## Analysis Info

**Analysis Name**: D:\Data\ESI\2016\2016-03\0315\C4-2_000002.d

**Sample Name**: C4-2

**Instrument**: solarIX

**Acquisition Date**: 3/15/2016 10:56:48 AM

### Acquisition Parameter

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
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</thead>
<tbody>
<tr>
<td>Acquisition Mode</td>
<td>Single MS</td>
</tr>
<tr>
<td>Polarity</td>
<td>Positive</td>
</tr>
<tr>
<td>Broadband Low Mass</td>
<td>57.7 m/z</td>
</tr>
<tr>
<td>Broadband High Mass</td>
<td>250.0 m/z</td>
</tr>
<tr>
<td>Acquired Scans</td>
<td>20</td>
</tr>
<tr>
<td>No. of Cell Fills</td>
<td>1</td>
</tr>
<tr>
<td>Source Accumulation</td>
<td>0.001 sec</td>
</tr>
<tr>
<td>Ion Accumulation Time</td>
<td>0.200 sec</td>
</tr>
<tr>
<td>Calibration Date</td>
<td>Thu Mar 10 09:43:56</td>
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<tr>
<td>Data Acquisition Size</td>
<td>2048576</td>
</tr>
<tr>
<td>Data Processing Size</td>
<td>2097152</td>
</tr>
<tr>
<td>Apodization</td>
<td>Sine-Bell Multiplication</td>
</tr>
</tbody>
</table>

### Mass Spectrogram

![Mass Spectrogram](image)

### Measured m/z, Formula, Score, m/z err [ppm], Mean err [ppm], mSigma, rdb, e- Conf, N-Rule

<table>
<thead>
<tr>
<th>m/z</th>
<th>Formula</th>
<th>Score</th>
<th>m/z err [ppm]</th>
<th>Mean err [ppm]</th>
<th>mSigma</th>
<th>rdb</th>
<th>e- Conf</th>
<th>N-Rule</th>
</tr>
</thead>
<tbody>
<tr>
<td>183.045004</td>
<td>C7H12NaO2S</td>
<td>100.00</td>
<td>-0.1</td>
<td>-0.0</td>
<td>26.2</td>
<td>1.5</td>
<td>even</td>
<td>ck</td>
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</table>
ESI(P), d4-1, 20160315

Analysis Info
Analysis Name: D:\Data\ESI\2016\2016-03\0315\d4-1_000001.d
Acquisition Date: 3/15/2016 11:10:40 AM
Sample Name: d4-1
Instrument: solarX

Acquisition Parameter:
Acquisition Mode: Single MS
Polarity: Positive
Broadband Low Mass: 57.7 m/z
Broadband High Mass: 500.0 m/z
Acquired Scans: 4
No. of Cell Fills: 1
Source Accumulation: 0.001 sec
Ion Accumulation Time: 0.100 sec
Calibration Date: Thu Mar 10 09:43:56
Data Acquisition Size: 2048576
Data Processing Size: 2097152
Apodization: Sine-Bell Multiplication

Meas. m/z  #  Ion Formula  Score  m/z  err [ppm]  Mean err [ppm]  mSigma  rdb  e−  Conf  N-Rule
253.123087  1  C12H22NaO2S  100.00  253.123272  -0.7  0.6  27.0  1.5  even  ok
ESI(P), d4-2, 20160315

Analysis Info
Analysis Name D:\Data\ESI\2016\2016-030315\d4-2_000002.d
Sample Name d4-2

Acquisition Parameter
Acquisition Mode Single MS
Polarity Positive
Broadband Low Mass 57.7 m/z
Broadband High Mass 500.0 m/z
Acquired Scans 10
No. of Cell Fills 1
Source Accumulation 0.001 sec
Ion Accumulation Time 0.100 sec
Calibration Date Thu Mar 10 09:43:56
Data Acquisition Size 2048576
Data Processing Size 2097152
Apodization Sine-Bell Multiplication

Intens. x10^3

trans-4b

Intens. x10^3

Measurements:

<table>
<thead>
<tr>
<th>Meas. m/z</th>
<th>Score</th>
<th>m/z</th>
<th>err [ppm]</th>
<th>Mean err [ppm]</th>
<th>mSigma</th>
<th>rdb</th>
<th>e^-</th>
<th>Conf</th>
<th>N-Rule</th>
</tr>
</thead>
<tbody>
<tr>
<td>253.123104</td>
<td>1</td>
<td>C12H22NaO2S</td>
<td>100.00</td>
<td>253.123272</td>
<td>-0.7</td>
<td>0.6</td>
<td>27.9</td>
<td>1.5</td>
<td>even</td>
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+MS
Analysis Info
Analysis Name: D:\Data\ESI\2016\2016-08\0804\F4-1_000002.d
Acquisition Date: 8/4/2016 9:20:11 AM
Sample Name: F4-1
Instrument: solariX

Acquisition Parameter
Polarity: Positive
Acquired Scans: 4
Broadband Low Mass: 57.7 m/z
Broadband High Mass: 300.0 m/z

<table>
<thead>
<tr>
<th>Meas. m/z</th>
<th>Ion Formula</th>
<th>Score</th>
<th>m/z</th>
<th>err [ppm]</th>
<th>Mean err [ppm]</th>
<th>mSigma</th>
<th>rdb</th>
<th>e⁻ Conf</th>
<th>N-Rule</th>
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</thead>
<tbody>
<tr>
<td>211.076337</td>
<td>C9H16NaO2S</td>
<td>100.00</td>
<td>211.076321</td>
<td>0.1</td>
<td>-0.2</td>
<td>26.0</td>
<td>1.5</td>
<td>even</td>
<td>ok</td>
</tr>
<tr>
<td>227.053578</td>
<td>C9H16NaO2S2</td>
<td>100.00</td>
<td>227.053478</td>
<td>0.1</td>
<td>-0.1</td>
<td>9.2</td>
<td>1.6</td>
<td>even</td>
<td>ok</td>
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<tr>
<td>269.064004</td>
<td>C11H16NaO2S2</td>
<td>100.00</td>
<td>269.064043</td>
<td>-0.1</td>
<td>0.4</td>
<td>2.4</td>
<td>2.5</td>
<td>even</td>
<td>ok</td>
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<tr>
<td>Meas. m/z</td>
<td>#</td>
<td>Ion Formula</td>
<td>Score</td>
<td>m/z</td>
<td>err [ppm]</td>
<td>Mean err [ppm]</td>
<td>mSigma</td>
<td>rdb</td>
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<tr>
<td>231.104814</td>
<td>1</td>
<td>C11H19O3S</td>
<td>100.00</td>
<td>231.104942</td>
<td>0.6</td>
<td>0.3</td>
<td>19.8</td>
<td>2.5</td>
<td>even</td>
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<td>253.086752</td>
<td>1</td>
<td>C11H18NaO3S</td>
<td>100.00</td>
<td>253.086886</td>
<td>0.5</td>
<td>0.2</td>
<td>2.7</td>
<td>2.5</td>
<td>even</td>
</tr>
<tr>
<td>269.061043</td>
<td>1</td>
<td>C11H18KO3S</td>
<td>100.00</td>
<td>269.060824</td>
<td>-0.8</td>
<td>-1.1</td>
<td>15.0</td>
<td>2.5</td>
<td>even</td>
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</table>
ESI(P), B2-S, 20171025

Analysis Info
Analysis Name: Data_ESI2017/2017-10/1025/B2-S_000001.d
Sample Name: B2-S

Acquisition Parameter
Polarity: Positive
Broadband Low Mass: 57.7 m/z
Broadband High Mass: 400.0 m/z

Acquisition Date: 10/25/2017 10:56:48 AM
Operator: solarix
Instrument: solariX
Calibration Date: Fri Sep 22 03:00:05 2017
Acquired Scans: 10

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Intens. x10^2

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Meas. m/z  Ion Formula  Score  m/z  err [ppm]  Mean err [ppm]  mSigma  rdb  e- Conf  N-Rule
203.050162  C10H12NO5  100.00  203.050107  0.4  -0.2  5.8  4.5  even  ek
ESI(P), B3-S, 20171025

Analysis Info
Analysis Name: D:\Data\ESI\2017\2017-10\01029\B3-S_000002.d
Sample Name: B3-S

Acquisition Date: 10/25/2017 10:50:53 AM
Operator: 
Instrument: solarIX

Acquisition Parameter
Polarity: Positive
Broadband Low Mass: 67.7 m/z
Broadband High Mass: 205.0 m/z

Calibration Date: Fri Sep 22 03:00:05 2017
Acquired Scans: 10

Chemical structure:

Measurements:

<table>
<thead>
<tr>
<th>m/z</th>
<th>Score</th>
<th>m/z</th>
<th>err [ppm]</th>
<th>Mean err [ppm]</th>
<th>mSigma</th>
<th>rdb</th>
<th>Conf</th>
<th>N-Rule</th>
</tr>
</thead>
<tbody>
<tr>
<td>281.027657</td>
<td>100.00</td>
<td>281.027509</td>
<td>0.5</td>
<td>-0.3</td>
<td>10.6</td>
<td>4.5</td>
<td>even</td>
<td>ok</td>
</tr>
</tbody>
</table>

Scanned by CamScanner
cis-4b
trans-4d