

## Supporting Information

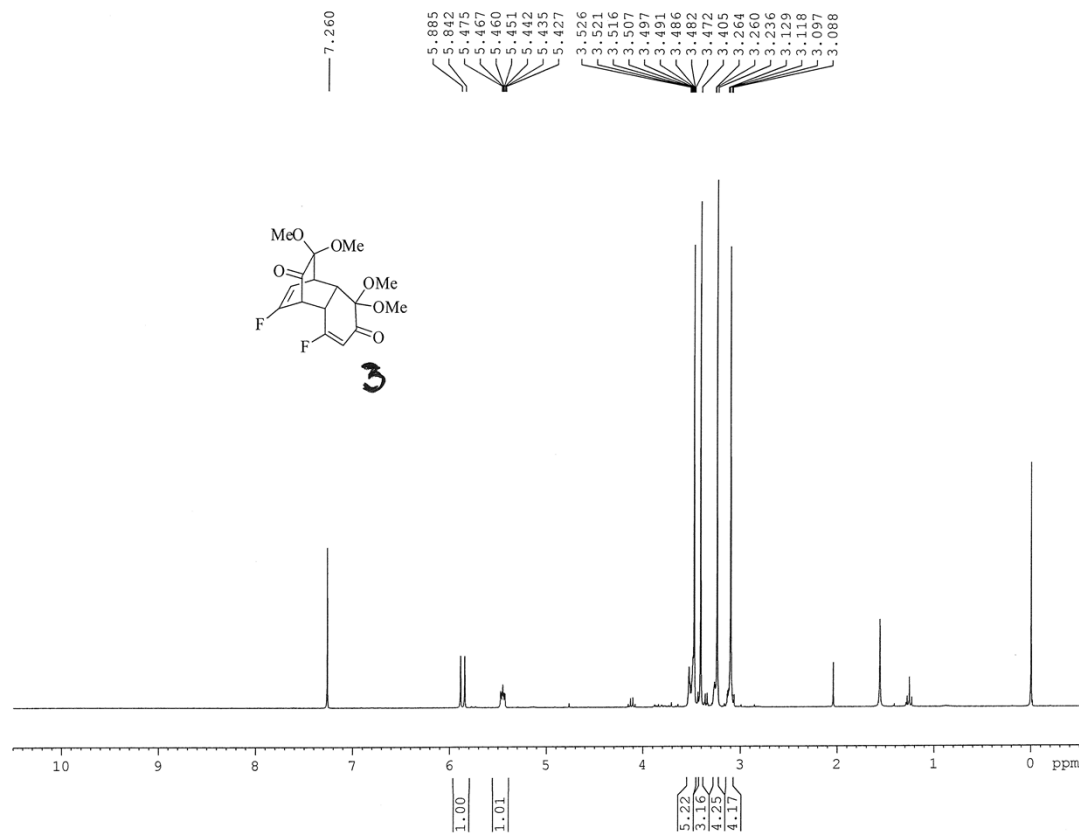
### **An Approach Towards Expanding the Scope of Masked *o*-Benzoquinone dimers to Generate Diverse Compound Libraries**

Santhosh Kumar Chittimalla,<sup>\*,[a]</sup> Shoba Laxmi,<sup>[b][‡]</sup> Amerlyn Chong Ming Liing,<sup>[b][‡]</sup> Jerald Lam Kai Jun,<sup>[b][‡]</sup> Rajesh Kuppusamy,<sup>[a]</sup> Sireesha Putturu,<sup>[a]</sup> and Chennakesavulu Bandi<sup>[a]</sup>

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[b] School of Chemical & Life Sciences, Singapore Polytechnic, 500 Dover Road, Singapore 139651.



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 CDCl<sub>3</sub>  
 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  
 FL1 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

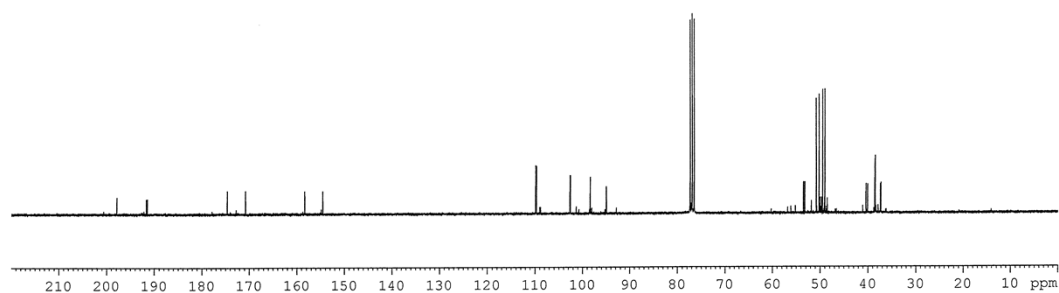
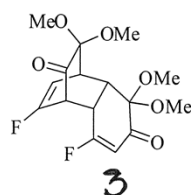


197.945  
191.743  
191.521

174.710  
170.873

158.431  
154.618

109.937  
109.759  
102.728  
102.643  
98.444  
98.435  
95.086  
95.035  
77.421  
76.997  
76.573  
53.563  
53.546  
53.292  
53.275  
50.885  
50.292  
49.551  
49.080  
40.462  
40.434  
40.162  
40.133  
38.621  
38.532  
37.483  
37.459  
37.369  
37.346



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

Current Data Parameters  
NAME SG-SIR-5F-Dim  
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

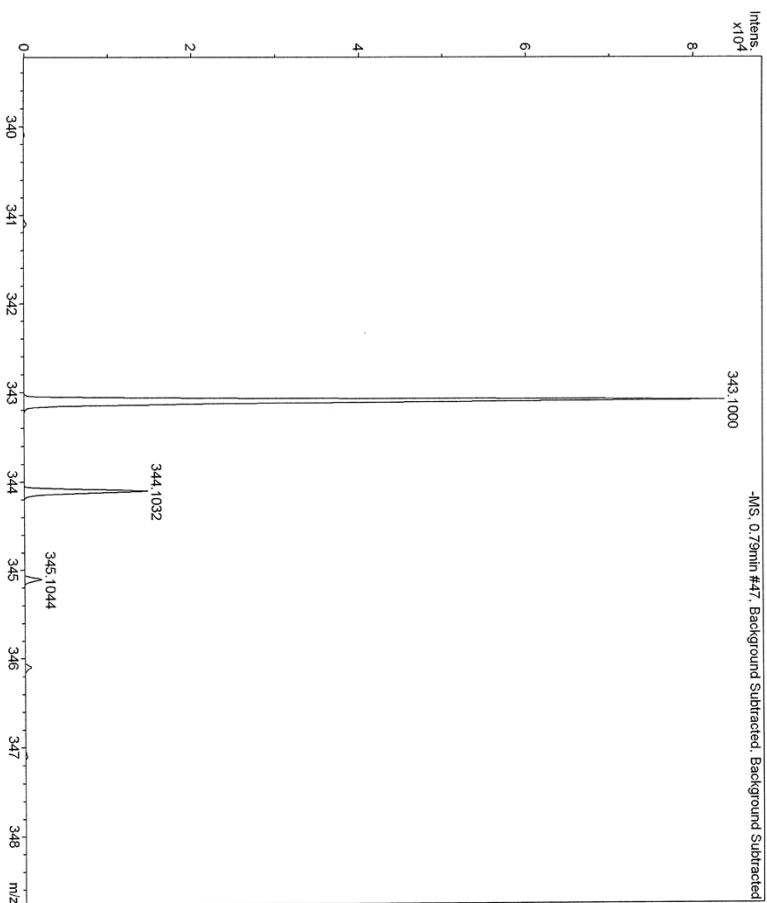
### Analysis Info

Analysis Name	D:\Data\Chemistry\Outside\AMRI\SF-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 / Set#	micrOTOF-Q II 10269
Comment	AMRI		

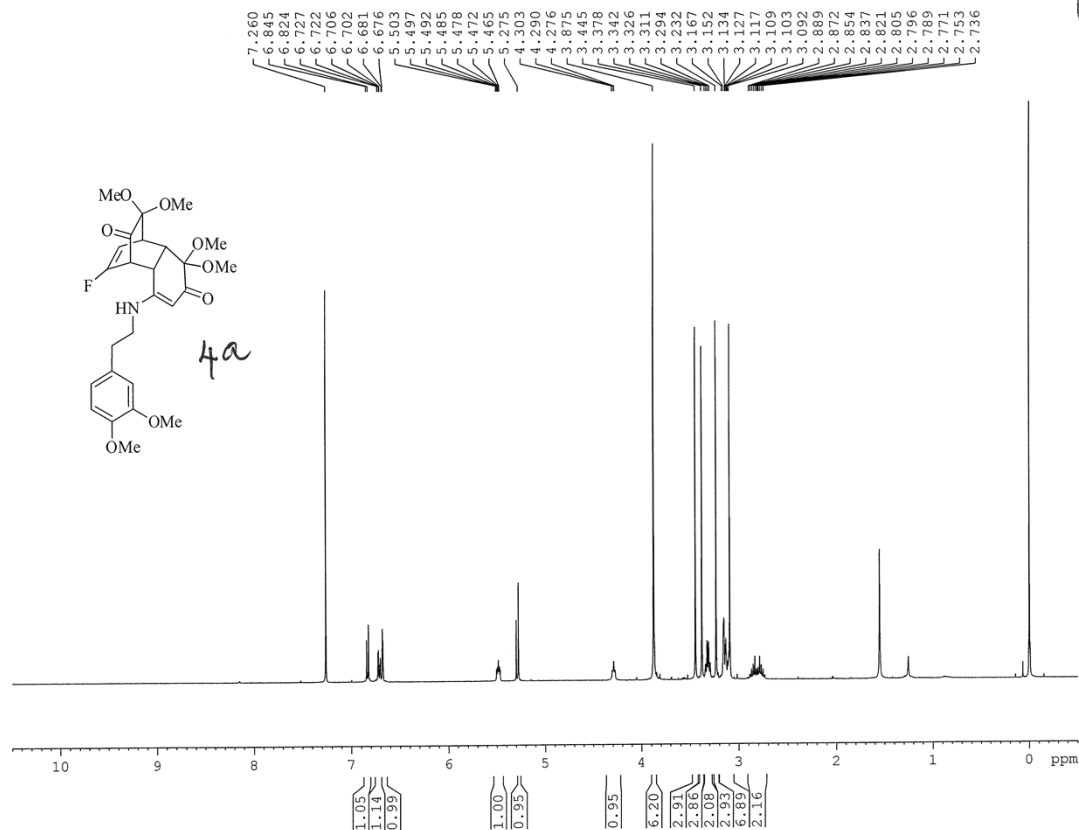
### Acquisition Parameter

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 <sup>-</sup> Conf	N-Rule
343.1000	1	C <sub>16</sub> H <sub>17</sub> F <sub>2</sub> O <sub>6</sub>	343.0999	-0.4	7.5	even	ok







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 BH-  
 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  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.70 usec  
 PL1 -2.00 dB  
 PL1W 14.33185768 W  
 SFO1 400.2330883 MHz

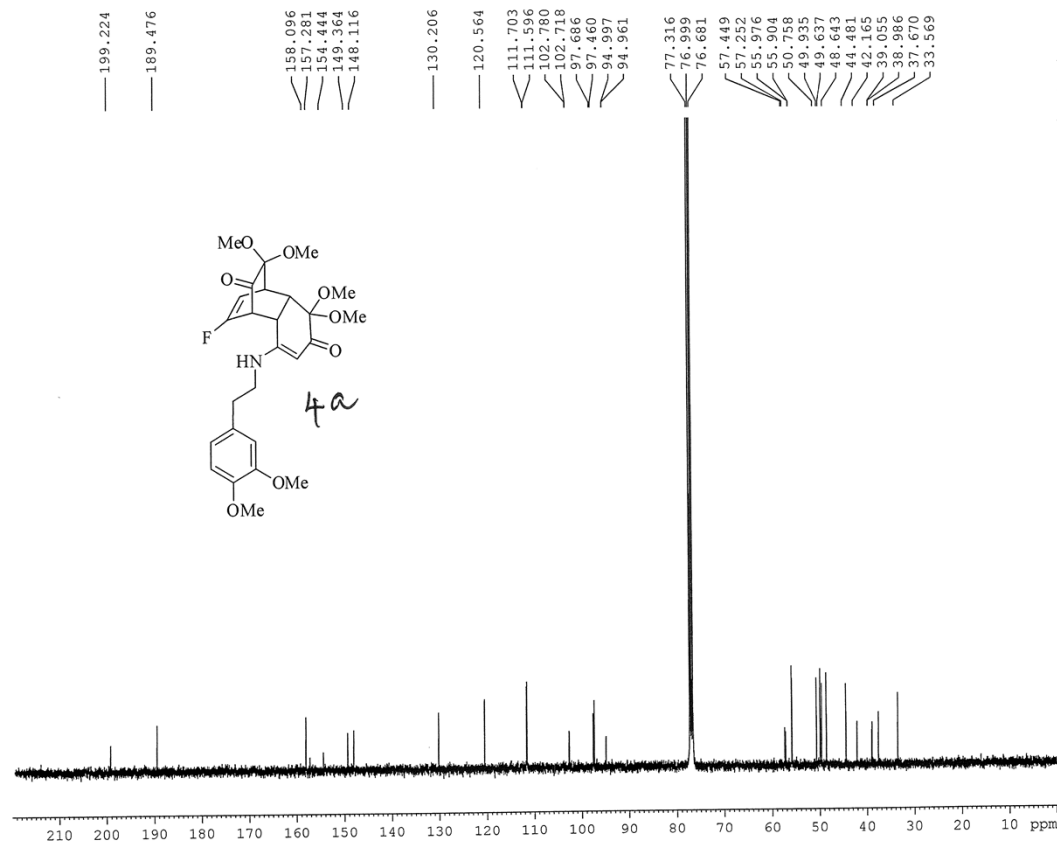
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 SI 32768  
 SF 400.2300118 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

Name \_\_\_\_\_

Date \_\_\_\_\_

NB # \_\_\_\_\_

AMRI; SRC AV400  
location; 18



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

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

F2 - Acquisition Parameters  
Date\_ 20140929  
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 0.23662708 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\F-3,4-DIOMe-PhEt-NH2-1.d  
 Method YCH\_Pos-150-1800.m  
 Sample Name 5F-3,4-DIOMe-PhEt-NH2  
 Comment AMRI  
 Santhosh Kumar Chittinalla

Acquisition Date 11/3/2014 2:55:55 PM

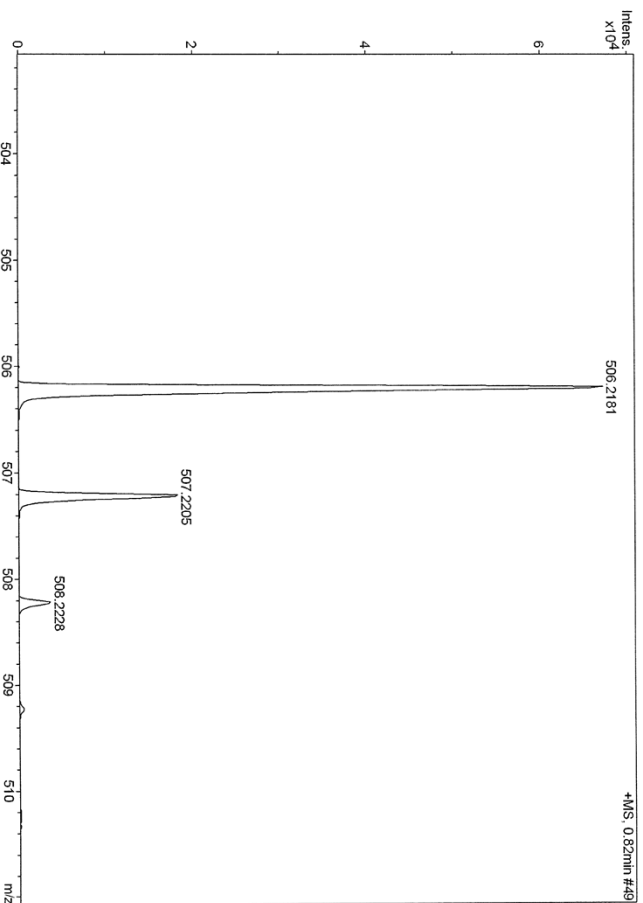
Operator

Instrument/ Ser# micrOTOF-Q II 10269

### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 W
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	1800 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste

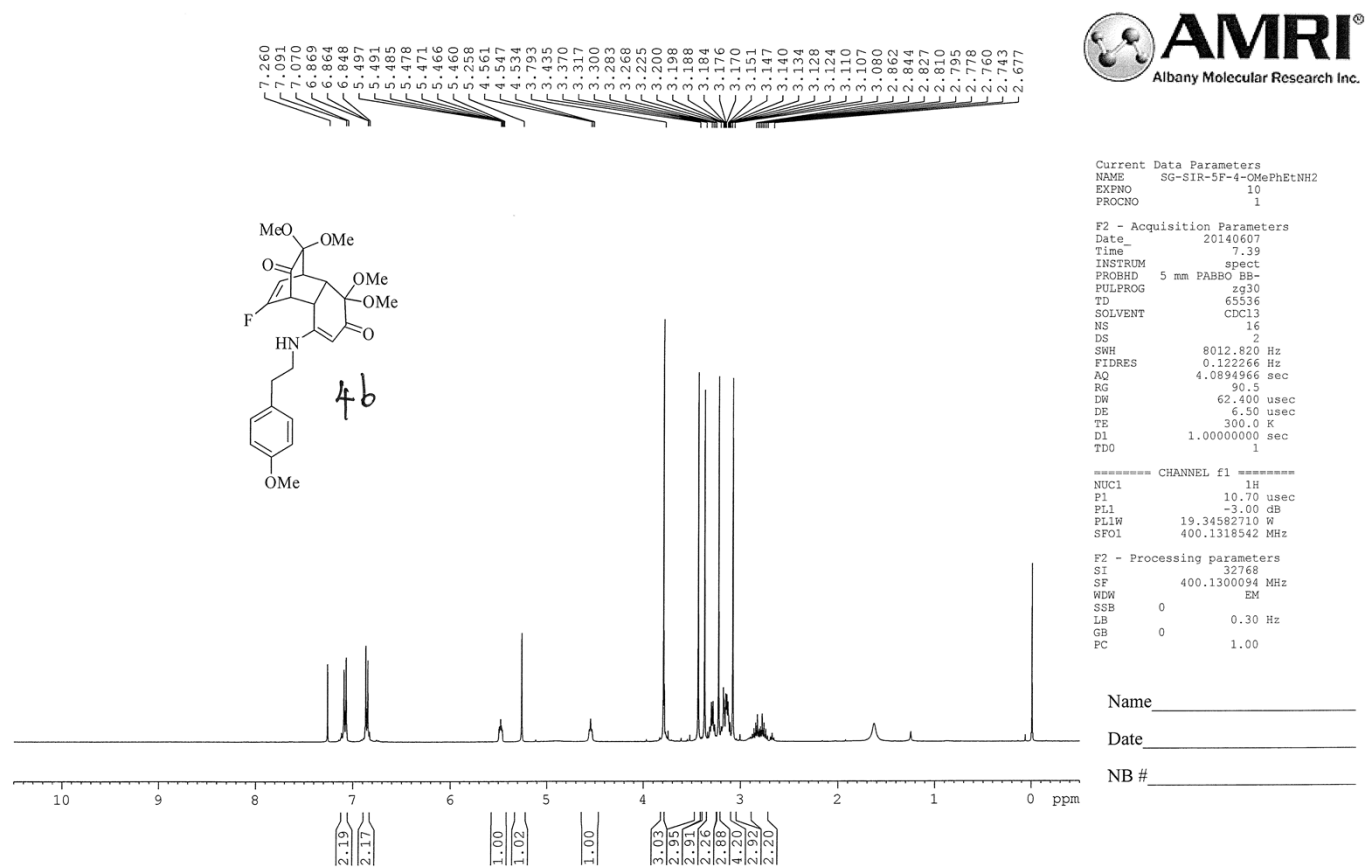
Meas. m/z	#	Formula	m/z	err [ppm]	rd	e <sup>-</sup>	Conf	N-Rule
506.2181	1	C <sub>26</sub> H <sub>33</sub> F <sub>3</sub> N <sub>2</sub> O <sub>8</sub>	506.2185	0.7	10.5	even		ok



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printed: 11/3/2014 2:58:40 PM

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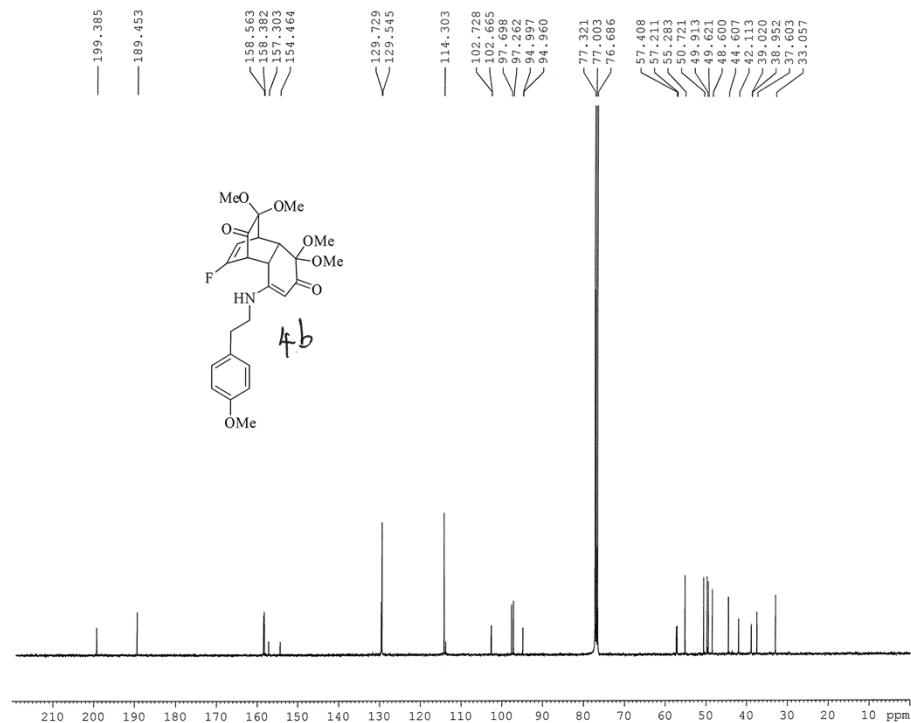


Name \_\_\_\_\_

Date \_\_\_\_\_

NB # \_\_\_\_\_

AMRI SRC  
location; 17



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

Current Data Parameters  
NAME SG-21R-5P-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 0.63000000 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  
PL12W 19.34582710 W  
PL13W 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

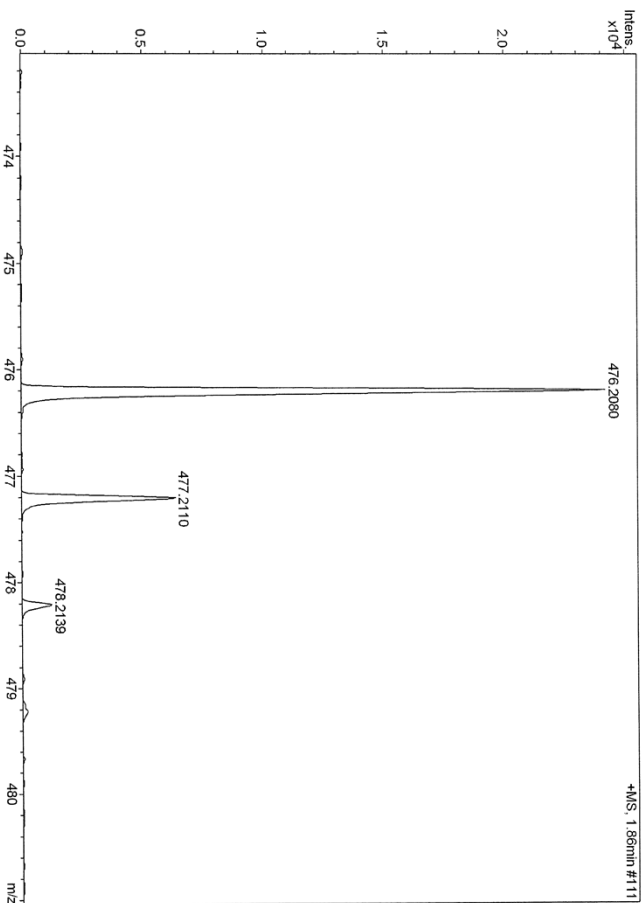
Analysis Name D:\Data\Chemistry\Outside\AMRI\20141103\SF-4-OMe-Phe-NH<sub>2</sub>-1.d  
 Method YCH\_Pos-150-1800.m  
 Sample Name SF-4-OMe-Phe-NH<sub>2</sub>  
 Comment AMRI  
 Santhosh Kumar Chittinalla

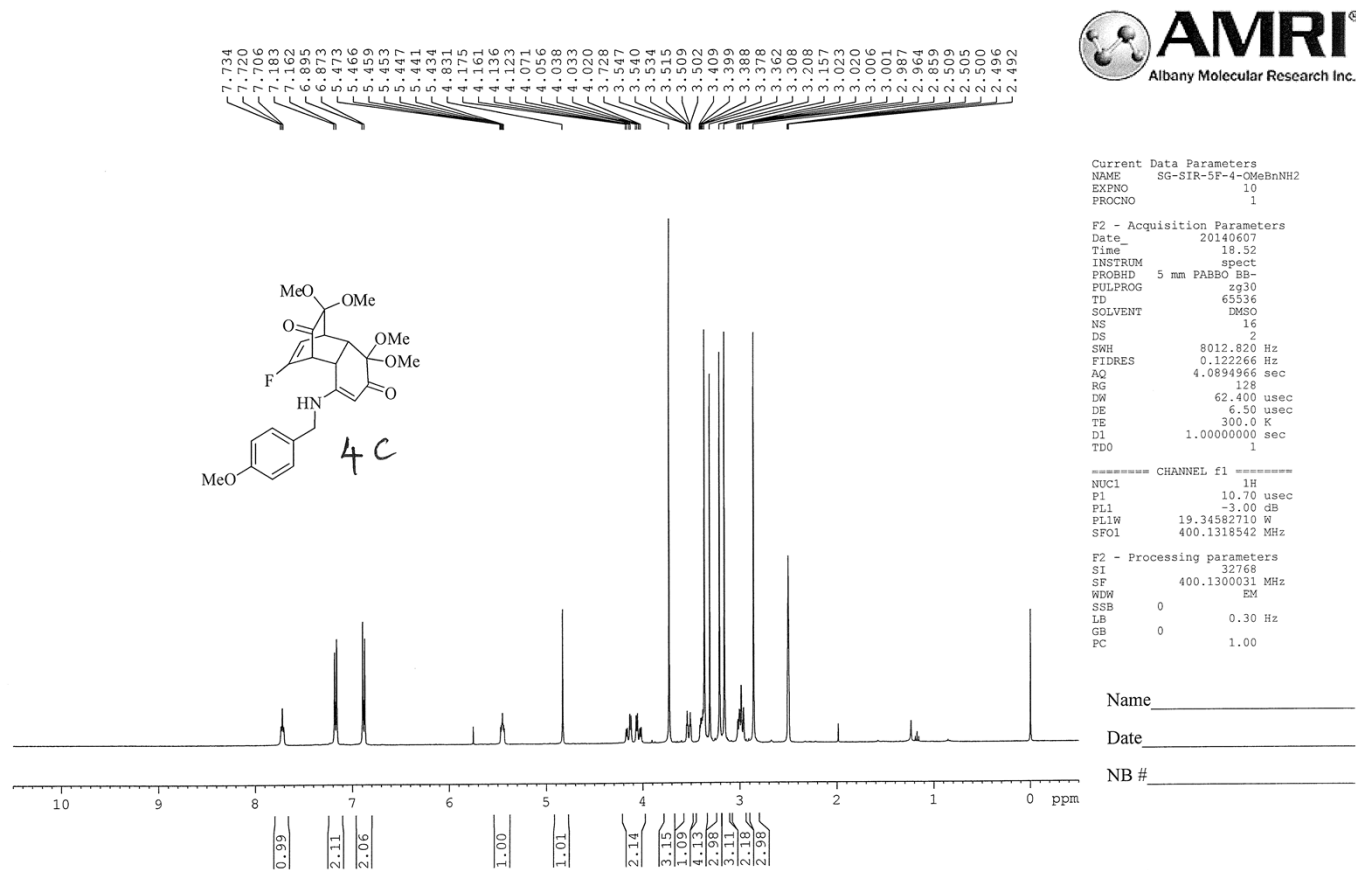
Acquisition Date 11/3/2014 11:32:00 AM  
 Operator default user  
 Instrument/ Ser# microTOF-Q II 10269

### Acquisition Parameter

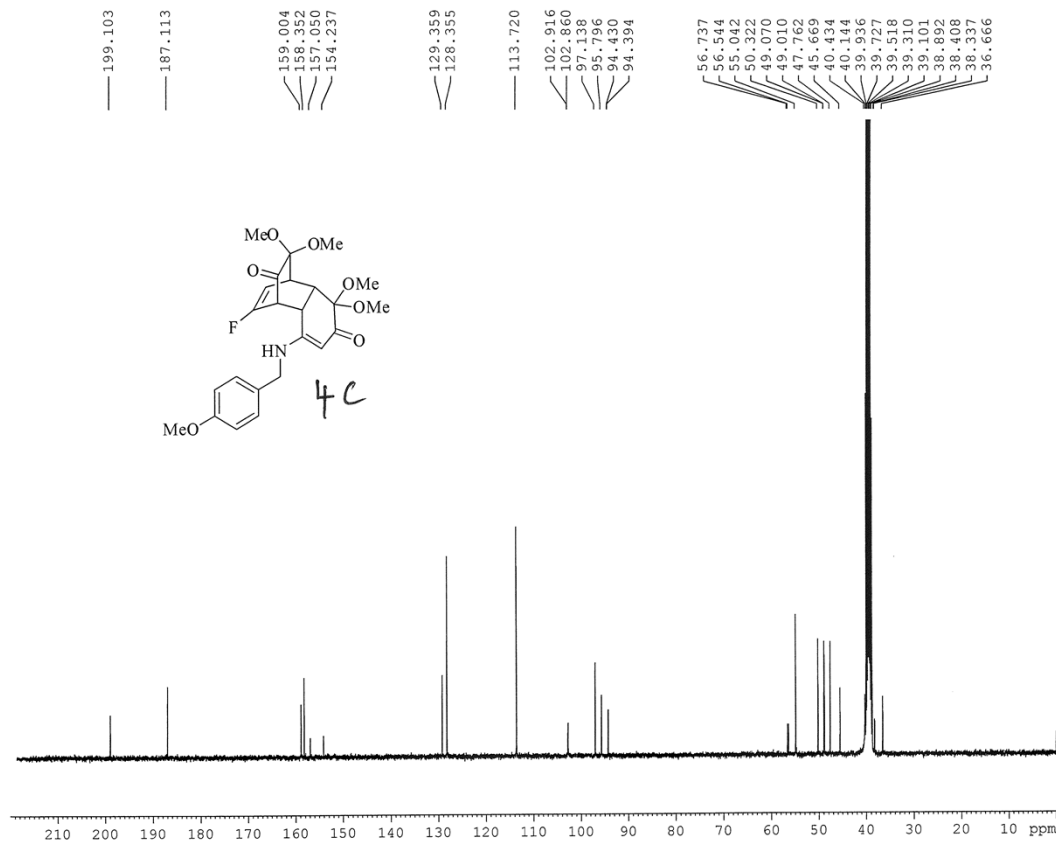
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	500 V	Set Dry Gas	6.0 l/min
Scan End	1800 m/z	Set Collision Cell RF	200.0 Vpp	Set Divergent Valve	Source

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdB	e <sup>-</sup> Conf	N-Rule
476.2080	1	C <sub>25</sub> H <sub>31</sub> N O <sub>7</sub>	100.00	476.2079	-0.1	-0.2	7.4	10.5	even	OK





# AMRI SRC location; 17



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

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

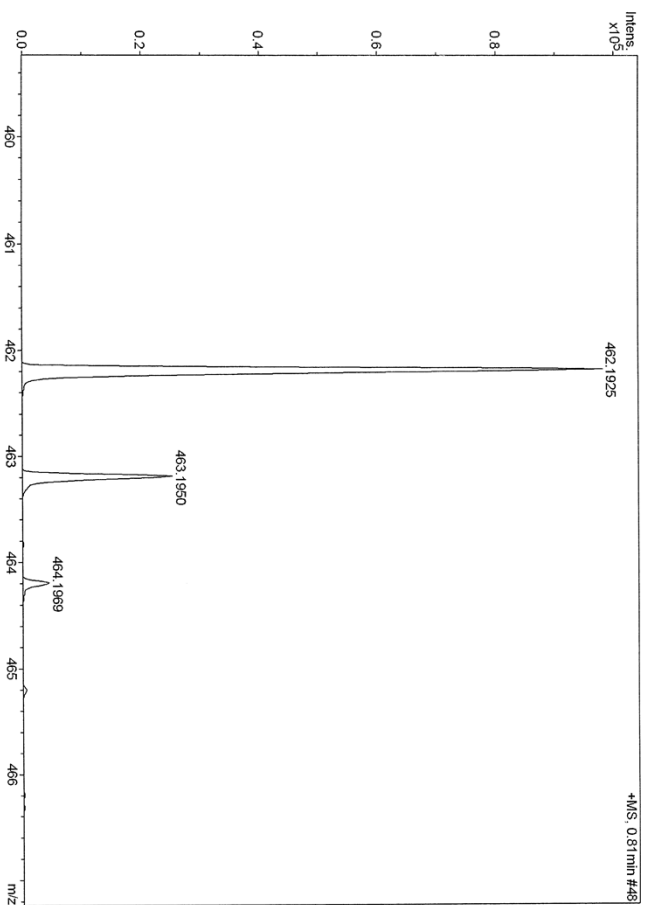
### Analysis Info

Analysis Name D:\Data\Chemistry\Outside\AMRI\20141103\SF-PMB-NH2-1.d Acquisition Date 11/3/2014 12:12:32 PM  
 Method YCH\_Pos-150-1800.m Operator default user  
 Sample Name SF-PMB-NH2 Instrument/Ser# microTOF-Q II 10269  
 Comment AMRI  
 Santhosh Kumar Chittinalla

### 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

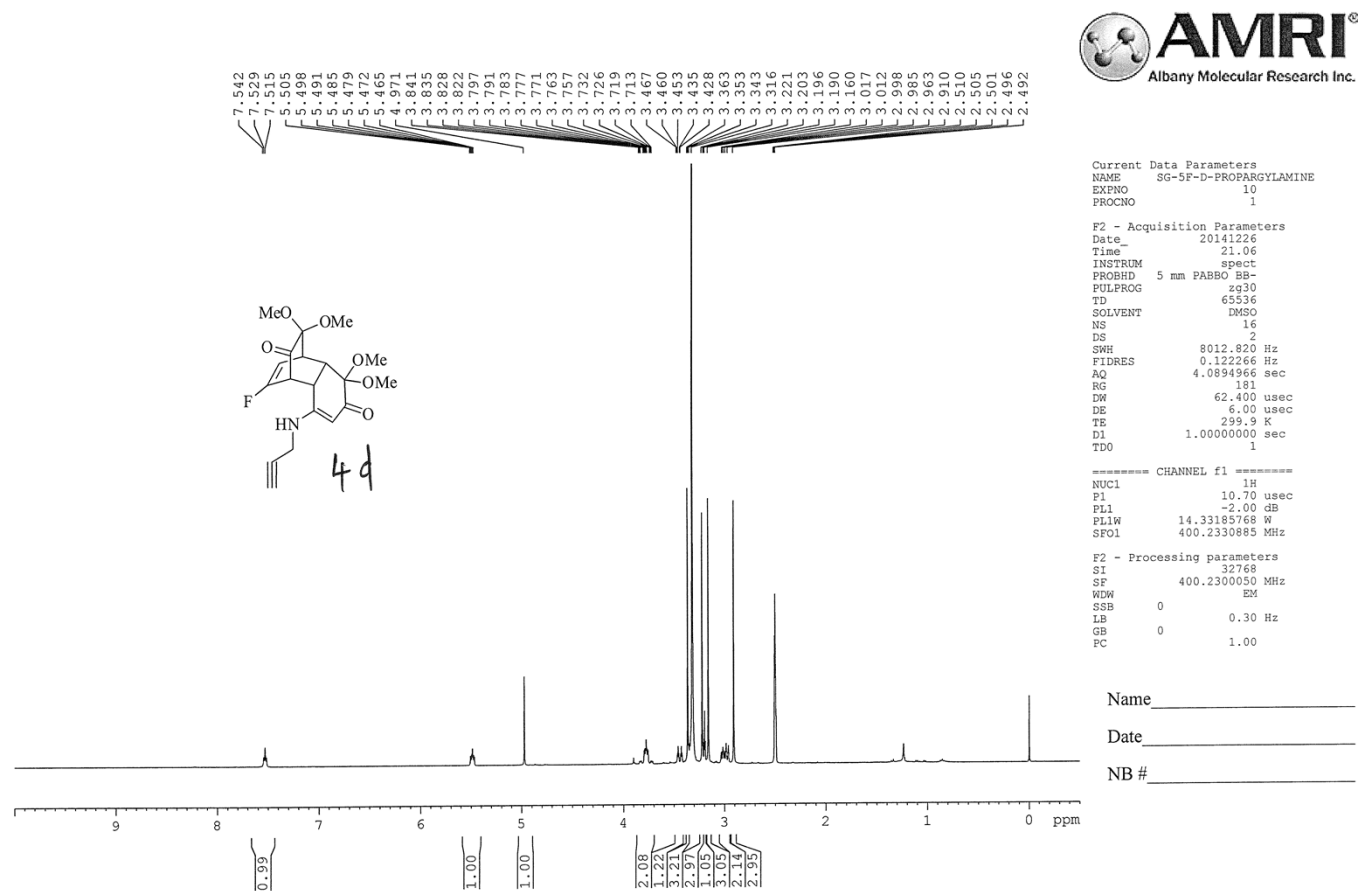
Meas m/z # Formula m/z err [ppm] rdb e<sup>-</sup> Conf N-Rule  
 462.1925 1 C<sub>24</sub>H<sub>29</sub>F<sub>3</sub>N<sub>3</sub>O<sub>7</sub> 462.1923 -0.6 10.5 even ok



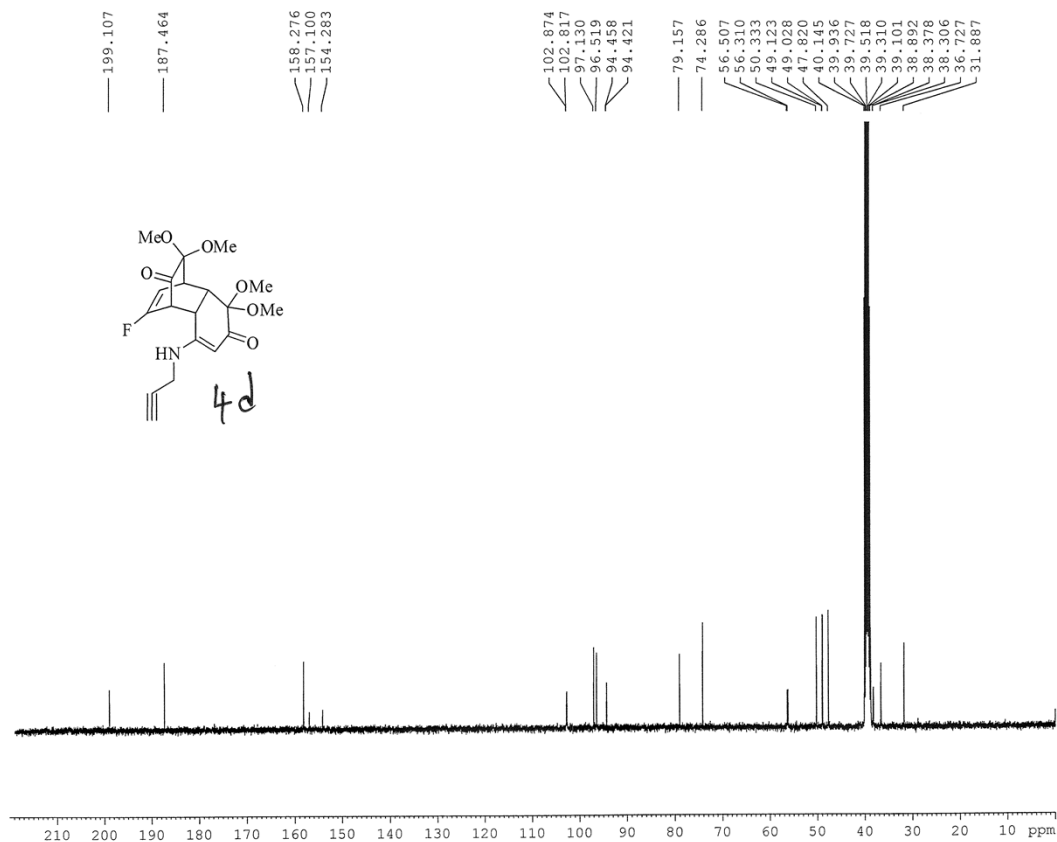
Bruker Compass DataAnalysis 4.0

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AMRI; SRC AV400  
location; 18



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

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 0.5000000 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  
PL1W 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

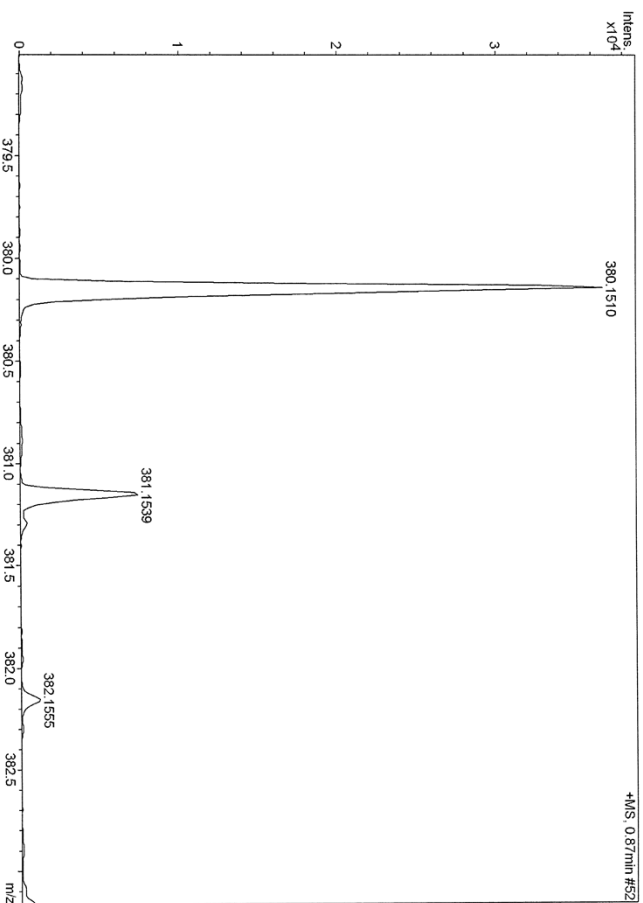
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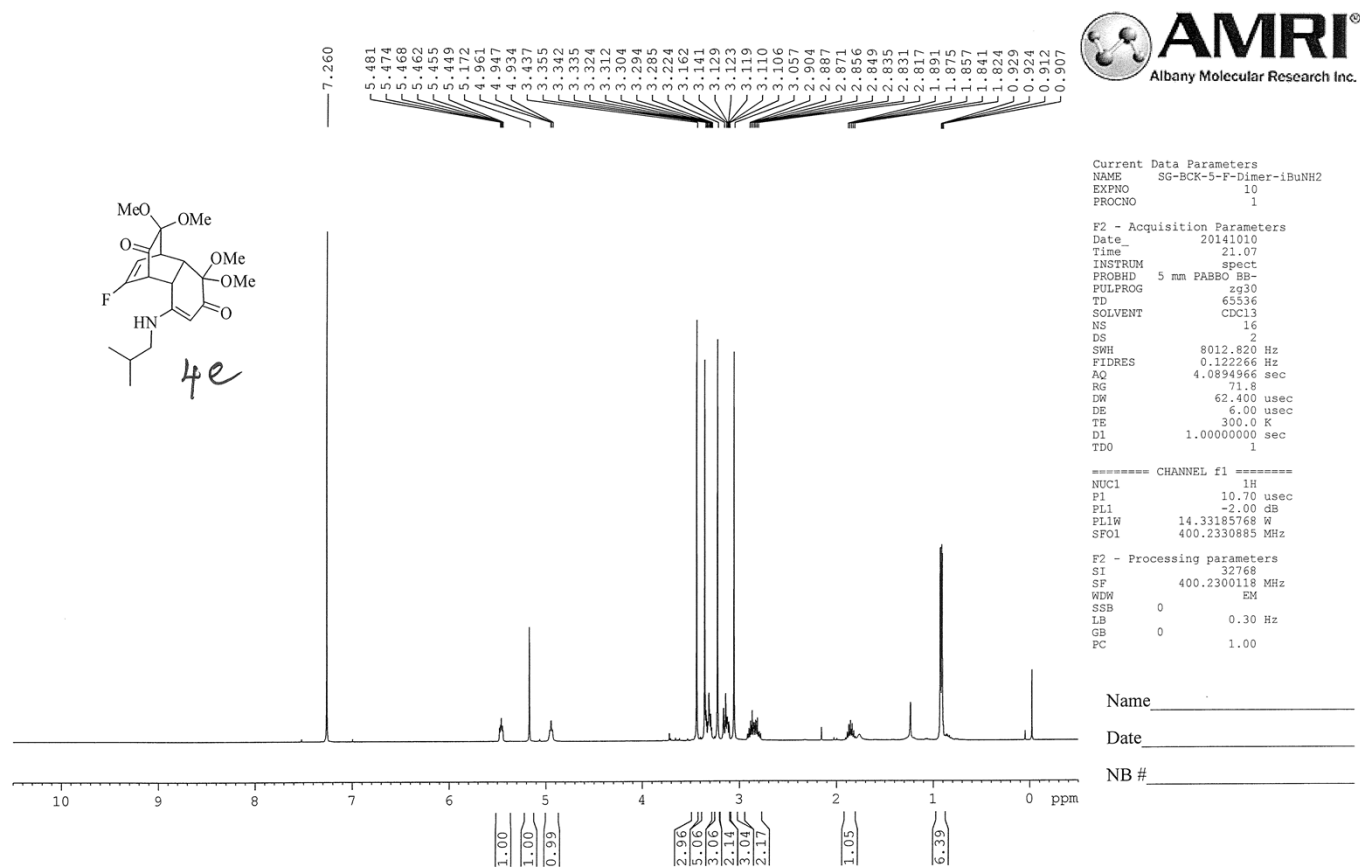
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 Method YCH\_Pos-150-1800.m Operator default user  
 Sample Name SF-Prg-Amine Instrument / Ser# microTOF-Q II 10269  
 Comment AMRI  
 Santhosh Kumar Chittinalla

### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4.500 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<sup>-</sup> Conf N-Rule  
 380.1510 1 C<sub>19</sub>H<sub>23</sub>F<sub>3</sub>N<sub>2</sub>O<sub>6</sub> 380.1504 -1.5 8.5 even N-Rule  
 ok





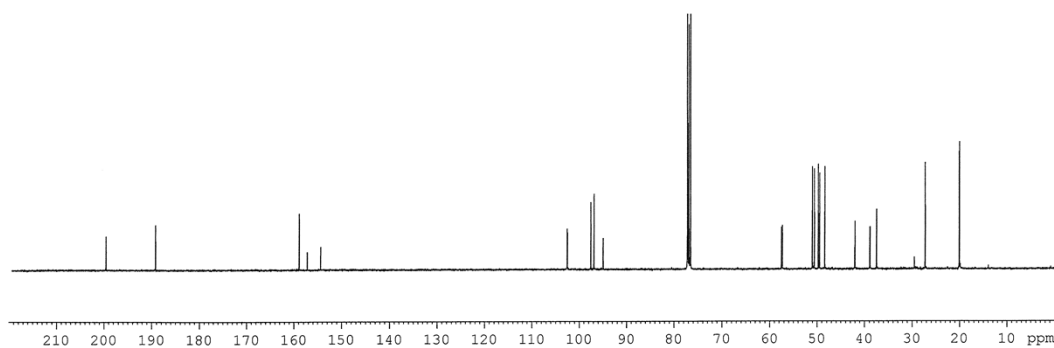
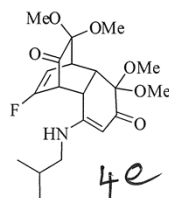
AMRI; SRC AV400  
location; 18



199.661  
189.287  
158.994  
157.294  
154.455

102.648  
102.586  
97.656  
96.985  
95.060  
95.023  
77.318  
77.202  
77.000  
76.683  
57.622  
57.425  
51.142  
50.703  
49.867  
49.567  
48.193  
48.117  
39.010  
38.941  
37.566  
27.379  
20.212  
20.154

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

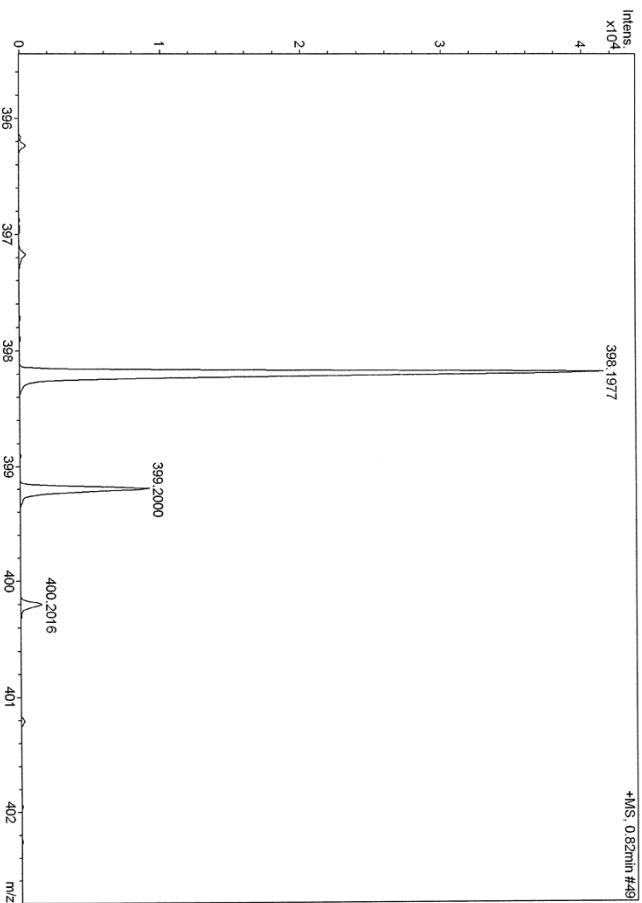
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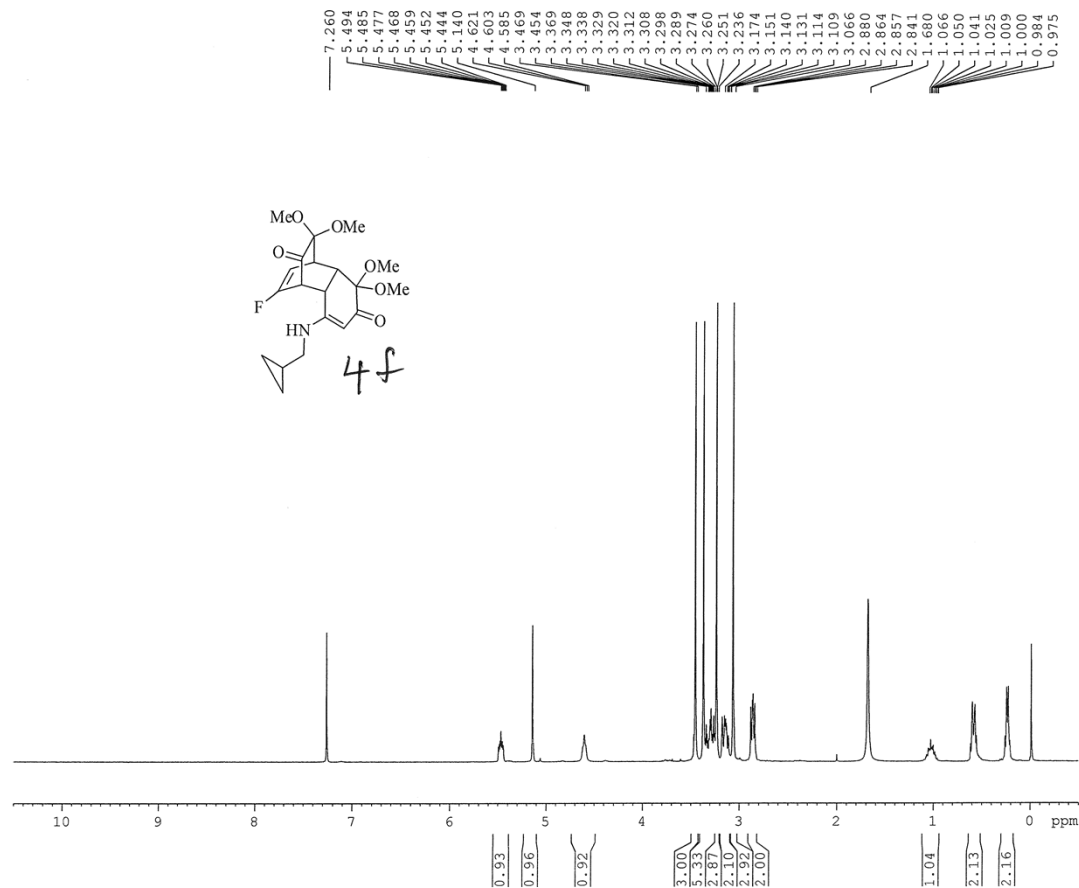
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 Method YCH\_Pos-150-1800.m Operator default user  
 Sample Name SF-IBu-NH2 Instrument / Ser# microTOF-Q II 10269  
 Comment AMRI  
 Santhosh Kumar Chittinalla

### 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





Current Data Parameters  
NAME SG-RKP-CYCLOPROPYLMETHAMINE-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  
DM 83.400 usec  
DE 6.00 usec  
TE 300.2 K  
D1 1.00000000 sec  
MCREST 0 sec  
MCRESK 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

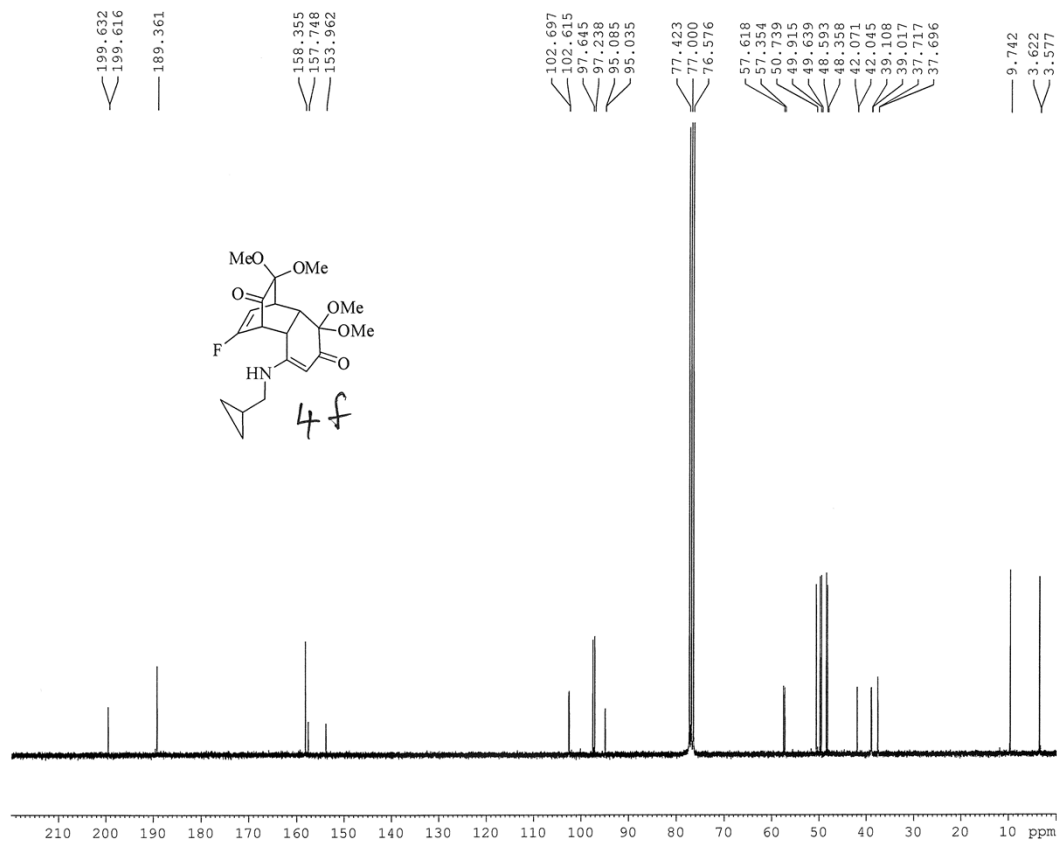
Name \_\_\_\_\_

Date \_\_\_\_\_

NB # \_\_\_\_\_



AMRI; SRC  
location; 15



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

Current Data Parameters  
NAME 5g-RKF-CYCLOPROPYLMETHAMINE-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

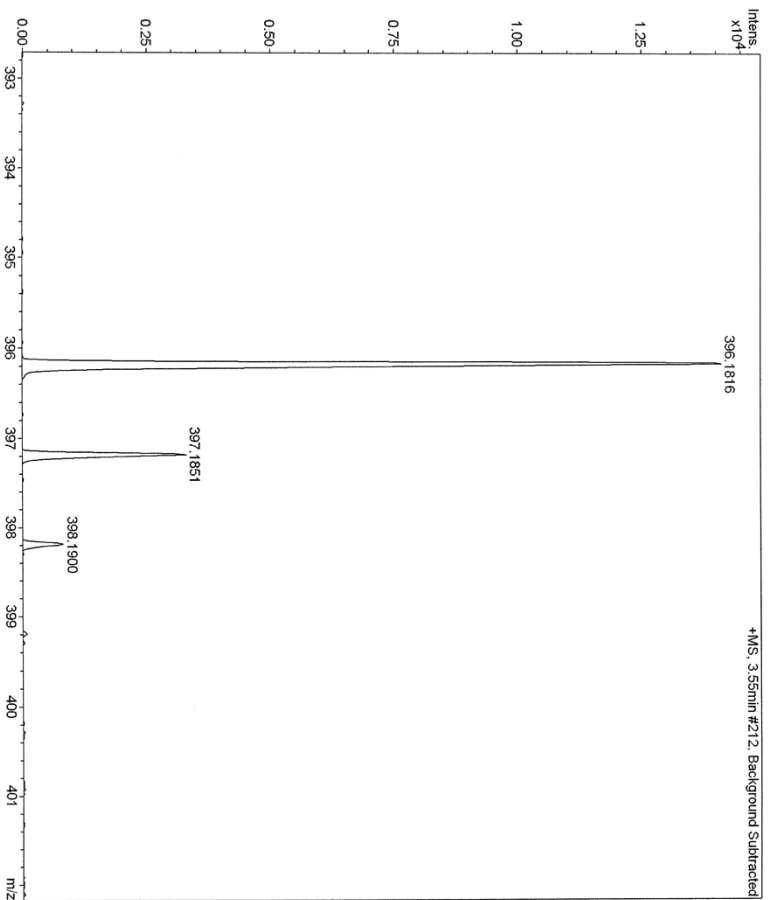
### Analysis Info

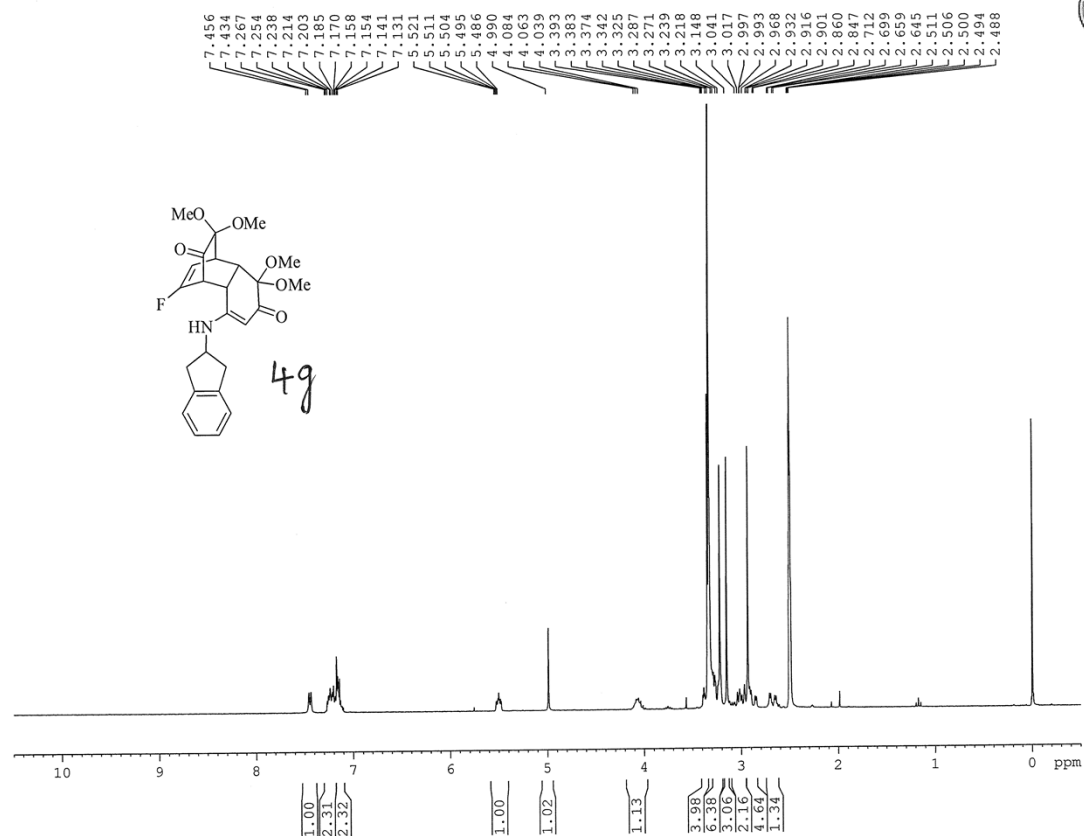
Analysis Name D:\Data\Chemistry\Outside\AMRI\20150107\5F-Cyp-Me-Amine.d Acquisition Date 1/7/2015 2:56:25 PM  
 Method YCH\_Pos-150-1800 m Operator default user  
 Sample Name 5F-Cyp-Me-Amine Instrument / Set# microTOF-Q II 10269  
 Comment AMRI

### 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

Mass. m/z	#	Formula	m/z	err [ppm]	rdB	e <sup>-</sup> Conf	N-Rule
396.1816	1	C <sub>20</sub> H <sub>27</sub> FNO <sub>6</sub>	396.1817	0.2	7.5	even	ok





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

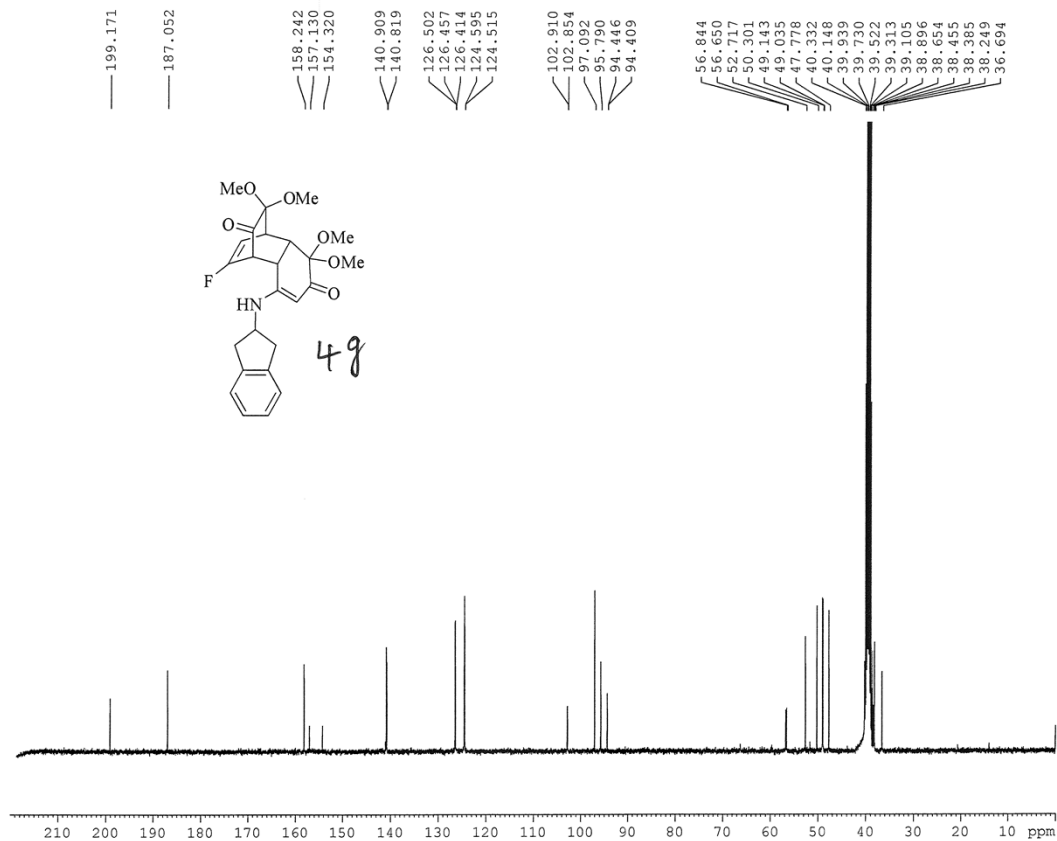
F2 - Acquisition Parameters  
 Date\_ 20140619  
 Time 20.11  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/13  
 PULPROG zg30  
 TD 32768  
 SOLVENT DMSO  
 NS 32  
 DS 2  
 SWH 5995.204 Hz  
 FIDRES 0.182959 Hz  
 AQ 2.7329011 sec  
 RG 812.7  
 DW 83.400 usec  
 DE 6.00 usec  
 TE 296.2 K  
 D1 1.00000000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

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 12.20 usec  
 PL1 0 dB  
 SF01 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 23980.614 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  
PL1W 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  
FC 1.40

## Mass Spectrum SmartFormula Report

### Analysis Info

Analysis Name D:\Data\Chemistry\Outiside\AMRI\20141103\F-Ar-Indane-1.d  
 Method YCH\_Pos-150-1800.m  
 Sample Name 5F-Ar-Indane  
 Comment AMRI  
 Santhosh Kumar Chittinalla

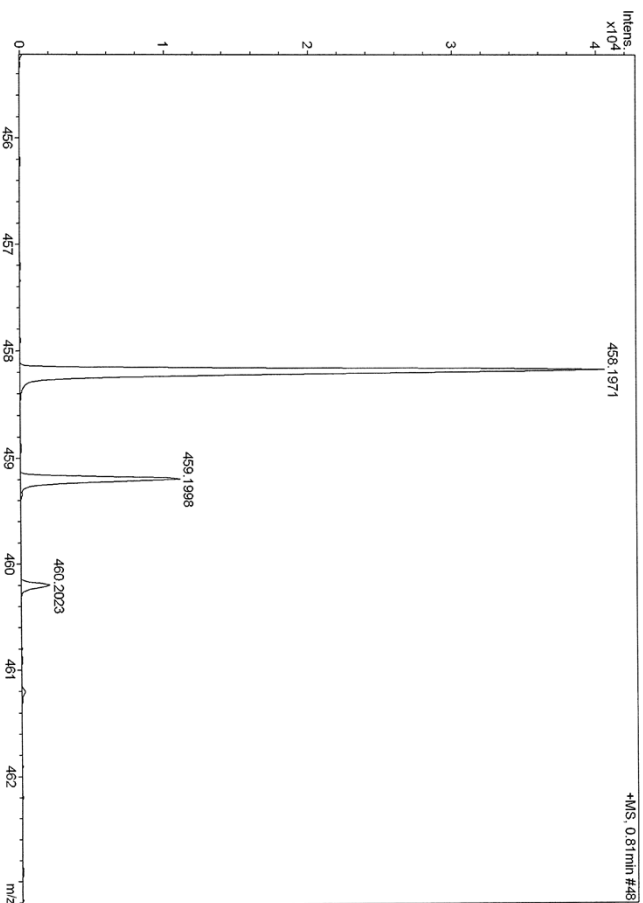
Acquisition Date 11/3/2014 3:09:03 PM

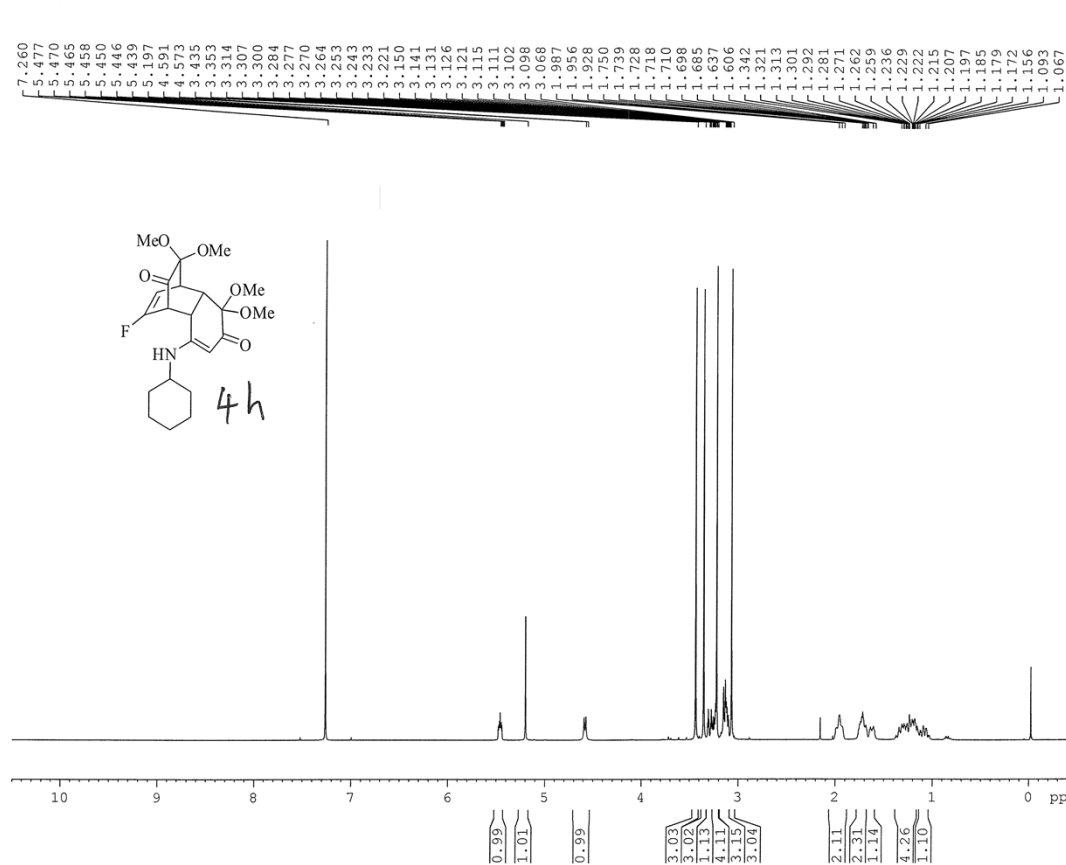
Operator default user  
 Instrument/ Ser# microTOF-Q II 10269

### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 W
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<sup>-</sup> Conf N-Rule  
 458.1971 1 C<sub>25</sub>H<sub>29</sub>F<sub>3</sub>N<sub>2</sub>O<sub>6</sub> 458.1973 0.6 11.5 even ok





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 4.089496 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

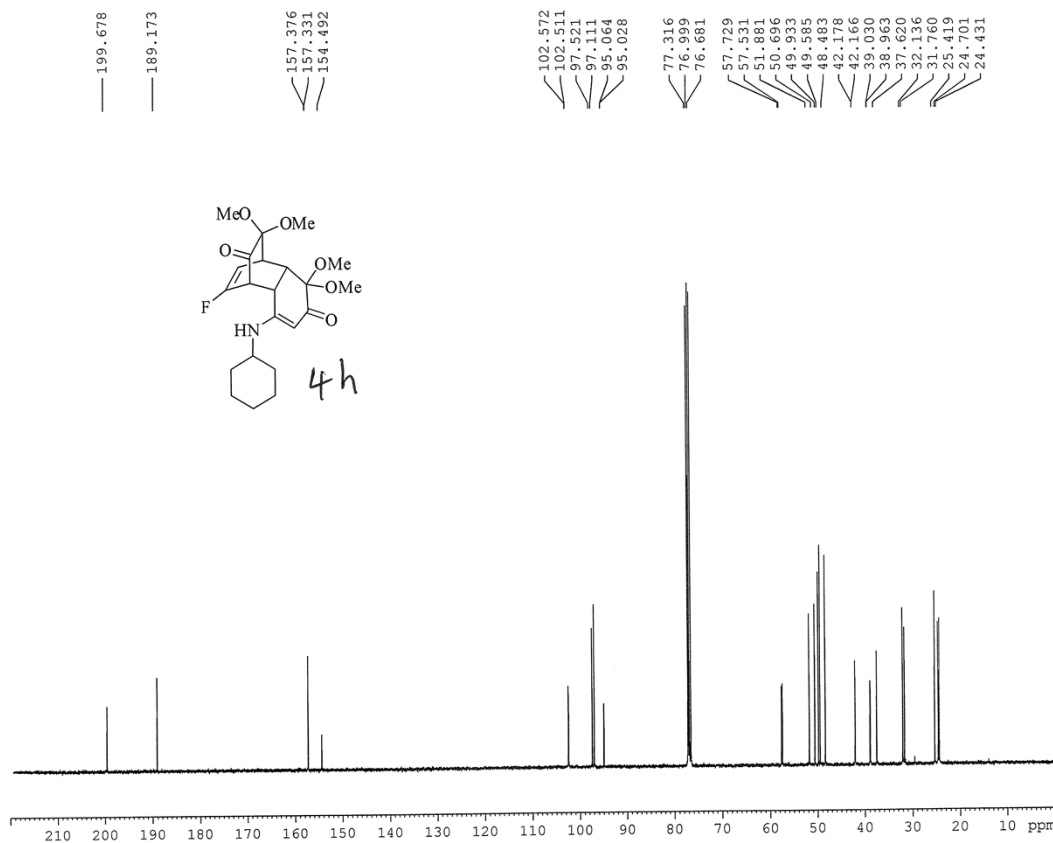
F2 - Processing parameters  
SI 32768  
SF 400.2300118 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

Name \_\_\_\_\_

Date \_\_\_\_\_

NB # \_\_\_\_\_

AMRI; SRC AV400  
location; 18



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

Current Data Parameters  
NAME SG-BCK-5-F-Dimer-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 0.23662708 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

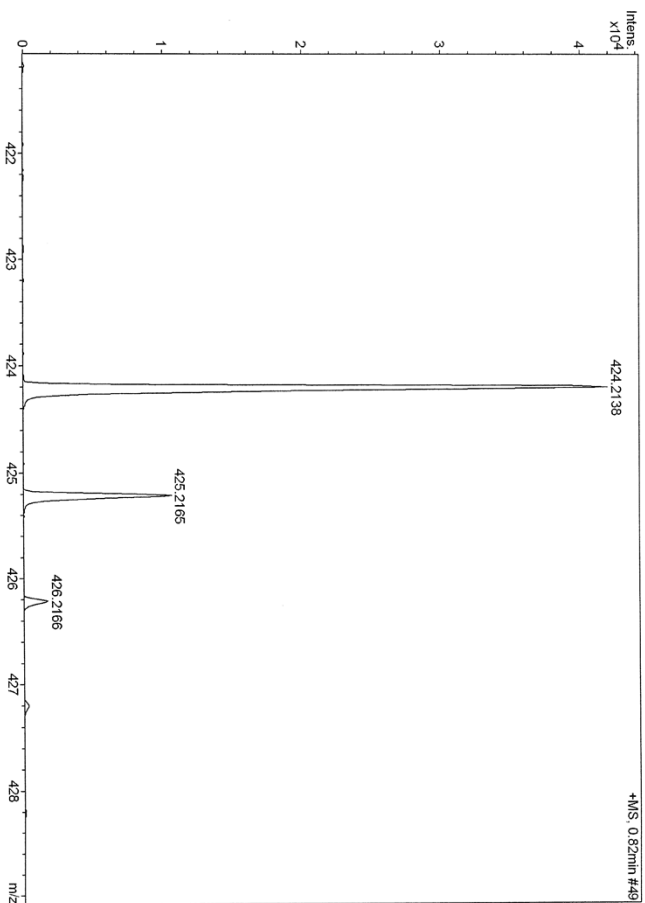
### Analysis Info

Analysis Name D:\Data\Chemistry\Outside\AMRI\20141103\SF-Cychex-NH2-1.d Acquisition Date 11/3/2014 11:39:56 AM  
 Method YCH\_Pos-150-1800.m Operator default user  
 Sample Name SF-Cychex-NH2 Instrument/Ser# microTOF-Q II 10269  
 Comment AMRI  
 Santhosh Kumar Chittinalla

### Acquisition Parameter

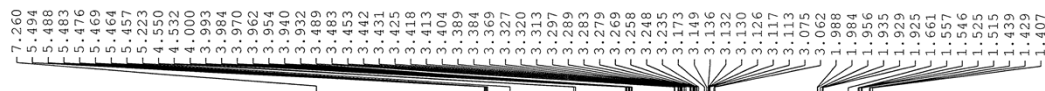
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1800 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste

Meas. m/z # Formula m/z err [ppm] rdb e<sup>-</sup> Conf N-Rule  
 424.2138 1 C<sub>22</sub>H<sub>31</sub>N<sub>3</sub>O<sub>6</sub> 424.2130 -1.9 7.5 even ok





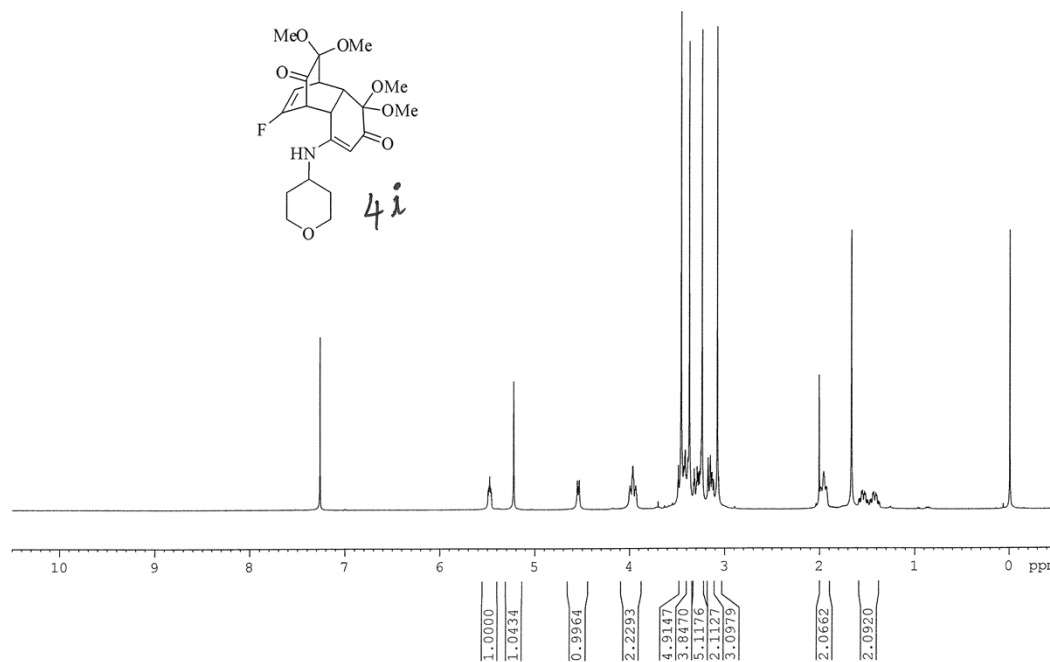
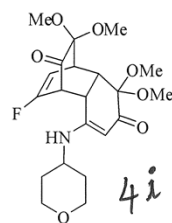
AMRI SRC  
location; 17



Name \_\_\_\_\_

Date \_\_\_\_\_

NB # \_\_\_\_\_



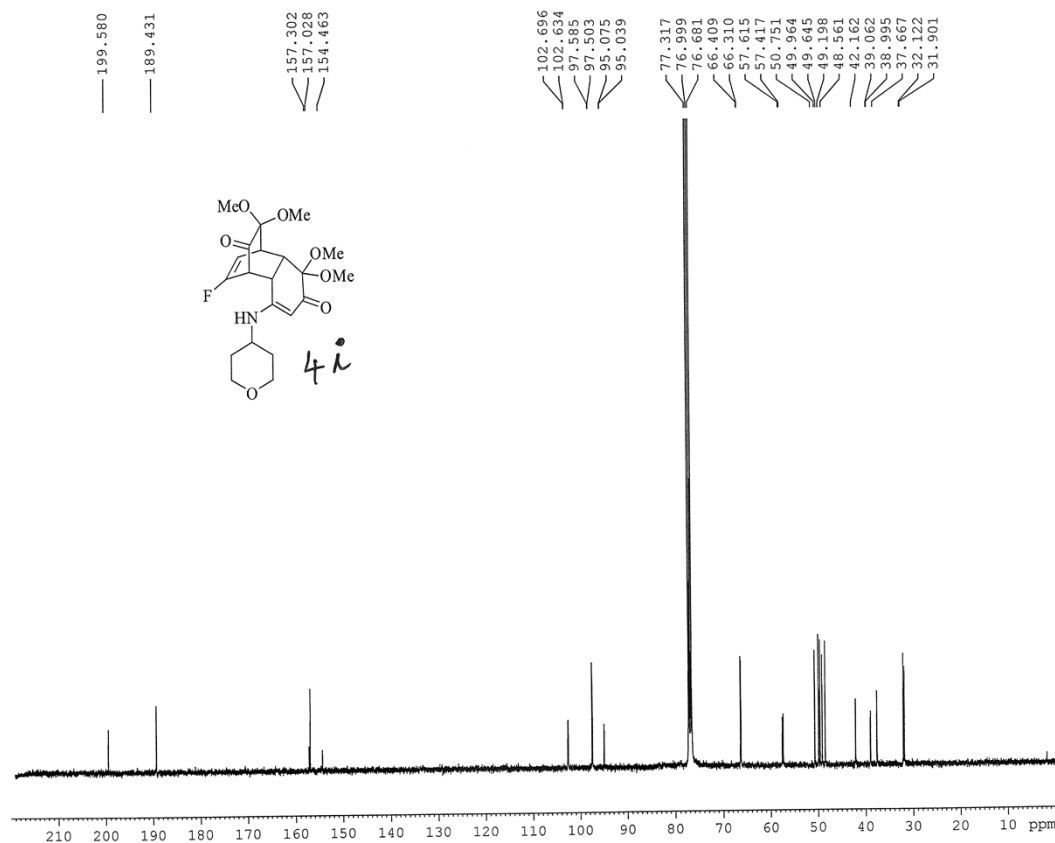
Current Data Parameters  
NAME SG-RKP-H-3-I  
EXPNO 10  
PROCNO 1

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-3-1  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20140621  
Time 8.35  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
FULPROG 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

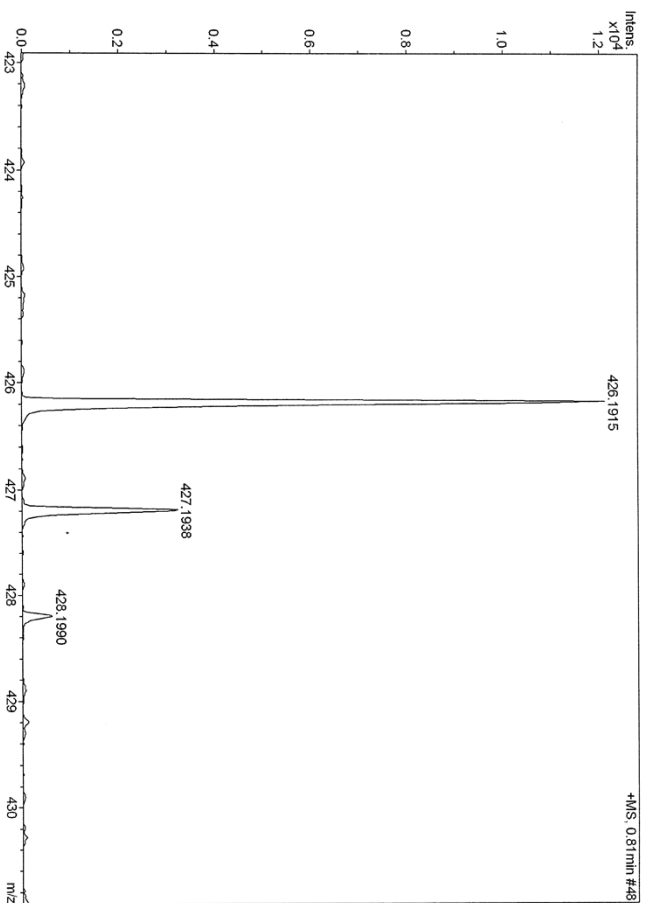
### Analysis Info

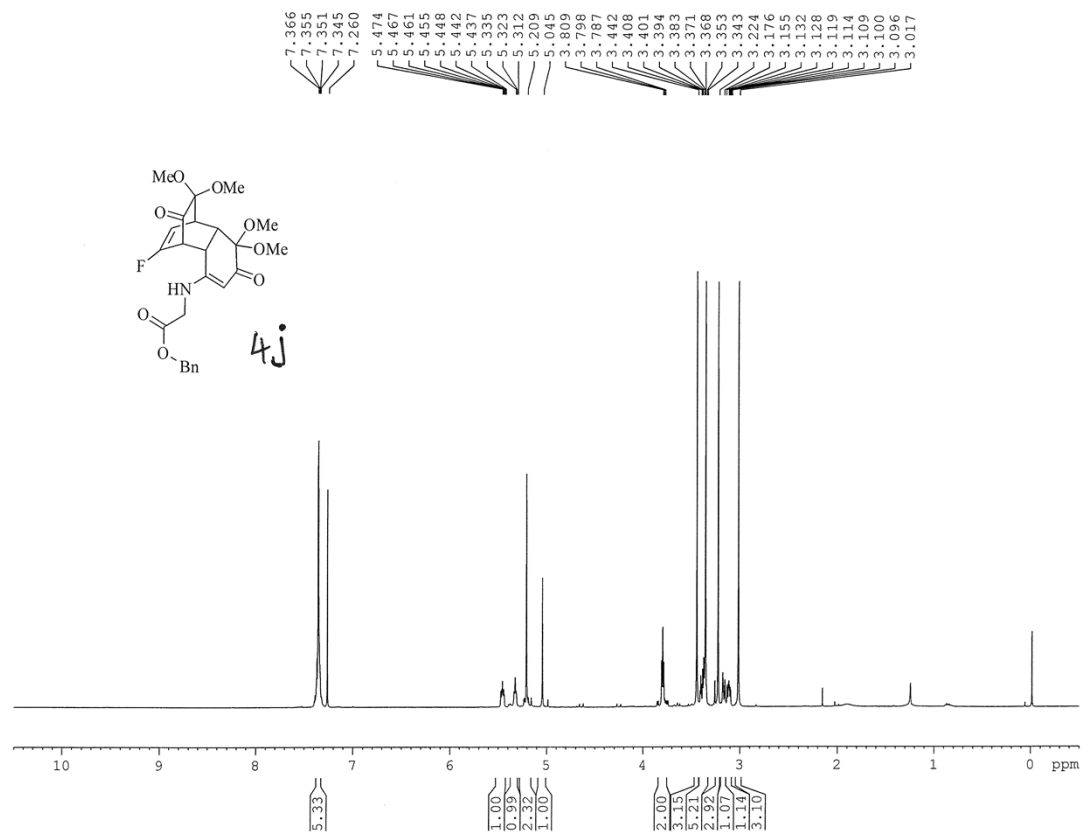
Analysis Name D:\Data\Chemistry\Outside\AMRI\20141103\SF-4Am-Pyrene-1.d Acquisition Date 11/3/2014 3:02:22 PM  
 Method YCH\_Pos-150-1800.m Operator default user  
 Sample Name SF-4Am-Pyrene Instrument / Ser# microTOF-Q II 10269  
 Comment AMRI  
 Santhosh Kumar Chittinalla

### 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 Mode	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]	rtb	e <sup>-</sup> Conf	N-Rule
426.1915	1	C <sub>21</sub> H <sub>29</sub> FNO <sub>7</sub>	426.1923	1.8	7.5	even	ok





Current Data Parameters  
 NAME SG-BCK-S-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 CDCl<sub>3</sub>  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894366 sec  
 RG 71.8  
 DW 62.400 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.70 usec  
 PL1 -2.00 dB  
 PL1W 14.33185768 W  
 SF01 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 \_\_\_\_\_

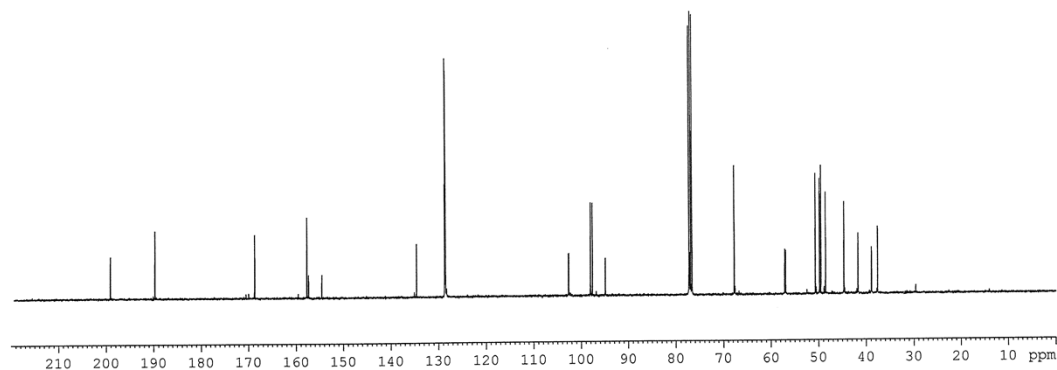
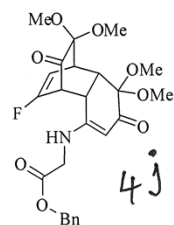
NB # \_\_\_\_\_

AMRI; SRC AV400  
location; 18



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

199.147  
189.754  
168.728  
157.776  
157.420  
154.577  
134.630  
128.774  
128.602  
128.593  
102.709  
102.646  
98.080  
97.681  
94.946  
94.910  
77.317  
77.000  
76.681  
67.766  
57.137  
56.939  
50.722  
49.842  
49.564  
48.597  
44.692  
41.739  
41.728  
38.956  
38.889  
37.650



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

F2 - Acquisition Parameters  
Date\_ 20141011  
Time 9.51  
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  
PL2 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

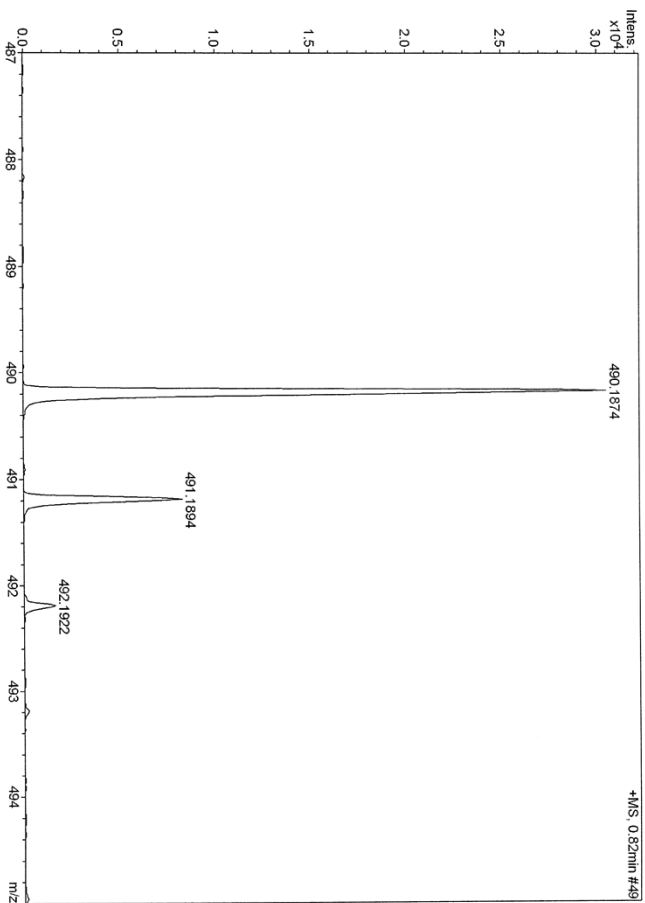
### Analysis Info

Analysis Name D:\Data\Chemistry\Outside\AMRI\20141103\F-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  
 Santhosh Kumar Chittinalla

### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 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

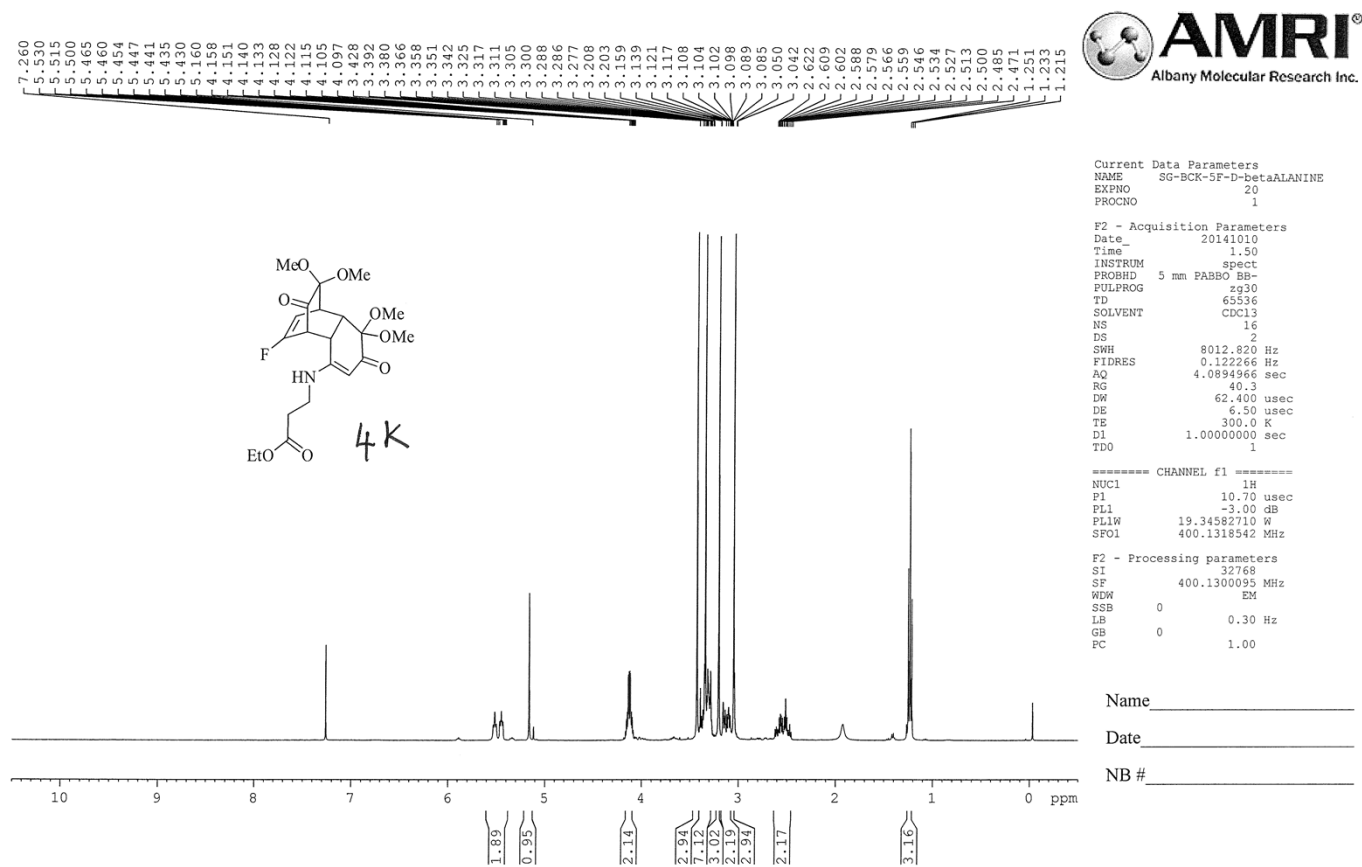
Meas m/z # Formula m/z err [ppm] rdb e<sup>-</sup> Conf N-Rule  
 490.1874 1 C<sub>25</sub>H<sub>29</sub>F<sub>3</sub>N<sub>3</sub>O<sub>8</sub> 490.1872 -0.4 11.5 even ok



Bruker Compass DataAnalysis 4.0

printed: 11/3/2014 11:55:54 AM

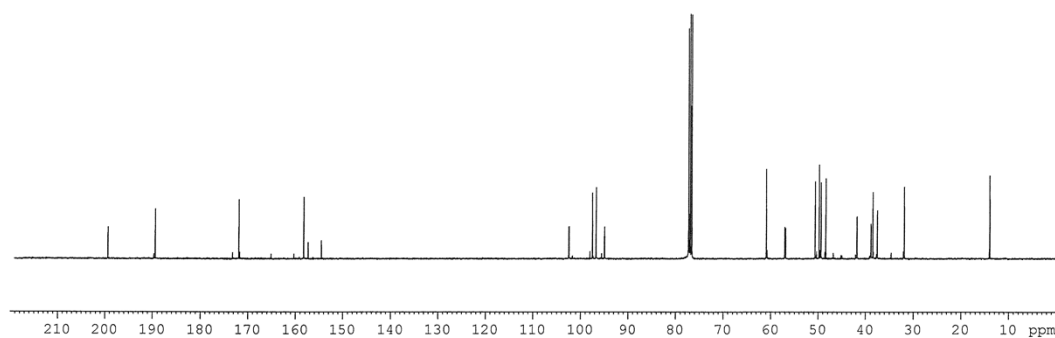
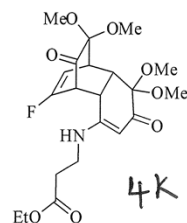
Page 1 of 1



# AMRI SRC location; 17



199.423  
 189.474  
 171.939  
 158.336  
 157.413  
 154.576  
 102.529  
 102.467  
 97.580  
 96.800  
 95.019  
 94.982  
 77.316  
 76.999  
 76.680  
 60.978  
 57.112  
 56.913  
 50.732  
 49.869  
 49.479  
 48.453  
 41.863  
 38.937  
 38.869  
 38.525  
 37.588  
 31.944  
 14.042



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 CDCl3  
 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  
 TDO 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

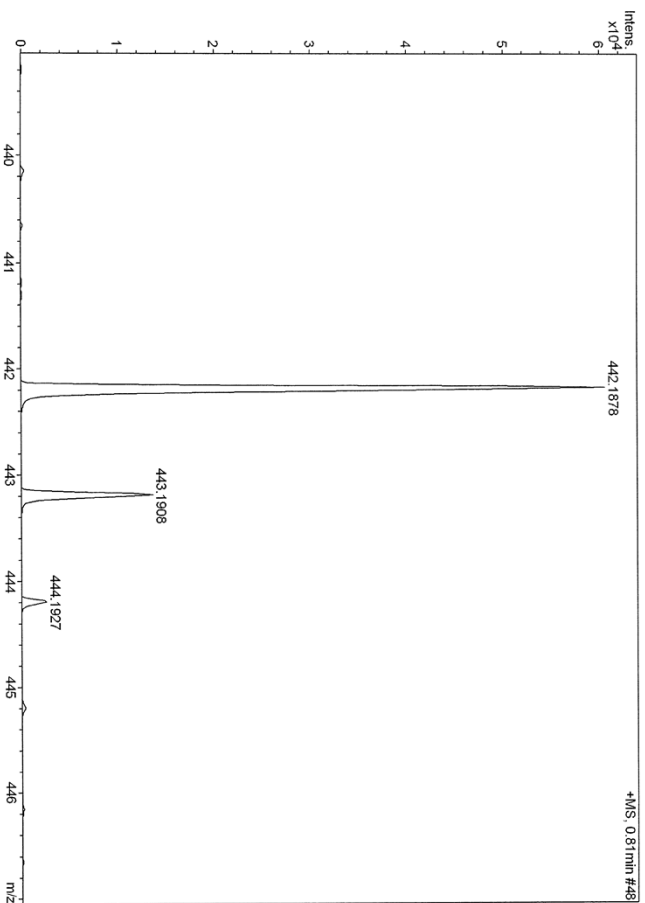
### Analysis Info

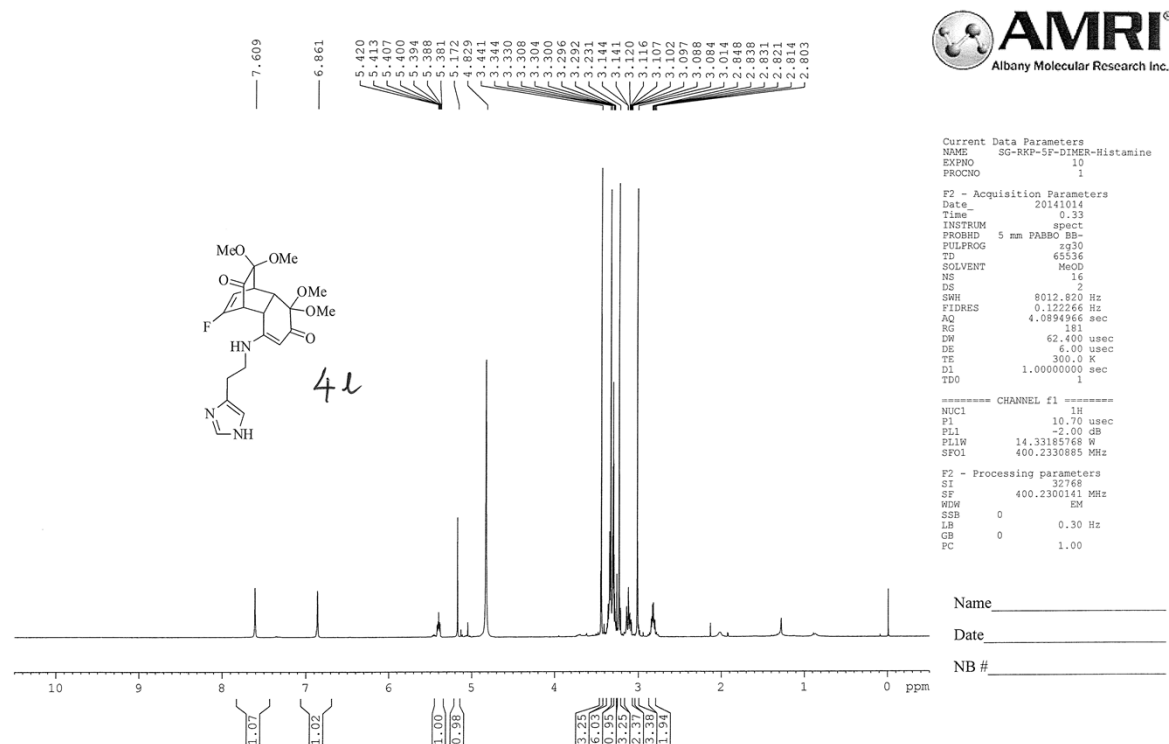
Analysis Name D:\Data\Chemistry\Outside\MMR120141103\SF-Beta-Alanine-1.d	Acquisition Date 11/3/2014 12:33:52 PM
Method YCH_Pos-150-1800.m	Operator default user
Sample Name SF-Beta-Alanine	Instrument / Ser# micrOTOF-Q II 10269
Comment Santhosh Kumar Chittinalla	

### Acquisition Parameter

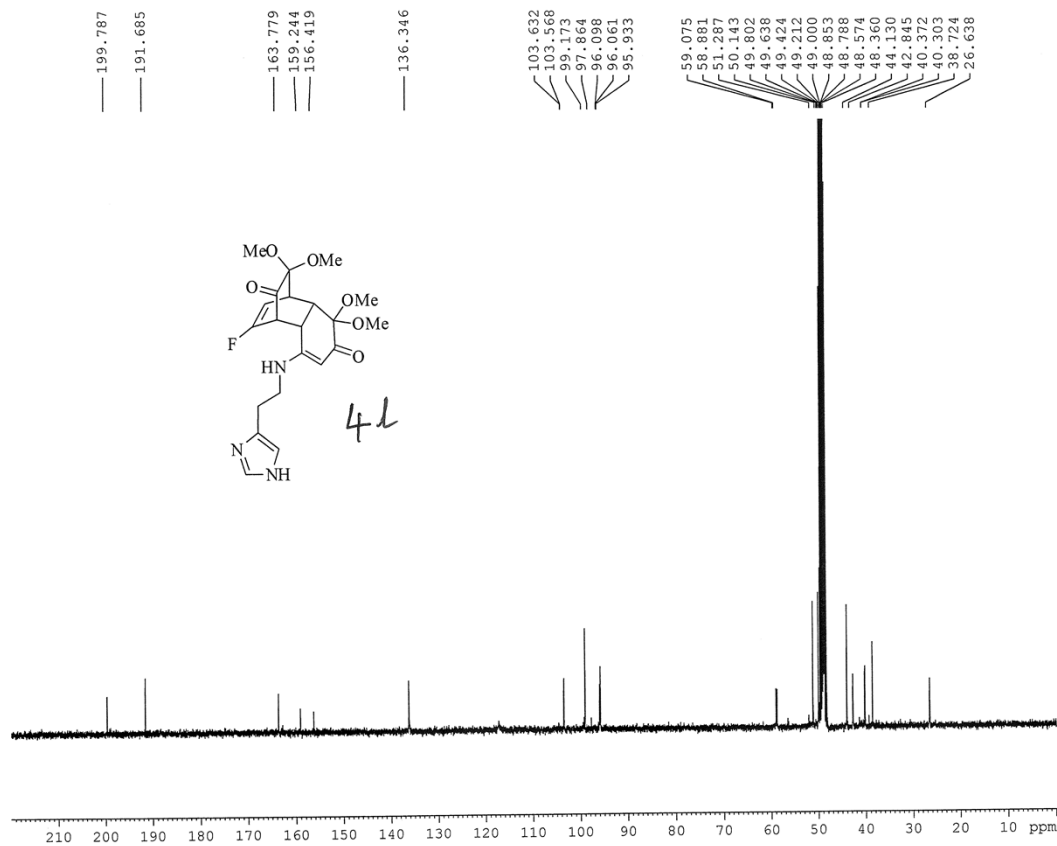
Source Type ESI	Ion Polarity Positive	Set Nebulizer 2.0 Bar
Focus Not active	Set Capillary 4500 V	Set Dry Heater 200 °C
Scan Begin 50 m/z	Set End Plate Offset -500 V	Set Dry Gas 6.0 l/min
Scan End 1800 m/z	Set Collision Cell Rf 200.0 Vpp	Set Divert Valve Waste

Meas m/z 442.1878	Formula C <sub>21</sub> H <sub>29</sub> F <sub>3</sub> N <sub>2</sub> O <sub>8</sub>	m/z err [ppm] -1.5
		rdB e <sup>-</sup> Conf N-Rule 7.5 even ok





AMRI; SRC AV400  
location; 18



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

Current Data Parameters  
NAME SG-RKP-5F-DIMER-Histamine  
EXFNO 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  
S1 32768  
SF 100.6377729 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

## Mass Spectrum SmartFormula Report

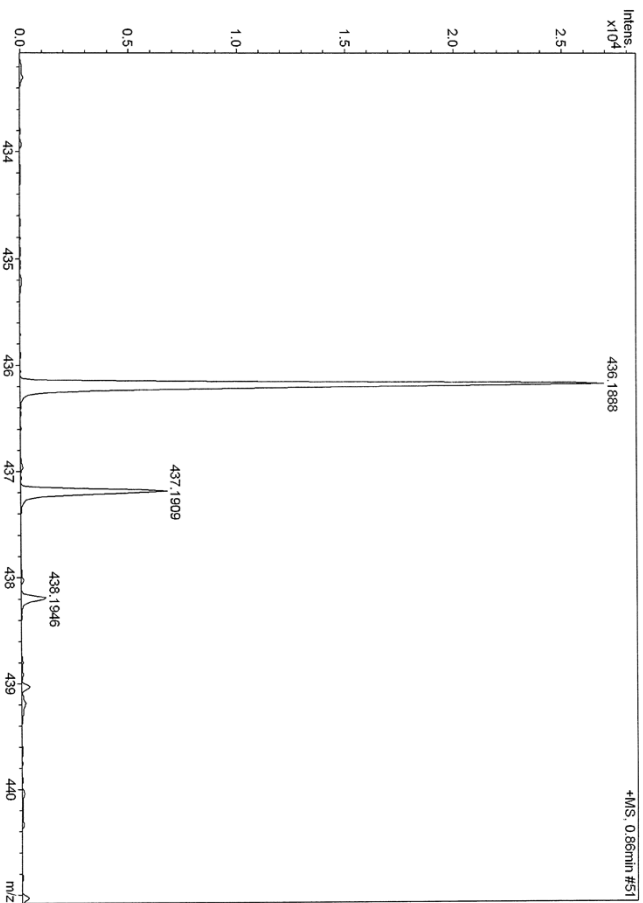
### Analysis Info

Analysis Name D:\Data\Chemistry\Outside\AMRI\20141103\SF-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 Santhosh Kumar Chittinalla	

### 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 5.0 l/min
Scan End 1800 m/z	Set Collision Cell RF 200.0 Vpp	Set Divert Valve Waste

Mass m/z 436.1888	Formula C <sub>21</sub> H <sub>27</sub> N <sub>3</sub> O <sub>6</sub>	m/z err [ppm] -2.2
		rdg 9.5
		e <sup>-</sup> Conf even
		N-Rule ok



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printed: 11/3/2014 11:49:46 AM

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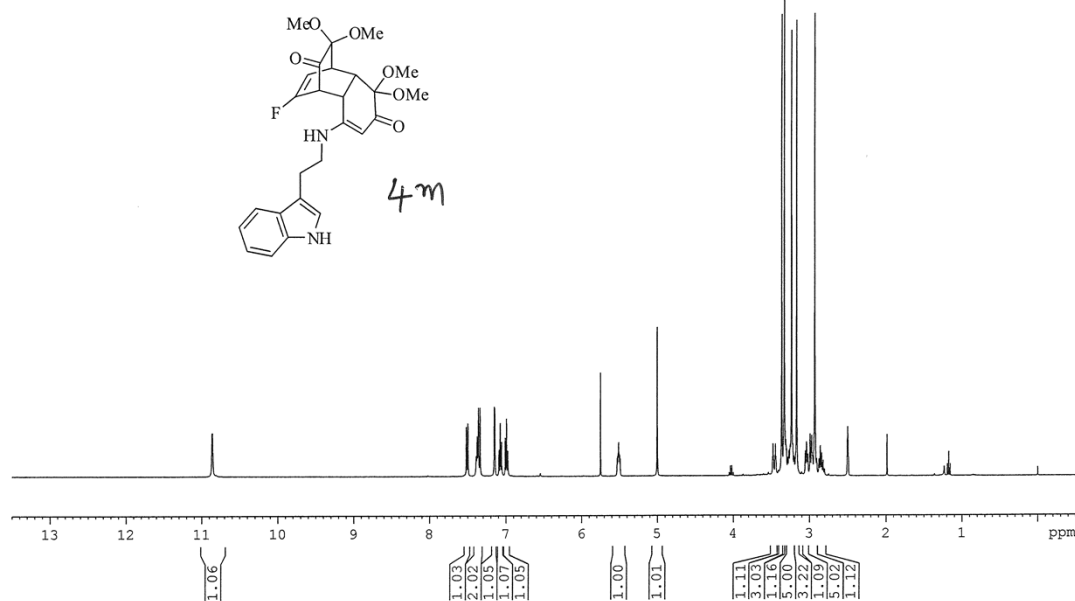
Current Data Parameters  
 NAME 5F-D-TRYPTAMINE  
 EXPNO 10  
 PROCNO 1

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  
 TDO 1

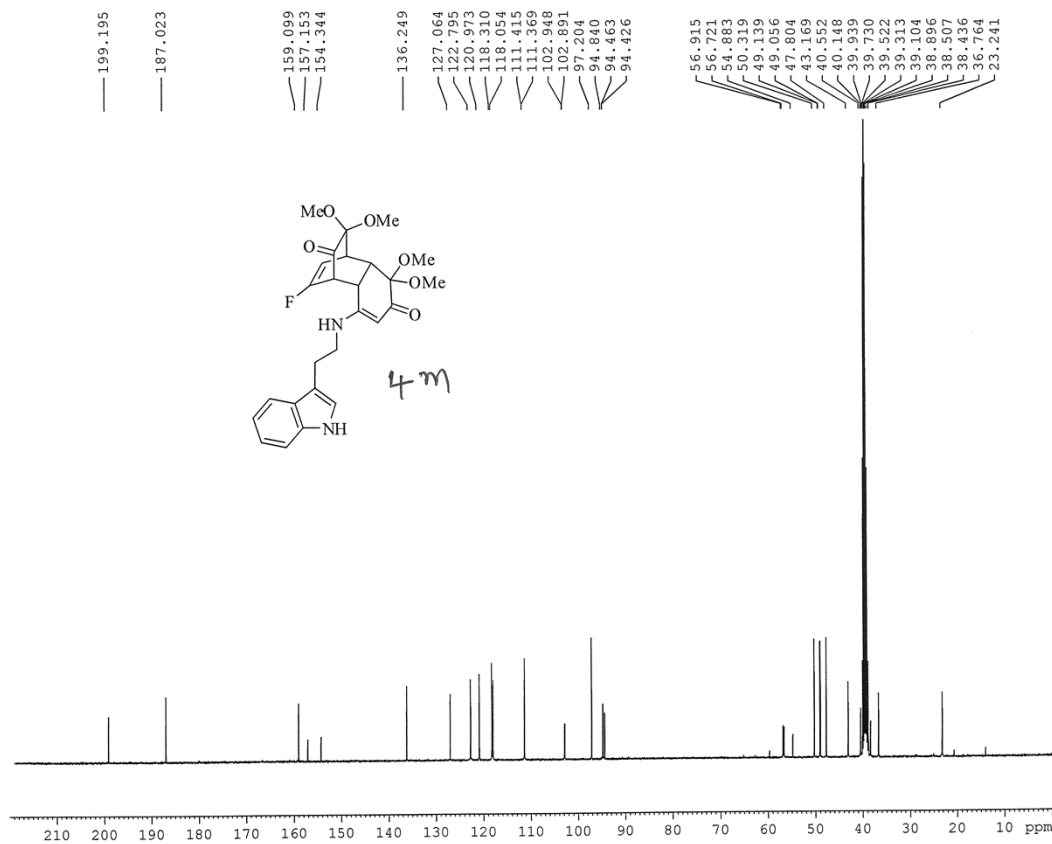
===== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.70 usec  
 PL1 -2.00 dB  
 PL1W 14.33185768 W  
 SFO1 400.2330885 MHz

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 SF-D-TRYPTAMINE  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date 20141221  
Time 0.32  
INSTRUM spect  
PROBHD 5 mm FAPBO 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

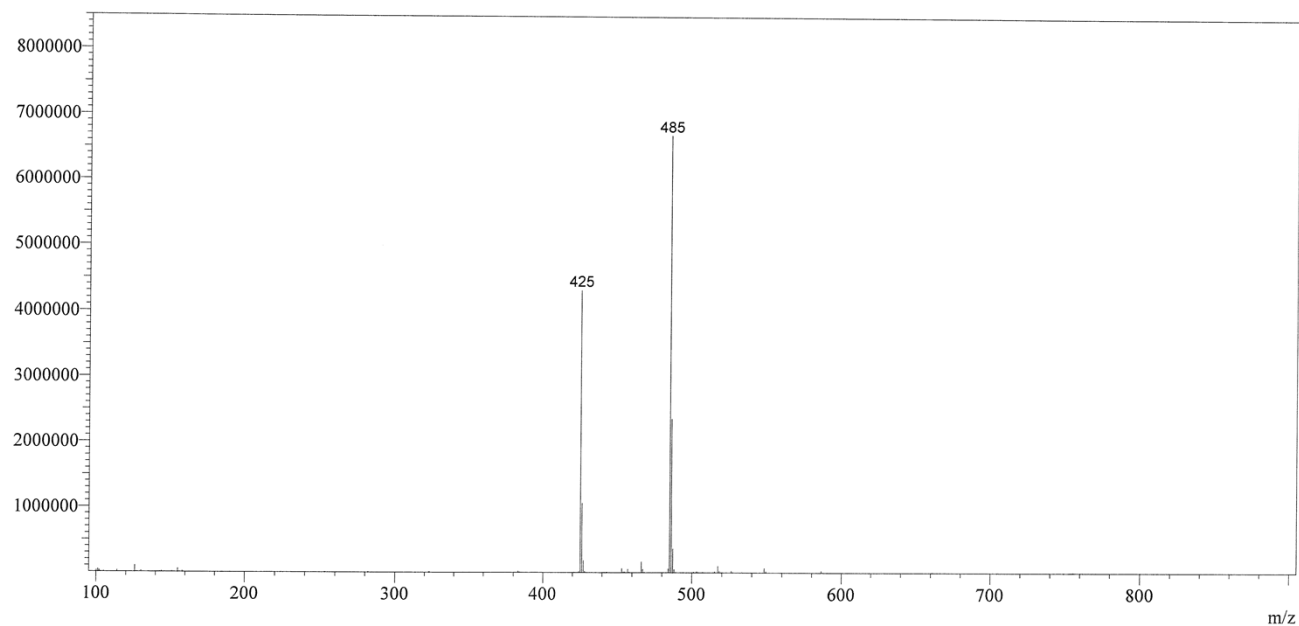
## AMRI Direct MS Analysis Report

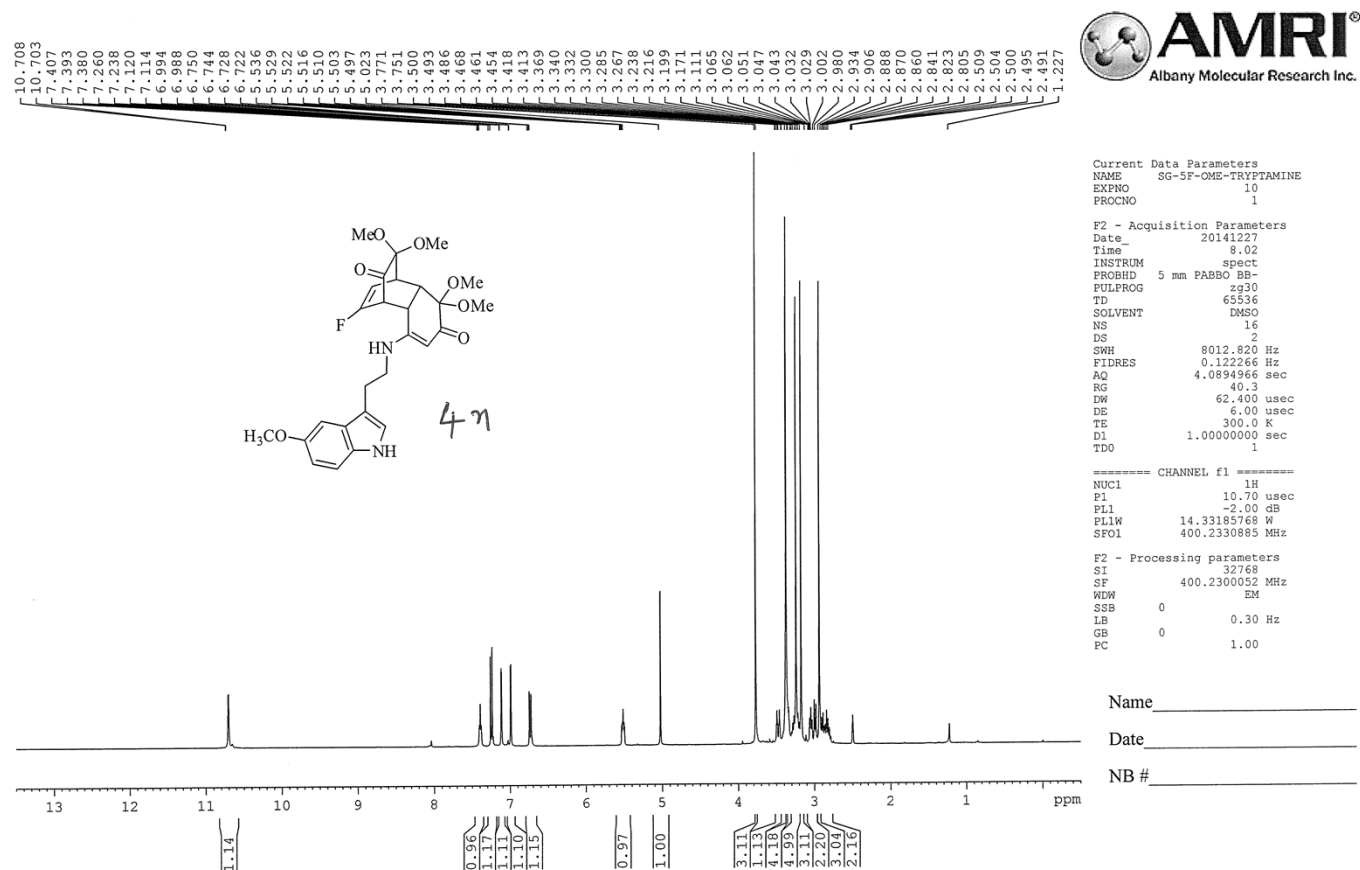
Acquired by : System Administrator  
Sample Name : SG-RKP-5F-TRYPTAMINE  
Data File : SG-RKP-5F-TRYPTAMINE.lcd  
Method File : ESI-LCMS Method3.lcm  
Month-Day Acquired : 2/4/2015



Mass Spectrum

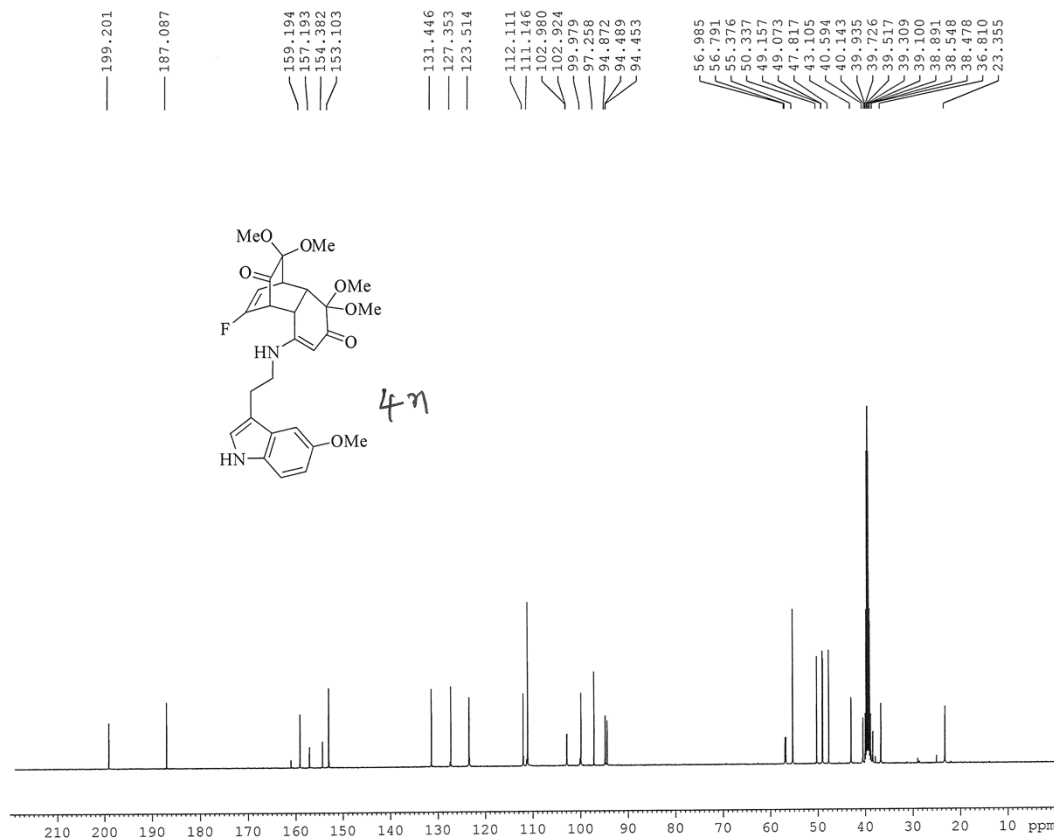
Peak # : 1, Retention Time : 2.867 min  
Base Peak m/z : 485, Base Peak Intensity : 66882376688237  
Polarity : Positive, Event : 1 - 1







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

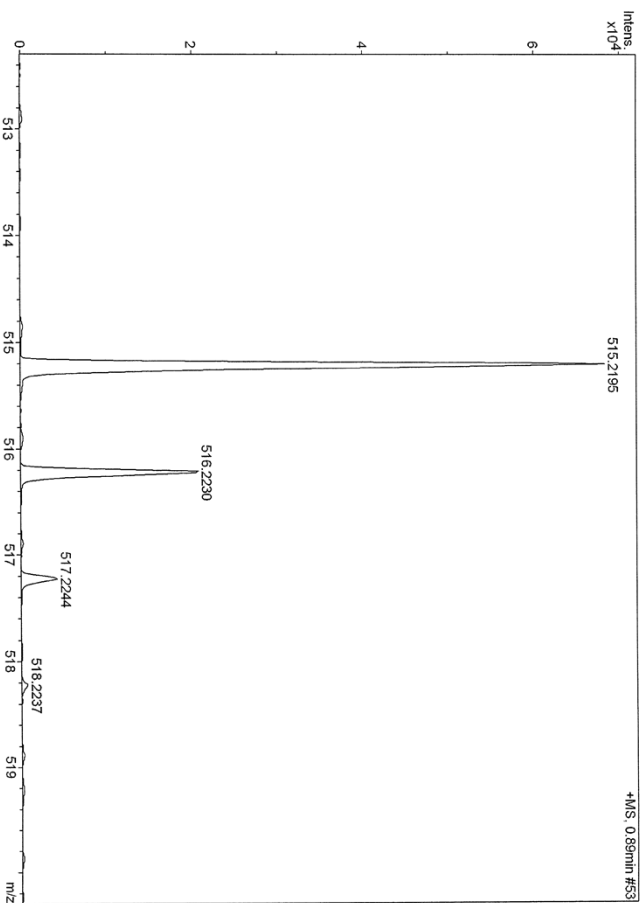
### Analysis Info

Analysis Name D:\Data\Chemistry\Outside\AMR120141218\SF-OMe-Tryp-1.d Acquisition Date 12/18/2014 4:44:46 PM  
 Method YCH\_Pos-150-1800.m  
 Sample Name SF-OMe-Tryp  
 Comment AMRI  
 Santhosh Kumar Chittinalla

### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 W
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1800 m/z	Set Collision Cell Rf	200.0 Vpp	Set Divert Valve	Waste

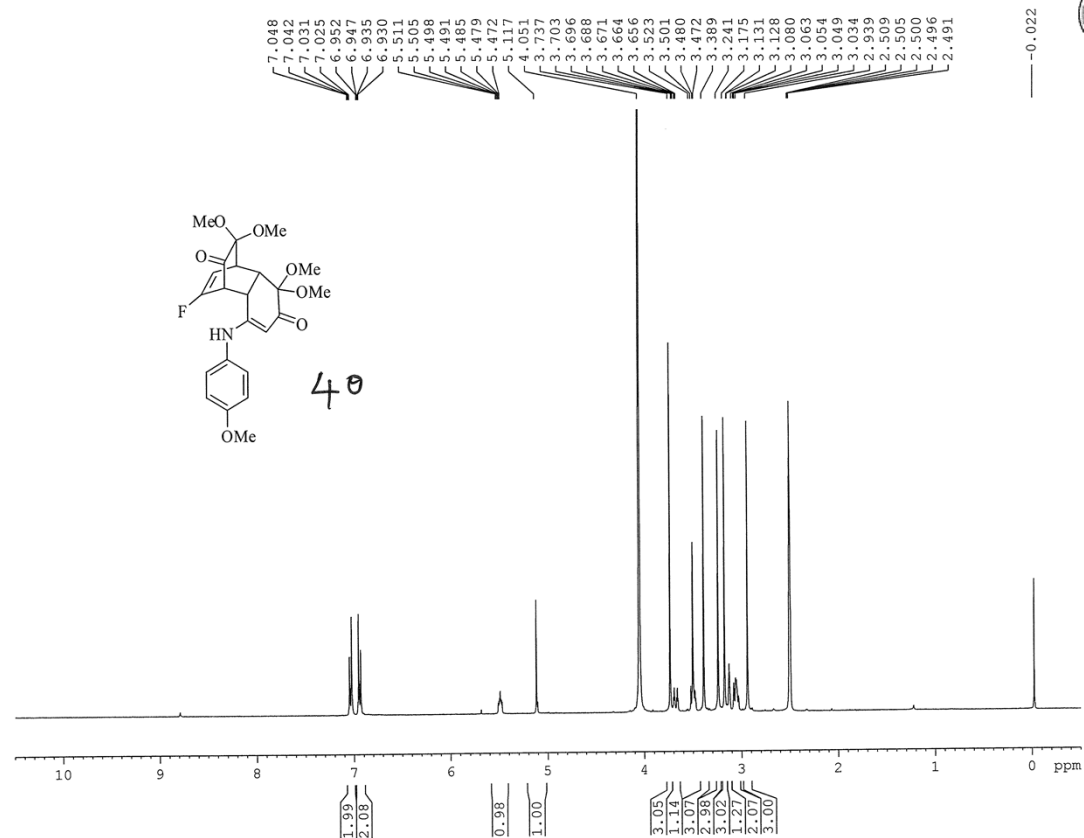
Meas. m/z # Formula m/z err [ppm] rdb e<sup>-</sup> Conf N-Rule  
 515.2195 1 C<sub>27</sub>H<sub>32</sub>F<sub>2</sub>N<sub>2</sub>O<sub>7</sub> 515.2188 -1.4 12.5 even ok



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printed: 12/18/2014 4:47:46 PM

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Current Data Parameters  
NAME SG-SIR-E-SF-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

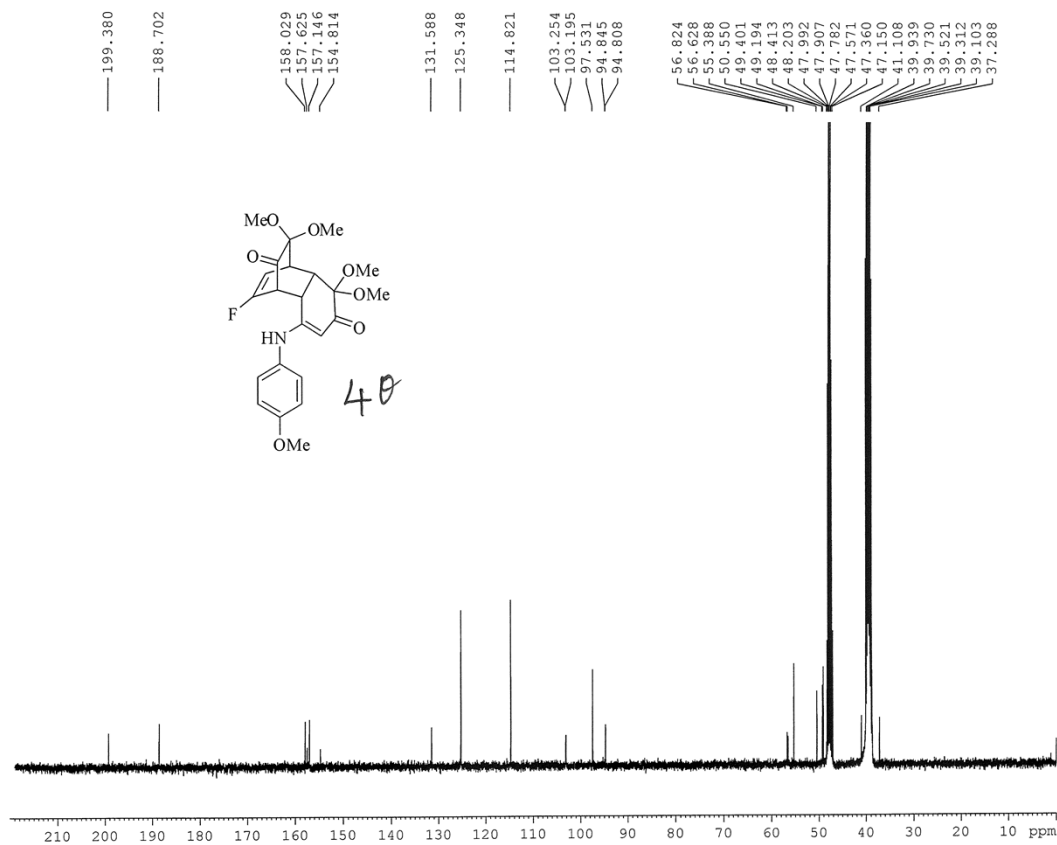
F2 - Processing parameters  
SI 32768  
SF 400.1300031 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

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  
S1 32768  
SF 100.6127805 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

## Mass Spectrum SmartFormula Report

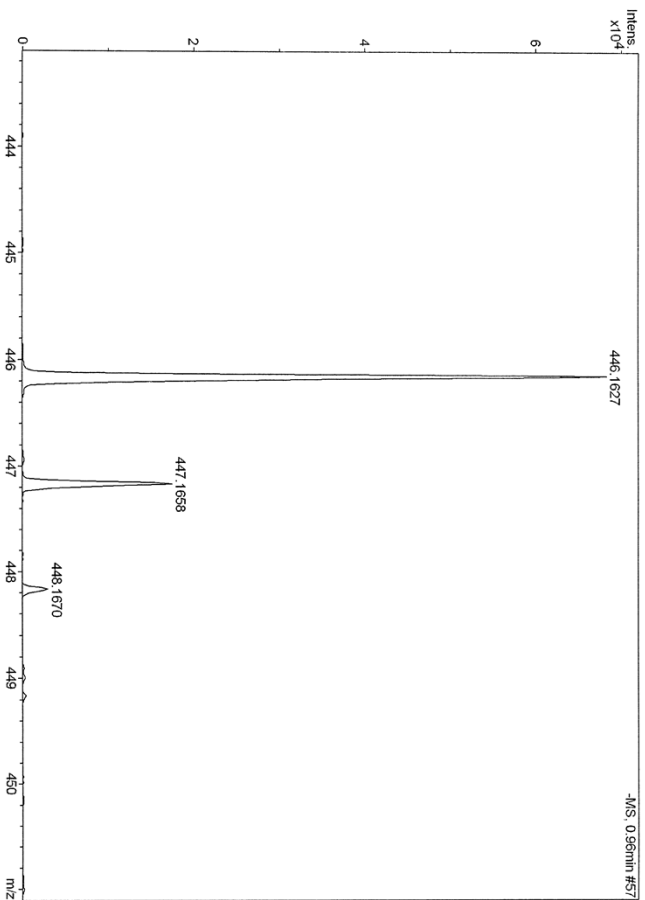
### Analysis Info

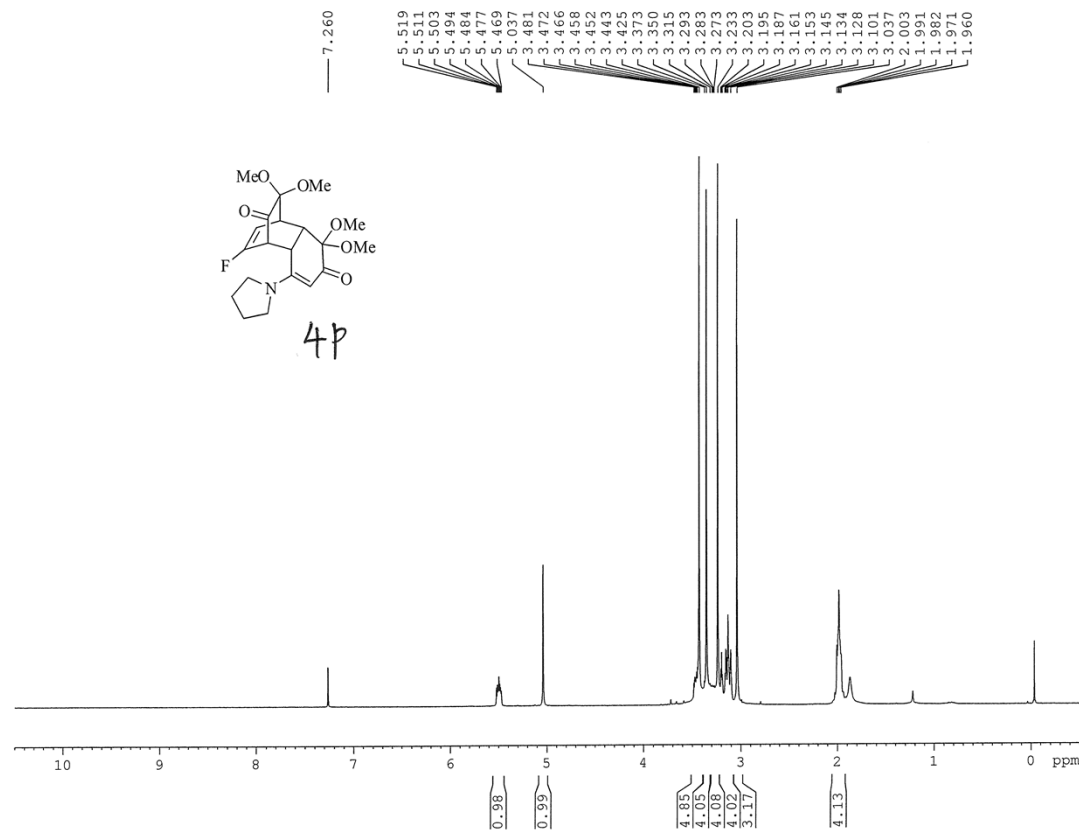
Analysis Name	D:\Data\Chemistry\Outside\AMRI\20141103\5F-Anisidine-1n.d	Acquisition Date	11/3/2014 11:04:33 AM
Method	YCH_Pos-150-1800.m	Operator	default user
Sample Name	5F-Anisidine	Instrument / Ser#	micrOTOF-Q II 10269
Comment	AMRI Santhosh Kumar Chittinalla		

### 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

Mass m/z	#	Formula	m/z	err [ppm]	rdp	e <sup>-</sup> Conf	N-Rule
446.1627	1	C <sub>23</sub> H <sub>25</sub> FNO <sub>7</sub>	446.1621	-1.5	11.5	even	OK





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 CDCl<sub>3</sub>  
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



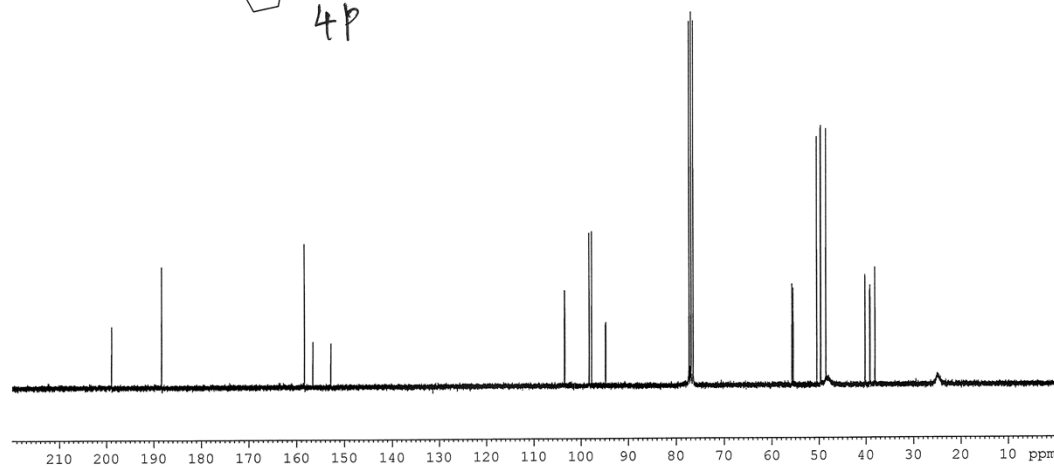
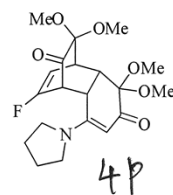
198.975  
198.959  
188.423

158.479  
156.710  
152.932

103.634  
103.552  
98.377  
97.824  
94.925  
94.875

77.424  
77.001  
76.577

55.860  
55.598  
50.612  
49.821  
49.736  
48.648  
48.132  
40.350  
40.325  
39.336  
39.244  
38.236  
38.215  
25.131



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 1.445188 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

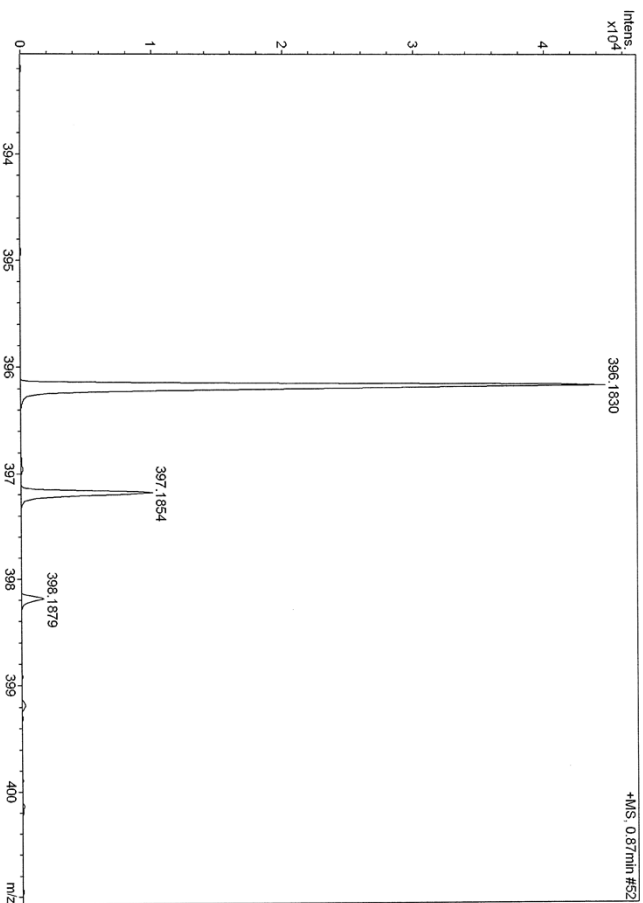
### Analysis Info

Analysis Name D:\Data\Chemistry\Outside\AMRI\20141103\SF-Pyrroldine-1.d Acquisition Date 11/3/2014 12:18:47 PM  
 Method YCH\_Pos-150-1800.m Operator default user  
 Sample Name SF-Pyrroldine Instrument/Ser# microTOF-Q II 10269  
 Comment AMRI  
 Santhosh Kumar Chittinalla

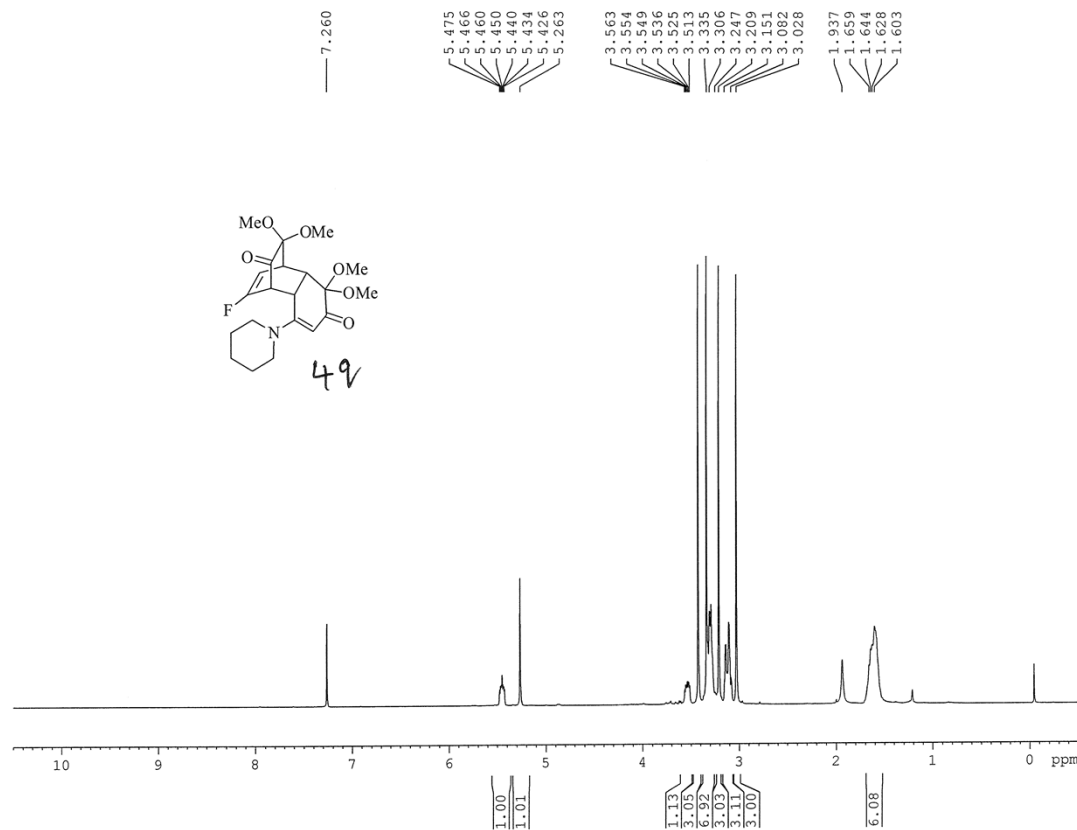
### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 W
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<sup>-</sup> Conf N-Rule  
 396.1830 1 C<sub>20</sub>H<sub>27</sub>N<sub>3</sub>O<sub>6</sub> 396.1817 -3.2 7.5 even ok







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

F2 - Acquisition Parameters  
 Date\_ 20141122  
 Time\_ 18.17  
 INSTRUM spect  
 FROBHD 5 mm QNP 1H/13  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl<sub>3</sub>  
 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



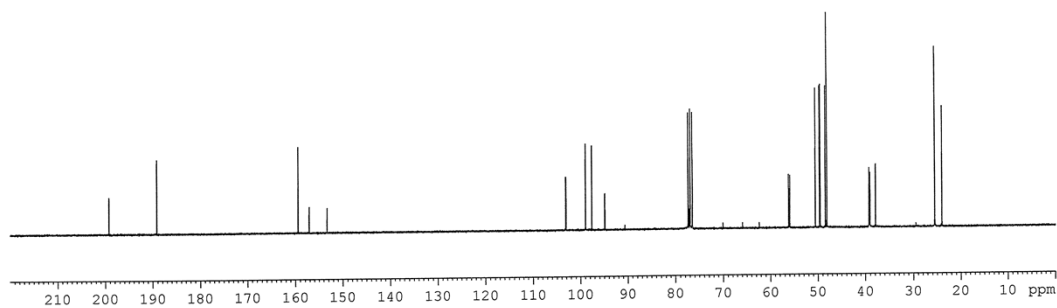
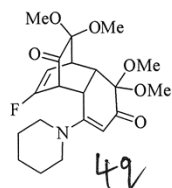
199.278  
199.261  
189.192

159.446  
157.153  
153.375

103.221  
103.137  
99.015  
97.705  
94.990  
94.940

77.425  
77.001  
76.576

56.255  
55.991  
50.632  
49.740  
49.596  
48.509  
48.199  
39.328  
39.304  
39.202  
39.110  
37.979  
37.959  
25.581  
24.060



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

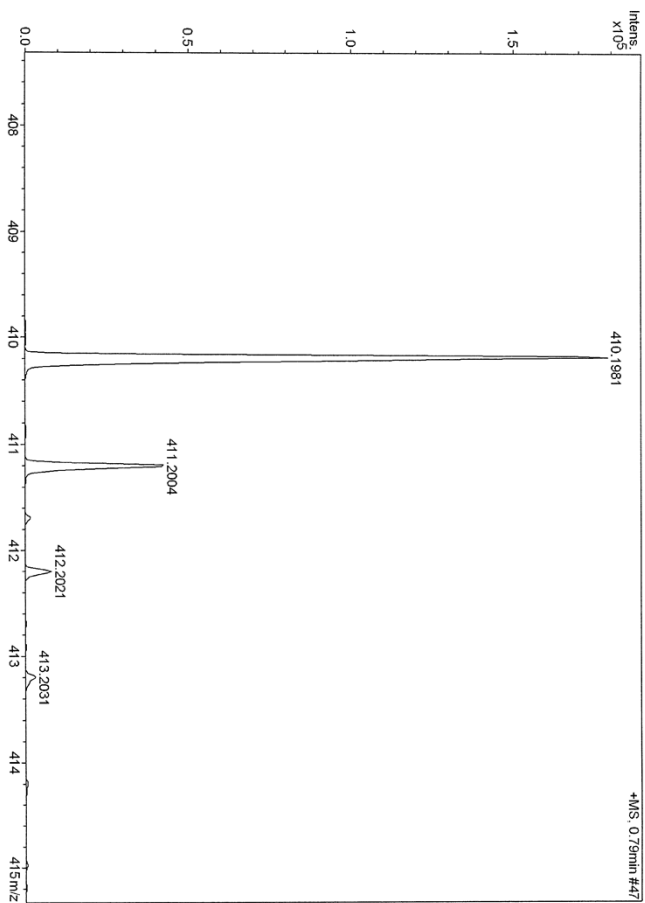
Analysis Name D:\Data\Chemistry\Outside\AMRI\20141218\SF-Piperidine-1.d Acquisition Date 12/18/2014 5:04:57 PM  
 Method YCH\_Pos-150-1800.m  
 Sample Name SF-Piperidine Operator default user  
 Comment AMRI Instrument / Ser# microTOF-Q II 10269  
 Santhosh Kumar Chittinalla

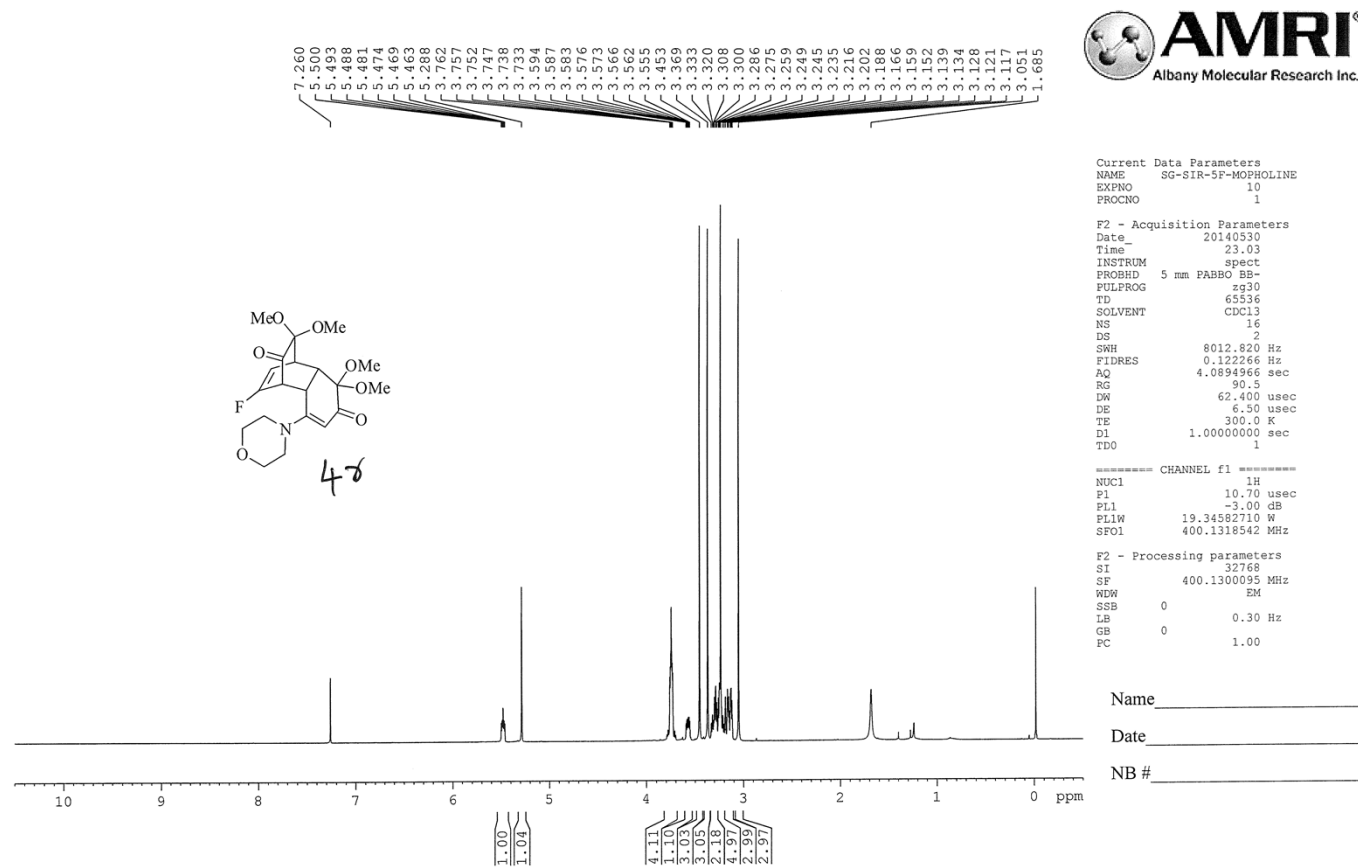
### Acquisition Parameter

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

Mass m/z	#	Formula	m/z	err [ppm]	rd	e <sup>-</sup> Conf	N-Rule
410.1981	1	C <sub>21</sub> H <sub>29</sub> FNO <sub>6</sub>	410.1973	-1.9	7.5	even	OK

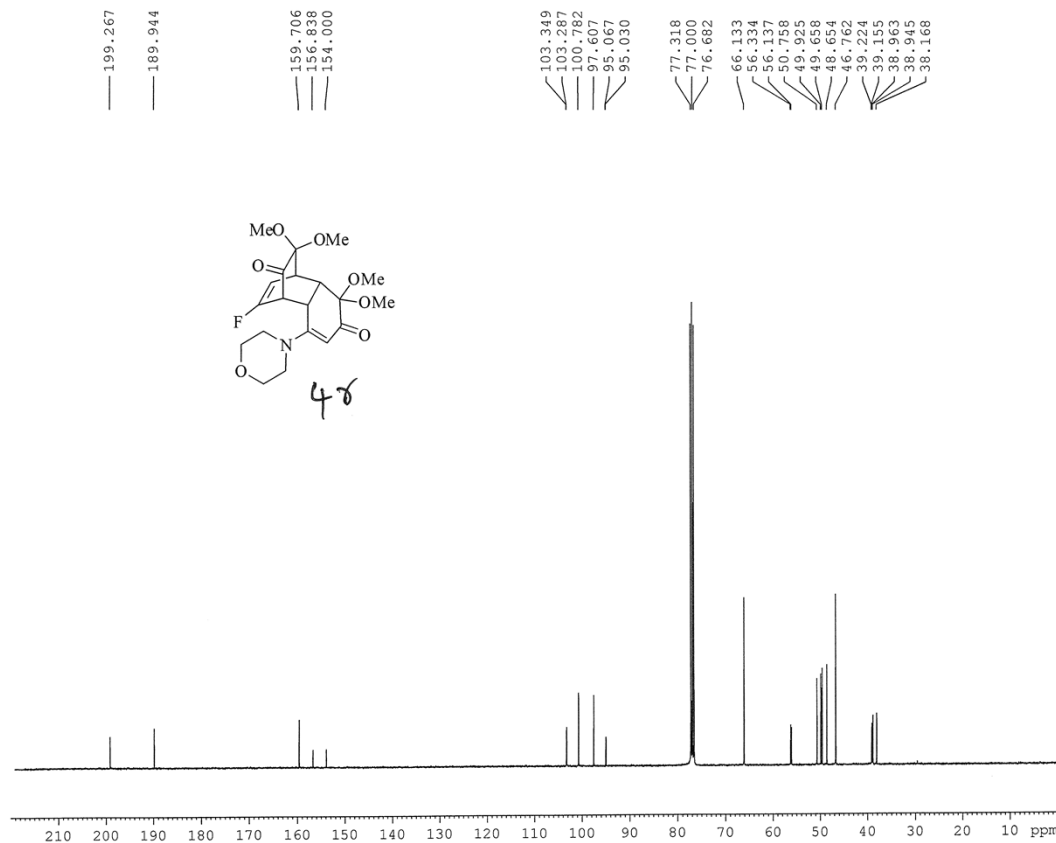




# AMRI SRC location; 17



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

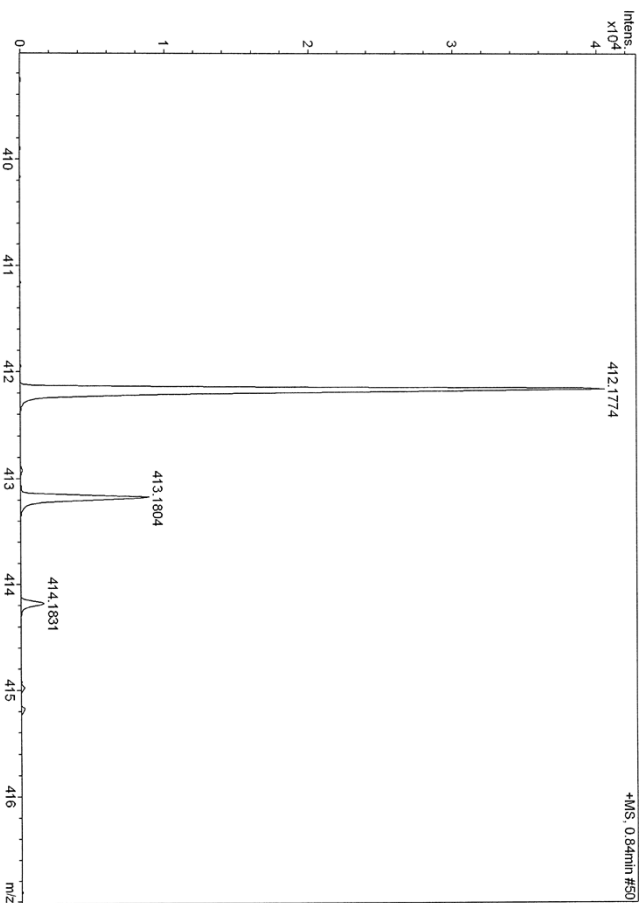
### Analysis Info

Analysis Name D:\Data\Chemistry\Outside\AMRI\20141103\SF-Morpholine-1.d Acquisition Date 11/3/2014 12:06:04 PM  
 Method YCH\_Pos-150-1800.m  
 Sample Name SF-Morpholine Operator default user  
 Comment AMRI Instrument / Ser# microTOF-Q II 10269  
 Santhosh Kumar Chittinalla

### 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 Diver Valve	Waste

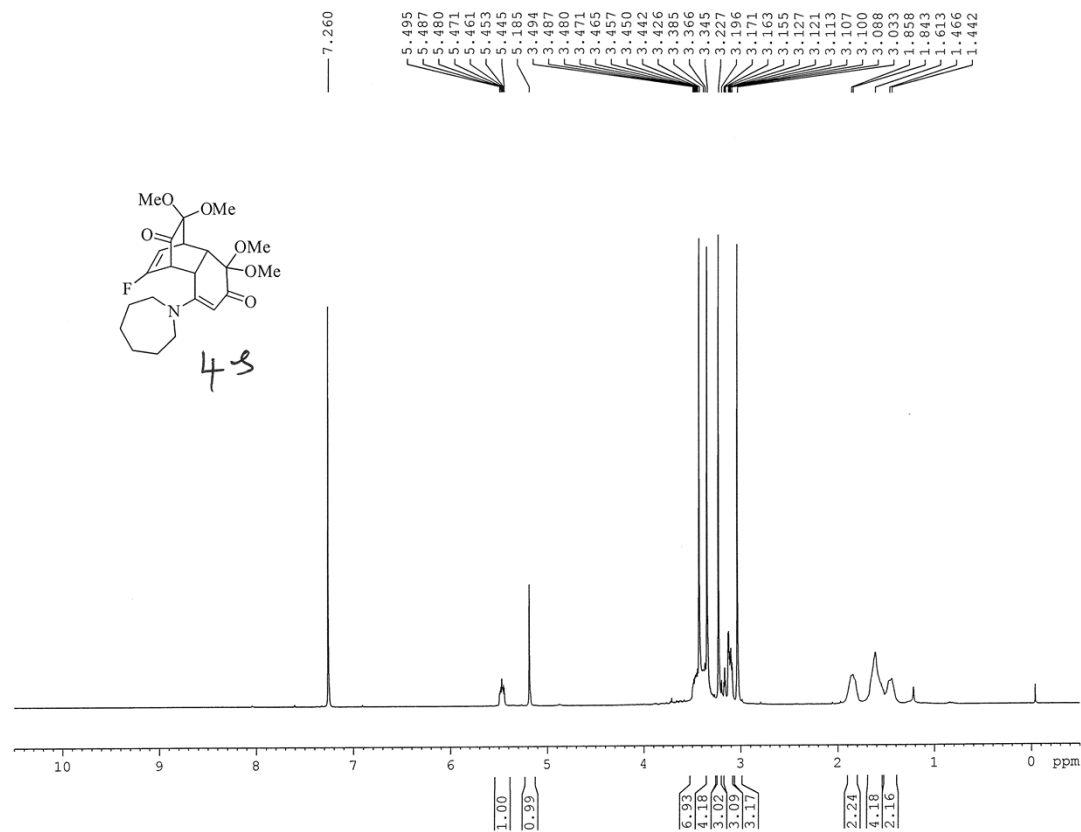
Meas. m/z # Formula m/z err [ppm] rdb e<sup>-</sup> Conf N-Rule  
 412.1774 1 C<sub>20</sub>H<sub>27</sub>FNO<sub>7</sub> 412.1766 -2.0 7.5 even ok



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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  
MCNRRK 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  
GB 0  
PC 1.00

Name \_\_\_\_\_

Date \_\_\_\_\_

NB # \_\_\_\_\_

AMRI; SRC  
location; 15



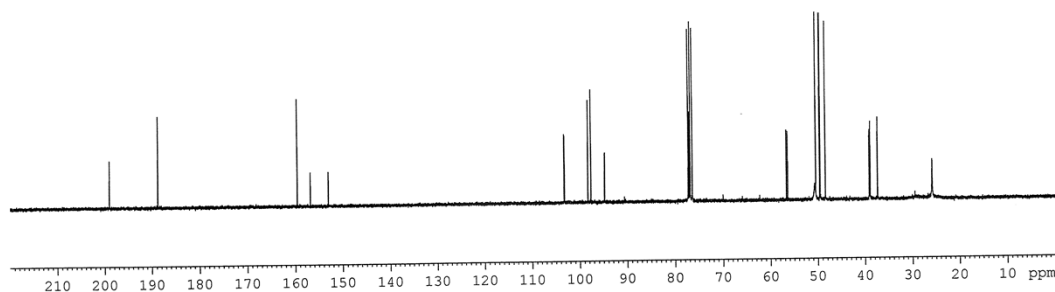
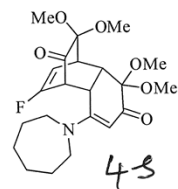
199.078  
199.062  
188.798

159.716  
156.933  
153.157

103.416  
103.332  
98.391  
97.773  
94.918  
94.868

77.424  
77.000  
76.576

56.765  
56.501  
50.770  
50.565  
49.739  
49.621  
48.541  
39.240  
39.147  
39.039  
39.015  
37.493  
37.473  
25.969



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 zgpg30  
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\AMR120141218SF-Azep-2.d  
 Method YCH\_Pos-150-1800.m  
 Sample Name 5F-Azep  
 Comment AMRI  
 Santhosh Kumar Chittinalla

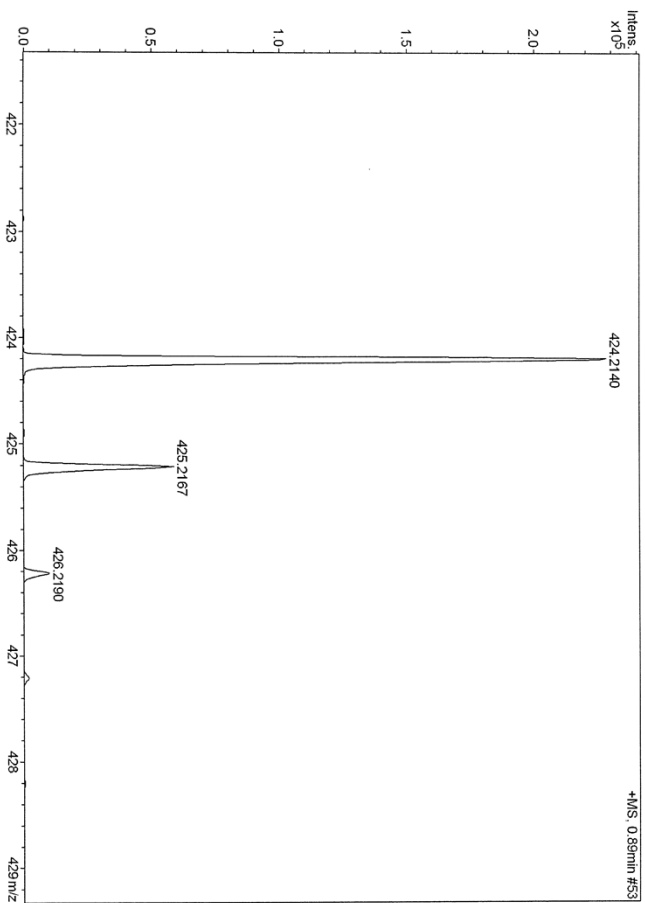
Acquisition Date 12/18/2014 4:38:03 PM

Operator default user  
 Instrument/ Ser# microTOF-Q II 10269

### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 W
Scan Begin	50 m/z	Set End Plate Offset	-500.0 Vpp	Set Dry Gas	6.0 l/min
Scan End	1800 m/z	Set Collision Cell RF	200.0 Vpp	Set Diverter Valve	Waste

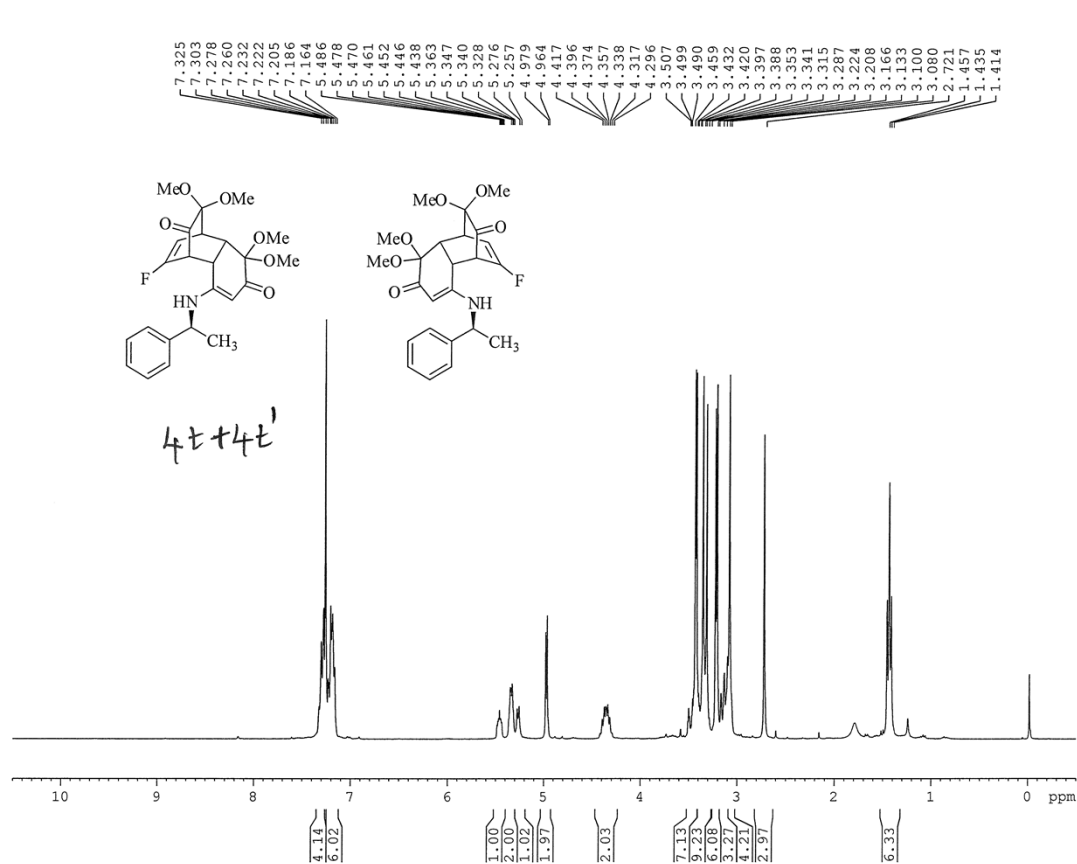
Meas. m/z	#	Formula	m/z	err [ppm]	rdB	e <sup>-</sup> Conf	N-Rule
424.2140	1	C <sub>22</sub> H <sub>31</sub> F <sub>3</sub> N <sub>3</sub> O <sub>6</sub>	424.2130	-2.3	7.5	even	ok



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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  
 MCWRR 0.01500000 sec

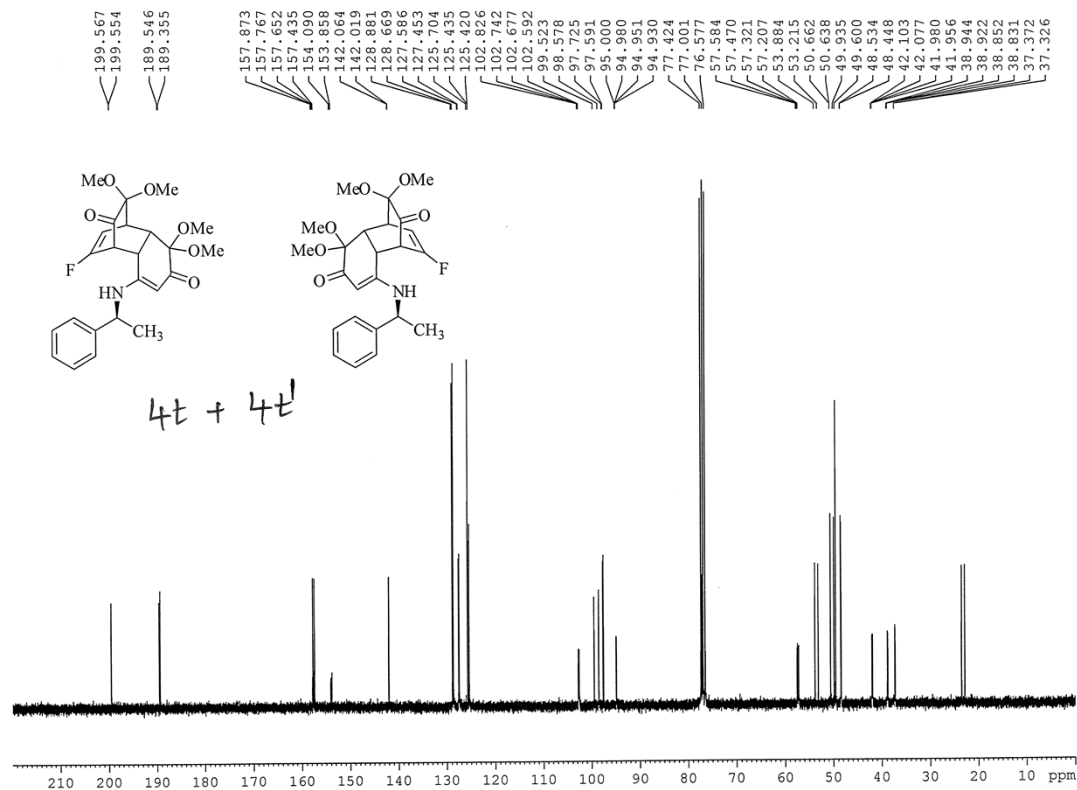
CHANNEL f1  
 NUC1 1H  
 P1 12.20 usec  
 PL1 0 dB  
 SFO1 300.1319508 MHz

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 # \_\_\_\_\_



Current Data Parameters  
NAME SS-BCK-SPH-St-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  
P2 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

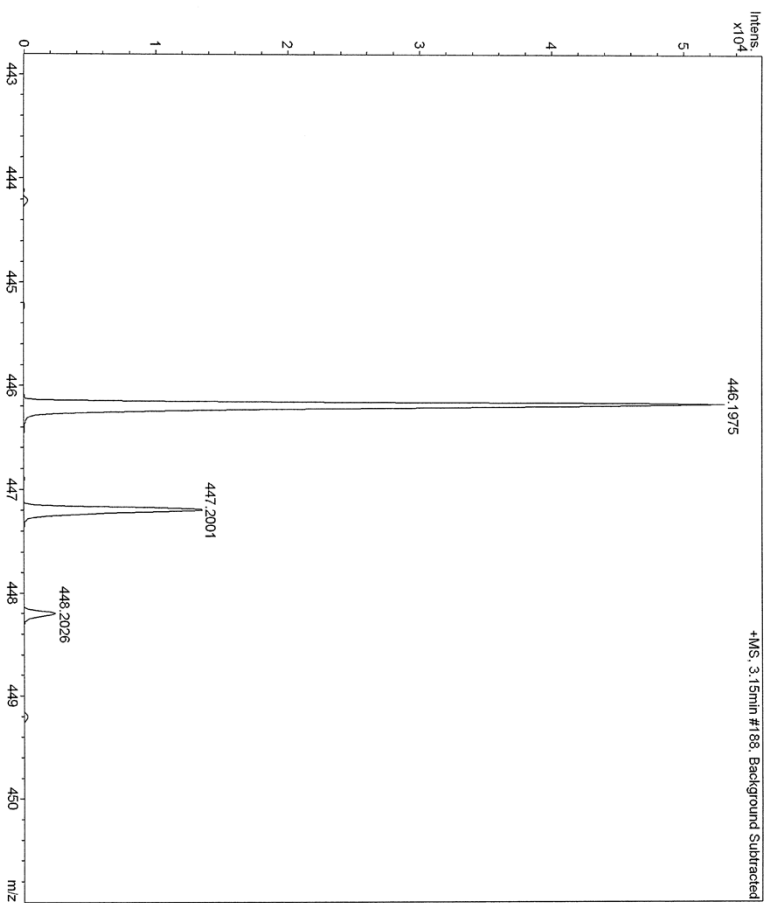
### Analysis Info

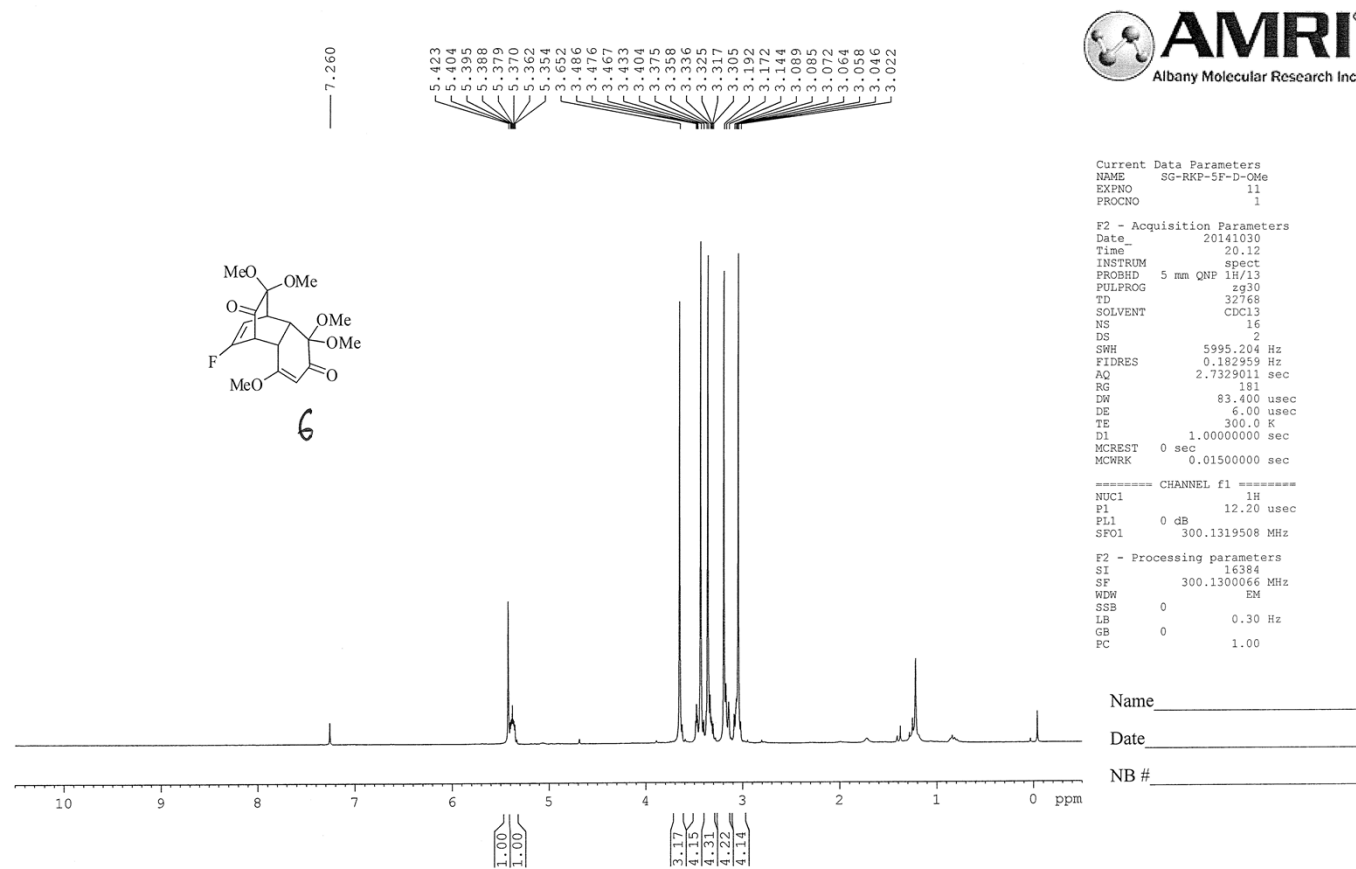
Analysis Name D:\Data\Chemistry\Outside\AMR120150107\6F-Ph-Et-NH2.d Acquisition Date 1/7/2015 3:08:50 PM  
 Method YCH\_Pos-150-1800 m Operator default user  
 Sample Name 6F-Ph-Et-NH2 Instrument / Ser# microTOF-Q II 10269  
 Comment AMRI

### 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 <sup>-</sup> Conf	N-Rule
446.1975	1	C <sub>24</sub> H <sub>29</sub> FNO <sub>6</sub>	446.1973	-0.3	10.5	even	ok





AMRI; SRC  
location; 15



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

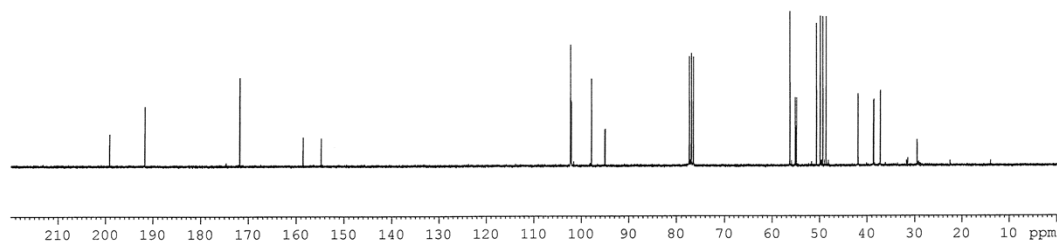
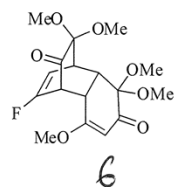
199.173  
199.155  
191.723

171.805  
158.642  
154.843

102.352  
102.247  
102.162  
97.945  
95.116  
95.065

77.424  
77.000  
76.576

56.359  
55.229  
54.962  
50.753  
49.975  
49.440  
48.743  
41.975  
41.948  
38.762  
38.671  
37.325  
37.303  
29.590



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 CDC13  
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  
FC 1.40

## Mass Spectrum SmartFormula Report

### Analysis Info

Analysis Name D:\Data\Chemistry\Outside\AMRI\20141218\SF-OMe-1.d  
 Method YCH\_Pos-150-1800.m  
 Sample Name SF-OMe  
 Comment AMRI  
 Santhosh Kumar Chittinalla

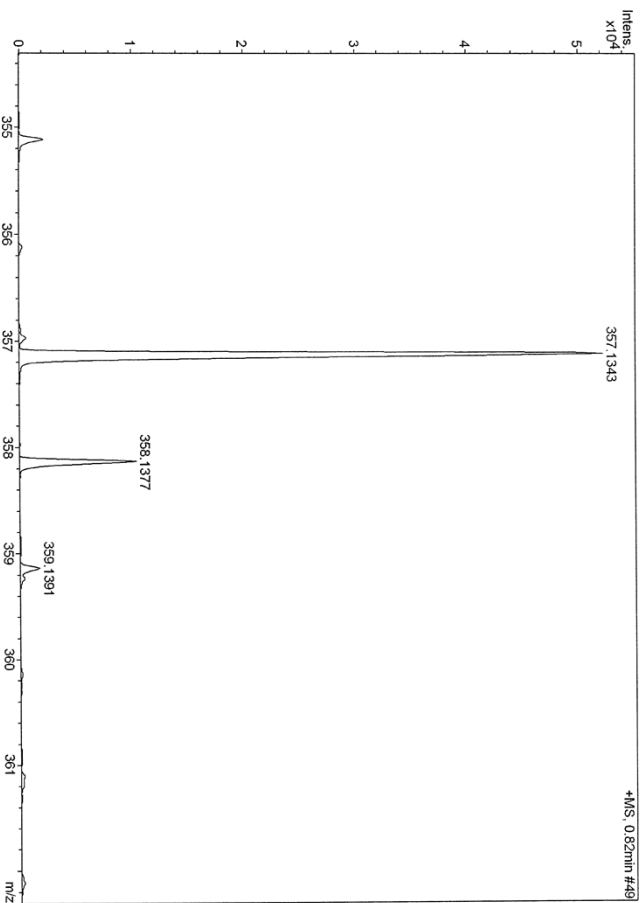
Acquisition Date 12/18/2014 4:51:27 PM

Operator default user  
 Instrument/ Ser# microTOF-Q II 10269

### 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

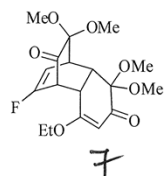
Meas m/z # Formula m/z err [ppm] rdb e<sup>-</sup> Conf N-Rule  
 357.1343 1 C<sub>17</sub>H<sub>22</sub>O<sub>7</sub> 357.1344 0.3 6.5 even ok



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AMRI; SRC  
location; 15



199.343  
199.326  
191.816

170.946

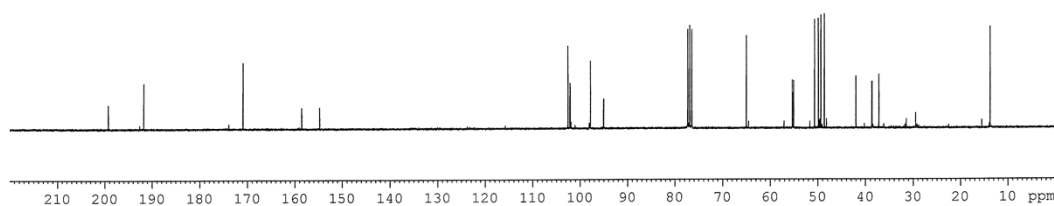
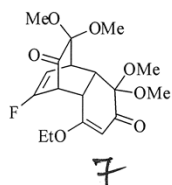
158.668  
154.869

102.660  
102.268  
102.183  
97.899  
95.156  
95.106

77.424  
77.000  
76.576

65.090  
55.454  
55.187  
50.769  
49.986  
49.463  
48.737  
42.116  
42.089  
38.792  
38.701  
37.293  
37.270

13.835



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

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  
MCWRR 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  
FC 1.40

## Mass Spectrum SmartFormula Report

### Analysis Info

Analysis Name D:\Data\Chemistry\Outsides\AMR120141218\SF-OEt-1.d  
 Method YCH\_Pos-150-1800.m  
 Sample Name SF-OEt  
 Comment AMRI  
 Santhosh Kumar Chittinalla

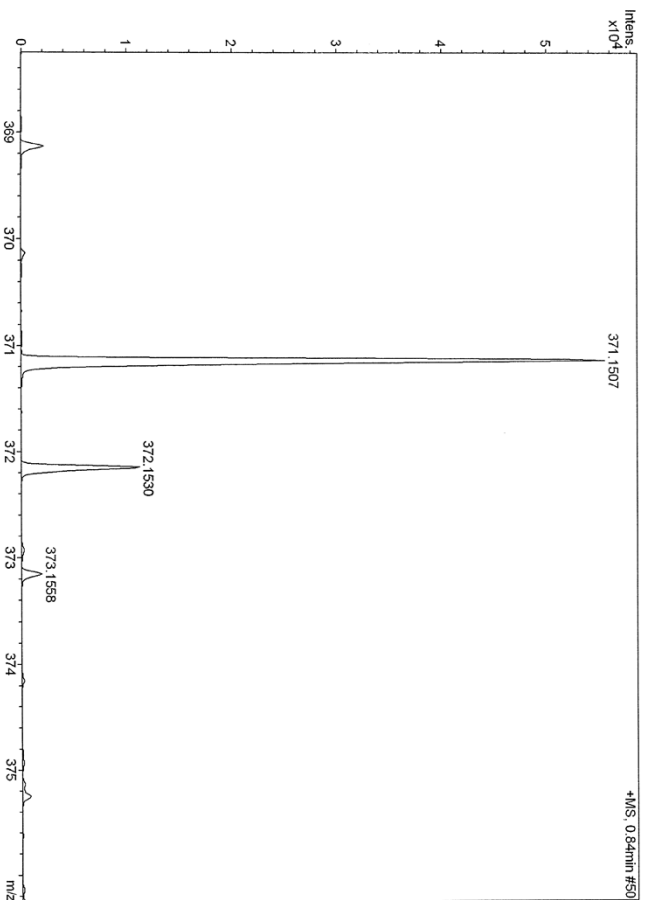
Acquisition Date 12/18/2014 4:58:38 PM

Operator default user  
 Instrument / Ser# micrOTOF-Q II 10269

### 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

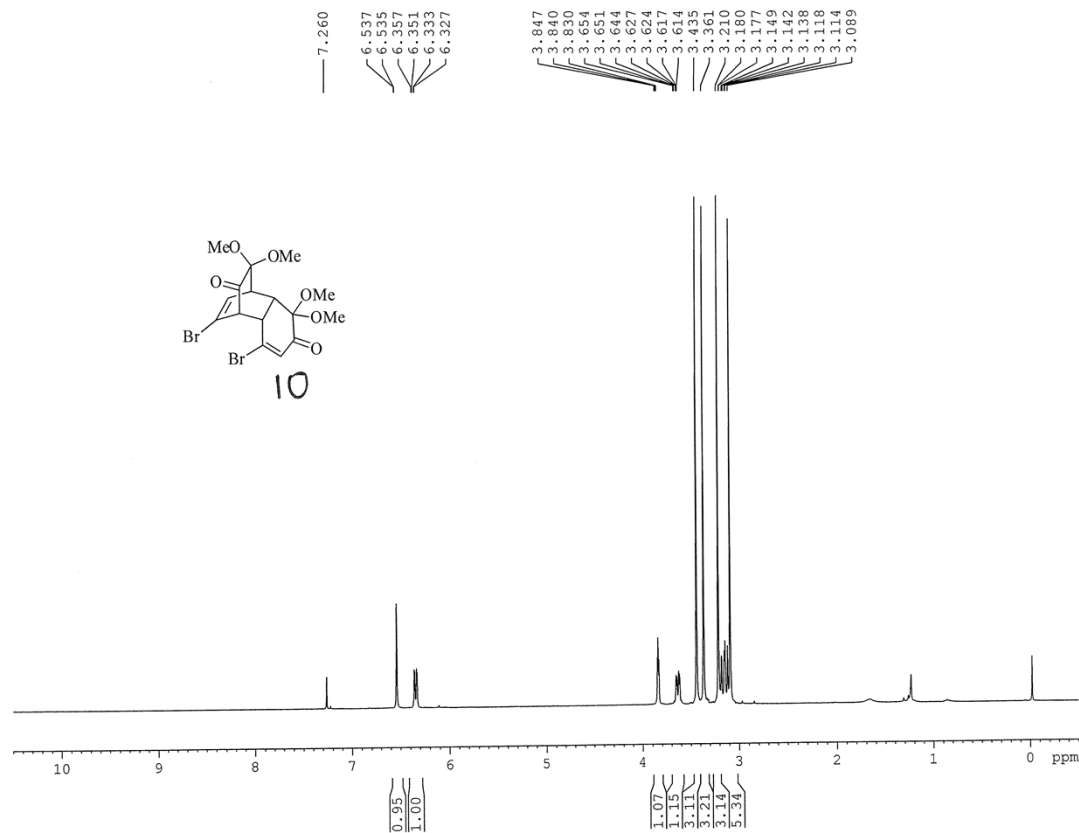
Meas. m/z	#	Formula	m/z	err [ppm]	rd	e <sup>-</sup>	Conf	N-Rule
371.1507	1	C <sub>18</sub> H <sub>24</sub> F <sub>2</sub> O <sub>7</sub>	371.1501	-1.7	6.5	even		ok



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Current Data Parameters  
 NAME SG-RKF-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 CDCl<sub>3</sub>  
 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  
 DL 1.00000000 sec  
 MCREST 0 sec  
 MCWRR 0.01500000 sec

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 12.20 usec  
 PL1 0 dB  
 SF01 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

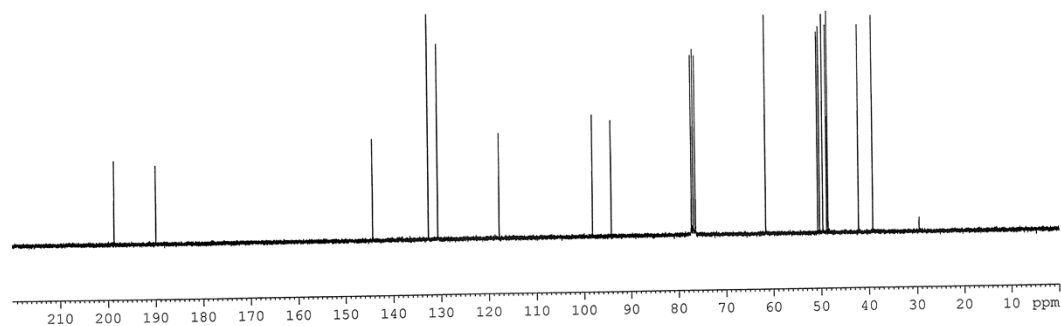
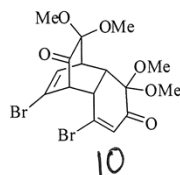
Name \_\_\_\_\_  
 Date \_\_\_\_\_  
 NB # \_\_\_\_\_

AMRI; SRC  
location; 15



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

198.778  
190.013  
144.395  
132.706  
130.768  
117.903  
98.256  
94.315  
77.423  
76.999  
76.575  
61.697  
50.782  
50.409  
49.736  
48.956  
48.642  
42.245  
39.295



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\SB-Dimer-2n.d  
 Method YCH\_Pos-150-1800.m  
 Sample Name SB-Dimer  
 Comment AMRI  
 Santosh Kumar Chittinalla

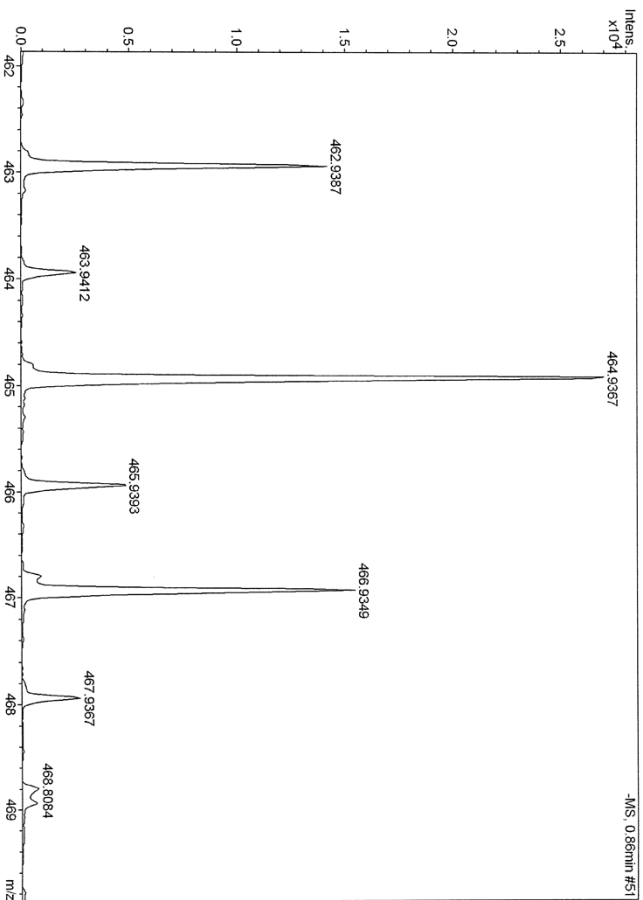
Acquisition Date 12/18/2014 2:52:36 PM

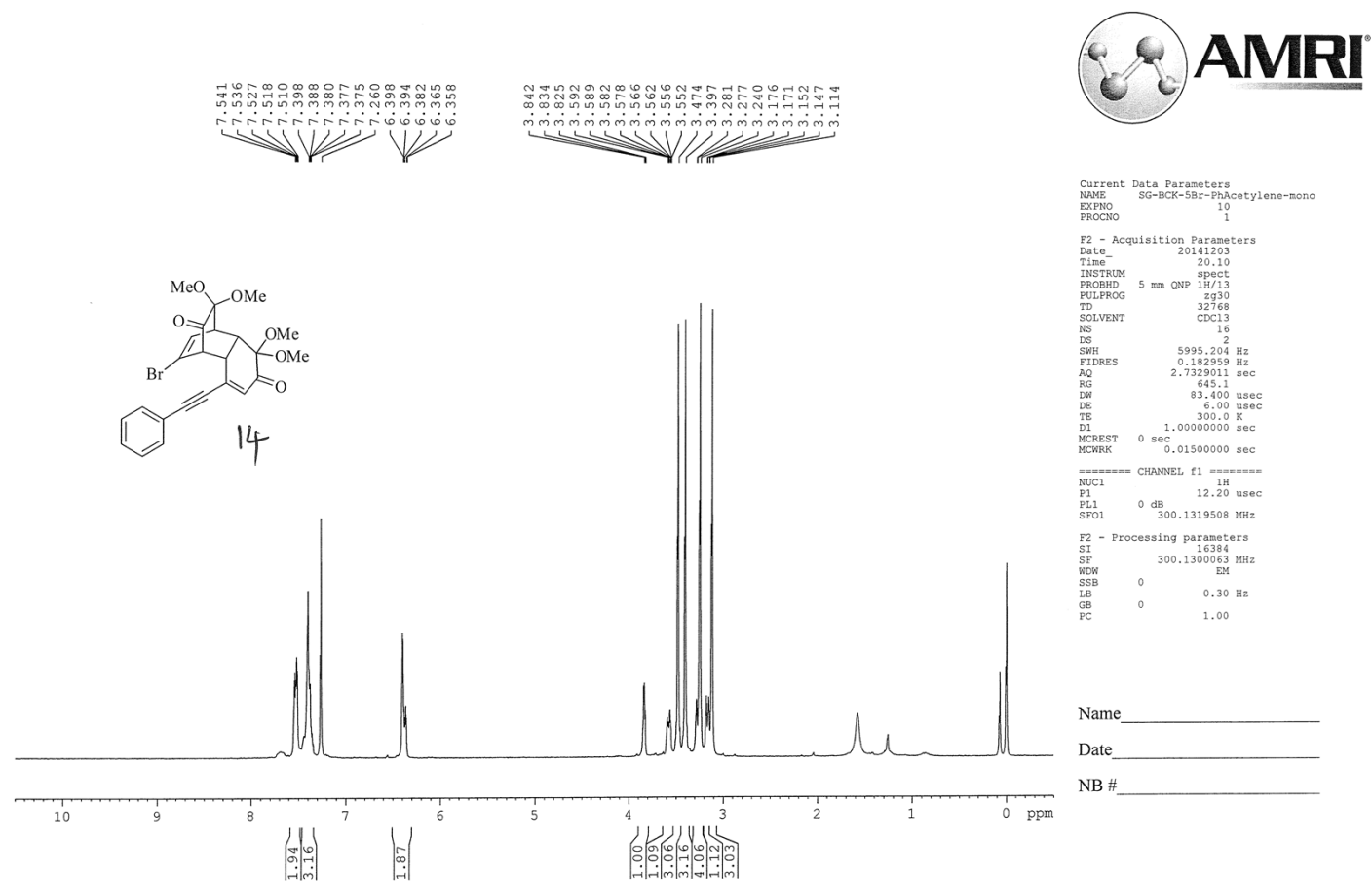
Operator default user  
 Instrument/ Ser# microTOF-Q II 10269

### Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	2.0 Bar
Focus	Not active	Set Collisity	3500 V	Set Dry Heater	200 °C
Scan Begin	500 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

Mass m/z	#	Formula	m/z	err [ppm]	rdB	e <sup>-</sup> Conf	N-Rule
462.9387	1	C <sub>16</sub> H <sub>17</sub> Br <sub>2</sub> O <sub>6</sub>	462.9397	2.2	7.5	even	ok





AMRI; SRC  
location; 15



Name \_\_\_\_\_

Date \_\_\_\_\_

NB # \_\_\_\_\_

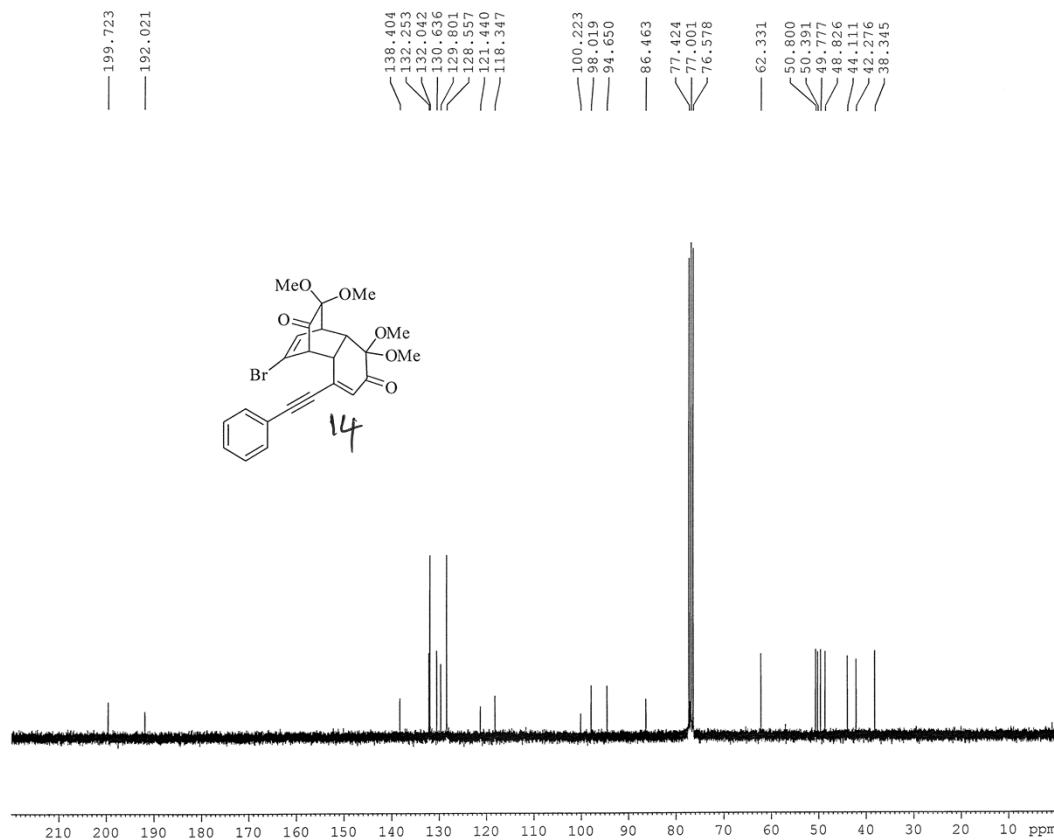
Current Data Parameters  
NAME SG-BCK-5Br-PhAcetylene-mono  
EXPNO 11  
PROCNO 1

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

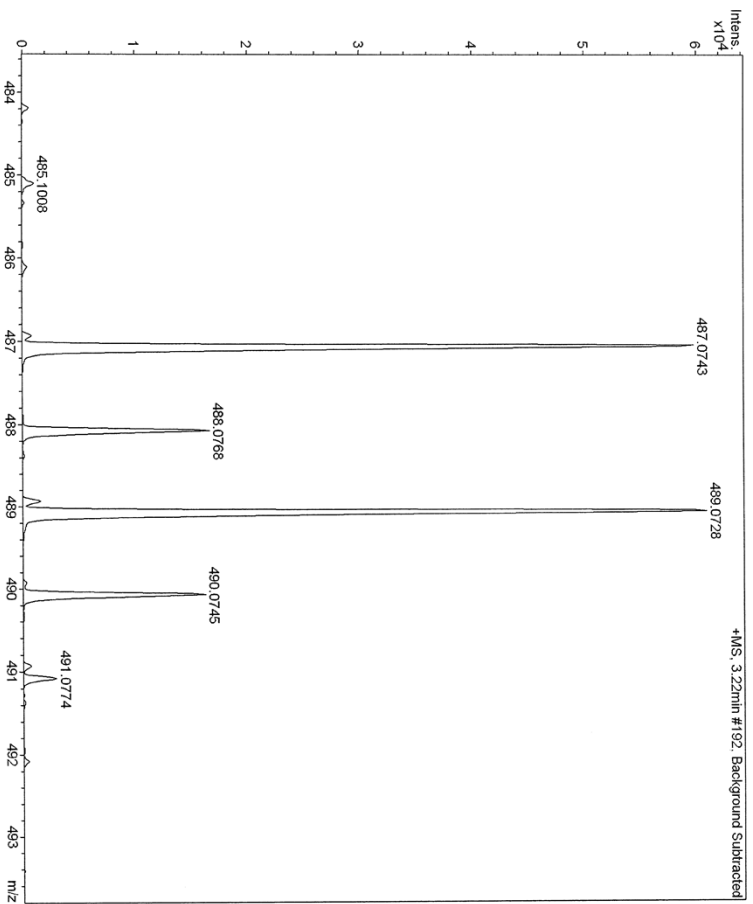
### Analysis Info

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

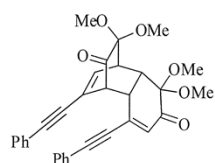
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste

Mass m/z	#	Formula	m/z	err [ppm]	rdp	e <sup>-</sup> Conf	N-Rule
487.0743	1	C <sub>24</sub> H <sub>24</sub> BrO <sub>6</sub>	487.0751	1.5	12.5	even	OK
	2	C <sub>37</sub> H <sub>41</sub> O <sub>2</sub>	487.0794	2.1	32.5	even	OK

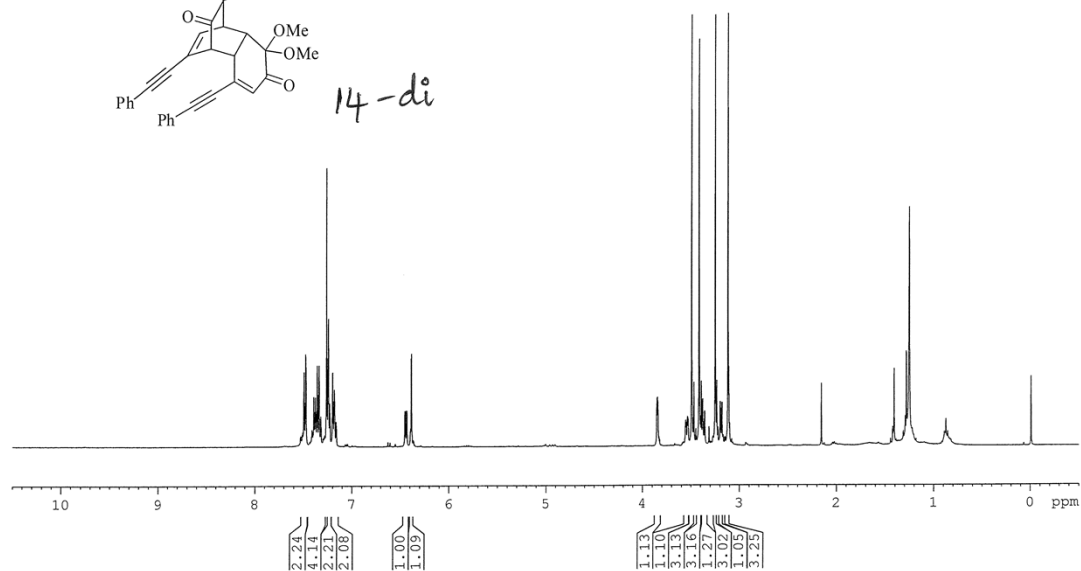




7.492  
7.489  
7.481  
7.475  
7.471  
7.392  
7.386  
7.378  
7.375  
7.370  
7.356  
7.342  
7.338  
7.321  
7.316  
7.260  
7.249  
7.241  
7.226  
7.220  
7.199  
7.197  
7.191  
7.183  
7.180  
7.176  
7.165  
7.161  
7.158  
6.450  
6.446  
6.433  
6.429  
6.385  
6.382  
3.853  
3.849  
3.845  
3.841  
3.559  
3.555  
3.551  
3.547  
3.539  
3.535  
3.531  
3.527  
3.492  
3.469  
3.414  
3.391  
3.378  
3.358  
3.249  
3.233  
3.199  
3.196  
3.182  
3.179  
3.117  
3.108



14-di



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 9012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894966 sec  
RG 40.3  
LW 62.400 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TDO 1

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
NUC1 1H  
P1 10.70 usec  
PL1 -3.00 dB  
FLW 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

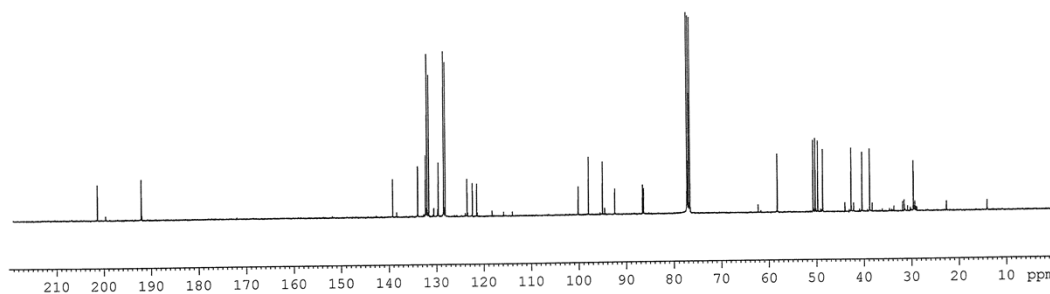
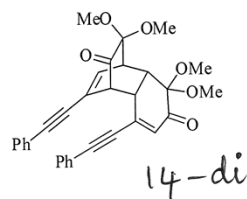


— 201.419  
— 192.136

139.221  
133.942  
132.324  
131.957  
131.619  
129.642  
128.471  
128.134  
123.586  
122.453  
121.545

100.145  
97.985  
95.059  
92.419  
86.617  
86.386  
77.319  
77.001  
76.684

58.297  
50.772  
50.332  
49.779  
48.737  
42.760  
40.454  
38.834  
29.640



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

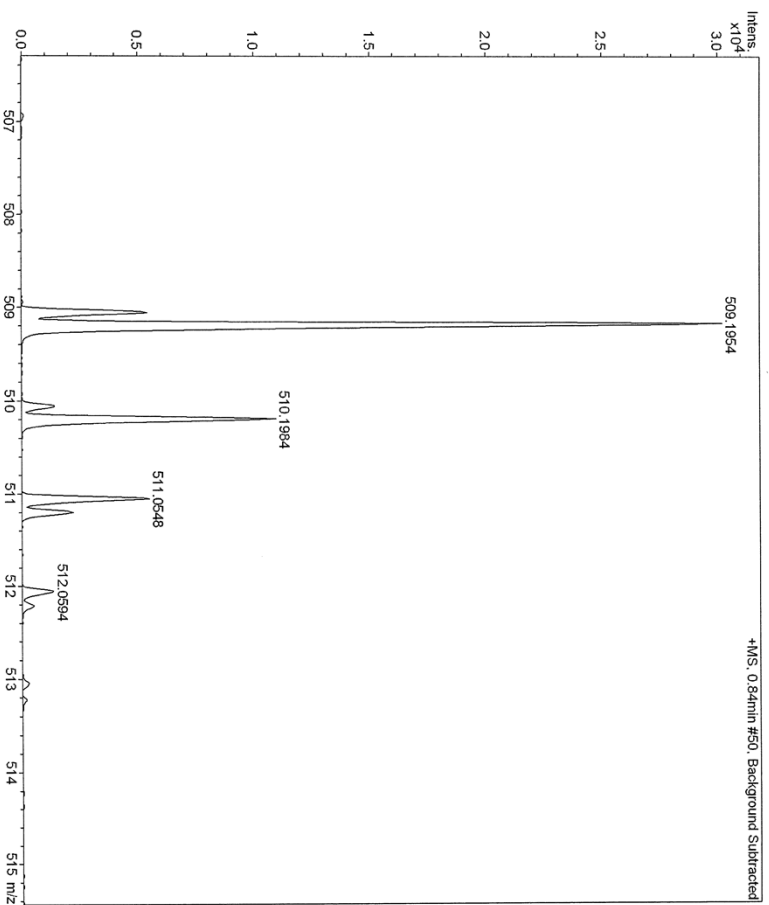
### Analysis Info

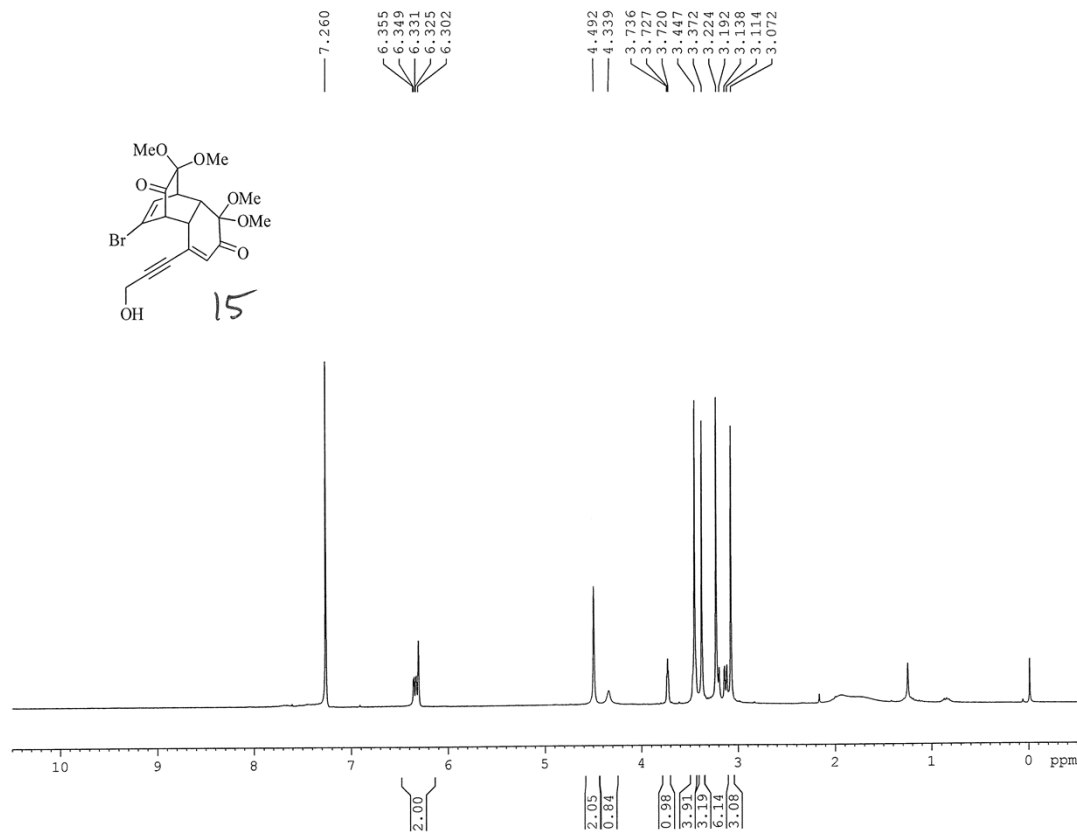
Analysis Name D:\Data\Chemistry\Outside\AMRI\20150107\5Br-DI-Phe-Acet.d Acquisition Date 1/7/2015 3:43:08 PM  
 Method YCH\_Pos-150-1800.m Operator default user  
 Sample Name 5Br-DI-Phe-Acet Instrument / Ser# microTOF-Q II 10269  
 Comment AMRI

### 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

Mass m/z # Formula m/z err [ppm] rdb e<sup>-</sup> Conf N-Rule  
 509.1954 1 C<sub>32</sub>H<sub>29</sub>O<sub>6</sub> 509.1959 0.8 18.5 even OK





Current Data Parameters  
NAME SG-BCK-G-SF-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 # \_\_\_\_\_

— 199.548  
— 192.118

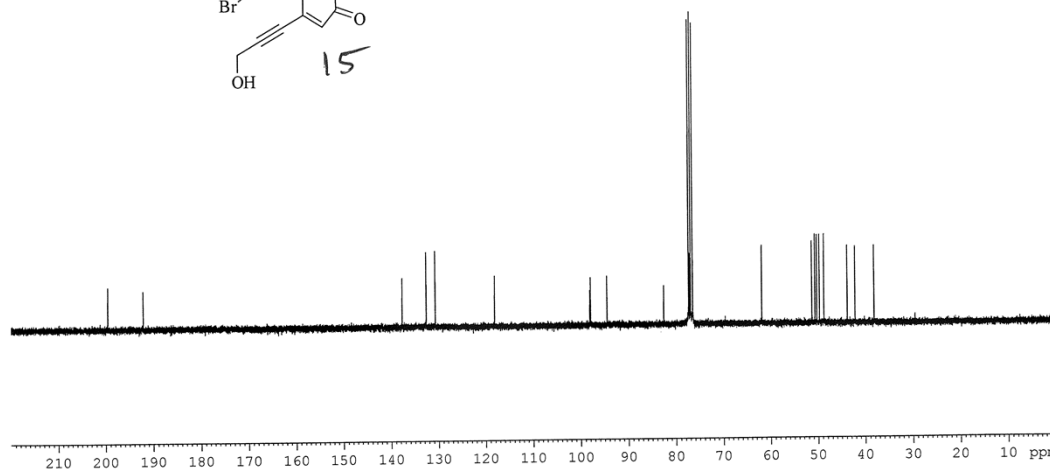
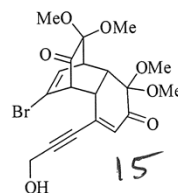
— 137.739  
— 132.675  
— 130.789

— 118.188

— 98.159  
— 98.006  
— 94.560

— 82.654  
— 77.424  
— 77.001  
— 76.577

— 61.948  
— 51.420  
— 50.760  
— 50.358  
— 49.807  
— 48.849  
— 43.932  
— 42.258  
— 38.265



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 1.445188 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\SB-Propargylalcol-mono-1n.d  
 Method YCH\_Pos-150-1800.m  
 Sample Name SB-Propargylalcol-mono  
 Comment AMRI  
 Santhosh Kumar Chittinalla

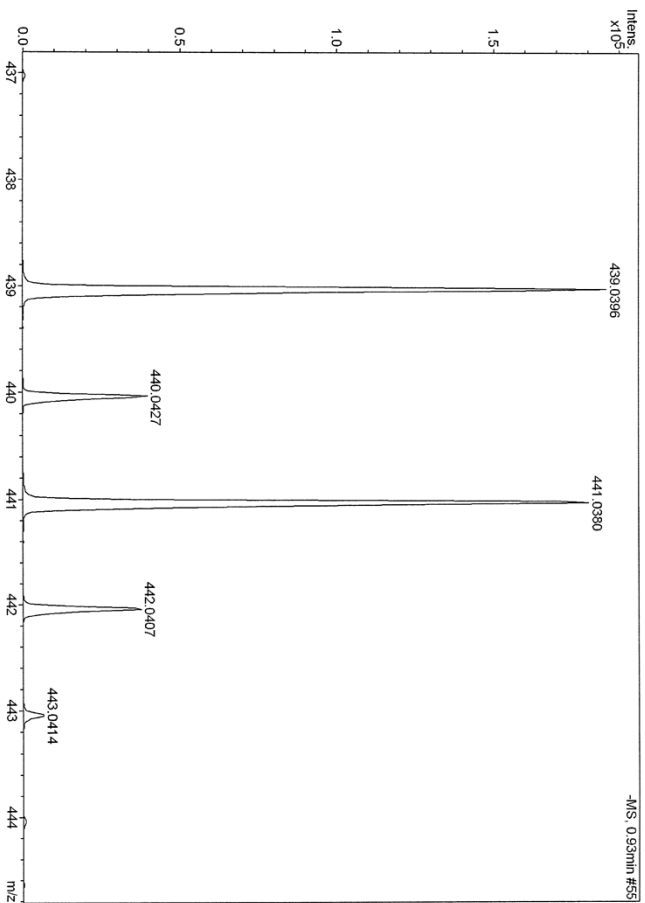
Acquisition Date 12/18/2014 2:39:49 PM

Operator default user  
 Instrument / Ser# micrOTOF-Q II 10269

### 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

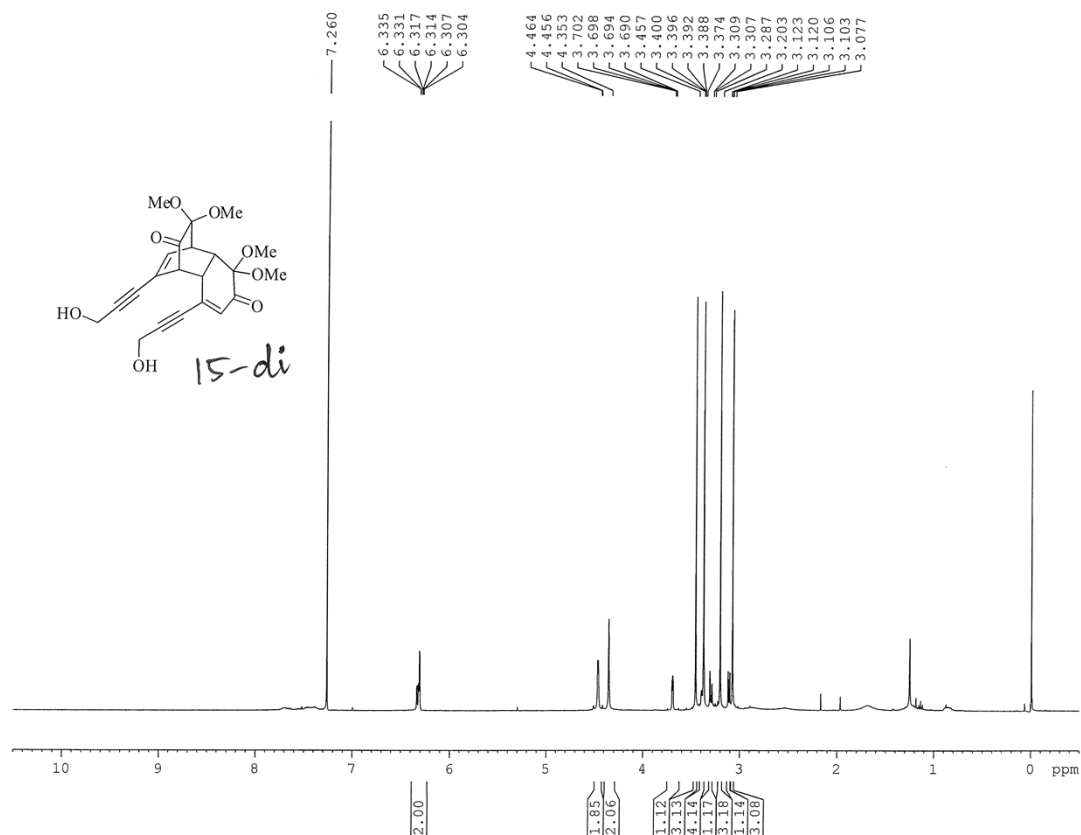
Meas m/z	#	Formula	m/z	err [ppm]	rd	e <sup>-</sup>	Conf	N-Rule
439.0396	1	C <sub>19</sub> H <sub>20</sub> BrO <sub>7</sub>	439.0396	0.5	9.5	even		OK



Brucker Compass DataAnalysis 4.0

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Page 1 of 1



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

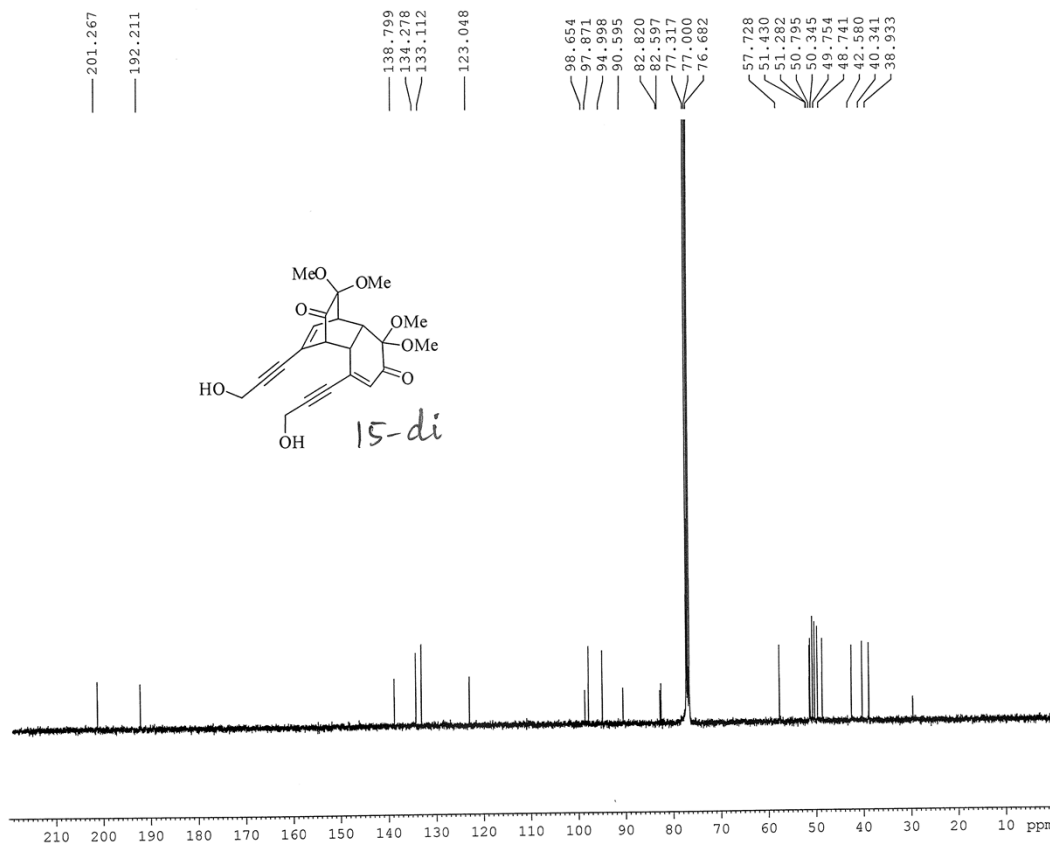
F2 - Acquisition Parameters  
 Date\_ 20141031  
 Time 20.13  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894966 sec  
 RG 128  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 1.00000000 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



Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

Current Data Parameters  
NAME SG-BCK-5Br-D-Prg-sonag-Di  
EXFNO 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

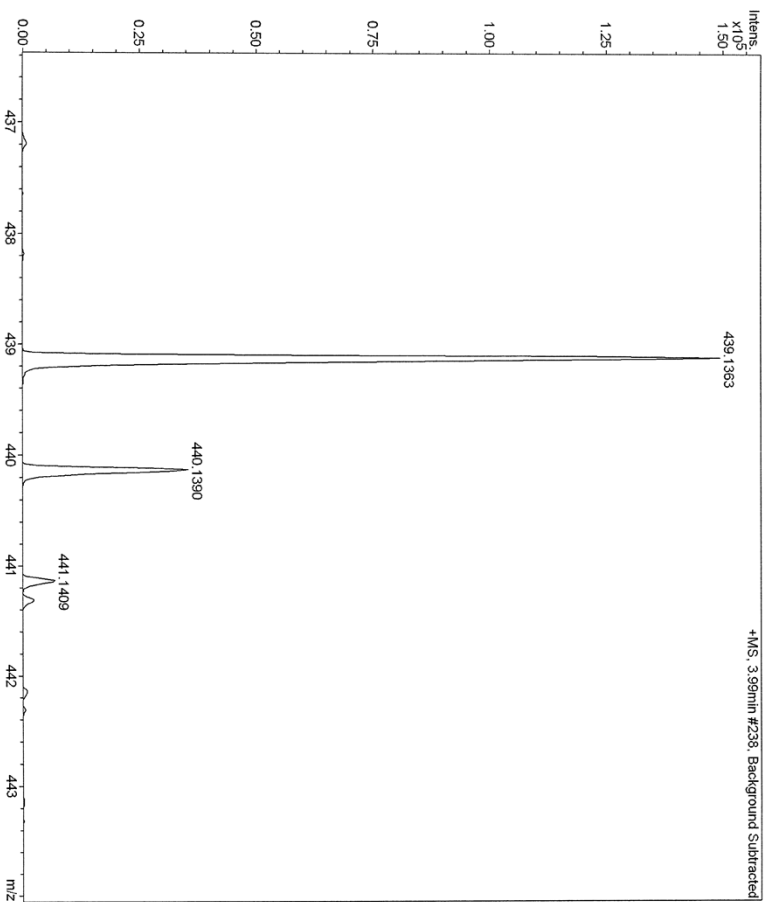
### Analysis Info

Analysis Name D:\Data\Chemistry\Outside\AMRI\20150107\5Br-DI-Pg-Alc.d Acquisition Date 1/7/2015 3:50:48 PM  
 Method YCH\_Pos-150-1800 m Operator default user  
 Sample Name 5Br-DI-Pg-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

Mass m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdp	e <sup>-</sup> Conf	N-Rule
439.1363	1	C <sub>22</sub> H <sub>24</sub> NaO <sub>8</sub>	100.00	439.1363	0.1	0.2	1.7	10.5	even	ok



AMRI SRC  
location; 17



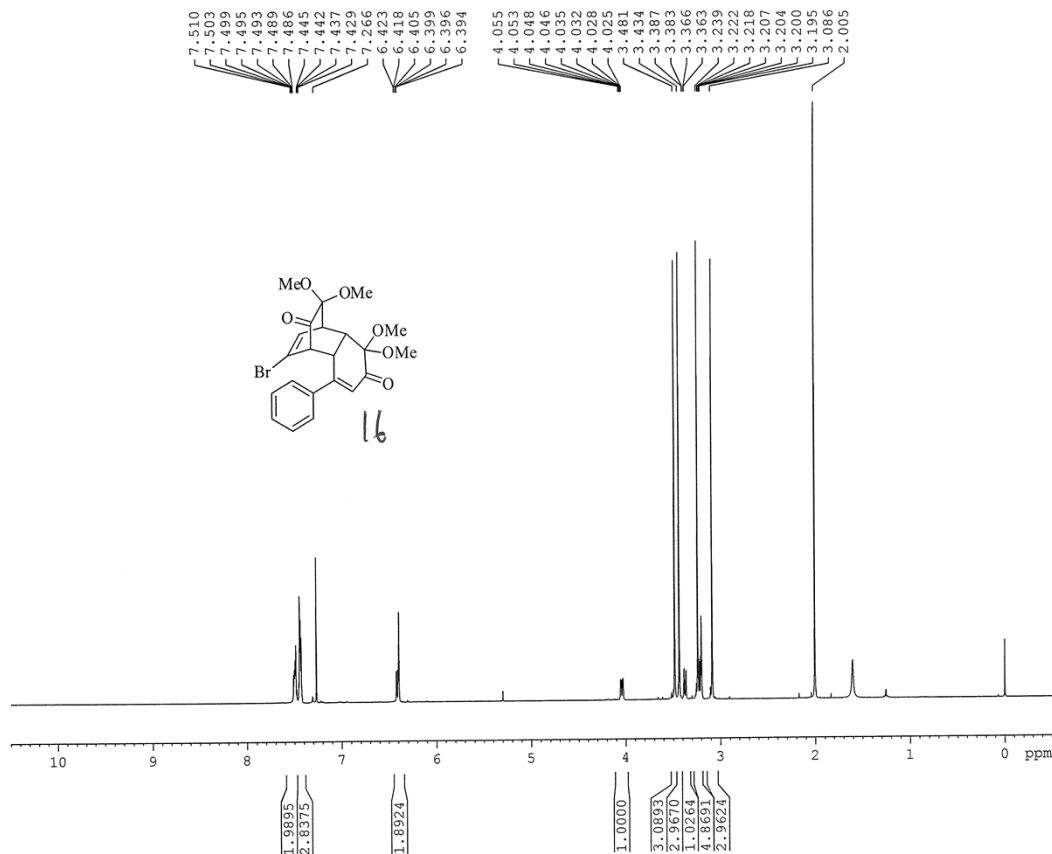
Name \_\_\_\_\_  
Date \_\_\_\_\_  
NB # \_\_\_\_\_

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

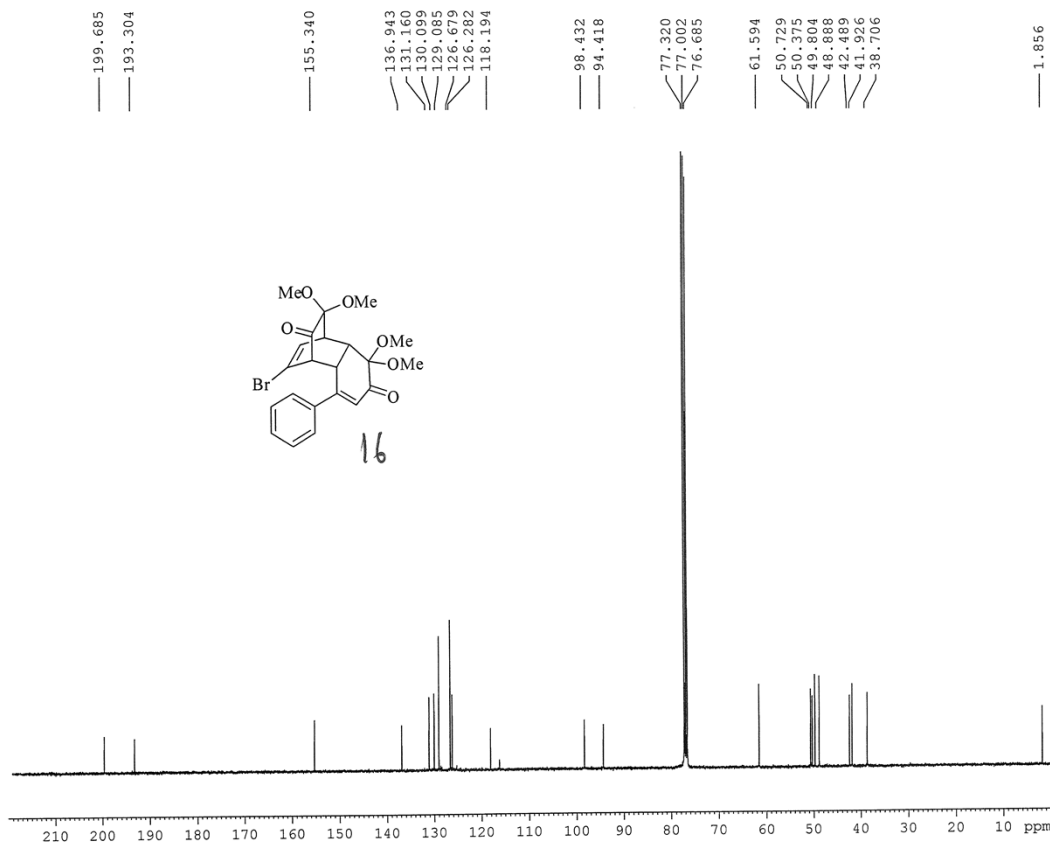
F2 - Acquisition Parameters  
Date\_ 20150119  
Time 20.10  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894966 sec  
RG 128  
DW 62.400 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

===== 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

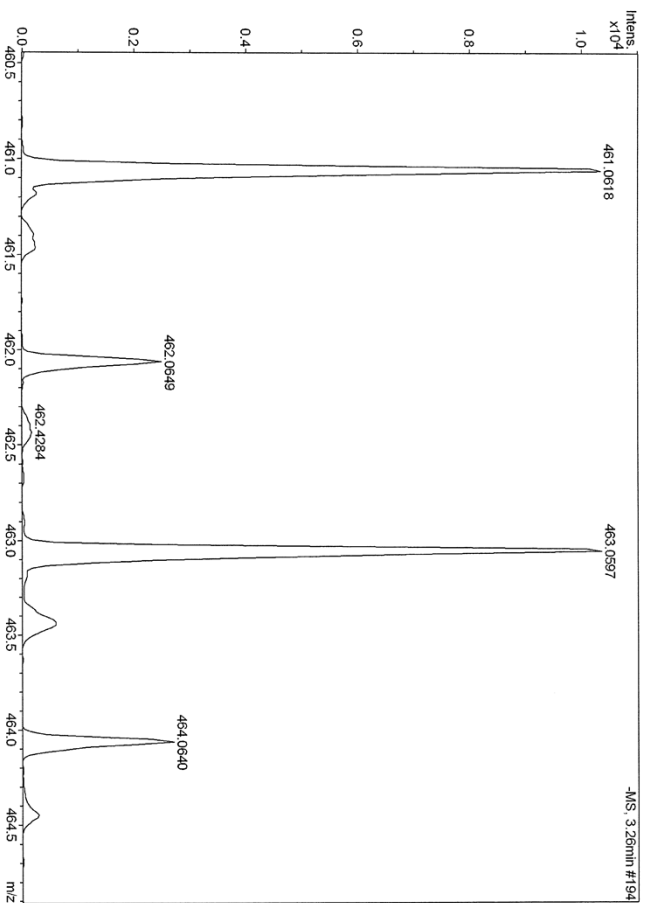
Analysis Name D:\Data\Chemistry\Outside\AMRI\20141218\SBF-Suz-mono-1n.d Acquisition Date 12/18/2014 3:48:33 PM  
 Method YCH\_Pos-300-2500.m Operator default user  
 Sample Name SBF-Suz-mono Instrument / Ser# microTOF-Q II 10269  
 Comment AMRI  
 Santhosh Kumar Chittinalla

### 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

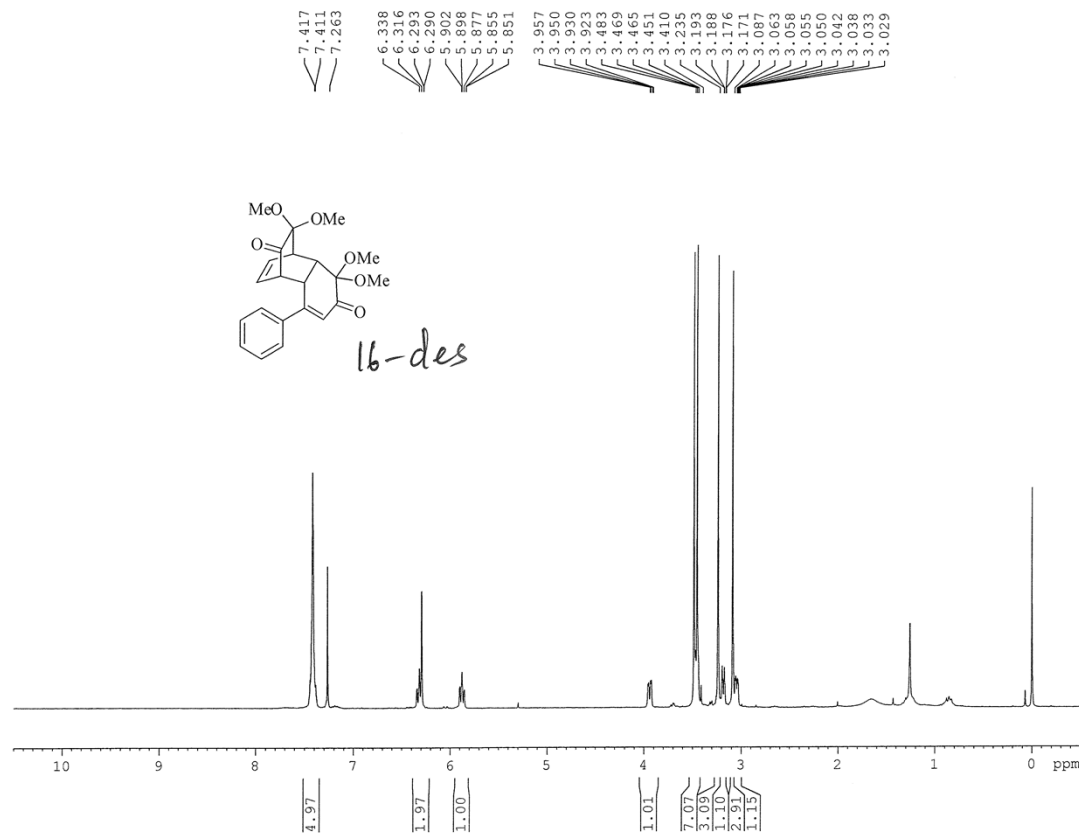
Mass m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdB	e <sup>-</sup> Conf	N-Rule
461.0618	1	C <sub>22</sub> H <sub>22</sub> BrO <sub>6</sub>	100.00	461.0605	-1.3	-2.9	15.4	11.5	even	OK



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Current Data Parameters  
 NAME SG-RKP-5F-D-phauz-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  
 MCWRRK 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



— 202.570  
— 194.008

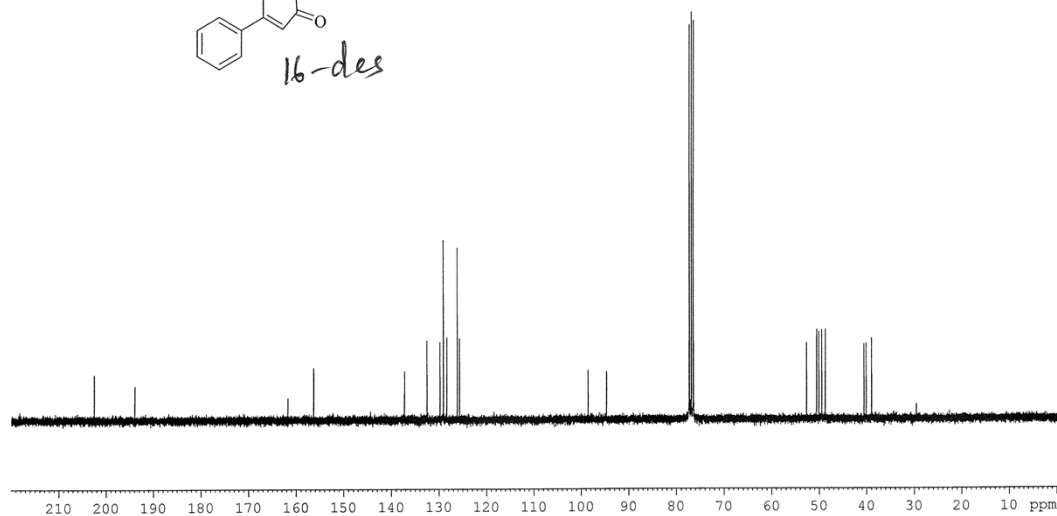
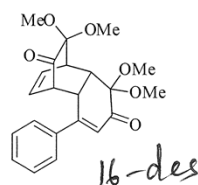
— 161.861  
— 156.452

137.354  
132.625  
129.941  
129.226  
128.488  
126.262  
125.786

— 98.666  
— 94.783

77.423  
76.999  
76.576

52.820  
50.687  
50.231  
49.626  
48.880  
40.725  
40.251  
39.119



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 2560.3  
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