Mass Spectrum SmartFormula Report

Analysis Info
Analysis Name: D:\Data\Mass Spectrometry Service\70127-000002.d
Method: LM MS 50 to 1100 m/z
Sample Name: Goldwell SC-5-2
Comment:

Acquisition Data: 3/23/2018 9:53:49 AM
Operator: user
Instrument/Ser# microOTOF-Q 74

Acquisition Parameter
Source Type: ESI
Ion Polarity: Positive
Scan Begin: 50 m/z
Scan End: 1100 m/z

Formula: C_{59} H_{84} O_{4} S Na

<table>
<thead>
<tr>
<th>z</th>
<th>m/z</th>
<th>Meas. m/z</th>
<th>err [ppm]</th>
<th>err [mDa]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1^+</td>
<td>891.7129</td>
<td>891.7129</td>
<td>-1.3</td>
<td>-1.2</td>
</tr>
</tbody>
</table>

Bruker Compass DataAnalysis 4.0
printed: 3/23/2018 10:03:06 AM
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Accurate Mass