Small Molecule Synthesis Report

Analysis Information

Item name: CA_32785_Small Molecules Direct Infusion Sep 01, 2016 11:58:56 GMT Daylight Time

Analysis Method Item name: Small Molecules Direct Infusion

Version: 1

Modified date: Sep 01, 2016 12:04:09 GMT Daylight Time

Modified by: Boodhun, Asha

Folder: Company/Training

Sample List

<table>
<thead>
<tr>
<th>Item name</th>
<th>Sample type</th>
<th>Run time</th>
<th>Replicates</th>
</tr>
</thead>
<tbody>
<tr>
<td>CA_32785_AT110</td>
<td>Unknown</td>
<td>1.000</td>
<td>1</td>
</tr>
</tbody>
</table>

Item name: CA_32785_AT110, Sample position: 1:A,1, Replicate number: 1

<table>
<thead>
<tr>
<th>Component name</th>
<th>Formula</th>
<th>Neutral mass (Da)</th>
<th>Observed neutral mass (Da)</th>
<th>Observed m/z</th>
<th>Mass error (mDa)</th>
<th>Mass error (ppm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CA_32785_AT110</td>
<td>C9H8IN3</td>
<td>284.97629</td>
<td>284.9773</td>
<td>285.9846</td>
<td>1.0</td>
<td>3.5</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Component name</th>
<th>Observed CCS (Å)</th>
<th>Detector counts</th>
<th>Adducts</th>
<th>Charge</th>
</tr>
</thead>
<tbody>
<tr>
<td>CA_32785_AT110</td>
<td>147.88</td>
<td>33160816</td>
<td>+H, +Na</td>
<td>1</td>
</tr>
</tbody>
</table>

Item name: CA_32785_AT110

Item description:

UNIFI page 1 of 2
Item name: CA_32785_AT110
Item description:

Channel name: High energy : Time 0.5009 +/- 0.4760 minutes

Observed mass [m/z]: 159.07947, 285.98439, 406.29458, 407.29749, 512.28869, 499.91193, 606.92209, 729.37302, 815.65896, 931.74443