# Mass Spectrum SmartFormula Report

**Analysis Info**
- **Analysis Name**: D:\Data\SongMarch2017\CF-0382.d
- **Method**: lowpositive.m
- **Sample Name**: PA
- **Comment**

**Acquisition Parameter**
- **Source Type**: ESI
- **Focus**: Not active
- **Scan Begin**: 50 m/z
- **Scan End**: 2400 m/z
- **Ion Polarity**: Positive
- **Set Capillary**: 4000 V
- **Set Charging Voltage**: 0 V
- **Set Corona**: 0 nA
- **Set Nebulizer**: 0.5 Bar
- **Set Dry Gas**: 4.0 L/min
- **Set Dry Heater**: 180 °C
- **Set Divert Valve**: Source
- **Set APCI Heater**: 0 °C

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**Graph**

![Mass Spectrum Graph]

+C^20H^40^3^5N^5O, 784.1483

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**Printed Information**
- **Bruker Compass DataAnalysis 4.2**
- **Printed**: 3/20/2017 1:56:00 PM
- **By**: Lijiang Song

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**Page 1 of 2**
**Mass Spectrum SmartFormula Report**

**Analysis Info**
- Analysis Name: lowpositive.m
- Sample Name: LS
- Comment: 
- Acquisition Date: 3/5/2017 2:54:40 PM
- Operator: Lijiang Song
- Instrument: maXis plus
- Instrument ID: 255552.00050

**Acquisition Parameter**

<table>
<thead>
<tr>
<th>Source Type</th>
<th>ESI</th>
<th>Ion Polarity</th>
<th>Positive</th>
<th>Set Nebulizer</th>
<th>0.5 Bar</th>
</tr>
</thead>
<tbody>
<tr>
<td>Focus</td>
<td>Not active</td>
<td>Set Capillary</td>
<td>4000 V</td>
<td>Set Dry Heater</td>
<td>180 °C</td>
</tr>
<tr>
<td>Scan Begin</td>
<td>50 m/z</td>
<td>Set End Plate Offset</td>
<td>-500 V</td>
<td>Set Dry Gas</td>
<td>4.0 l/min</td>
</tr>
<tr>
<td>Scan End</td>
<td>2400 m/z</td>
<td>Set Charging Voltage</td>
<td>0 V</td>
<td>Set Divert Valve</td>
<td>Source</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Set Corona</td>
<td>0 nA</td>
<td>Set APCI Heater</td>
<td>0 °C</td>
</tr>
</tbody>
</table>

**DIAGRAM**

![Mass Spectrum Diagram]

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CF0369.d

Bruker Compass DataAnalysis 4.2

printed: 3/5/2017 3:03:22 PM

by: Lijiang Song

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Mass Spectrum SmartFormula Report

Analysis Info
Analysis Name: D:\Data\SongMarch2017\CF0375.d
Method: lowpositive.m
Sample Name: LS
Comment:

Acquisition Parameter
Source Type: ESI
Focus: Not active
Scan Begin: 50 m/z
Scan End: 2400 m/z
Ion Polarity: Positive
Set Capillary: 4000 V
Set End Plate Offset: -500 V
Set Charging Voltage: 0 V
Set Corona: 0 nA
Set Nebulizer: 0.5 Bar
Set Dry Heater: 180 °C
Set Dry Gas: 4.0 l/min
Set Divert Valve: Source
Set APCI Heater: 0 °C

Graphical Representation:

intens. 5000 4000 3000 2000 1000 0


+MS, 0.8min #47

C_{49}H_{64}BrI\text{N}_{6}O_{5}, 888.1553

Graph 1:

Graph 2:

CF0375.d
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Mass Spectrum SmartFormula Report

Analysis Info
Analysis Name: D:\Data\SongMarch2017\CF0376.d
Method: lowpositive.m
Sample Name: LS
Comment:

Acquisition Date: 3/5/2017 2:57:22 PM
Operator: Lijiang Song
Instrument: maXis plus
Instrument ID: 255552.00050

Acquisition Parameter
Source Type: ESI
Focus: Not active
Scan Begin: 50 m/z
Scan End: 2400 m/z

Ion Polarity: Positive
Set Capillary: 4000 V
Set End Plate Offset: -500 V
Set Charging Voltage: 0 V
Set Corona: 0 nA
Set Nebulizer: 0.5 Bar
Set Dry Heater: 180 °C
Set Dry Gas: 4.0 l/min
Set Divert Valve: Source
Set APCI Heater: 0 °C

Intens.

4000
3000
2000
1000
0

4000
3000
2000
1000
0

838 840 842 844 846 848 m/z

CF0376.d
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Mass Spectrum SmartFormula Report

Analysis Info
Analysis Name: D:\Data\SongMarch2017\CF0380.d
Method: lowpositive.m
Sample Name: LS
Comment:

Acquisition Date: 3/10/2017 8:48:41 AM
Operator: Lijiang Song
Instrument: maXis plus
Indicate: 255552.00050

Acquisition Parameter
Source Type: ESI
Focus: Not active
Scan Begin: 50 m/z
Scan End: 2400 m/z
Ion Polarity: Positive
Set Capillary: 4000 V
Set End Plate Offset: -500 V
Set Charging Voltage: 0 V
Set Corona: 0 nA
Set Nebulizer: 0.5 Bar
Set Dry Heater: 180 °C
Set Dry Gas: 4.0 l/min
Set Divert Valve: Source
Set APCI Heater: 0 °C

Intens.
8000
6000
4000
2000
0

+MS, 0.1-0.7min #S-43

Complex 14

C42H44IrN4O5, 889.2870

CF0380.d
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