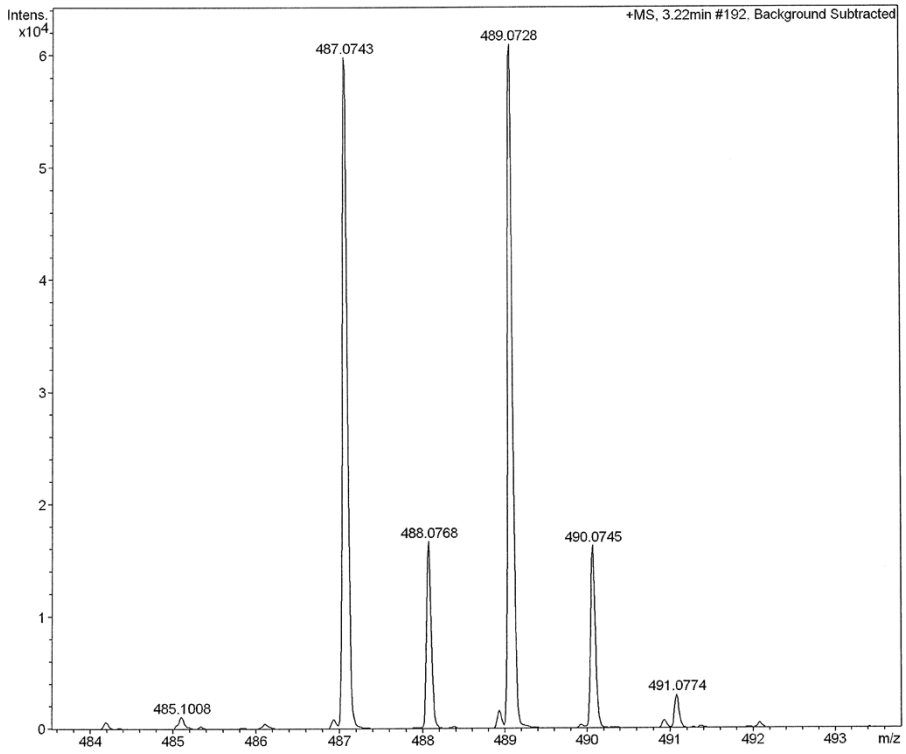
**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Chemistry\Outside\AMRI\20150107\5Br-Mono-Phen-Ace.d | Acquisition Date | 1/7/2015 3:22:22 PM |
| Method | YCH_Pos-150-1800.m | Operator | default user |
| Sample Name | 5Br-Mono-Phen-Ace | Instrument / Ser# | micrOTOF-Q II 10269 |
| Comment | AMRI | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 2.0 Bar |
| Focus | Not active | Set Capillary | 4500 V | Set Dry Heater | 200 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 6.0 l/min |
| Scan End | 1200 m/z | Set Collision Cell RF | 200.0 Vpp | Set Divert Valve | Waste |

| Meas. m/z | # | Formula | m/z | err [ppm] | rdb | e⁻ Conf | N-Rule |
|---|---|---|---|---|---|---|---|
| 487.0743 | 1 | C 24 H 24 Br O 6 | 487.0751 | 1.5 | 12.5 | even | ok |
| | 2 | C 37 H 11 O 2 | 487.0754 | 2.1 | 32.5 | even | ok |

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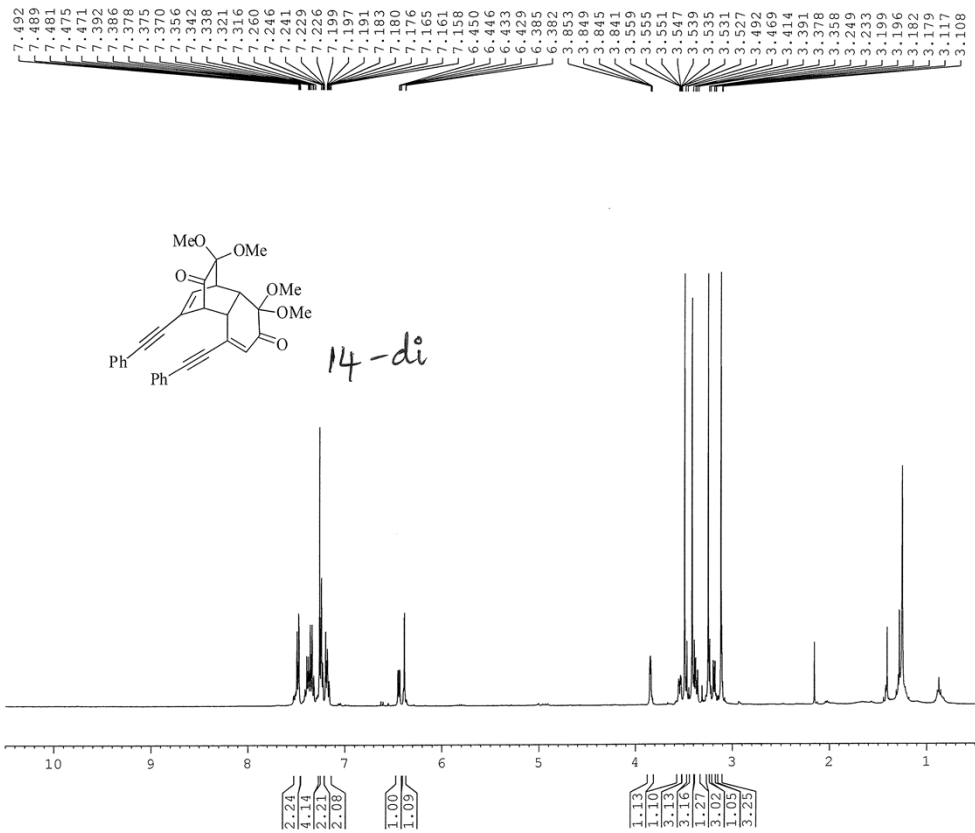



AMRI®
Albany Molecular Research Inc.

```
Current Data Parameters
NAME      SG-BCK-5Br-D-PhAcet-sonag-Di
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20141101
Time_               4.37
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              4.0894966 sec
RG                  40.3
DW                 62.400 usec
DE                  6.50 usec
TE                300.0 K
D1              1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                   1H
P1                 10.70 usec
PL1                -3.00 dB
PL1W         19.34582710 W
SFO1         400.1318542 MHz

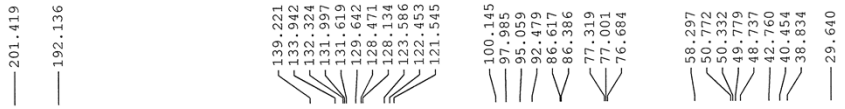
F2 - Processing parameters
SI                 32768
SF           400.1300095 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Name_____

Date_____

NB #_____

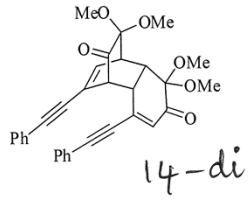
AMRI SRC
location; 17

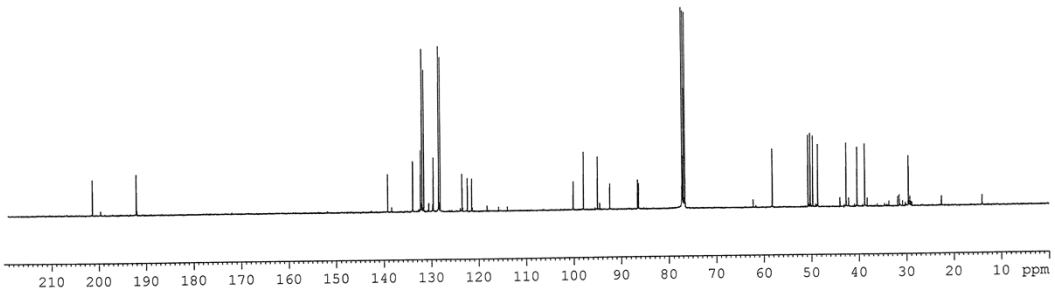



Name_____

Date_____

NB #_____




```
Current Data Parameters
NAME      SG-BCK-5Br-D-PhAcet-sonag-Di
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20141101
Time              8.29
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                 4000
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                9195.2
DW               20.850 usec
DE                6.50 usec
TE               300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                  7.10 usec
PL1                -4.00 dB
PL1W        82.02445221 W
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              80.00 usec
PL2                -3.00 dB
PL12               14.47 dB
PL13               15.06 dB
PL2W        19.34582710 W
PL12W        0.34640750 W
PL13W        0.30240381 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF         100.6127734 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

# Mass Spectrum SmartFormula Report

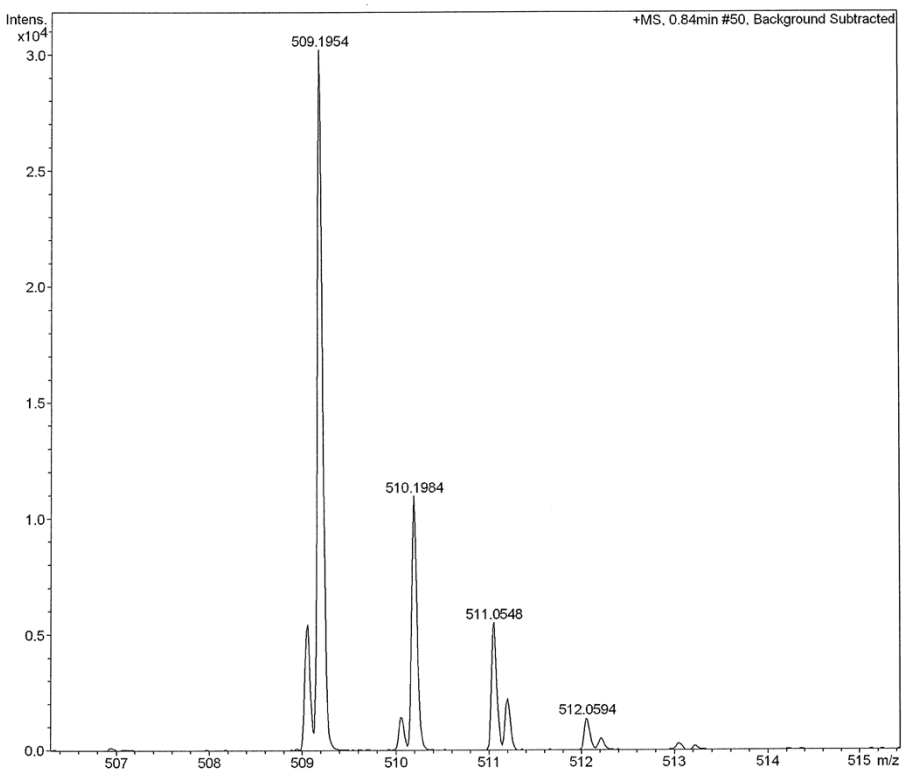
**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Chemistry\Outside\AMRI\20150107\5Br-Di-Phe-Acet.d | Acquisition Date | 1/7/2015 3:43:08 PM |
| Method | YCH_Pos-150-1800.m | Operator | default user |
| Sample Name | 5Br-Di-Phe-Acet | Instrument / Ser# | micrOTOF-Q II 10269 |
| Comment | AMRI | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 2.0 Bar |
| Focus | Not active | Set Capillary | 4500 V | Set Dry Heater | 200 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 6.0 l/min |
| Scan End | 1200 m/z | Set Collision Cell RF | 200.0 Vpp | Set Divert Valve | Waste |

| Meas. m/z | # | Formula | m/z | err [ppm] | rdb | $e^-$ Conf | N-Rule |
|---|---|---|---|---|---|---|---|
| 509.1954 | 1 | C 32 H 29 O 6 | 509.1959 | 0.8 | 18.5 | even | ok |

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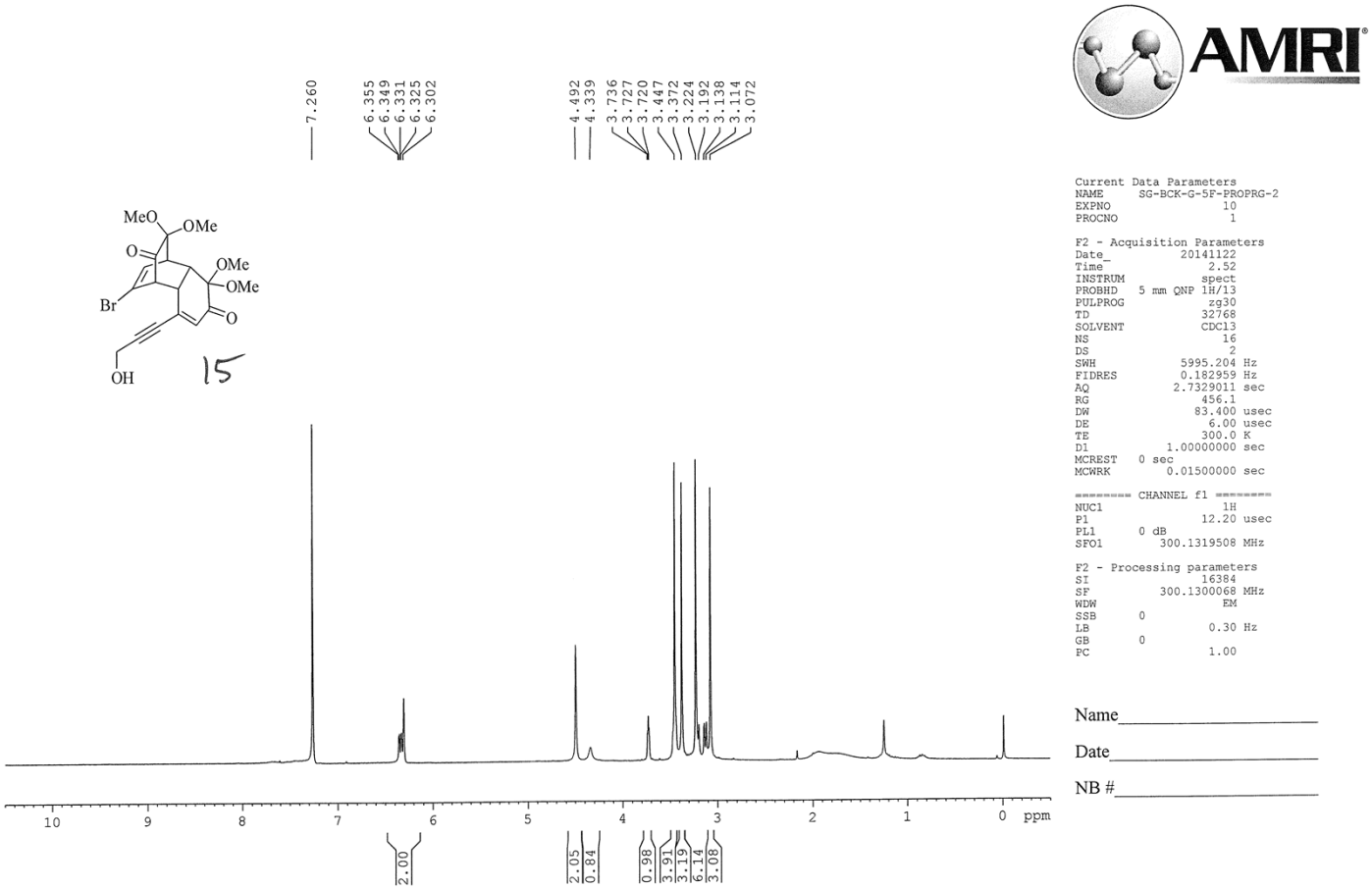



AMRI

```
Current Data Parameters
NAME      SG-BCK-G-5F-PROPRG-2
EXPNO                       10
PROCNO                       1

F2 - Acquisition Parameters
Date_              20141122
Time                   2.52
INSTRUM               spect
PROBHD   5 mm QNP 1H/13
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                5995.204 Hz
FIDRES            0.182959 Hz
AQ                2.7329011 sec
RG                     456.1
DW                  83.400 usec
DE                   6.00 usec
TE                   300.0 K
D1                1.00000000 sec
MCREST    0 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                    12.20 usec
PL1       0 dB
SFO1           300.1319508 MHz

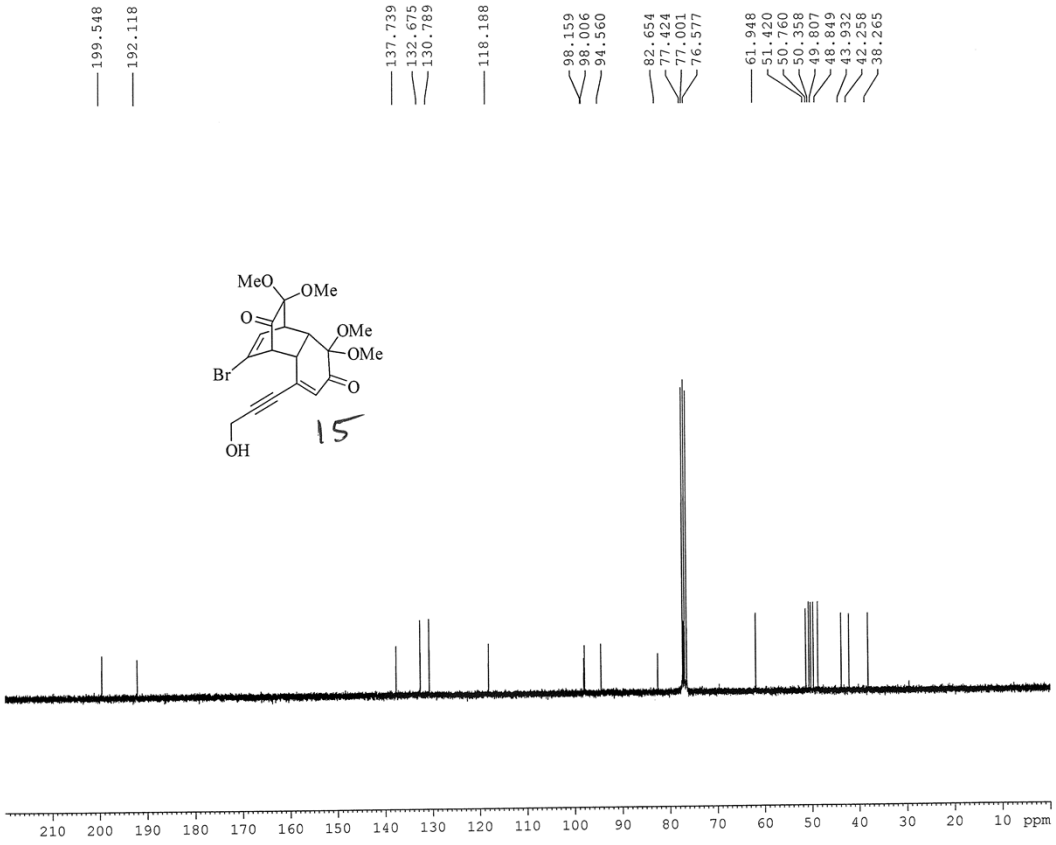
F2 - Processing parameters
SI                        16384
SF             300.1300068 MHz
WDW                         EM
SSB       0
LB                     0.30 Hz
GB        0
PC                     1.00
```

Name_____

Date_____

NB #_____

AMRI; SRC
location; 15




Name_____

Date_____

NB #_____

```
Current Data Parameters
NAME       SG-BCK-G-5F-PROPRG-2
EXPNO                        11
PROCNO                        1

F2 - Acquisition Parameters
Date_              20141122
Time                   5.07
INSTRUM               spect
PROBHD   5 mm QNP 1H/13
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   4000
DS                      0
SWH            22675.736 Hz
FIDRES          0.346004 Hz
AQ              1.4451188 sec
RG                   3251
DW                 22.050 usec
DE                  6.00 usec
TE                 300.0 K
D1            0.50000000 sec
d11           0.03000000 sec
DELTA         0.40000001 sec
MCREST   0 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                   8.00 usec
PL1                 -2.00 dB
SFO1          75.4767751 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2                80.00 usec
PL2       0 dB
PL12                16.33 dB
PL13                16.00 dB
SFO2         300.1315007 MHz

F2 - Processing parameters
SI                  131072
SF            75.4677497 MHz
WDW                     EM
SSB       0
LB                   0.30 Hz
GB        0
PC                   1.40
```

# Mass Spectrum SmartFormula Report

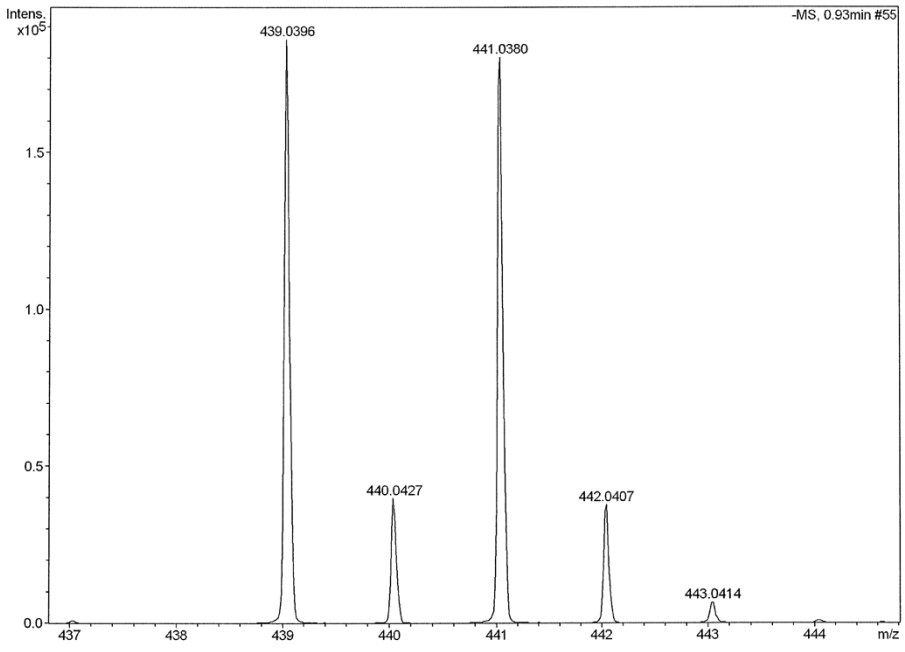
**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Chemistry\Outside\AMRI\20141218\5Br-Propargylalcol-mono-1n.d | Acquisition Date | 12/18/2014 2:39:49 PM |
| Method | YCH_Pos-150-1800.m | Operator | default user |
| Sample Name | 5Br-Propargylalcol-mono | Instrument / Ser# | micrOTOF-Q II 10269 |
| Comment | AMRI<br>Santhosh Kumar Chittimalla | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Negative | Set Nebulizer | 2.0 Bar |
| Focus | Not active | Set Capillary | 3500 V | Set Dry Heater | 200 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 6.0 l/min |
| Scan End | 1800 m/z | Set Collision Cell RF | 200.0 Vpp | Set Divert Valve | Waste |

| Meas. m/z | # | Formula | m/z | err [ppm] | rdb | $e^-$ Conf | N-Rule |
|---|---|---|---|---|---|---|---|
| 439.0396 | 1 | C 19 H 20 Br O 7 | 439.0398 | 0.5 | 9.5 | even | ok |

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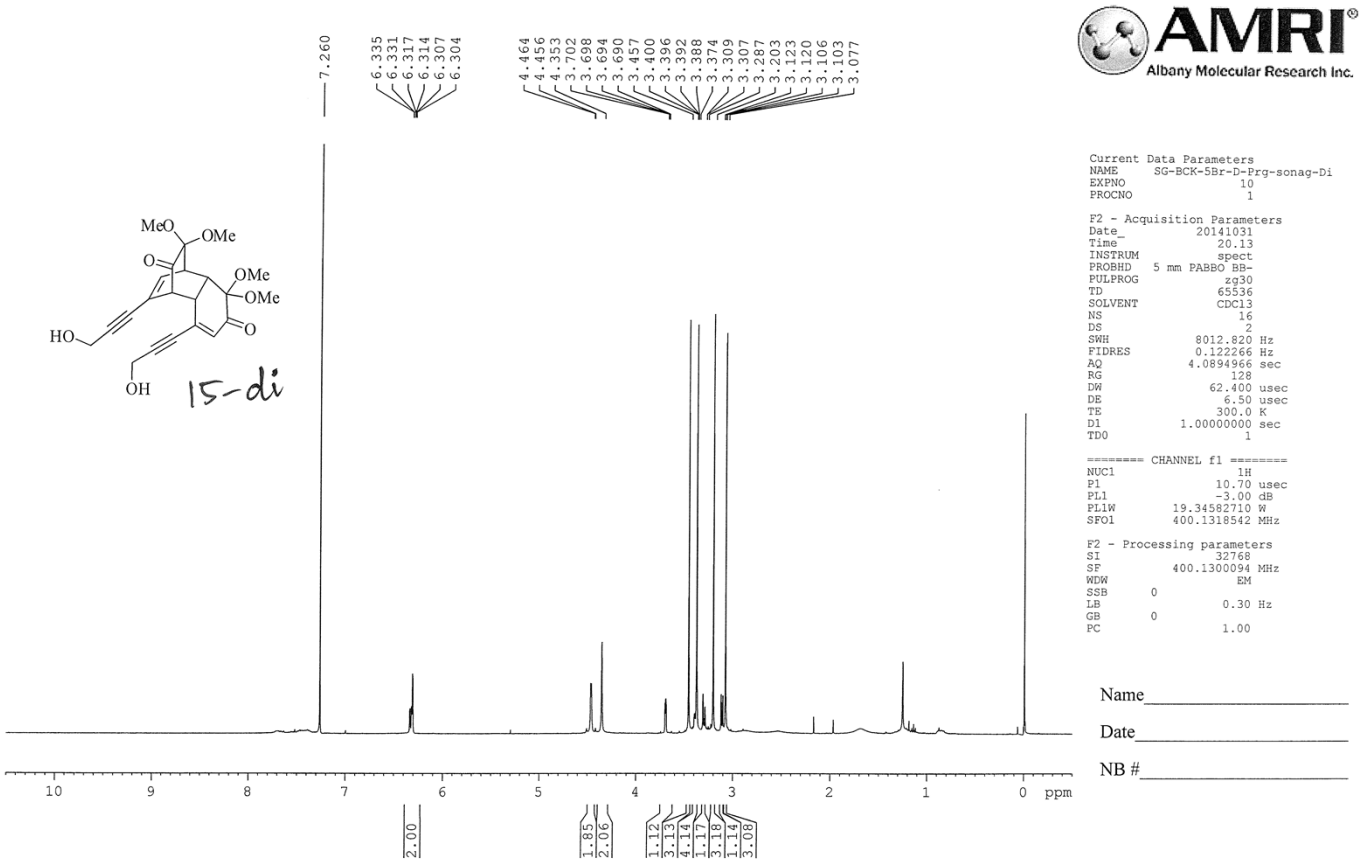



AMRI
Albany Molecular Research Inc.

```
Current Data Parameters
NAME        SG-BCK-5Br-D-Prg-sonag-Di
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20141031
Time                20.13
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               4.0894966 sec
RG                   128
DW                  62.400 usec
DE                   6.50 usec
TE                 300.0 K
D1              1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 10.70 usec
PL1                -3.00 dB
PL1W          19.34582710 W
SFO1          400.1318542 MHz

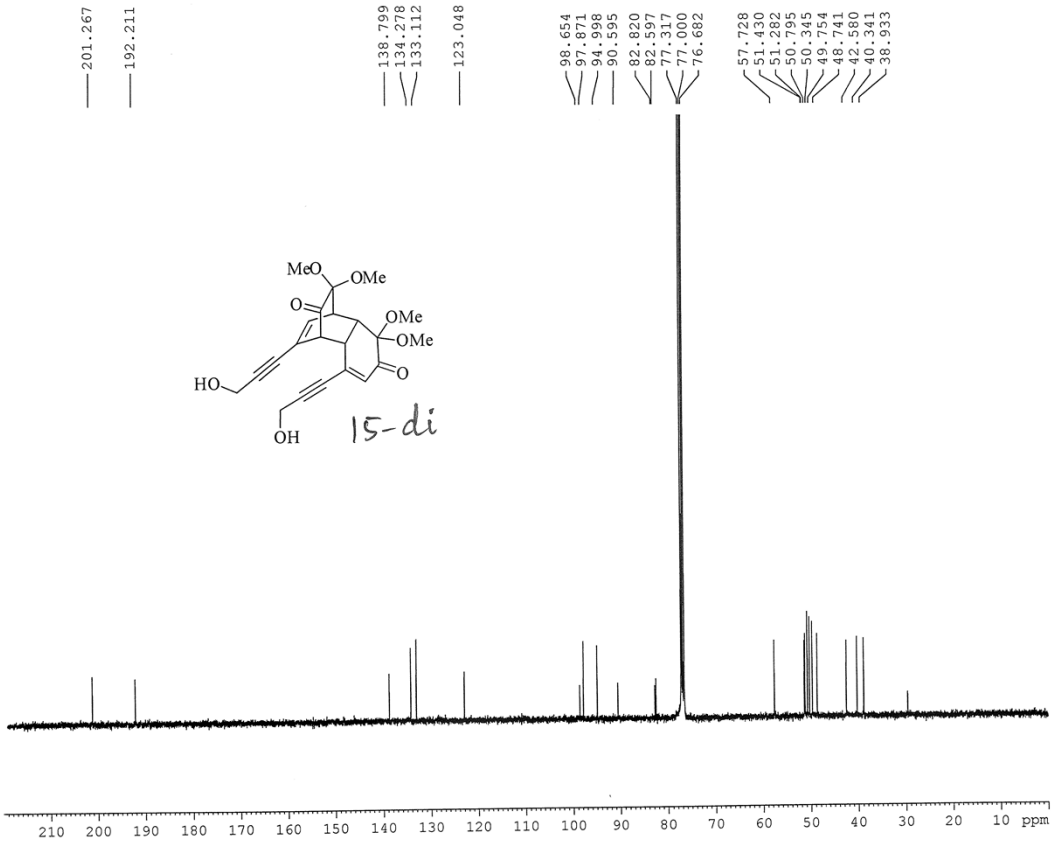
F2 - Processing parameters
SI                 32768
SF            400.1300094 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Name_____

Date_____

NB #_____

AMRI SRC
location; 17




AMRI

Name_____

Date_____

NB #_____

```
Current Data Parameters
NAME       SG-BCK-5Br-D-Prg-sonag-Di
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_          20141101
Time               0.05
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                4000
DS                   4
SWH          23980.814 Hz
FIDRES        0.365918 Hz
AQ            1.3664756 sec
RG              20642.5
DW               20.850 usec
DE                6.50 usec
TE               300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1                 7.10 usec
PL1               -4.00 dB
PL1W        82.02445221 W
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             80.00 usec
PL2               -3.00 dB
PL12              14.47 dB
PL13              15.06 dB
PL2W        19.34582710 W
PL12W        0.34640750 W
PL13W        0.30240381 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                32768
SF         100.6127701 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

# Mass Spectrum SmartFormula Report

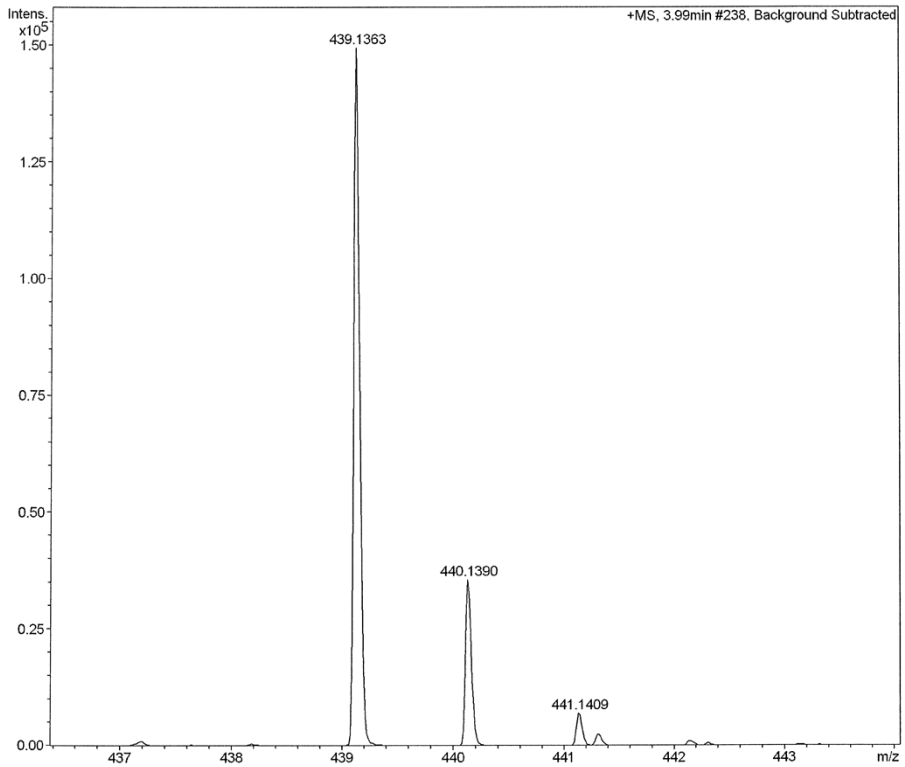
**Analysis Info**

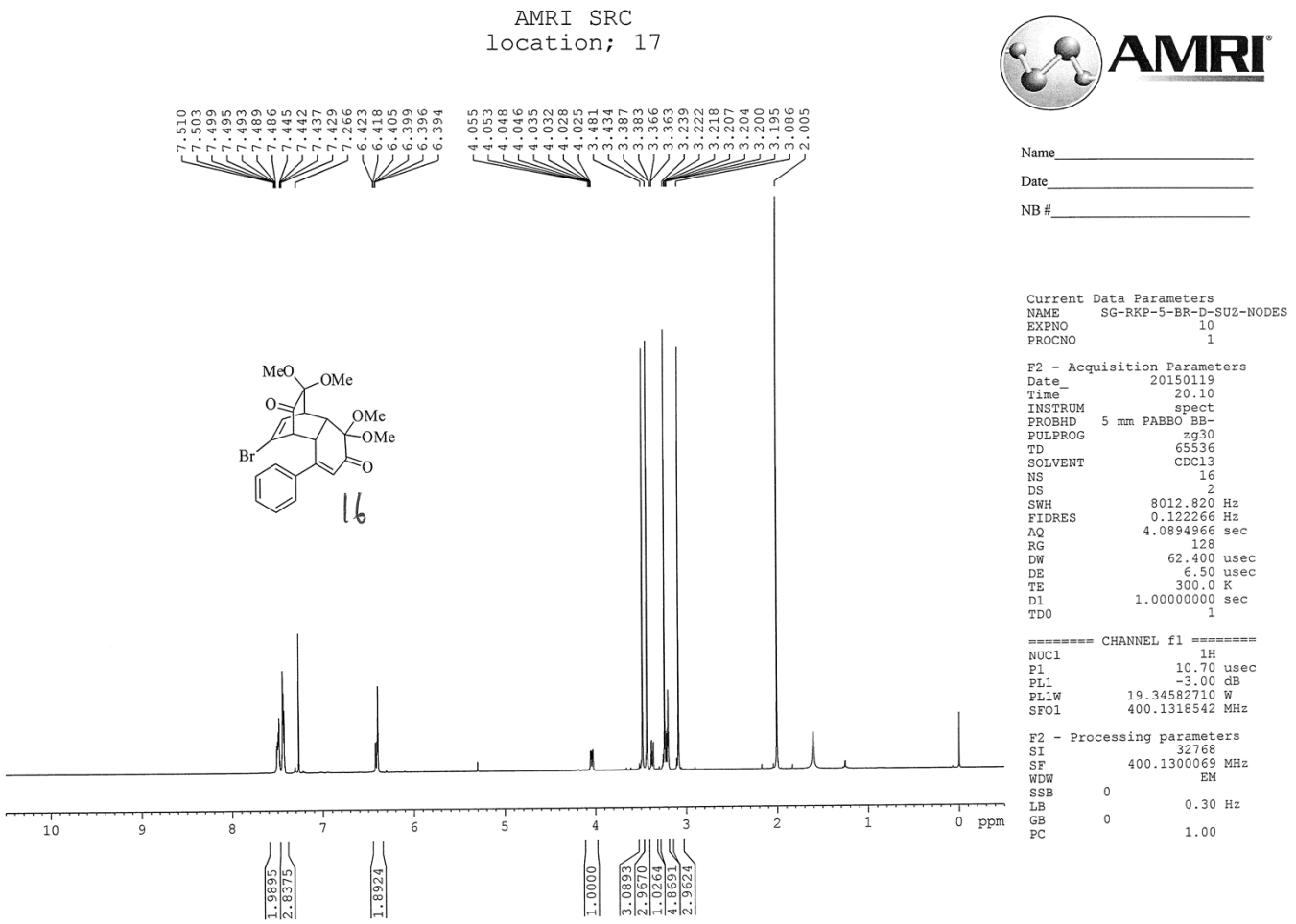
| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Chemistry\Outside\AMRI\20150107\5Br-Di-Prg-Alc.d | Acquisition Date | 1/7/2015 3:50:48 PM |
| Method | YCH_Pos-150-1800.m | Operator | default user |
| Sample Name | 5Br-Di-Prg-Alc | Instrument / Ser# | micrOTOF-Q II 10269 |
| Comment | AMRI | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 2.0 Bar |
| Focus | Not active | Set Capillary | 4500 V | Set Dry Heater | 200 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 6.0 l/min |
| Scan End | 1500 m/z | Set Collision Cell RF | 200.0 Vpp | Set Divert Valve | Waste |

| Meas. m/z | # | Formula | Score | m/z | err [mDa] | err [ppm] | mSigma | rdb | e¯ Conf | N-Rule |
|---|---|---|---|---|---|---|---|---|---|---|
| 439.1363 | 1 | C 22 H 24 Na O 8 | 100.00 | 439.1363 | 0.1 | 0.2 | 1.7 | 10.5 | even | ok |






AMRI

Name_____

Date_____

NB #_____

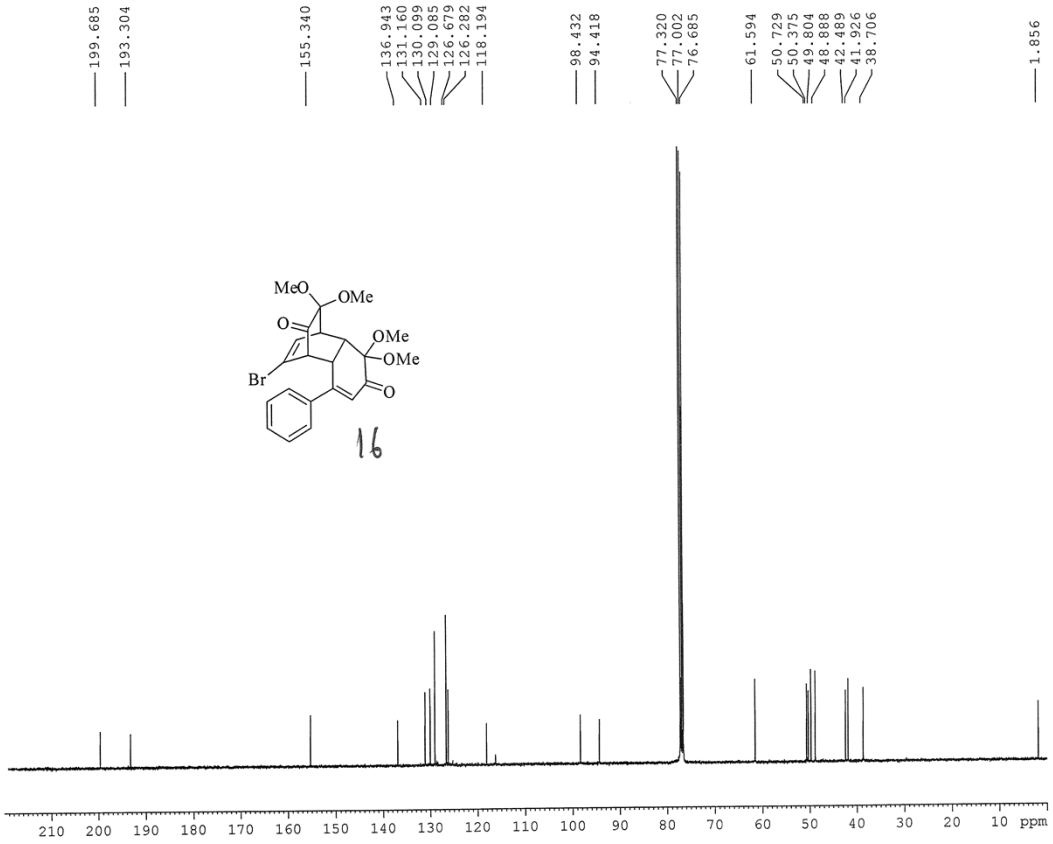
```
Current Data Parameters
NAME      SG-RKP-5-BR-D-SUZ-NODES
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_               20150119
Time                   20.10
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                 4.0894966 sec
RG                      128
DW                    62.400 usec
DE                     6.50 usec
TE                    300.0 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                    10.70 usec
PL1                   -3.00 dB
PL1W          19.34582710 W
SFO1          400.1318542 MHz

F2 - Processing parameters
SI                    32768
SF            400.1300069 MHz
WDW                      EM
SSB       0
LB                     0.30 Hz
GB        0
PC                     1.00
```

AMRI SRC
location; 17




Name_____

Date_____

NB #_____

```
Current Data Parameters
NAME       SG-RKP-5-BR-D-SUZ-NODES
EXPNO                   11
PROCNO                   1

F2 - Acquisition Parameters
Date_              20150120
Time                   1.56
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    6000
DS                       4
SWH               23980.814 Hz
FIDRES             0.365918 Hz
AQ                1.3664756 sec
RG                  14596.5
DW                   20.850 usec
DE                    6.50 usec
TE                   300.0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    13C
P1                     7.10 usec
PL1                   -4.00 dB
PL1W           82.02445221 W
SFO1           100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                   -3.00 dB
PL12                  14.47 dB
PL13                  15.06 dB
PL2W           19.34582710 W
PL12W           0.34640750 W
PL13W           0.30240381 W
SFO2           400.1316005 MHz

F2 - Processing parameters
SI                      32768
SF             100.6127710 MHz
WDW                        EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

# Mass Spectrum SmartFormula Report

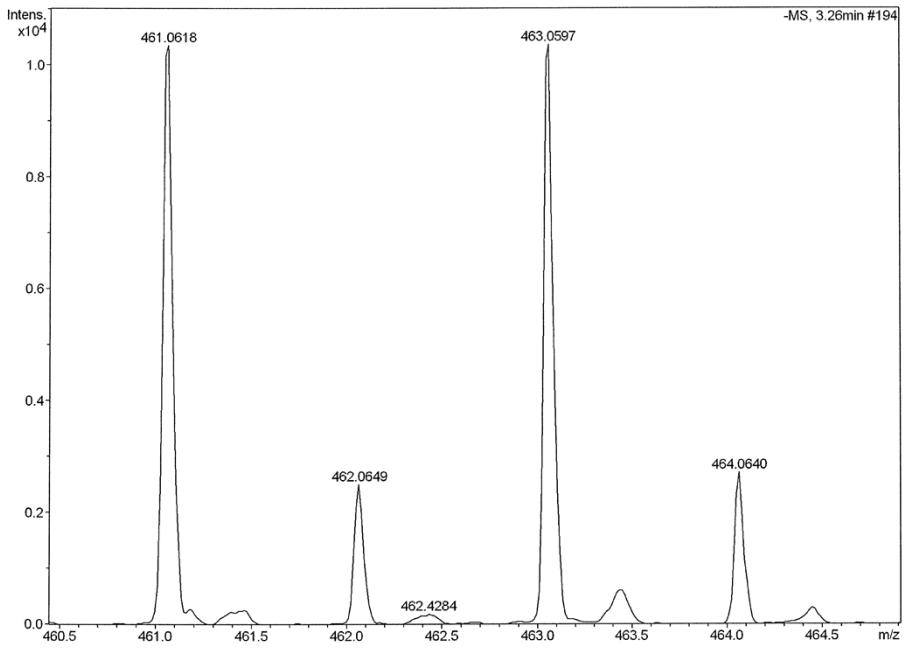
**Analysis Info**

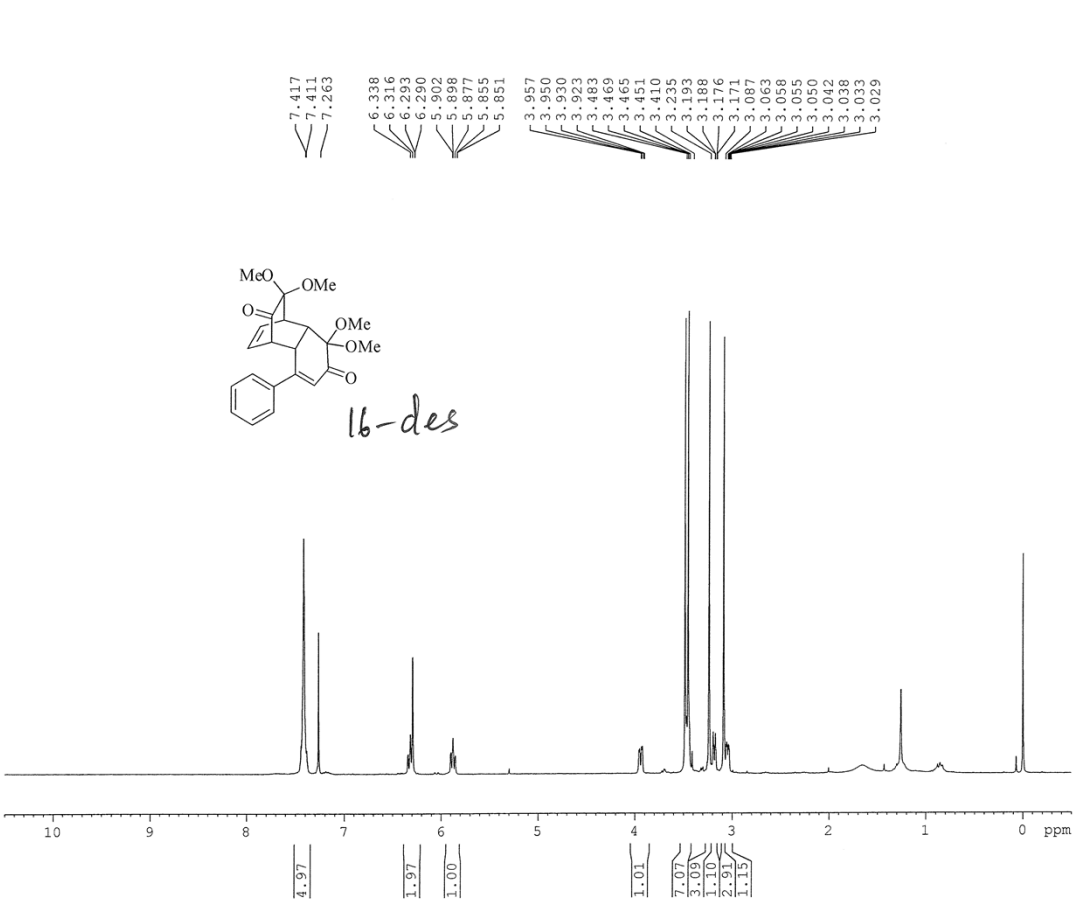
| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Chemistry\Outside\AMRI\20141218\5Br-Suz-mono-1n.d | Acquisition Date | 12/18/2014 3:48:33 PM |
| Method | YCH_Pos-300-2500.m | Operator | default user |
| Sample Name | 5Br-Suz-mono | Instrument / Ser# | micrOTOF-Q II 10269 |
| Comment | AMRI<br>Santhosh Kumar Chittimalla | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | APCI | Ion Polarity | Negative | Set Nebulizer | 3.0 Bar |
| Focus | Not active | Set Capillary | 3500 V | Set Dry Heater | 200 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 6.0 l/min |
| Scan End | 2500 m/z | Set Collision Cell RF | 300.0 Vpp | Set Divert Valve | Waste |

| Meas. m/z | # | Formula | Score | m/z | err [mDa] | err [ppm] | mSigma | rdb | e¯ Conf | N-Rule |
|---|---|---|---|---|---|---|---|---|---|---|
| 461.0618 | 1 | C 22 H 22 Br O 6 | 100.00 | 461.0605 | -1.3 | -2.9 | 15.4 | 11.5 | even | ok |






AMRI

```
Current Data Parameters
NAME      SG-RKP-5F-D-phsuz-Mono
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20141031
Time              20.09
INSTRUM           spect
PROBHD   5 mm QNP 1H/13
PULPROG           zg30
TD               32768
SOLVENT           CDCl3
NS                  16
DS                   2
SWH            5995.204 Hz
FIDRES         0.182959 Hz
AQ             2.7329011 sec
RG                645.1
DW               83.400 usec
DE                6.00 usec
TE               300.0 K
D1            1.00000000 sec
MCREST    0 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                12.20 usec
PL1       0 dB
SFO1         300.1319508 MHz

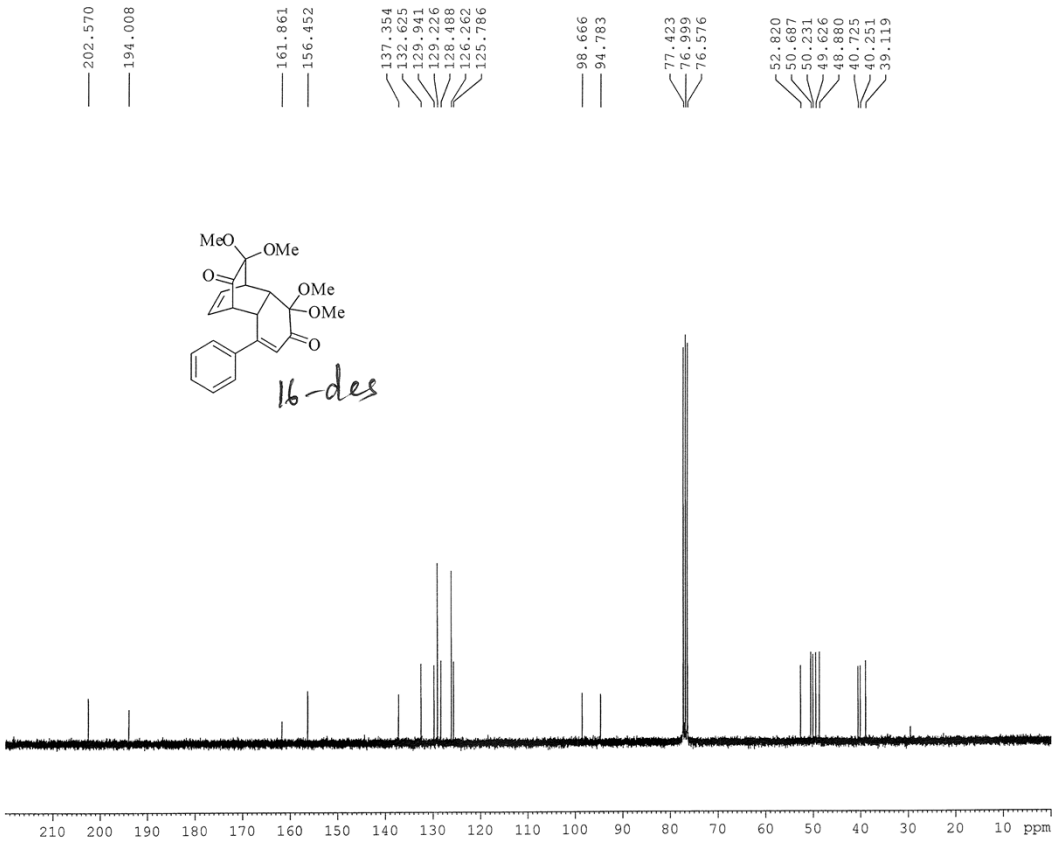
F2 - Processing parameters
SI                16384
SF          300.1300057 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

Name_____

Date_____

NB #_____

AMRI; SRC
location; 15




AMRI

Name_____

Date_____

NB #_____

```
Current Data Parameters
NAME      SG-RKP-5F-D-phsuz-Mono
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20141031
Time              21.50
INSTRUM           spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3000
DS                    0
SWH           22675.736 Hz
FIDRES         0.346004 Hz
AQ             1.4451188 sec
RG                2580.3
DW                22.050 usec
DE                 6.00 usec
TE                300.0 K
D1            0.50000000 sec
d11           0.03000000 sec
DELTA         0.40000001 sec
MCREST   0 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                 8.00 usec
PL1               -2.00 dB
SFO1         75.4767751 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2              80.00 usec
PL2       0 dB
PL12              16.33 dB
PL13              16.00 dB
SFO2        300.1315007 MHz

F2 - Processing parameters
SI                131072
SF           75.4677497 MHz
WDW                 EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.40
```