<table>
<thead>
<tr>
<th>Peak ID</th>
<th>Measured mass [Da]</th>
<th>Tentative empirical formula (measured mass minus exact ion mass in mDa)</th>
<th>Temp largest signal</th>
<th>Concentration (mean, 10, 50, 90% percentiles) [ng/m³]</th>
<th>LOD [ng/m³]</th>
<th>Fraction of total burden (rank)</th>
</tr>
</thead>
<tbody>
<tr>
<td>m18.0085</td>
<td>18.010</td>
<td></td>
<td>200</td>
<td>0.32, (0.01, 0.23, 0.75)</td>
<td>0.015</td>
<td>0.029% (346)</td>
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<tr>
<td>m18.0321</td>
<td>18.033</td>
<td>NH₃H⁺ (-0.5)</td>
<td>150</td>
<td>90, (2.4, 79, 177)</td>
<td>n.c.</td>
<td>8.06% (1)</td>
</tr>
<tr>
<td>m18.0817</td>
<td>18.083</td>
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<td>150</td>
<td>0.101, (0.004, 0.061, 0.267)</td>
<td>0.003</td>
<td>0.0090% (458)</td>
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<tr>
<td>m28.0054</td>
<td>28.006</td>
<td></td>
<td>300</td>
<td>0.034, (0.000, 0.027, 0.068)</td>
<td>0.009</td>
<td>0.0031% (550)</td>
</tr>
<tr>
<td>m28.0175</td>
<td>28.018</td>
<td>CHNH⁺ (0.1)</td>
<td>300</td>
<td>1.16, (0.01, 1.05, 2.29)</td>
<td>0.267</td>
<td>0.104% (173)</td>
</tr>
<tr>
<td>m28.0301</td>
<td>28.031</td>
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<td>300</td>
<td>0.058, (0.003, 0.050, 0.129)</td>
<td>0.003</td>
<td>0.0052% (506)</td>
</tr>
<tr>
<td>m31.0174</td>
<td>31.018</td>
<td>CH₂OH⁺ (0.2)</td>
<td>300</td>
<td>4.0, (0.26, 3.8, 7.3)</td>
<td>0.961</td>
<td>0.36% (58)</td>
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<tr>
<td>m32.0519</td>
<td>32.053</td>
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<td>0.039, (0.002, 0.028, 0.083)</td>
<td>0.004</td>
<td>0.0035% (542)</td>
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<tr>
<td>m33.0332</td>
<td>33.034</td>
<td>CH₄OH⁺ (0.3)</td>
<td>200</td>
<td>1.22, (0.06, 1.11, 2.18)</td>
<td>0.089</td>
<td>0.109% (163)</td>
</tr>
<tr>
<td>m34.0358</td>
<td>34.036</td>
<td>CH₄OH⁺ (-0.5)</td>
<td>200</td>
<td>0.017, (0.002, 0.014, 0.031)</td>
<td>0.003</td>
<td>0.00148% (606)</td>
</tr>
<tr>
<td>m36.0442</td>
<td>36.045</td>
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<td>0.28, (0.01, 0.16, 0.59)</td>
<td>0.111</td>
<td>0.025% (361)</td>
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<tr>
<td>m42.0339</td>
<td>42.034</td>
<td>C₂H₃NH⁺ (0.3)</td>
<td>250</td>
<td>2.2, (0.03, 1.7, 4.7)</td>
<td>n.c.</td>
<td>0.20% (101)</td>
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<tr>
<td>m43.0180</td>
<td>43.018</td>
<td>C₂H₂OH⁺ (0.3)</td>
<td>150</td>
<td>7.0, (0.19, 5.8, 15.9)</td>
<td>0.365</td>
<td>0.63% (39)</td>
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<tr>
<td>m44.0131</td>
<td>44.013</td>
<td>CHNOH⁺ (0.2)</td>
<td>300</td>
<td>3.6, (0.14, 2.7, 8.6)</td>
<td>0.313</td>
<td>0.33% (65)</td>
</tr>
<tr>
<td>m44.0495</td>
<td>44.050</td>
<td>C₂H₃NH⁺ (0.2)</td>
<td>200</td>
<td>0.25, (0.01, 0.22, 0.54)</td>
<td>0.008</td>
<td>0.023% (376)</td>
</tr>
<tr>
<td>m44.9972</td>
<td>44.997</td>
<td>CO₂H⁺ (0.2)</td>
<td>200</td>
<td>0.071, (0.003, 0.054, 0.158)</td>
<td>0.005</td>
<td>0.0064% (497)</td>
</tr>
<tr>
<td>m45.0336</td>
<td>45.034</td>
<td>C₂H₄OH⁺ (0.2)</td>
<td>200</td>
<td>9.3, (0.53, 9.1, 17.9)</td>
<td>0.419</td>
<td>0.83% (27)</td>
</tr>
<tr>
<td>m45.9925</td>
<td>45.993</td>
<td>NO₂⁺ (0.2)</td>
<td>150</td>
<td>0.42, (0.00, 0.20, 0.90)</td>
<td>0.017</td>
<td>0.038% (313)</td>
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<tr>
<td>m46.0291</td>
<td>46.029</td>
<td>CH₃NOH⁺ (0.4)</td>
<td>200</td>
<td>3.3, (0.08, 2.8, 7.0)</td>
<td>0.031</td>
<td>0.29% (75)</td>
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<tr>
<td>m46.0648</td>
<td>46.065</td>
<td>C₂H₇NH⁺ (-0.3)</td>
<td>200</td>
<td>0.090, (0.002, 0.070, 0.207)</td>
<td>0.002</td>
<td>0.0081% (470)</td>
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<tr>
<td>m</td>
<td>m/p</td>
<td>CH</td>
<td>H</td>
<td>O</td>
<td>H</td>
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<tr>
<td>m47.0133</td>
<td>47.013</td>
<td>CH₂O₂H⁺ (0.6)</td>
<td>150</td>
<td>10.4, (0.46, 10.5, 18.7)</td>
<td></td>
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<tr>
<td>m47.0233</td>
<td>47.023</td>
<td>H₂N₂OH⁺ (-0.7)</td>
<td>150</td>
<td>1.18, (0.08, 1.08, 2.24)</td>
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<tr>
<td>m47.0485</td>
<td>47.049</td>
<td>C₂H₆OH⁺ (-0.6)</td>
<td>150</td>
<td>0.22, (0.01, 0.23, 0.42)</td>
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<tr>
<td>m47.9673</td>
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<tr>
<td>m48.0087</td>
<td>48.009</td>
<td>HNO₂H⁺ (0.7)</td>
<td>150</td>
<td>0.149, (0.009, 0.149, 0.277)</td>
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<tr>
<td>m48.9845</td>
<td>48.985</td>
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<tr>
<td>m49.0072</td>
<td>49.007</td>
<td>HNO₂H⁺ (2.1)</td>
<td>150</td>
<td>0.031, (0.001, 0.028, 0.059)</td>
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<td>m49.0285</td>
<td>49.028</td>
<td>CH₄O₂H⁺ (0.1)</td>
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<td>0.21, (0.01, 0.15, 0.48)</td>
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<td>m51.0446</td>
<td>51.044</td>
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<td>m51.9955</td>
<td>51.995</td>
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<td>m52.0184</td>
<td>52.018</td>
<td>C₃HNH⁺ (0.1)</td>
<td>350</td>
<td>0.070, (0.004, 0.065, 0.132)</td>
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<tr>
<td>m53.0027</td>
<td>53.003</td>
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<tr>
<td>m53.0390</td>
<td>53.039</td>
<td>C₄H₄⁺ (0.3)</td>
<td>150</td>
<td>0.122, (0.001, 0.090, 0.307)</td>
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<tr>
<td>m53.9927</td>
<td>53.993</td>
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<tr>
<td>m54.0344</td>
<td>54.034</td>
<td>C₃H₃NH⁺ (0.4)</td>
<td>300</td>
<td>0.83, (0.01, 0.62, 1.78)</td>
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<tr>
<td>m54.0551</td>
<td>54.055</td>
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<td>m55.1067</td>
<td>55.106</td>
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<tr>
<td>m56.0233</td>
<td>56.023</td>
<td>C₂H₂OH⁺ (1.8), CHN₃H⁺ (-1.3)</td>
<td>150</td>
<td>0.057, (0.002, 0.041, 0.136)</td>
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<tr>
<td>m56.0454</td>
<td>56.045</td>
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<td>m56.0552</td>
<td>56.055</td>
<td>C₄H₈⁺ (-2.6)</td>
<td>350</td>
<td>0.25, (0.00, 0.20, 0.57)</td>
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<td>57.035</td>
<td>C₃H₄OH⁺ (1.0)</td>
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<td>3.5, (0.14, 3.1, 6.6)</td>
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<td>0.31% (69)</td>
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<td>m</td>
<td>Mass</td>
<td>Formula</td>
<td>Intensity</td>
<td>Coordinates</td>
<td>Width</td>
<td>Peak Area</td>
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<td>m58.0314</td>
<td>58.031</td>
<td>C₂H₃NOH⁺ (2.3)</td>
<td>200</td>
<td>0.44, (0.02, 0.39, 0.86)</td>
<td>0.005</td>
<td>0.039% (305)</td>
</tr>
<tr>
<td>m58.0733</td>
<td>58.073</td>
<td>C₄H₈⁺ (-0.3)</td>
<td>150</td>
<td>0.22, (-0.03, 0.08, 0.59)</td>
<td>0.047</td>
<td>0.0194% (395)</td>
</tr>
<tr>
<td>m58.9812</td>
<td>58.981</td>
<td>C₃N⁺ (-1.6)</td>
<td>100</td>
<td>0.022, (0.001, 0.019, 0.050)</td>
<td>0.001</td>
<td>0.00194% (591)</td>
</tr>
<tr>
<td>m59.0496</td>
<td>59.049</td>
<td>C₃H₆OH⁺ (0.1)</td>
<td>100</td>
<td>0.011, (0.001, 0.007, 0.023)</td>
<td>0.002</td>
<td>0.00095% (626)</td>
</tr>
<tr>
<td>m59.9319</td>
<td>59.932</td>
<td></td>
<td>100</td>
<td>0.007, (0.000, 0.005, 0.017)</td>
<td>0.001</td>
<td>0.00065% (630)</td>
</tr>
<tr>
<td>m59.9671</td>
<td>59.967</td>
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<td>100</td>
<td>0.007, (0.000, 0.005, 0.017)</td>
<td>0.001</td>
<td>0.00065% (630)</td>
</tr>
<tr>
<td>m60.0226</td>
<td>60.022</td>
<td>HN₃OH⁺ (3.0)</td>
<td>200</td>
<td>0.052, (0.002, 0.036, 0.123)</td>
<td>0.002</td>
<td>0.0046% (515)</td>
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<tr>
<td>m60.0473</td>
<td>60.047</td>
<td>C₂H₅NO⁺ (2.5)</td>
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<td>3.5, (0.09, 2.9, 7.5)</td>
<td>0.026</td>
<td>0.31% (57)</td>
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<tr>
<td>m60.0809</td>
<td>60.081</td>
<td>C₃H₇NH⁺ (-0.3)</td>
<td>200</td>
<td>0.176, (0.003, 0.143, 0.390)</td>
<td>0.003</td>
<td>0.0158% (415)</td>
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<tr>
<td>m60.9869</td>
<td>60.987</td>
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<td>200</td>
<td>0.28, (0.02, 0.24, 0.57)</td>
<td>0.003</td>
<td>0.025% (363)</td>
</tr>
<tr>
<td>m61.0291</td>
<td>61.029</td>
<td>C₃H₈O₂⁺ (0.3)</td>
<td>200</td>
<td>33, (1.6, 30, 65)</td>
<td>0.214</td>
<td>2.99% (3)</td>
</tr>
<tr>
<td>m61.9805</td>
<td>61.980</td>
<td>CH(OS)⁺ (-2.0)</td>
<td>200</td>
<td>0.024, (0.001, 0.019, 0.056)</td>
<td>0.005</td>
<td>0.021% (583)</td>
</tr>
<tr>
<td>m62.0298</td>
<td>62.029</td>
<td>C₂H₄O₂⁺ (-2.4)</td>
<td>200</td>
<td>0.92, (0.03, 0.86, 1.79)</td>
<td>0.009</td>
<td>0.082% (199)</td>
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<tr>
<td>m63.0015</td>
<td>63.001</td>
<td></td>
<td>300</td>
<td>0.045, (0.003, 0.039, 0.093)</td>
<td>0.006</td>
<td>0.0040% (527)</td>
</tr>
<tr>
<td>m63.0256</td>
<td>63.025</td>
<td>CH₃NO₂⁺ (-1.9), C₃H₆SH⁺ (-1.2)</td>
<td>150</td>
<td>0.082, (0.001, 0.074, 0.179)</td>
<td>0.008</td>
<td>0.0074% (481)</td>
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<tr>
<td>m63.0438</td>
<td>63.043</td>
<td>C₂H₆O₂⁺ (-0.7)</td>
<td>200</td>
<td>0.26, (0.00, 0.20, 0.57)</td>
<td>0.025</td>
<td>0.023% (375)</td>
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<td>m64.0042</td>
<td>64.004</td>
<td>HNO₃⁺ (0.8)</td>
<td>150</td>
<td>0.007, (0.000, 0.004, 0.014)</td>
<td>0.002</td>
<td>0.00061% (531)</td>
</tr>
<tr>
<td>m64.0421</td>
<td>64.042</td>
<td>CH₅NO₂⁺ (2.3)</td>
<td>200</td>
<td>0.022, (0.000, 0.014, 0.046)</td>
<td>0.002</td>
<td>0.0020% (588)</td>
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<tr>
<td>m64.9703</td>
<td>64.970</td>
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<td>250</td>
<td>0.028, (0.001, 0.021, 0.058)</td>
<td>0.001</td>
<td>0.0025% (569)</td>
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<tr>
<td>m65.0244</td>
<td>65.024</td>
<td>CH₄O₂⁺ (0.5), C₄H₇NH⁺ (2.3)</td>
<td>150</td>
<td>1.02, (0.03, 0.77, 2.24)</td>
<td>0.008</td>
<td>0.091% (185)</td>
</tr>
<tr>
<td>m65.0601</td>
<td>65.060</td>
<td></td>
<td>150</td>
<td>0.038, (0.002, 0.035, 0.074)</td>
<td>0.003</td>
<td>0.0034% (544)</td>
</tr>
<tr>
<td>m</td>
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<td>Error</td>
<td>Standard Deviation</td>
<td>Uncertainty</td>
<td>Uncertainty Percentage</td>
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<tr>
<td>65.978</td>
<td>0.011, (0.000, 0.008, 0.024)</td>
<td>0.001</td>
<td>0.0009% (625)</td>
<td></td>
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<tr>
<td>66.028</td>
<td>0.031, (0.001, 0.032, 0.061)</td>
<td>0.002</td>
<td>0.0028% (559)</td>
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<td>67.030</td>
<td>0.025, (0.001, 0.020, 0.056)</td>
<td>0.003</td>
<td>0.0023% (579)</td>
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<tr>
<td>67.054</td>
<td>0.91, (0.01, 0.70, 2.06)</td>
<td>0.028</td>
<td>0.081% (202)</td>
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<tr>
<td>68.027</td>
<td>0.017, (0.002, 0.016, 0.033)</td>
<td>0.004</td>
<td>0.00156% (605)</td>
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<tr>
<td>68.051</td>
<td>0.52, (0.01, 0.43, 1.08)</td>
<td>0.012</td>
<td>0.047% (275)</td>
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<td>68.998</td>
<td>0.039, (0.001, 0.025, 0.088)</td>
<td>0.002</td>
<td>0.0035% (541)</td>
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<td>69.034</td>
<td>1.49, (0.03, 1.16, 3.33)</td>
<td>0.080</td>
<td>0.134% (136)</td>
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<tr>
<td>70.006</td>
<td>0.004, (0.000, 0.003, 0.009)</td>
<td>0.002</td>
<td>0.00035% (638)</td>
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<tr>
<td>70.031</td>
<td>0.27, (0.01, 0.27, 0.51)</td>
<td>0.006</td>
<td>0.024% (368)</td>
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<tr>
<td>70.071</td>
<td>0.34, (-0.01, 0.24, 0.80)</td>
<td>0.021</td>
<td>0.030% (335)</td>
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<tr>
<td>71.016</td>
<td>0.26, (0.01, 0.19, 0.64)</td>
<td>0.008</td>
<td>0.024% (373)</td>
<td></td>
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</tr>
<tr>
<td>71.049</td>
<td>5.4, (0.23, 4.8, 10.6)</td>
<td>0.092</td>
<td>0.49% (46)</td>
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<td>72.008</td>
<td>0.044, (0.001, 0.031, 0.099)</td>
<td>0.002</td>
<td>0.0040% (528)</td>
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<td>72.047</td>
<td>0.86, (0.02, 0.73, 1.79)</td>
<td>0.014</td>
<td>0.077% (214)</td>
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<td>73.029</td>
<td>13.1, (1.22, 13.6, 23.9)</td>
<td>0.125</td>
<td>1.18% (17)</td>
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<td>73.051</td>
<td>0.72, (0.03, 0.59, 1.66)</td>
<td>0.016</td>
<td>0.064% (240)</td>
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<td>73.064</td>
<td>1.41, (-0.05, 1.23, 3.00)</td>
<td>0.140</td>
<td>0.126% (143)</td>
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<tr>
<td>74.026</td>
<td>0.91, (0.06, 0.92, 1.74)</td>
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<td>0.082% (201)</td>
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<td>74.062</td>
<td>0.35, (0.01, 0.31, 0.73)</td>
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<td>0.031% (333)</td>
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<tr>
<td>75.009</td>
<td>0.161, (0.004, 0.146, 0.350)</td>
<td>0.006</td>
<td>0.0144% (424)</td>
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<tr>
<td>75.044</td>
<td>5.5, (0.07, 5.5, 0.293</td>
<td>0.50% (45)</td>
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</table>
m75.9962 75.995 150 0.016, (0.001, 0.011, 0.040) 0.005 0.00143% (612)
m76.0429 76.042 C₂H₅NO₂H⁺ (2.8) 200 0.47, (0.01, 0.32, 1.09) 0.006 0.042% (291)
m76.9808 76.980 150 0.038, (0.002, 0.026, 0.096) 0.002 0.0034% (543)
m77.0609 77.060 C₃H₈O₂H⁺ (0.4) 150 0.155, (0.003, 0.099, 0.371) 0.006 0.0139% (429)
m77.9933 77.992 N₂O₃H⁺ (-2.7) 150 0.005, (0.000, 0.003, 0.011) 0.002 0.00042% (636)
m78.9962 78.995 150 0.185, (0.016, 0.165, 0.353) 0.063 0.0166% (406)
m79.0415 79.041 C₂H₆O₃H⁺ (1.7) 200 0.94, (0.00, 0.51, 2.32) 0.013 0.084% (193)
m79.9998 79.992 HNO₄H⁺ (1.1) 150 0.004, (0.000, 0.003, 0.009) 0.001 0.00039% (637)
m80.0149 80.014 C₃HNOH⁺ (0.9) 300 0.040, (0.001, 0.026, 0.108) 0.005 0.0036% (538)
m80.0515 80.051 C₃H₅NH⁺ (1.2), CH₆N₂O₂H⁺ (-2.9) 300 0.42, (0.01, 0.37, 0.86) 0.033 0.038% (312)
m80.9934 80.993 HNO₄H⁺ (-2.4) 150 0.048, (0.002, 0.039, 0.099) 0.012 0.0043% (522)
m81.0359 81.035 C₃H₄OH⁺ (1.5), CH₅NO₃H⁺ (-2.6) 250 0.88, (0.02, 0.63, 2.00) 0.033 0.079% (209)
m81.0707 81.070 C₅H₈H⁺ (-0.1) 150 1.22, (-0.02, 0.89, 3.10) 0.116 0.109% (162)
m82.0060 82.005 150 0.006, (0.000, 0.005, 0.014) 0.001 0.00057% (633)
m82.0333 82.032 300 0.36, (0.02, 0.34, 0.72) 0.009 0.033% (327)
m82.0693 82.068 300 0.58, (0.01, 0.44, 1.32) 0.008 0.052% (266)
m82.9464 82.946 200 0.016, (0.001, 0.009, 0.038) 0.007 0.00140% (614)
m83.0152 83.014 C₄H₂O₂H⁺ (1.5) 150 0.50, (0.00, 0.36, 1.09) 0.025 0.044% (283)
m83.0503 83.049 C₅H₆OH⁺ (0.2) 150 8.6, (0.27, 6.7, 16.9) 0.189 0.77% (33)
m84.0227 84.022 C₂HN₃OH⁺ (2.5) 150 0.012, (-0.001, 0.006, 0.034) 0.004 0.00106% (623)
<table>
<thead>
<tr>
<th>m</th>
<th>m</th>
<th>C_6H_{10}^+ (-2.0)</th>
<th>150</th>
<th>1.15, (0.03, 0.96, 2.35)</th>
<th>0.001</th>
<th>0.103% (175)</th>
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<td>m</td>
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<td>C_6H_4O_2^+ (0.3)</td>
<td>150</td>
<td>8.2, (0.33, 7.4, 16.3)</td>
<td>0.175</td>
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<td>m</td>
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<td>C_3H_8OH^+ (0.1)</td>
<td>150</td>
<td>4.6, (0.15, 4.0, 9.4)</td>
<td>0.098</td>
<td>0.41% (55)</td>
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<td>m</td>
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<td>C_4H_10O^+ (-0.3)</td>
<td>200</td>
<td>0.65, (0.01, 0.59, 1.32)</td>
<td>0.006</td>
<td>0.058% (255)</td>
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<td>m</td>
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<td>C_5H_10O^+ (1.7)</td>
<td>200</td>
<td>0.97, (0.03, 0.81, 2.05)</td>
<td>0.014</td>
<td>0.087% (191)</td>
</tr>
<tr>
<td>m</td>
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<td>C_4H_10O^+ (0.2)</td>
<td>150</td>
<td>12.9, (0.42, 11.5, 25.4)</td>
<td>0.080</td>
<td>1.15% (19)</td>
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<tr>
<td>m</td>
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<td>C_3H_10OH^+ (-0.3)</td>
<td>200</td>
<td>1.90, (0.01, 1.83, 3.96)</td>
<td>0.060</td>
<td>0.170% (109)</td>
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<td>m</td>
<td>m</td>
<td>C_6H_10O_2^+ (0.1)</td>
<td>150</td>
<td>0.90, (0.00, 0.005, 0.016)</td>
<td>0.002</td>
<td>0.00061% (632)</td>
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<tr>
<td>m</td>
<td>m</td>
<td>C_4H_8O_2H^+ (-0.6)</td>
<td>150</td>
<td>0.94, (0.01, 0.86, 2.06)</td>
<td>0.099</td>
<td>0.084% (194)</td>
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<tr>
<td>m</td>
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<td>C_3H_7NOH^+ (0.7)</td>
<td>150</td>
<td>0.103, (0.001, 0.048, 0.279)</td>
<td>0.029</td>
<td>0.0092% (457)</td>
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<td>m</td>
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<td>C_4H_8O_2H^+ (-1.9)</td>
<td>150</td>
<td>0.179, (-0.006, 0.118, 0.441)</td>
<td>0.007</td>
<td>0.0161% (410)</td>
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<tr>
<td>m</td>
<td>m</td>
<td>C_3H_8O_2^+ (2.8)</td>
<td>250</td>
<td>0.128, (0.000, 0.043, 0.363)</td>
<td>n.c.</td>
<td>0.0114% (440)</td>
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<tr>
<td>m</td>
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<td>C_7H_8H^+ (0.1)</td>
<td>100</td>
<td>0.021, (0.000, 0.017, 0.043)</td>
<td>0.008</td>
<td>0.00187% (595)</td>
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<td>Mass (m)</td>
<td>Mol. Wt (M)</td>
<td>Figures</td>
<td>T (K)</td>
<td>Intensity (a.u.)</td>
<td>Relative Intensity (%)</td>
<td></td>
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<td>m92.9588</td>
<td>92.958</td>
<td>150</td>
<td>0.014, (0.000, 0.012, 0.031)</td>
<td>0.003</td>
<td>0.00127% (618)</td>
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<tr>
<td>m93.0123</td>
<td>93.011</td>
<td>150</td>
<td>0.48, (0.03, 0.45, 0.93)</td>
<td>0.018</td>
<td>0.043% (288)</td>
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<tr>
<td>m93.0380</td>
<td>93.037</td>
<td>150</td>
<td>0.24, (0.00, 0.24, 0.48)</td>
<td>0.031</td>
<td>0.021% (385)</td>
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<td>m93.0705</td>
<td>93.069</td>
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<td>1.20, (0.01, 0.94, 2.84)</td>
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<td>0.107% (167)</td>
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<tr>
<td>m94.0086</td>
<td>94.008</td>
<td>150</td>
<td>0.037, (0.002, 0.030, 0.076)</td>
<td>0.001</td>
<td>0.0033% (547)</td>
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<tr>
<td>m94.0338</td>
<td>94.033</td>
<td>300</td>
<td>0.23, (0.02, 0.21, 0.42)</td>
<td>0.039</td>
<td>0.020% (387)</td>
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<tr>
<td>m94.0682</td>
<td>94.067</td>
<td>300</td>
<td>0.57, (0.00, 0.46, 1.36)</td>
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<td>0.051% (267)</td>
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<tr>
<td>m94.9929</td>
<td>94.992</td>
<td>150</td>
<td>0.90, (0.01, 0.66, 1.94)</td>
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<td>0.081% (204)</td>
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<tr>
<td>m95.047</td>
<td>95.047</td>
<td>250</td>
<td>2.5, (0.05, 1.9, 5.2)</td>
<td>0.242</td>
<td>0.22% (95)</td>
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<td>m95.0861</td>
<td>95.085</td>
<td>150</td>
<td>1.26, (-0.07, 0.91, 3.11)</td>
<td>0.264</td>
<td>0.113% (156)</td>
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<tr>
<td>m95.9523</td>
<td>95.951</td>
<td>150</td>
<td>0.012, (0.001, 0.010, 0.027)</td>
<td>0.003</td>
<td>0.00109% (621)</td>
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<tr>
<td>m96.046</td>
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<td>150</td>
<td>1.31, (0.02, 1.21, 2.62)</td>
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<td>0.118% (149)</td>
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<tr>
<td>m96.0879</td>
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<td>0.34, (0.00, 0.28, 0.77)</td>
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<td>0.031% (334)</td>
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<td>m96.9621</td>
<td>96.961</td>
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<td>0.040, (0.001, 0.033, 0.092)</td>
<td>0.011</td>
<td>0.0036% (537)</td>
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<td>m96.9909</td>
<td>96.990</td>
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<td>0.23, (0.00, 0.14, 0.59)</td>
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<td>0.020% (389)</td>
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<td>m97.0297</td>
<td>97.029</td>
<td>250</td>
<td>13.4, (0.88, 13.7, 25.4)</td>
<td>0.193</td>
<td>1.20% (16)</td>
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<td>m97.0652</td>
<td>97.064</td>
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<td>5.7, (0.21, 4.3, 12.9)</td>
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<td>0.51% (44)</td>
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<td>m97.9474</td>
<td>97.946</td>
<td>200</td>
<td>0.025, (0.000, 0.019, 0.055)</td>
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<td>0.0022% (582)</td>
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<td>m98.0263</td>
<td>98.025</td>
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<td>2.7, (0.13, 2.8, 5.1)</td>
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<td>m98.0623</td>
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<td>1.42, (0.03, 1.13, 3.00)</td>
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<td>Formula</td>
<td>Charge</td>
<td>Temperature</td>
<td>Retention</td>
<td>Width</td>
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<td>m98.1042</td>
<td>98.103</td>
<td>C₇H₁₂H⁺ (-1.4)</td>
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<td>300</td>
<td>0.138, (-0.006, 0.112, 0.293)</td>
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<tr>
<td>m98.960</td>
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<td>C₇H₂O₃H⁺ (0.4), H₃NO₃H⁺ (2.6)</td>
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<td>200</td>
<td>0.44, (0.02, 0.41, 0.88)</td>
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<td>m99.0091</td>
<td>99.008</td>
<td>C₃H₆O₂H⁺ (-0.2)</td>
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<td>200</td>
<td>20, (0.9, 20, 37)</td>
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<td>m99.0449</td>
<td>99.044</td>
<td>C₆H₁₀OH⁺ (-1.2)</td>
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<td>3.2, (0.06, 2.9, 7.3)</td>
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<td>m99.9479</td>
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<td>C₄H₂O₃H⁺ (-1.9), C₂H₂N₃O₂H⁺ (-1.2)</td>
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<td>200</td>
<td>0.84, (0.03, 0.85, 1.61)</td>
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<td>m100.014</td>
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<td>C₃H₆O₂H⁺ (0.6), C₂H₂N₃H⁺ (2.4)</td>
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<td>200</td>
<td>4.0, (0.04, 3.2, 8.3)</td>
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<td>C₅H₈O₂H⁺ (0.2)</td>
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<td>9.2, (0.12, 8.8, 19.7)</td>
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<td>C₇H₉NO₂H⁺ (0.6)</td>
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<td>C₇H₆O₂H⁺ (1.0), C₂H₃NH⁺ (2.8)</td>
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<tr>
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<td>104.050</td>
<td>C&lt;sub&gt;2&lt;/sub&gt;H&lt;sub&gt;3&lt;/sub&gt;NH&lt;sup&gt;+&lt;/sup&gt; (0.5), C&lt;sub&gt;4&lt;/sub&gt;H&lt;sub&gt;9&lt;/sub&gt;NSH&lt;sup&gt;+&lt;/sup&gt; (-2.9)</td>
<td>300</td>
<td>0.47, (0.03, 0.39, 0.99)</td>
<td>0.016</td>
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<tr>
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<td>104.932</td>
<td>150</td>
<td>C&lt;sub&gt;2&lt;/sub&gt;H&lt;sub&gt;3&lt;/sub&gt;NO&lt;sub&gt;3&lt;/sub&gt;H&lt;sup&gt;+&lt;/sup&gt; (-1.6), C&lt;sub&gt;4&lt;/sub&gt;H&lt;sub&gt;9&lt;/sub&gt;OSH&lt;sup&gt;+&lt;/sup&gt; (-0.9)</td>
<td>150</td>
<td>0.005, (-0.001, 0.003, 0.011)</td>
<td>0.002</td>
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<tr>
<td>m104.959</td>
<td>104.958</td>
<td>150</td>
<td>C&lt;sub&gt;2&lt;/sub&gt;H&lt;sub&gt;3&lt;/sub&gt;OH&lt;sup&gt;+&lt;/sup&gt; (1.1), C&lt;sub&gt;3&lt;/sub&gt;H&lt;sub&gt;5&lt;/sub&gt;N&lt;sub&gt;3&lt;/sub&gt;H&lt;sup&gt;+&lt;/sup&gt; (-2.0)</td>
<td>150</td>
<td>0.121, (0.004, 0.104, 0.240)</td>
<td>0.008</td>
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<tr>
<td>m105.037</td>
<td>105.036</td>
<td>150</td>
<td>C&lt;sub&gt;2&lt;/sub&gt;H&lt;sub&gt;2&lt;/sub&gt;NH&lt;sup&gt;+&lt;/sup&gt; (1.2), C&lt;sub&gt;3&lt;/sub&gt;H&lt;sub&gt;5&lt;/sub&gt;N&lt;sub&gt;3&lt;/sub&gt;H&lt;sup&gt;+&lt;/sup&gt; (-2.9)</td>
<td>200</td>
<td>0.146, (0.000, 0.118, 0.312)</td>
<td>0.016</td>
</tr>
<tr>
<td>m106.039</td>
<td>106.038</td>
<td>150</td>
<td>C&lt;sub&gt;2&lt;/sub&gt;H&lt;sub&gt;3&lt;/sub&gt;OH&lt;sup&gt;+&lt;/sup&gt; (-0.5)</td>
<td>300</td>
<td>0.25, (0.02, 0.22, 0.45)</td>
<td>0.044</td>
</tr>
<tr>
<td>m106.072</td>
<td>106.071</td>
<td>150</td>
<td>C&lt;sub&gt;2&lt;/sub&gt;H&lt;sub&gt;3&lt;/sub&gt;NH&lt;sup&gt;+&lt;/sup&gt; (1.2), C&lt;sub&gt;3&lt;/sub&gt;H&lt;sub&gt;5&lt;/sub&gt;N&lt;sub&gt;3&lt;/sub&gt;H&lt;sup&gt;+&lt;/sup&gt; (-2.9)</td>
<td>200</td>
<td>0.52, (0.01, 0.34, 1.27)</td>
<td>0.014</td>
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<tr>
<td>m106.939</td>
<td>106.938</td>
<td>150</td>
<td>C&lt;sub&gt;2&lt;/sub&gt;H&lt;sub&gt;3&lt;/sub&gt;OH&lt;sup&gt;+&lt;/sup&gt; (0.5)</td>
<td>200</td>
<td>0.32, (0.001, 0.030, 0.068)</td>
<td>0.005</td>
</tr>
<tr>
<td>m107.085</td>
<td>107.084</td>
<td>150</td>
<td>C&lt;sub&gt;2&lt;/sub&gt;H&lt;sub&gt;2&lt;/sub&gt;NH&lt;sup&gt;+&lt;/sup&gt; (1.2), C&lt;sub&gt;3&lt;/sub&gt;H&lt;sub&gt;5&lt;/sub&gt;N&lt;sub&gt;3&lt;/sub&gt;H&lt;sup&gt;+&lt;/sup&gt; (-2.9)</td>
<td>200</td>
<td>1.86, (0.08, 1.68, 3.77)</td>
<td>0.016</td>
</tr>
<tr>
<td>m108.053</td>
<td>108.052</td>
<td>150</td>
<td>C&lt;sub&gt;2&lt;/sub&gt;H&lt;sub&gt;2&lt;/sub&gt;NH&lt;sup&gt;+&lt;/sup&gt; (1.2), C&lt;sub&gt;3&lt;/sub&gt;H&lt;sub&gt;5&lt;/sub&gt;N&lt;sub&gt;3&lt;/sub&gt;H&lt;sup&gt;+&lt;/sup&gt; (-2.9)</td>
<td>150</td>
<td>3.8, (0.12, 2.8, 8.8)</td>
<td>0.155</td>
</tr>
<tr>
<td>m108.961</td>
<td>108.960</td>
<td>200</td>
<td>C&lt;sub&gt;2&lt;/sub&gt;H&lt;sub&gt;2&lt;/sub&gt;NH&lt;sup&gt;+&lt;/sup&gt; (0.2)</td>
<td>200</td>
<td>0.88, (-0.05, 0.69, 1.99)</td>
<td>0.245</td>
</tr>
<tr>
<td>m109.031</td>
<td>109.030</td>
<td>200</td>
<td>C&lt;sub&gt;2&lt;/sub&gt;H&lt;sub&gt;2&lt;/sub&gt;NH&lt;sup&gt;+&lt;/sup&gt; (1.2), C&lt;sub&gt;3&lt;/sub&gt;H&lt;sub&gt;5&lt;/sub&gt;N&lt;sub&gt;3&lt;/sub&gt;H&lt;sup&gt;+&lt;/sup&gt; (-2.9)</td>
<td>150</td>
<td>0.009, (0.001, 0.006, 0.021)</td>
<td>0.002</td>
</tr>
<tr>
<td>m109.066</td>
<td>109.065</td>
<td>150</td>
<td>C&lt;sub&gt;2&lt;/sub&gt;H&lt;sub&gt;2&lt;/sub&gt;NH&lt;sup&gt;+&lt;/sup&gt; (0.2)</td>
<td>200</td>
<td>0.185, (0.008, 0.177, 0.357)</td>
<td>0.002</td>
</tr>
<tr>
<td>m110.035</td>
<td>110.034</td>
<td>200</td>
<td>C&lt;sub&gt;2&lt;/sub&gt;H&lt;sub&gt;2&lt;/sub&gt;NH&lt;sup&gt;+&lt;/sup&gt; (2.9), C&lt;sub&gt;3&lt;/sub&gt;H&lt;sub&gt;5&lt;/sub&gt;N&lt;sub&gt;3&lt;/sub&gt;H&lt;sup&gt;+&lt;/sup&gt; (-0.9)</td>
<td>150</td>
<td>1.29, (0.02, 0.93, 2.90)</td>
<td>0.028</td>
</tr>
<tr>
<td>m</td>
<td>110.105</td>
<td>C₇H₁₂H⁺ (-0.6)</td>
<td>150</td>
<td>0.25, (-0.01, 0.18, 0.59)</td>
<td>0.029</td>
<td>0.022% (382)</td>
</tr>
<tr>
<td>-----</td>
<td>---------</td>
<td>----------------</td>
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<td>--------------------------</td>
<td>-------</td>
<td>---------------</td>
</tr>
<tr>
<td>m</td>
<td>111.046</td>
<td>C₆H₁₀₂H⁺ (0.9)</td>
<td>200</td>
<td>17.6, (0.54, 15.3, 38.0)</td>
<td>0.132</td>
<td>1.57% (12)</td>
</tr>
<tr>
<td>m</td>
<td>111.081</td>
<td>C₇₁₀OH⁺ (-0.5)</td>
<td>150</td>
<td>4.9, (0.10, 3.7, 11.3)</td>
<td>0.091</td>
<td>0.44% (51)</td>
</tr>
<tr>
<td>m</td>
<td>111.956</td>
<td>C₆H₁₂H⁺ (-0.6)</td>
<td>150</td>
<td>0.029, (0.001, 0.020, 0.067)</td>
<td>0.003</td>
<td>0.0026% (566)</td>
</tr>
<tr>
<td>m</td>
<td>112.043</td>
<td>C₇H₁₂NO₂H⁺ (2.7), CH₅N₂O₄H⁺ (-1.4)</td>
<td>300</td>
<td>0.74, (0.03, 0.56, 1.73)</td>
<td>n.c.</td>
<td>0.066% (235)</td>
</tr>
<tr>
<td>m</td>
<td>112.079</td>
<td>C₆H₁₀NO⁺ (2.3)</td>
<td>150</td>
<td>1.02, (0.01, 0.78, 2.27)</td>
<td>0.013</td>
<td>0.092% (184)</td>
</tr>
<tr>
<td>m</td>
<td>112.961</td>
<td>C₅H₁₀NO₂H⁺ (-0.7)</td>
<td>150</td>
<td>0.27, (0.01, 0.25, 0.54)</td>
<td>0.021</td>
<td>0.024% (369)</td>
</tr>
<tr>
<td>m</td>
<td>113.026</td>
<td>C₆H₁₂NO₂H⁺ (1.7), CH₅NO₃H⁺ (-2.4)</td>
<td>200</td>
<td>15.3, (0.71, 15.2, 29.3)</td>
<td>0.308</td>
<td>1.37% (14)</td>
</tr>
<tr>
<td>m</td>
<td>113.059</td>
<td>C₆H₁₂OH⁺ (-0.1)</td>
<td>150</td>
<td>19.4, (0.38, 16.4, 38.8)</td>
<td>0.521</td>
<td>1.74% (11)</td>
</tr>
<tr>
<td>m</td>
<td>113.097</td>
<td>C₇H₁₂OH⁺ (-0.1)</td>
<td>150</td>
<td>2.8, (0.00, 2.3, 6.2)</td>
<td>0.090</td>
<td>0.25% (85)</td>
</tr>
<tr>
<td>m</td>
<td>114.025</td>
<td>C₅H₁₀NO⁺ (2.7)</td>
<td>200</td>
<td>0.93, (0.03, 0.92, 1.86)</td>
<td>0.019</td>
<td>0.084% (195)</td>
</tr>
<tr>
<td>m</td>
<td>114.057</td>
<td>C₇H₁₂NO₂H⁺ (2.0)</td>
<td>150</td>
<td>1.47, (0.05, 1.11, 3.40)</td>
<td>n.c.</td>
<td>0.132% (137)</td>
</tr>
<tr>
<td>m</td>
<td>114.092</td>
<td>C₇H₁₁NO₂H⁺ (-0.4)</td>
<td>150</td>
<td>0.43, (0.01, 0.32, 1.02)</td>
<td>0.019</td>
<td>0.039% (309)</td>
</tr>
<tr>
<td>m</td>
<td>114.958</td>
<td>C₇H₁₁OH⁺ (-0.4)</td>
<td>150</td>
<td>0.081, (0.002, 0.056, 0.189)</td>
<td>0.002</td>
<td>0.0073% (485)</td>
</tr>
<tr>
<td>m</td>
<td>115.040</td>
<td>C₅H₁₀NO₂H⁺ (0.0), C₅H₁₀NH⁺ (1.8)</td>
<td>150</td>
<td>13.6, (0.04, 12.1, 31.5)</td>
<td>0.132</td>
<td>1.22% (15)</td>
</tr>
<tr>
<td>m</td>
<td>115.076</td>
<td>C₆H₁₀O₂H⁺ (-0.4)</td>
<td>150</td>
<td>8.9, (0.09, 7.9, 18.9)</td>
<td>0.099</td>
<td>0.80% (31)</td>
</tr>
<tr>
<td>m</td>
<td>115.112</td>
<td>C₇H₁₄OH⁺ (-0.7)</td>
<td>150</td>
<td>0.53, (-0.07, 0.36, 1.41)</td>
<td>0.065</td>
<td>0.048% (273)</td>
</tr>
<tr>
<td>m</td>
<td>116.039</td>
<td>C₇H₁₄OH⁺ (-0.7)</td>
<td>150</td>
<td>1.22, (0.00, 0.92, 2.85)</td>
<td>0.005</td>
<td>0.110% (160)</td>
</tr>
<tr>
<td>m</td>
<td>116.078</td>
<td>C₇H₁₄OH⁺ (-1.7)</td>
<td>150</td>
<td>0.86, (0.01, 0.74, 1.93)</td>
<td>0.008</td>
<td>0.077% (213)</td>
</tr>
<tr>
<td>m</td>
<td>116.115</td>
<td>C₇H₁₄OH⁺ (-1.1)</td>
<td>150</td>
<td>0.98, (-0.007, 0.083, 0.234)</td>
<td>0.008</td>
<td>0.0088% (460)</td>
</tr>
<tr>
<td>m</td>
<td>116.909</td>
<td>C₇H₁₄OH⁺ (-1.1)</td>
<td>150</td>
<td>0.041, (0.000, 0.028, 0.095)</td>
<td>0.014</td>
<td>0.0037% (535)</td>
</tr>
<tr>
<td>m</td>
<td>m+1</td>
<td>C/H/O/H+</td>
<td>m</td>
<td>m+1</td>
<td>C/H/O/H+</td>
<td>m</td>
</tr>
<tr>
<td>-----</td>
<td>-----</td>
<td>----------</td>
<td>-----</td>
<td>-----</td>
<td>----------</td>
<td>-----</td>
</tr>
<tr>
<td>117.021</td>
<td>117.020</td>
<td>C₂H₄O₄H⁺ (1.8)</td>
<td>200</td>
<td>1.52, (0.06, 1.17, 3.35)</td>
<td>0.021</td>
<td>0.136% (130)</td>
</tr>
<tr>
<td>117.056</td>
<td>117.055</td>
<td>C₃H₆O₃H⁺ (0.4), C₅H₅NH⁺ (2.2)</td>
<td>150</td>
<td>3.7, (0.03, 3.0, 8.5)</td>
<td>0.007</td>
<td>0.33% (63)</td>
</tr>
<tr>
<td>117.091</td>
<td>117.090</td>
<td>C₆H₁₂O₂H⁺ (-1.0)</td>
<td>150</td>
<td>0.35, (0.01, 0.30, 0.80)</td>
<td>0.037</td>
<td>0.032% (330)</td>
</tr>
<tr>
<td>117.959</td>
<td>117.958</td>
<td>C₇H₈O₃H⁺ (2.4), C₈H₇N₃O₃H⁺ (-0.7)</td>
<td>150</td>
<td>0.016, (0.000, 0.012, 0.036)</td>
<td>0.002</td>
<td>0.00145% (609)</td>
</tr>
<tr>
<td>118.025</td>
<td>118.024</td>
<td>C₄H₂O₄H⁺ (1.8), C₈H₅NH⁺ (2.2)</td>
<td>150</td>
<td>0.21, (0.01, 0.18, 0.47)</td>
<td>0.007</td>
<td>0.0192% (397)</td>
</tr>
<tr>
<td>118.078</td>
<td>118.077</td>
<td>C₅H₈O₃H⁺ (2.4)</td>
<td>150</td>
<td>0.50, (0.00, 0.36, 1.15)</td>
<td>0.084</td>
<td>0.045% (280)</td>
</tr>
<tr>
<td>118.995</td>
<td>118.994</td>
<td>C₆H₁₀O₂H⁺ (-1.0)</td>
<td>150</td>
<td>0.31, (0.04, 0.24, 0.66)</td>
<td>0.041</td>
<td>0.028% (350)</td>
</tr>
<tr>
<td>119.038</td>
<td>119.037</td>
<td>C₇H₉O₂H⁺ (2.4), C₈H₉N₃O₃H⁺ (-0.7)</td>
<td>150</td>
<td>1.57, (-0.02, 0.92, 3.63)</td>
<td>0.502</td>
<td>0.140% (126)</td>
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<tr>
<td>120.048</td>
<td>120.047</td>
<td>C₈H₁₀O₂H⁺ (2.4), C₉H₆N₂O₃H⁺ (-1.4), C₉H₆N₂O₃H⁺ (-0.7)</td>
<td>300</td>
<td>0.33, (0.01, 0.29, 0.68)</td>
<td>0.046</td>
<td>0.030% (340)</td>
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<tr>
<td>120.091</td>
<td>120.090</td>
<td>C₉H₁₀H⁺ (1.2)</td>
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<td>0.46, (-0.02, 0.19, 0.84)</td>
<td>0.097</td>
<td>0.041% (298)</td>
</tr>
<tr>
<td>120.903</td>
<td>120.902</td>
<td>C₂H₆N₂O₃H⁺ (-1.4)</td>
<td>150</td>
<td>0.013, (-0.001, 0.008, 0.034)</td>
<td>0.006</td>
<td>0.00118% (619)</td>
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<tr>
<td>121.066</td>
<td>121.065</td>
<td>C₇H₈O₂H⁺ (2.4)</td>
<td>150</td>
<td>3.6, (0.12, 1.6, 8.9)</td>
<td>1.005</td>
<td>0.32% (66)</td>
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<tr>
<td>122.967</td>
<td>122.966</td>
<td>C₈H₁₀O₂H⁺ (2.4), C₈H₁₀N₂O₃H⁺ (-2.4)</td>
<td>150</td>
<td>0.079, (0.003, 0.057, 0.201)</td>
<td>0.012</td>
<td>0.0070% (488)</td>
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<tr>
<td>123.046</td>
<td>123.045</td>
<td>C₉H₆O₂H⁺ (1.0), C₉H₁₀O₂H⁺ (-2.4)</td>
<td>150</td>
<td>4.9, (0.06, 4.5, 10.2)</td>
<td>0.079</td>
<td>0.44% (53)</td>
</tr>
<tr>
<td>123.079</td>
<td>123.078</td>
<td>C₉H₁₀OH⁺ (-2.4), C₉H₁₀N₂O₃H⁺ (1.6)</td>
<td>150</td>
<td>3.4, (0.13, 2.9, 7.8)</td>
<td>0.024</td>
<td>0.31% (70)</td>
</tr>
<tr>
<td>123.118</td>
<td>123.117</td>
<td>C₉H₁₄H⁺ (0.2)</td>
<td>150</td>
<td>0.40, (-0.03, 0.30, 0.96)</td>
<td>0.241</td>
<td>0.036% (317)</td>
</tr>
<tr>
<td>124.046</td>
<td>124.045</td>
<td>C₉H₆O₂H⁺ (-2.3), C₉H₆N₂O₃H⁺ (1.7), C₉H₆NO₂SH⁺ (2.4)</td>
<td>150</td>
<td>1.21, (0.02, 1.18, 2.37)</td>
<td>0.010</td>
<td>0.109% (165)</td>
</tr>
<tr>
<td>124.079</td>
<td>124.078</td>
<td>C₉H₆NOH⁺ (2.4), C₉H₁₀N₂O₃H⁺ (-1.7)</td>
<td>150</td>
<td>0.88, (0.01, 0.63, 2.00)</td>
<td>0.017</td>
<td>0.079% (211)</td>
</tr>
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</table>
m124.120 124.119 $C_9H_{14}H^+$ (-1.1) 150 0.117, (-0.006, 0.085, 0.273) 0.029 0.0105% (449)  
124.950 124.949 $C_9S_{2}H^+$ (-2.3) 150 0.086, (0.006, 0.069, 0.181) 0.006 0.0077% (474)  
m125.026 125.025 $C_7H_{9}O_{3}H^+$ (1.8), $C_9H_{9}NO_{3}H^+$ (-2.3), $C_9H_{9}O_{3}SH^+$ (-1.6) 250 4.3, (0.34, 4.6, 7.1) 0.097 0.38% (57)  
m125.061 125.060 $C_9H_{8}O_{2}H^+$ (0.4) 150 12.1, (0.31, 9.3, 25.2) 0.161 1.08% (20)  
m125.096 125.095 $C_8H_{12}OH^+$ (-1.0) 150 3.4, (0.02, 2.7, 8.3) 0.101 0.30% (71)  
m125.963 125.962 $C_7H_{7}N_{2}O_{5}H^+$ (0.5), $C_2H_{7}NO_{5}H^+$ (-2.9) 250 0.36, (0.02, 0.37, 0.66) 0.010 0.033% (328)  
m126.024 126.023 $C_8H_{9}N_{2}O_{4}H^+$ (0.1) 200 2.2, (0.04, 1.8, 4.6) 0.009 0.20% (103)  
m126.097 126.096 $C_9H_{9}N_{2}O_{5}H^+$ (1.1), $C_2H_{7}NO_{5}SH^+$ (-2.9) 150 0.61, (0.00, 0.46, 1.37) 0.012 0.055% (261)  
m126.908 126.907 $C_8H_{8}N_{2}O_{4}H^+$ (0.1) 150 0.028, (0.001, 0.019, 0.062) 0.002 0.0025% (568)  
m126.971 126.970 $C_9H_{8}O_{5}SH^+$ (0.5), $C_2H_{7}NO_{5}SH^+$ (-2.9) 150 0.21, (0.00, 0.17, 0.44) 0.008 0.0184% (400)  
m127.041 127.040 $C_8H_{8}O_{3}H^+$ (1.1), $C_2H_{7}NO_{3}H^+$ (-2.9) 150 8.4, (0.06, 7.8, 17.0) 0.155 0.75% (34)  
m127.076 127.075 $C_9H_{10}O_{2}H^+$ (-0.2) 200 20, (0.4, 17, 43) 0.492 1.83% (9)  
m127.112 127.111 $C_8H_{14}OH^+$ (-0.6) 150 1.62, (-0.07, 1.33, 4.16) 0.094 0.145% (123)  
m127.949 127.948 $C_9H_{9}N_{2}O_{5}H^+$ (-0.2) 150 0.033, (0.001, 0.024, 0.074) 0.002 0.0029% (553)  
m127.994 127.993 $CH_{2}O_{2}H^+$ (2.4) 150 0.042, (0.002, 0.030, 0.094) 0.006 0.0037% (532)  
m128.039 128.038 $CH_{6}N_{2}O_{5}H^+$ (-0.2) 200 0.92, (0.01, 0.73, 2.02) 0.009 0.082% (200)  
m128.076 128.075 $CH_{6}N_{2}O_{5}H^+$ (-0.2) 150 2.3, (0.03, 1.9, 5.1) 0.049 0.20% (99)  
m128.115 128.114 $C_9H_{14}OH^+$ (-1.0) 150 0.31, (0.00, 0.24, 0.73) 0.012 0.028% (351)  
m128.897 128.896 $C_9H_{14}OH^+$ (-1.0) 200 0.012, (0.001, 0.009, 0.025) 0.004 0.00108% (622)  
m128.973 128.972 $C_9H_{14}OH^+$ (-1.0) 150 0.158, (0.003, 0.131, 0.348) 0.025 0.0141% (426)
<table>
<thead>
<tr>
<th>Mass (m)</th>
<th>Abundance (I)</th>
<th>Retention Time (r)</th>
<th>M/Z Value (m/z)</th>
<th>Mass Difference (Δm)</th>
<th>Compound Description</th>
<th>Relative Abundance (%)</th>
<th>Figures and Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>129.056</td>
<td>0.362</td>
<td>150</td>
<td>129.055</td>
<td>0.5</td>
<td>C₂H₃O₂H⁺ (0.5), C₂H₃NH⁺ (2.3)</td>
<td>0.99% (23)</td>
<td>(0.10, 9.2, 24.3)</td>
</tr>
<tr>
<td>129.090</td>
<td>0.055</td>
<td>150</td>
<td>129.089</td>
<td>-1.9</td>
<td>C₆H₁₂O₂H⁺ (-1.9)</td>
<td>0.51% (43)</td>
<td>(0.01, 4.6, 13.2)</td>
</tr>
<tr>
<td>130.055</td>
<td>0.016</td>
<td>200</td>
<td>130.054</td>
<td>-0.3</td>
<td>C₆H₁₀OH⁺ (-0.3)</td>
<td>0.027% (356)</td>
<td>(0.04, 0.19, 0.81)</td>
</tr>
<tr>
<td>130.091</td>
<td>0.009</td>
<td>150</td>
<td>130.090</td>
<td>-1.9</td>
<td>C₆H₁₀OH⁺ (-1.9)</td>
<td>0.065% (238)</td>
<td>(0.00, 0.57, 1.75)</td>
</tr>
<tr>
<td>131.036</td>
<td>0.014</td>
<td>150</td>
<td>131.035</td>
<td>-1.4</td>
<td>C₅H₆N₂O₂H⁺ (-1.4)</td>
<td>0.040% (493)</td>
<td>(0.00, 0.35, 1.08)</td>
</tr>
<tr>
<td>131.085</td>
<td>0.007</td>
<td>150</td>
<td>131.084</td>
<td>-2.3</td>
<td>C₅H₉N₂O₂H⁺ (-2.3)</td>
<td>0.028% (352)</td>
<td>(0.00, 0.24, 0.67)</td>
</tr>
<tr>
<td>132.047</td>
<td>0.005</td>
<td>150</td>
<td>132.046</td>
<td>-1.7</td>
<td>C₅H₉N₂O₂H⁺ (-1.7)</td>
<td>0.043% (290)</td>
<td>(0.00, 0.33, 1.11)</td>
</tr>
<tr>
<td>132.084</td>
<td>0.023</td>
<td>150</td>
<td>132.083</td>
<td>-1.0</td>
<td>C₅H₁₀N₂O₂H⁺ (-1.0)</td>
<td>0.087% (190)</td>
<td>(0.01, 0.79, 2.17)</td>
</tr>
<tr>
<td>132.976</td>
<td>0.031</td>
<td>150</td>
<td>132.975</td>
<td>-2.4</td>
<td>C₅H₉N₂O₂H⁺ (-2.4)</td>
<td>0.031% (332)</td>
<td>(0.02, 0.24, 0.81)</td>
</tr>
<tr>
<td>133.007</td>
<td>0.053</td>
<td>150</td>
<td>133.006</td>
<td>-1.1</td>
<td>C₅H₁₀N₂O₂H⁺ (-1.1)</td>
<td>0.046% (49)</td>
<td>(0.01, 2.6, 14.6)</td>
</tr>
<tr>
<td>133.028</td>
<td>0.007</td>
<td>50</td>
<td>133.027</td>
<td>-1.2</td>
<td>C₅H₁₀N₂O₂H⁺ (-1.2)</td>
<td>0.040% (301)</td>
<td>(0.00, 0.025)</td>
</tr>
<tr>
<td>133.052</td>
<td>0.046</td>
<td>150</td>
<td>133.051</td>
<td>1.7</td>
<td>C₅H₁₀N₂O₂H⁺ (1.7)</td>
<td>0.114% (154)</td>
<td>(0.01, 2.6, 14.6)</td>
</tr>
<tr>
<td>133.066</td>
<td>0.242</td>
<td>350</td>
<td>133.065</td>
<td>-3.0</td>
<td>C₅H₁₀N₂O₂H⁺ (-3.0)</td>
<td>0.040% (301)</td>
<td>(0.02, 0.34, 0.81)</td>
</tr>
<tr>
<td>133.100</td>
<td>0.057</td>
<td>150</td>
<td>133.099</td>
<td>-2.0</td>
<td>C₅H₁₀N₂O₂H⁺ (-2.0)</td>
<td>0.114% (154)</td>
<td>(0.02, 0.99, 2.93)</td>
</tr>
<tr>
<td>m133.985</td>
<td>133.984</td>
<td>150</td>
<td>0.095, (0.005, 0.076, 0.188)</td>
<td>0.003</td>
<td>0.0085% (463)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>m134.066</td>
<td>134.065</td>
<td>150</td>
<td>0.80, (0.01, 0.61, 1.87)</td>
<td>0.008</td>
<td>0.071% (223)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>m134.102</td>
<td>134.101</td>
<td>150</td>
<td>0.23, (0.00, 0.15, 0.59)</td>
<td>0.012</td>
<td>0.021% (386)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>m134.966</td>
<td>134.965</td>
<td>150</td>
<td>0.193, (0.007, 0.159, 0.434)</td>
<td>0.007</td>
<td>0.0173% (404)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>m135.047</td>
<td>135.046</td>
<td>250</td>
<td>0.79, (0.03, 0.65, 1.64)</td>
<td>0.054</td>
<td>0.071% (225)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>m135.117</td>
<td>135.116</td>
<td>150</td>
<td>0.73, (-0.02, 0.53, 1.68)</td>
<td>0.137</td>
<td>0.065% (237)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>m136.044</td>
<td>136.043</td>
<td>250</td>
<td>0.45, (0.01, 0.41, 0.91)</td>
<td>0.013</td>
<td>0.040% (302)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>m136.083</td>
<td>136.082</td>
<td>150</td>
<td>0.99, (0.07, 0.80, 2.22)</td>
<td>0.009</td>
<td>0.089% (187)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>m136.960</td>
<td>136.959</td>
<td>150</td>
<td>0.122, (0.005, 0.106, 0.243)</td>
<td>0.024</td>
<td>0.0109% (445)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>m137.029</td>
<td>137.028</td>
<td>150</td>
<td>0.48, (0.01, 0.33, 0.96)</td>
<td>0.008</td>
<td>0.043% (286)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>m137.061</td>
<td>137.060</td>
<td>250</td>
<td>5.1, (0.18, 4.4, 11.3)</td>
<td>0.136</td>
<td>0.46% (47)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>m137.095</td>
<td>137.094</td>
<td>150</td>
<td>2.8, (0.06, 2.4, 7.0)</td>
<td>0.025</td>
<td>0.25% (84)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>m137.965</td>
<td>137.964</td>
<td>150</td>
<td>0.031, (0.001, 0.026, 0.064)</td>
<td>0.004</td>
<td>0.0028% (557)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>m138.015</td>
<td>138.014</td>
<td>300</td>
<td>0.115, (0.003, 0.084, 0.262)</td>
<td>0.021</td>
<td>0.0103% (451)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>m138.059</td>
<td>138.058</td>
<td>200</td>
<td>1.50, (0.02, 1.30, 3.02)</td>
<td>0.011</td>
<td>0.135% (133)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>m138.094</td>
<td>138.093</td>
<td>150</td>
<td>0.70, (0.01, 0.52, 1.46)</td>
<td>0.006</td>
<td>0.062% (243)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>m</td>
<td>138.136</td>
<td>138.135</td>
<td>C\textsubscript{10}H\textsubscript{16}H\textsuperscript{+} (-0.5)</td>
<td>300</td>
<td>0.026, (-0.003, 0.020, 0.060)</td>
<td>0.016</td>
<td>0.0024% (573)</td>
</tr>
<tr>
<td>m</td>
<td>138.965</td>
<td>138.964</td>
<td></td>
<td>150</td>
<td>0.34, (0.01, 0.28, 0.70)</td>
<td>0.006</td>
<td>0.030% (337)</td>
</tr>
<tr>
<td>m</td>
<td>139.041</td>
<td>139.040</td>
<td>C\textsubscript{7}H\textsubscript{6}O\textsubscript{3}H\textsuperscript{+} (1.3), C\textsubscript{3}H\textsubscript{7}NO\textsubscript{3}H\textsuperscript{+} (-2.8), C\textsubscript{3}H\textsubscript{10}O\textsubscript{3}SH\textsuperscript{+} (-2.0)</td>
<td>150</td>
<td>9.8, (0.39, 8.6, 19.3)</td>
<td>0.183</td>
<td>0.88% (25)</td>
</tr>
<tr>
<td>m</td>
<td>139.074</td>
<td>139.073</td>
<td>C\textsubscript{8}H\textsubscript{10}O\textsubscript{2}H\textsuperscript{+} (-1.1), C\textsubscript{3}H\textsubscript{10}N\textsubscript{2}O\textsubscript{4}H\textsuperscript{+} (3.0)</td>
<td>200</td>
<td>11.5, (0.35, 9.3, 27.4)</td>
<td>0.442</td>
<td>1.03% (21)</td>
</tr>
<tr>
<td>m</td>
<td>139.112</td>
<td>139.111</td>
<td>C\textsubscript{9}H\textsubscript{14}OH\textsuperscript{+} (-0.4)</td>
<td>150</td>
<td>2.2, (0.01, 2.1, 5.0)</td>
<td>0.120</td>
<td>0.20% (102)</td>
</tr>
<tr>
<td>m</td>
<td>139.674</td>
<td>139.673</td>
<td></td>
<td>150</td>
<td>0.024, (0.000, 0.017, 0.053)</td>
<td>0.004</td>
<td>0.0021% (584)</td>
</tr>
<tr>
<td>m</td>
<td>139.979</td>
<td>139.978</td>
<td></td>
<td>150</td>
<td>0.093, (0.002, 0.077, 0.204)</td>
<td>0.008</td>
<td>0.0084% (467)</td>
</tr>
<tr>
<td>m</td>
<td>140.039</td>
<td>140.038</td>
<td>C\textsubscript{2}H\textsubscript{6}N\textsubscript{2}O\textsubscript{5}H\textsuperscript{+} (0.0)</td>
<td>150</td>
<td>1.10, (0.04, 0.98, 2.23)</td>
<td>0.008</td>
<td>0.099% (179)</td>
</tr>
<tr>
<td>m</td>
<td>140.074</td>
<td>140.073</td>
<td>C\textsubscript{7}H\textsubscript{9}NO\textsubscript{2}H\textsuperscript{+} (2.7), C\textsubscript{3}H\textsubscript{10}N\textsubscript{2}O\textsubscript{4}H\textsuperscript{+} (-1.4)</td>
<td>200</td>
<td>2.6, (0.03, 2.1, 5.7)</td>
<td>0.012</td>
<td>0.23% (94)</td>
</tr>
<tr>
<td>m</td>
<td>140.114</td>
<td>140.113</td>
<td>C\textsubscript{9}H\textsubscript{14}OH\textsuperscript{+} (-1.8)</td>
<td>150</td>
<td>0.46, (0.00, 0.36, 1.08)</td>
<td>0.010</td>
<td>0.041% (297)</td>
</tr>
<tr>
<td>m</td>
<td>140.982</td>
<td>140.981</td>
<td>C\textsubscript{8}H\textsubscript{3}S\textsubscript{2}H\textsuperscript{+} (-1.4)</td>
<td>150</td>
<td>0.43, (0.01, 0.34, 0.87)</td>
<td>0.035</td>
<td>0.039% (310)</td>
</tr>
<tr>
<td>m</td>
<td>141.056</td>
<td>141.055</td>
<td>C\textsubscript{7}H\textsubscript{8}O\textsubscript{3}H\textsuperscript{+} (0.7), C\textsubscript{10}H\textsubscript{5}NH\textsuperscript{+} (2.5)</td>
<td>150</td>
<td>23, (0.4, 18, 46)</td>
<td>0.261</td>
<td>2.02% (6)</td>
</tr>
<tr>
<td>m</td>
<td>141.090</td>
<td>141.089</td>
<td>C\textsubscript{8}H\textsubscript{12}O\textsubscript{2}H\textsuperscript{+} (-1.7)</td>
<td>150</td>
<td>7.3, (0.10, 5.4, 17.3)</td>
<td>0.074</td>
<td>0.65% (37)</td>
</tr>
<tr>
<td>m</td>
<td>141.126</td>
<td>141.125</td>
<td>C\textsubscript{9}H\textsubscript{16}OH\textsuperscript{+} (-1.1)</td>
<td>150</td>
<td>0.89, (-0.05, 0.77, 2.16)</td>
<td>0.055</td>
<td>0.080% (207)</td>
</tr>
<tr>
<td>m</td>
<td>141.960</td>
<td>141.959</td>
<td></td>
<td>150</td>
<td>0.057, (0.002, 0.042, 0.127)</td>
<td>0.005</td>
<td>0.0051% (509)</td>
</tr>
<tr>
<td>m</td>
<td>142.057</td>
<td>142.056</td>
<td>C\textsubscript{7}H\textsubscript{8}O\textsubscript{3}H\textsuperscript{+} (-1.6), C\textsubscript{2}H\textsubscript{8}N\textsubscript{2}O\textsubscript{3}H\textsuperscript{+} (2.4)</td>
<td>150</td>
<td>2.3, (0.02, 1.7, 5.2)</td>
<td>0.081</td>
<td>0.21% (96)</td>
</tr>
<tr>
<td>m</td>
<td>142.090</td>
<td>142.089</td>
<td></td>
<td>150</td>
<td>1.51, (0.01, 1.16, 3.26)</td>
<td>0.018</td>
<td>0.135% (132)</td>
</tr>
<tr>
<td>m</td>
<td>142.927</td>
<td>142.926</td>
<td></td>
<td>150</td>
<td>0.058, (0.001, 0.041, 0.126)</td>
<td>0.003</td>
<td>0.0052% (507)</td>
</tr>
<tr>
<td>m</td>
<td>142.996</td>
<td>142.995</td>
<td>C\textsubscript{3}H\textsubscript{2}O\textsubscript{3}H\textsuperscript{+} (-2.1)</td>
<td>150</td>
<td>0.23, (0.01, 0.20, 0.54)</td>
<td>0.009</td>
<td>0.020% (388)</td>
</tr>
<tr>
<td>m</td>
<td>143.038</td>
<td>143.037</td>
<td>C\textsubscript{4}H\textsubscript{8}N\textsubscript{4}SH\textsuperscript{+} (-1.2)</td>
<td>150</td>
<td>1.22, (0.00, 0.75, 2.76)</td>
<td>0.044</td>
<td>0.109% (161)</td>
</tr>
<tr>
<td>Formula</td>
<td>Mass</td>
<td>Charge</td>
<td>Mw</td>
<td>Mw</td>
<td>Mw</td>
<td>Mw</td>
<td></td>
</tr>
<tr>
<td>---------</td>
<td>------</td>
<td>--------</td>
<td>----</td>
<td>----</td>
<td>----</td>
<td>----</td>
<td></td>
</tr>
<tr>
<td>C₂H₁₀O₂H⁺ (1.1), C₁₀H₂NH⁺ (2.9)</td>
<td>143.072</td>
<td>9.5, (0.07, 8.3, 21.0)</td>
<td>0.271</td>
<td>0.85% (26)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C₈H₁₄O₂H⁺ (-1.3)</td>
<td>143.106</td>
<td>2.7, (-0.04, 2.0, 6.7)</td>
<td>0.009</td>
<td>0.24% (90)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C₈H₁₀OH⁺ + (1.1)</td>
<td>143.305</td>
<td>0.026, (0.000, 0.016, 0.050)</td>
<td>0.004</td>
<td>0.0023% (577)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C₉H₁₄O₂H⁺ (-0.9)</td>
<td>144.037</td>
<td>0.42, (0.00, 0.32, 0.89)</td>
<td>0.021</td>
<td>0.037% (315)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C₈H₁₄O₂H⁺ (-1.6)</td>
<td>144.109</td>
<td>1.19, (0.00, 0.93, 2.56)</td>
<td>0.033</td>
<td>0.107% (168)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C₈H₁₄OH⁺ (-1.0)</td>
<td>144.146</td>
<td>0.041, (-0.009, 0.030, 0.106)</td>
<td>0.022</td>
<td>0.0037% (308)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C₇HNO₂H⁺ (-3.0), C₇H₃N₂O₄H⁺ (1.1), C₅H₄N₃O₂SH⁺ (1.8)</td>
<td>145.009</td>
<td>0.155, (0.007, 0.100, 0.344)</td>
<td>0.046</td>
<td>0.0139% (428)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C₉H₁₄O₂H⁺ (-0.9)</td>
<td>145.052</td>
<td>0.085, (0.006, 0.072, 0.181)</td>
<td>0.004</td>
<td>0.0076% (477)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C₈H₁₄O₂H⁺ (2.9), C₈H₈N₄SH⁺ (-1.8)</td>
<td>145.053</td>
<td>3.3, (0.01, 2.2, 7.4)</td>
<td>0.122</td>
<td>0.30% (74)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C₈H₁₆O₂H⁺ (-0.9)</td>
<td>145.122</td>
<td>0.88, (0.00, 0.68, 2.02)</td>
<td>0.128</td>
<td>0.079% (208)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C₈H₁₆O₂H⁺ (-2.2)</td>
<td>146.124</td>
<td>0.28, (0.00, 0.20, 0.66)</td>
<td>0.012</td>
<td>0.026% (360)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C₉H₁₆O₂H⁺ (-2.2)</td>
<td>146.979</td>
<td>0.20, (0.01, 0.12, 0.47)</td>
<td>0.058</td>
<td>0.0181% (401)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C₈H₈O₂H⁺ (2.4), C₉H₇N₂O₃H⁺ (-1.7), C₈H₁₀O₂SH⁺ (-1.0)</td>
<td>147.047</td>
<td>1.51, (0.06, 1.45, 2.90)</td>
<td>0.023</td>
<td>0.135% (131)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C₁₀H₁₄OH⁺ (-3.0), C₉H₁₀N₂O₃H⁺ (1.0), C₈H₇N₃H⁺ (2.8)</td>
<td>147.078</td>
<td>1.90, (0.02, 1.49, 4.24)</td>
<td>0.014</td>
<td>0.170% (108)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C₁₁H₁₄H⁺ (-1.4), C₈H₁₄N₂O₂H⁺ (2.6)</td>
<td>147.115</td>
<td>0.31, (-0.02, 0.23, 0.75)</td>
<td>0.048</td>
<td>0.028% (349)</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
m147.982 147.981 150 0.042, (0.004, 0.029, 0.092) 0.004 0.0038% (531)

m148.042 148.041 300 1.25, (0.01, 1.08, 2.51) 0.029 0.112% (158)

m148.042 148.041 C₈H₇NO₂H⁺ (-1.2)

m149.026 149.025 150 0.024, (0.000, 0.012, 0.067) 0.005 0.0021% (585)

m149.094 149.094 150 0.077, (0.01, 0.57, 1.82) 0.009 0.069% (229)

m150.029 150.028 150 0.074, (-0.04, 0.69, 1.62) 0.004 0.067% (232)

m150.094 150.093 200 0.77, (0.00, 0.63, 1.65) 0.012 0.069% (226)

m150.135 150.134 150 0.097, (-0.001, 0.071, 0.209) 0.016 0.0087% (462)

m150.970 150.970 150 0.181, (0.007, 0.156, 0.387) 0.012 0.0162% (409)

m151.042 151.041 250 1.56, (0.03, 1.39, 3.02) 0.041 0.140% (128)

m151.076 151.075 150 4.5, (0.08, 3.3, 10.3) 0.074 0.41% (56)

m151.110 151.109 150 2.8, (0.04, 2.5, 6.0) 0.030 0.26% (83)

m151.939 151.938 150 0.012, (0.001, 0.008, 0.028) 0.003 0.00112% (620)

m151.978 151.977 150 0.050, (-0.001, 0.043, 0.107) 0.014 0.0045% (521)

m152.040 152.039 150 0.32, (0.00, 0.29, 0.64) 0.005 0.029% (344)

m152.076 152.075 200 1.30, (0.01, 0.95, 2.83) 0.011 0.117% (150)
<table>
<thead>
<tr>
<th>m152.114</th>
<th>152.114</th>
<th>C_{10}H_{14}OH^+ (-1.6), C_{3}H_{14}N_{2}O_{3}H^+ (2.5)</th>
<th>150</th>
<th>0.52, (0.01, 0.41, 1.09)</th>
<th>0.009</th>
<th>0.046% (278)</th>
</tr>
</thead>
<tbody>
<tr>
<td>m153.022</td>
<td>153.022</td>
<td>C_{6}H_{8}O_{4}SH^+ (-0.1)</td>
<td>250</td>
<td>0.69, (0.00, 0.74, 1.23)</td>
<td>0.035</td>
<td>0.062% (246)</td>
</tr>
<tr>
<td>m153.057</td>
<td>153.057</td>
<td>C_{3}H_{8}O_{3}H^+ (1.9), C_{3}H_{9}NO_{3}H^+ (-2.1), C_{3}H_{12}O_{3}SH^+ (-1.4)</td>
<td>150</td>
<td>6.9, (0.16, 5.6, 14.5)</td>
<td>0.137</td>
<td>0.62% (40)</td>
</tr>
<tr>
<td>m153.091</td>
<td>153.091</td>
<td>C_{3}H_{12}O_{2}H^+ (-0.5)</td>
<td>150</td>
<td>7.8, (0.03, 5.6, 18.1)</td>
<td>0.146</td>
<td>0.70% (36)</td>
</tr>
<tr>
<td>m153.126</td>
<td>153.126</td>
<td>C_{10}H_{16}OH^+ (-1.8)</td>
<td>150</td>
<td>1.37, (-0.03, 1.06, 3.22)</td>
<td>0.052</td>
<td>0.123% (146)</td>
</tr>
<tr>
<td>m153.692</td>
<td>153.692</td>
<td></td>
<td>150</td>
<td>0.026, (0.000, 0.019, 0.059)</td>
<td>0.005</td>
<td>0.0023% (578)</td>
</tr>
<tr>
<td>m153.923</td>
<td>153.923</td>
<td></td>
<td>150</td>
<td>0.026, (0.000, 0.018, 0.053)</td>
<td>0.004</td>
<td>0.0023% (576)</td>
</tr>
<tr>
<td>m154.013</td>
<td>154.013</td>
<td>C_{3}H_{3}NO_{4}H^+ (-0.9)</td>
<td>350</td>
<td>0.157, (0.000, 0.150, 0.305)</td>
<td>0.014</td>
<td>0.0141% (427)</td>
</tr>
<tr>
<td>m154.057</td>
<td>154.057</td>
<td>C_{3}H_{8}O_{3}H^+ (-1.4), C_{3}H_{8}N_{2}O_{3}H^+ (2.6)</td>
<td>150</td>
<td>1.07, (0.02, 0.80, 2.38)</td>
<td>0.023</td>
<td>0.096% (180)</td>
</tr>
<tr>
<td>m154.089</td>
<td>154.089</td>
<td>C_{3}H_{11}NO_{2}H^+ (2.3), C_{3}H_{12}N_{2}O_{4}H^+ (-1.8)</td>
<td>150</td>
<td>1.69, (0.01, 1.17, 3.91)</td>
<td>0.023</td>
<td>0.151% (119)</td>
</tr>
<tr>
<td>m154.930</td>
<td>154.930</td>
<td></td>
<td>150</td>
<td>0.094, (0.001, 0.063, 0.214)</td>
<td>0.003</td>
<td>0.0084% (466)</td>
</tr>
<tr>
<td>m155.031</td>
<td>155.031</td>
<td>C_{10}H_{3}NOH^+ (-1.5), C_{3}H_{3}N_{3}O_{3}H^+ (2.5)</td>
<td>150</td>
<td>1.59, (-0.01, 0.39, 4.86)</td>
<td>0.101</td>
<td>0.143% (125)</td>
</tr>
<tr>
<td>m155.072</td>
<td>155.072</td>
<td>C_{6}H_{10}O_{3}^{+} (1.3), C_{3}H_{11}NO_{3}H^+ (-2.8)</td>
<td>150</td>
<td>16.3, (0.09, 12.3, 37.7)</td>
<td>0.140</td>
<td>1.46% (13)</td>
</tr>
<tr>
<td>m155.143</td>
<td>155.143</td>
<td>C_{10}H_{18}OH^+ (-0.4)</td>
<td>150</td>
<td>3.1, (-0.06, 2.4, 7.3)</td>
<td>0.086</td>
<td>0.28% (80)</td>
</tr>
<tr>
<td>m155.921</td>
<td>155.921</td>
<td></td>
<td>150</td>
<td>0.032, (0.000, 0.021, 0.073)</td>
<td>0.004</td>
<td>0.0028% (556)</td>
</tr>
<tr>
<td>m156.032</td>
<td>156.032</td>
<td>C_{3}H_{3}NO_{4}H^{+} (2.5)</td>
<td>150</td>
<td>0.21, (0.00, 0.12, 0.63)</td>
<td>0.019</td>
<td>0.0192% (396)</td>
</tr>
<tr>
<td>m156.072</td>
<td>156.072</td>
<td>C_{3}H_{10}O_{3}H^+ (-2.0), C_{3}H_{10}N_{2}O_{3}H^+ (2.0)</td>
<td>150</td>
<td>2.7, (0.01, 1.8, 6.1)</td>
<td>0.016</td>
<td>0.24% (87)</td>
</tr>
<tr>
<td>m157.051</td>
<td>157.051</td>
<td>C_{3}H_{3}O_{2}H^{+} (1.1), C_{10}H_{3}NOH^+ (2.9)</td>
<td>150</td>
<td>21, (0.0, 16, 49)</td>
<td>0.164</td>
<td>1.86% (8)</td>
</tr>
<tr>
<td>m157.085</td>
<td>157.085</td>
<td>C\textsubscript{6}H\textsubscript{12}O\textsubscript{3}H\textsuperscript{+} (-1.3), C\textsubscript{11}H\textsubscript{9}NH\textsuperscript{+} (0.5)</td>
<td>150</td>
<td>7.1, (0.05, 5.8, 16.5)</td>
<td>0.374</td>
<td>0.64% (38)</td>
</tr>
<tr>
<td>m157.121</td>
<td>157.121</td>
<td>C\textsubscript{9}H\textsubscript{16}O\textsubscript{2}H\textsuperscript{+} (-1.7)</td>
<td>150</td>
<td>1.11, (-0.07, 0.87, 2.78)</td>
<td>0.196</td>
<td>0.099% (178)</td>
</tr>
<tr>
<td>m157.660</td>
<td>157.660</td>
<td></td>
<td>150</td>
<td>0.030, (0.000, 0.021, 0.069)</td>
<td>0.003</td>
<td>0.0027% (563)</td>
</tr>
<tr>
<td>m158.055</td>
<td>158.055</td>
<td>C\textsubscript{7}H\textsubscript{8}O\textsubscript{4}H\textsuperscript{+} (1.8), C\textsubscript{5}H\textsubscript{7}N\textsubscript{3}O\textsubscript{3}H\textsuperscript{+} (-1.4)</td>
<td>150</td>
<td>2.0, (0.02, 1.5, 4.6)</td>
<td>0.042</td>
<td>0.179% (105)</td>
</tr>
<tr>
<td>m158.094</td>
<td>158.094</td>
<td>C\textsubscript{11}H\textsubscript{11}NH\textsuperscript{+} (-2.8), C\textsubscript{6}H\textsubscript{11}N\textsubscript{3}O\textsubscript{2}H\textsuperscript{+} (1.2)</td>
<td>150</td>
<td>1.42, (0.00, 1.02, 3.34)</td>
<td>0.022</td>
<td>0.127% (141)</td>
</tr>
<tr>
<td>m158.158</td>
<td>158.158</td>
<td></td>
<td>150</td>
<td>0.072, (-0.004, 0.112, 0.488)</td>
<td>0.056</td>
<td>0.0164% (408)</td>
</tr>
<tr>
<td>m159.046</td>
<td>159.046</td>
<td>C\textsubscript{10}H\textsubscript{10}O\textsubscript{2}H\textsuperscript{+} (1.6), C\textsubscript{6}H\textsubscript{7}NO\textsubscript{2}H\textsuperscript{+} (-2.5), C\textsubscript{3}H\textsubscript{10}O\textsubscript{2}SH\textsuperscript{+} (-1.8)</td>
<td>150</td>
<td>0.183, (0.004, 0.112, 0.488)</td>
<td>0.056</td>
<td>0.0164% (408)</td>
</tr>
<tr>
<td>m159.066</td>
<td>159.066</td>
<td>C\textsubscript{7}H\textsubscript{10}O\textsubscript{2}H\textsuperscript{+} (0.5), C\textsubscript{10}H\textsubscript{2}NO\textsubscript{2}H\textsuperscript{+} (2.3)</td>
<td>150</td>
<td>4.9, (0.05, 2.2, 12.8)</td>
<td>0.031</td>
<td>0.44% (54)</td>
</tr>
<tr>
<td>m159.120</td>
<td>159.120</td>
<td>C\textsubscript{12}H\textsubscript{14}H\textsuperscript{+} (2.8), C\textsubscript{8}H\textsubscript{15}NO\textsubscript{2}H\textsuperscript{+} (-1.2), C\textsubscript{9}H\textsubscript{18}SH\textsuperscript{+} (-0.5)</td>
<td>150</td>
<td>0.76, (-0.03, 0.40, 2.05)</td>
<td>0.054</td>
<td>0.068% (230)</td>
</tr>
<tr>
<td>m159.982</td>
<td>159.982</td>
<td></td>
<td>100</td>
<td>0.037, (0.004, 0.034, 0.072)</td>
<td>0.002</td>
<td>0.0034% (545)</td>
</tr>
<tr>
<td>m160.071</td>
<td>160.071</td>
<td>C\textsubscript{7}H\textsubscript{10}O\textsubscript{2}H\textsuperscript{+} (2.2), C\textsubscript{5}H\textsubscript{9}N\textsubscript{3}O\textsubscript{3}H\textsuperscript{+} (-1.0)</td>
<td>150</td>
<td>0.75, (0.00, 0.47, 1.71)</td>
<td>0.029</td>
<td>0.067% (231)</td>
</tr>
<tr>
<td>m160.123</td>
<td>160.123</td>
<td>C\textsubscript{12}H\textsubscript{14}H\textsuperscript{+} (2.5)</td>
<td>150</td>
<td>0.27, (0.00, 0.16, 0.65)</td>
<td>0.014</td>
<td>0.024% (370)</td>
</tr>
<tr>
<td>m160.976</td>
<td>160.976</td>
<td></td>
<td>100</td>
<td>0.107, (0.008, 0.070, 0.223)</td>
<td>0.020</td>
<td>0.0096% (455)</td>
</tr>
<tr>
<td>m161.059</td>
<td>161.059</td>
<td>C\textsubscript{10}H\textsubscript{8}O\textsubscript{2}H\textsuperscript{+} (-1.0)</td>
<td>150</td>
<td>3.0, (0.13, 2.8, 5.8)</td>
<td>n.c.</td>
<td>0.27% (81)</td>
</tr>
<tr>
<td>m161.982</td>
<td>161.982</td>
<td></td>
<td>100</td>
<td>0.027, (0.004, 0.022, 0.056)</td>
<td>0.003</td>
<td>0.0024% (572)</td>
</tr>
<tr>
<td>m162.059</td>
<td>162.059</td>
<td>C\textsubscript{3}H\textsubscript{8}N\textsubscript{2}O\textsubscript{4}H\textsuperscript{+} (-0.3), C\textsubscript{8}H\textsubscript{11}NO\textsubscript{2}SH\textsuperscript{+} (0.4)</td>
<td>150</td>
<td>0.81, (0.01, 0.67, 1.65)</td>
<td>0.019</td>
<td>0.073% (222)</td>
</tr>
<tr>
<td>m162.098</td>
<td>162.098</td>
<td><strong>C_{11}H_{12}OH^+ (-1.7), C_{6}H_{12}N_{2}O_{3}H^+ (2.3)</strong></td>
<td>200</td>
<td>0.28, (-0.01, 0.22, 0.65)</td>
<td>0.066</td>
<td>0.025% (365)</td>
</tr>
<tr>
<td>m162.936</td>
<td>162.936</td>
<td></td>
<td>250</td>
<td>0.023, (-0.001, 0.018, 0.051)</td>
<td>0.013</td>
<td>0.0021% (586)</td>
</tr>
<tr>
<td>m163.043</td>
<td>163.043</td>
<td><strong>C_{2}H_{5}NO_{3}H^+ (-0.3)</strong></td>
<td>150</td>
<td>3.2, (0.07, 3.0, 6.0)</td>
<td>0.011</td>
<td>0.29% (78)</td>
</tr>
<tr>
<td>m163.075</td>
<td>163.075</td>
<td><strong>C_{10}H_{10}O_{2}H^+ (-0.6)</strong></td>
<td>150</td>
<td>2.7, (0.13, 2.3, 6.0)</td>
<td>0.199</td>
<td>0.24% (88)</td>
</tr>
<tr>
<td>m163.111</td>
<td>163.111</td>
<td><strong>C_{11}H_{14}OH^+ (-1.0)</strong></td>
<td>150</td>
<td>0.72, (0.00, 0.61, 1.60)</td>
<td>0.028</td>
<td>0.065% (239)</td>
</tr>
<tr>
<td>m163.979</td>
<td>163.979</td>
<td></td>
<td>150</td>
<td>0.033, (0.000, 0.025, 0.068)</td>
<td>0.001</td>
<td>0.0030% (551)</td>
</tr>
<tr>
<td>m164.042</td>
<td>164.042</td>
<td><strong>C_{5}H_{6}O_{3}H^+ (-0.5)</strong></td>
<td>150</td>
<td>0.47, (0.00, 0.43, 0.95)</td>
<td>0.038</td>
<td>0.042% (292)</td>
</tr>
<tr>
<td>m164.076</td>
<td>164.076</td>
<td><strong>C_{10}H_{10}O_{2}H^+ (-2.9), C_{5}H_{10}N_{2}O_{4}H^+ (1.1), C_{6}H_{13}NO_{2}SH^+ (1.8)</strong></td>
<td>200</td>
<td>0.99, (0.02, 0.79, 2.14)</td>
<td>0.028</td>
<td>0.089% (189)</td>
</tr>
<tr>
<td>m164.113</td>
<td>164.113</td>
<td><strong>C_{11}H_{14}OH^+ (-2.3), C_{6}H_{14}N_{2}O_{3}H^+ (1.7)</strong></td>
<td>150</td>
<td>0.27, (0.00, 0.19, 0.67)</td>
<td>0.006</td>
<td>0.025% (367)</td>
</tr>
<tr>
<td>m165.022</td>
<td>165.022</td>
<td></td>
<td>150</td>
<td>0.59, (0.00, 0.57, 1.24)</td>
<td>0.041</td>
<td>0.053% (265)</td>
</tr>
<tr>
<td>m165.057</td>
<td>165.057</td>
<td><strong>C_{5}H_{6}O_{3}H^+ (2.2), C_{5}H_{6}NO_{3}H^+ (-1.9), C_{6}H_{12}O_{3}SH^+ (-1.2)</strong></td>
<td>200</td>
<td>1.90, (0.05, 1.65, 3.66)</td>
<td>0.098</td>
<td>0.171% (107)</td>
</tr>
<tr>
<td>m165.091</td>
<td>165.091</td>
<td><strong>C_{10}H_{12}O_{2}H^+ (-0.2)</strong></td>
<td>150</td>
<td>5.1, (0.06, 3.7, 12.4)</td>
<td>0.106</td>
<td>0.46% (48)</td>
</tr>
<tr>
<td>m165.972</td>
<td>165.972</td>
<td></td>
<td>200</td>
<td>0.018, (0.000, 0.013, 0.039)</td>
<td>0.004</td>
<td>0.00166% (600)</td>
</tr>
<tr>
<td>m166.020</td>
<td>166.020</td>
<td><strong>C_{5}H_{4}O_{4}H^+ (-1.8), C_{3}H_{3}N_{3}S_{3}SH^+ (1.6)</strong></td>
<td>150</td>
<td>0.087, (0.001, 0.081, 0.171)</td>
<td>0.005</td>
<td>0.0078% (471)</td>
</tr>
<tr>
<td>m166.055</td>
<td>166.055</td>
<td><strong>C_{8}H_{8}N_{2}O_{3}H^+ (0.9), C_{5}H_{11}NO_{3}SH^+ (1.6)</strong></td>
<td>200</td>
<td>0.45, (0.00, 0.37, 0.95)</td>
<td>0.003</td>
<td>0.041% (299)</td>
</tr>
<tr>
<td>m166.091</td>
<td>166.091</td>
<td><strong>C_{3}H_{12}N_{2}O_{4}H^+ (0.5)</strong></td>
<td>150</td>
<td>1.18, (0.00, 0.74, 2.74)</td>
<td>0.014</td>
<td>0.106% (171)</td>
</tr>
<tr>
<td>m166.907</td>
<td>166.907</td>
<td></td>
<td>150</td>
<td>0.039, (0.001, 0.027, 0.092)</td>
<td>0.004</td>
<td>0.0035% (540)</td>
</tr>
<tr>
<td>m166.965</td>
<td>166.965</td>
<td></td>
<td>150</td>
<td>0.126, (0.002, 0.087, 0.298)</td>
<td>0.013</td>
<td>0.0113% (441)</td>
</tr>
<tr>
<td>m167.037</td>
<td>167.037</td>
<td>C₈H₆O₄H⁺ (3.0), C₅H₁₀O₄SH⁺ (-0.4)</td>
<td>200</td>
<td>1.01, (0.00, 0.96, 2.02)</td>
<td>0.022</td>
<td>0.090% (186)</td>
</tr>
<tr>
<td>m167.072</td>
<td>167.072</td>
<td>C₁₀H₁₀O₃H⁺ (1.6), C₉H₁₁NO₃H⁺ (-2.5), C₈H₁₄O₃SH⁺ (-1.8)</td>
<td>150</td>
<td>6.2, (0.07, 4.3, 13.6)</td>
<td>0.255</td>
<td>0.56% (42)</td>
</tr>
<tr>
<td>m167.104</td>
<td>167.104</td>
<td>C₁₀H₁₄O₃H⁺ (-2.8), C₅H₁₄N₂O₅H⁺ (1.2)</td>
<td>150</td>
<td>4.9, (-0.01, 3.8, 11.6)</td>
<td>0.112</td>
<td>0.44% (52)</td>
</tr>
<tr>
<td>m168.035</td>
<td>168.035</td>
<td>C₈H₆O₄H⁺ (-2.4)</td>
<td>150</td>
<td>0.165, (0.002, 0.145, 0.339)</td>
<td>0.006</td>
<td>0.0148% (419)</td>
</tr>
<tr>
<td>m168.073</td>
<td>168.073</td>
<td>C₅H₁₀O₃H⁺ (-0.8)</td>
<td>150</td>
<td>1.32, (0.01, 0.86, 2.84)</td>
<td>0.035</td>
<td>0.118% (147)</td>
</tr>
<tr>
<td>m168.104</td>
<td>168.104</td>
<td>C₁₃H₁₃NO₂H⁺ (2.0), C₅H₁₄N₂O₄H⁺ (-2.1)</td>
<td>150</td>
<td>0.93, (0.00, 0.62, 2.20)</td>
<td>0.021</td>
<td>0.083% (198)</td>
</tr>
<tr>
<td>m168.903</td>
<td>168.903</td>
<td></td>
<td>150</td>
<td>0.044, (0.001, 0.026, 0.098)</td>
<td>0.003</td>
<td>0.0039% (530)</td>
</tr>
<tr>
<td>m169.053</td>
<td>169.053</td>
<td>C₅H₁₂O₄SH⁺ (0.0), C₉H₁₂O₃H⁺ (-1.0), C₁₂H₉NH⁺ (0.8), C₃H₁₂N₂O₅H⁺ (3.0)</td>
<td>200</td>
<td>3.8, (0.01, 2.6, 8.4)</td>
<td>0.105</td>
<td>0.34% (60)</td>
</tr>
<tr>
<td>m169.085</td>
<td>169.085</td>
<td></td>
<td>150</td>
<td>9.1, (0.05, 6.4, 21.3)</td>
<td>0.045</td>
<td>0.82% (30)</td>
</tr>
<tr>
<td>m169.120</td>
<td>169.120</td>
<td>C₁₀H₁₆O₂H⁺ (-2.4)</td>
<td>150</td>
<td>1.72, (-0.03, 1.32, 4.22)</td>
<td>0.078</td>
<td>0.154% (118)</td>
</tr>
<tr>
<td>m169.158</td>
<td>169.158</td>
<td>C₁₁H₂₀OH⁺ (-0.8)</td>
<td>150</td>
<td>0.21, (0.00, 0.15, 0.49)</td>
<td>0.022</td>
<td>0.0188% (399)</td>
</tr>
<tr>
<td>m170.055</td>
<td>170.055</td>
<td>C₈H₆O₄H⁺ (2.0), C₆H₇N₃O₃H⁺ (-1.1)</td>
<td>200</td>
<td>0.71, (0.01, 0.43, 1.76)</td>
<td>0.013</td>
<td>0.064% (241)</td>
</tr>
<tr>
<td>m170.086</td>
<td>170.086</td>
<td>C₅H₁₂N₂O₅H⁺ (0.7)</td>
<td>150</td>
<td>1.83, (0.00, 1.11, 4.30)</td>
<td>0.025</td>
<td>0.164% (112)</td>
</tr>
<tr>
<td>m170.926</td>
<td>170.926</td>
<td></td>
<td>150</td>
<td>0.100, (0.003, 0.072, 0.222)</td>
<td>0.029</td>
<td>0.0090% (459)</td>
</tr>
<tr>
<td>m171.067</td>
<td>171.067</td>
<td>C₈H₁₀O₄H⁺ (1.7)</td>
<td>150</td>
<td>26, (0.0, 20, 58)</td>
<td>0.351</td>
<td>2.33% (4)</td>
</tr>
<tr>
<td>m171.137</td>
<td>171.137</td>
<td>C₁₀H₁₈O₂H⁺ (-1.0)</td>
<td>150</td>
<td>3.8, (-0.11, 2.9, 9.6)</td>
<td>0.278</td>
<td>0.34% (62)</td>
</tr>
<tr>
<td>m171.974</td>
<td>171.974</td>
<td></td>
<td>300</td>
<td>0.165, (0.013, 0.129, 0.363)</td>
<td>0.020</td>
<td>0.0148% (421)</td>
</tr>
<tr>
<td>m172.069</td>
<td>172.069</td>
<td>C₈H₁₀O₄H⁺ (0.4), C₆H₉N₃O₃H⁺ (-2.7)</td>
<td>150</td>
<td>3.2, (0.01, 2.3, 7.0)</td>
<td>0.058</td>
<td>0.29% (77)</td>
</tr>
<tr>
<td>m</td>
<td>172.140</td>
<td>172.140</td>
<td>C&lt;sub&gt;10&lt;/sub&gt;H&lt;sub&gt;18&lt;/sub&gt;O&lt;sub&gt;2&lt;/sub&gt;H&lt;sup&gt;+&lt;/sup&gt; (-1.4)</td>
<td>150</td>
<td>0.69, (-0.01, 0.46, 1.65)</td>
<td>0.036</td>
</tr>
<tr>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>m</td>
<td>172.959</td>
<td>172.959</td>
<td></td>
<td>150</td>
<td>0.33, (0.00, 0.23, 0.84)</td>
<td>0.032</td>
</tr>
<tr>
<td>m</td>
<td>173.049</td>
<td>173.049</td>
<td></td>
<td>150</td>
<td>3.3, (0.00, 1.5, 9.3)</td>
<td>0.034</td>
</tr>
<tr>
<td>m</td>
<td>173.077</td>
<td>173.077</td>
<td>C&lt;sub&gt;11&lt;/sub&gt;H&lt;sub&gt;9&lt;/sub&gt;NOH&lt;sup&gt;+&lt;/sup&gt; (-2.1), C&lt;sub&gt;6&lt;/sub&gt;H&lt;sub&gt;9&lt;/sub&gt;N&lt;sub&gt;3&lt;/sub&gt;O&lt;sub&gt;3&lt;/sub&gt;H&lt;sup&gt;+&lt;/sup&gt; (2.0), C&lt;sub&gt;7&lt;/sub&gt;H&lt;sub&gt;12&lt;/sub&gt;N&lt;sub&gt;2&lt;/sub&gt;OSH&lt;sup&gt;+&lt;/sup&gt; (2.7)</td>
<td>150</td>
<td>3.7, (-0.04, 2.1, 8.4)</td>
<td>0.050</td>
</tr>
<tr>
<td>m</td>
<td>173.153</td>
<td>173.153</td>
<td>C&lt;sub&gt;10&lt;/sub&gt;H&lt;sub&gt;20&lt;/sub&gt;O&lt;sub&gt;2&lt;/sub&gt;H&lt;sup&gt;+&lt;/sup&gt; (-0.6)</td>
<td>150</td>
<td>0.99, (-0.06, 0.91, 2.23)</td>
<td>0.184</td>
</tr>
<tr>
<td>m</td>
<td>173.970</td>
<td>173.970</td>
<td></td>
<td>150</td>
<td>0.143, (0.009, 0.113, 0.309)</td>
<td>0.004</td>
</tr>
<tr>
<td>m</td>
<td>174.054</td>
<td>174.054</td>
<td>C&lt;sub&gt;10&lt;/sub&gt;H&lt;sub&gt;7&lt;/sub&gt;NO&lt;sup&gt;2&lt;/sup&gt;H&lt;sup&gt;+&lt;/sup&gt; (-1.0)</td>
<td>150</td>
<td>0.39, (0.00, 0.24, 0.97)</td>
<td>0.023</td>
</tr>
<tr>
<td>m</td>
<td>174.080</td>
<td>174.080</td>
<td></td>
<td>150</td>
<td>0.90, (0.00, 0.50, 2.15)</td>
<td>0.011</td>
</tr>
<tr>
<td>m</td>
<td>174.155</td>
<td>174.155</td>
<td>C&lt;sub&gt;11&lt;/sub&gt;H&lt;sub&gt;20&lt;/sub&gt;O&lt;sub&gt;2&lt;/sub&gt;H&lt;sup&gt;+&lt;/sup&gt; (-2.0)</td>
<td>150</td>
<td>0.27, (0.00, 0.22, 0.61)</td>
<td>0.023</td>
</tr>
<tr>
<td>m</td>
<td>175.044</td>
<td>175.044</td>
<td>C&lt;sub&gt;6&lt;/sub&gt;H&lt;sub&gt;7&lt;/sub&gt;NO&lt;sup&gt;3&lt;/sup&gt;H&lt;sup&gt;+&lt;/sup&gt; (1.0)</td>
<td>150</td>
<td>0.74, (0.02, 0.68, 1.50)</td>
<td>0.018</td>
</tr>
<tr>
<td>m</td>
<td>175.067</td>
<td>175.067</td>
<td>C&lt;sub&gt;3&lt;/sub&gt;H&lt;sub&gt;7&lt;/sub&gt;N&lt;sub&gt;5&lt;/sub&gt;OH&lt;sup&gt;+&lt;/sup&gt; (-2.5), C&lt;sub&gt;3&lt;/sub&gt;H&lt;sub&gt;10&lt;/sub&gt;N&lt;sub&gt;4&lt;/sub&gt;OSH&lt;sup&gt;+&lt;/sup&gt; (2.2)</td>
<td>150</td>
<td>1.81, (0.01, 1.28, 4.27)</td>
<td>0.041</td>
</tr>
<tr>
<td>m</td>
<td>175.147</td>
<td>175.147</td>
<td>C&lt;sub&gt;13&lt;/sub&gt;H&lt;sub&gt;18&lt;/sub&gt;H&lt;sup&gt;+&lt;/sup&gt; (-1.1), C&lt;sub&gt;5&lt;/sub&gt;H&lt;sub&gt;18&lt;/sub&gt;N&lt;sub&gt;2&lt;/sub&gt;O&lt;sub&gt;2&lt;/sub&gt;H&lt;sup&gt;+&lt;/sup&gt; (2.9)</td>
<td>150</td>
<td>0.43, (-0.02, 0.34, 1.04)</td>
<td>0.071</td>
</tr>
<tr>
<td>m</td>
<td>175.975</td>
<td>175.975</td>
<td></td>
<td>300</td>
<td>0.020, (0.000, 0.016, 0.046)</td>
<td>0.011</td>
</tr>
<tr>
<td>m</td>
<td>176.042</td>
<td>176.042</td>
<td>C&lt;sub&gt;10&lt;/sub&gt;H&lt;sub&gt;6&lt;/sub&gt;O&lt;sub&gt;3&lt;/sub&gt;H&lt;sup&gt;+&lt;/sup&gt; (-0.3)</td>
<td>250</td>
<td>0.085, (0.002, 0.085, 0.174)</td>
<td>0.004</td>
</tr>
<tr>
<td>m</td>
<td>176.071</td>
<td>176.071</td>
<td>C&lt;sub&gt;10&lt;/sub&gt;H&lt;sub&gt;9&lt;/sub&gt;NO&lt;sub&gt;2&lt;/sub&gt;H&lt;sup&gt;+&lt;/sup&gt; (0.4)</td>
<td>150</td>
<td>0.63, (0.00, 0.43, 1.42)</td>
<td>0.009</td>
</tr>
<tr>
<td>m</td>
<td>176.151</td>
<td>176.151</td>
<td>C&lt;sub&gt;13&lt;/sub&gt;H&lt;sub&gt;18&lt;/sub&gt;H&lt;sup&gt;+&lt;/sup&gt; (-0.4)</td>
<td>150</td>
<td>0.165, (-0.005, 0.110, 0.407)</td>
<td>0.012</td>
</tr>
<tr>
<td>m</td>
<td>177.056</td>
<td>177.056</td>
<td>C&lt;sub&gt;10&lt;/sub&gt;H&lt;sub&gt;8&lt;/sub&gt;O&lt;sub&gt;3&lt;/sub&gt;H&lt;sup&gt;+&lt;/sup&gt; (1.4), C&lt;sub&gt;6&lt;/sub&gt;H&lt;sub&gt;9&lt;/sub&gt;No&lt;sub&gt;3&lt;/sub&gt;H&lt;sup&gt;+&lt;/sup&gt; (-2.6)</td>
<td>150</td>
<td>1.49, (-0.02, 1.41, 3.00)</td>
<td>0.110</td>
</tr>
<tr>
<td>m</td>
<td>177.087</td>
<td>177.087</td>
<td>C&lt;sub&gt;5&lt;/sub&gt;H&lt;sub&gt;12&lt;/sub&gt;N&lt;sub&gt;2&lt;/sub&gt;O&lt;sub&gt;4&lt;/sub&gt;H&lt;sup&gt;+&lt;/sup&gt; (0.1), C&lt;sub&gt;5&lt;/sub&gt;H&lt;sub&gt;9&lt;/sub&gt;N&lt;sub&gt;3&lt;/sub&gt;OH&lt;sup&gt;+&lt;/sup&gt; (1.9)</td>
<td>200</td>
<td>1.41, (0.00, 1.16, 3.18)</td>
<td>0.096</td>
</tr>
<tr>
<td>m</td>
<td>178.058</td>
<td>178.058</td>
<td>C&lt;sub&gt;10&lt;/sub&gt;H&lt;sub&gt;8&lt;/sub&gt;O&lt;sub&gt;3&lt;/sub&gt;H&lt;sup&gt;+&lt;/sup&gt; (0.1)</td>
<td>150</td>
<td>0.25, (0.00, 0.23, 0.49)</td>
<td>0.014</td>
</tr>
<tr>
<td>Mass (m)</td>
<td>Charge (z)</td>
<td>Molecular Formula</td>
<td>Retention Time</td>
<td>Coordinates</td>
<td>FID Peak</td>
<td>Mass Accuracy (ppm)</td>
</tr>
<tr>
<td>---------</td>
<td>-----------</td>
<td>-------------------</td>
<td>---------------</td>
<td>-------------</td>
<td>----------</td>
<td>---------------------</td>
</tr>
<tr>
<td>m178.083</td>
<td>178.083</td>
<td>C_5H_{11}N_3O_4H^+ (0.8)</td>
<td>150</td>
<td>0.66, (0.00, 0.45, 1.52)</td>
<td>0.009</td>
<td>0.059% (251)</td>
</tr>
<tr>
<td>m178.167</td>
<td>178.167</td>
<td>C_{13}H_{20}H^+ (0.0)</td>
<td>150</td>
<td>0.064, (-0.005, 0.044, 0.154)</td>
<td>0.026</td>
<td>0.0057% (503)</td>
</tr>
<tr>
<td>m178.908</td>
<td>178.908</td>
<td>C_{5}H_{11}N_{3}O_{4}H^+ (1.5), C_{11}H_{14}SH^+ (-1.8)</td>
<td>100</td>
<td>0.52, (0.00, 0.33, 1.18)</td>
<td>0.023</td>
<td>0.047% (276)</td>
</tr>
<tr>
<td>m179.039</td>
<td>179.039</td>
<td>C_{7}H_{6}N_{3}SH^+ (0.5)</td>
<td>200</td>
<td>1.15, (0.00, 1.00, 2.30)</td>
<td>0.026</td>
<td>0.103% (174)</td>
</tr>
<tr>
<td>m179.087</td>
<td>179.087</td>
<td>C_{14}H_{10}H^+ (2.3), C_{10}H_{11}NO_{2}H^+ (-2.5), C_{5}H_{11}N_{3}O_{4}H^+ (1.5), C_{11}H_{14}SH^+ (-1.8)</td>
<td>150</td>
<td>0.033, (0.00, 0.025, 0.078)</td>
<td>0.011</td>
<td>0.0030% (552)</td>
</tr>
<tr>
<td>m179.972</td>
<td>179.972</td>
<td>C_{14}H_{10}H^+ (2.3), C_{10}H_{11}NO_{2}H^+ (-2.5), C_{5}H_{11}N_{3}O_{4}H^+ (1.5), C_{11}H_{14}SH^+ (-1.8)</td>
<td>150</td>
<td>0.60, (0.00, 0.44, 1.37)</td>
<td>0.065</td>
<td>0.053% (264)</td>
</tr>
<tr>
<td>m180.091</td>
<td>180.091</td>
<td>C_{14}H_{10}H^+ (2.3), C_{10}H_{11}NO_{2}H^+ (-2.5), C_{5}H_{11}N_{3}O_{4}H^+ (1.5), C_{11}H_{14}SH^+ (-1.8)</td>
<td>150</td>
<td>1.27, (0.01, 1.06, 2.60)</td>
<td>0.011</td>
<td>0.114% (155)</td>
</tr>
<tr>
<td>m181.009</td>
<td>181.009</td>
<td>C_{14}H_{10}H^+ (-1.0), C_{9}H_{12}N_{2}O_{5}H^+ (3.0), C_{5}H_{13}N_{3}O_{4}H^+ (-1.1)</td>
<td>150</td>
<td>8.8, (0.16, 7.1, 20.6)</td>
<td>0.510</td>
<td>0.79% (32)</td>
</tr>
<tr>
<td>m182.008</td>
<td>182.008</td>
<td>C_{7}H_{3}NO_{3}H^+ (-0.2)</td>
<td>150</td>
<td>0.33, (0.01, 0.28, 0.65)</td>
<td>0.035</td>
<td>0.030% (339)</td>
</tr>
<tr>
<td>m182.104</td>
<td>182.104</td>
<td>C_{14}H_{12}H^+ (-0.3), C_{9}H_{15}NO_{2}H^+ (1.9)</td>
<td>150</td>
<td>1.76, (0.02, 1.23, 3.81)</td>
<td>0.090</td>
<td>0.157% (116)</td>
</tr>
<tr>
<td>m182.937</td>
<td>182.937</td>
<td>C_{13}H_{10}OH^+ (2.8), C_{9}H_{11}NO_{3}H^+ (-1.3), C_{8}H_{11}N_{3}O_{4}H^+ (2.7), C_{10}H_{14}SH^+ (-0.6)</td>
<td>150</td>
<td>12.9, (0.15, 7.9, 30.0)</td>
<td>0.138</td>
<td>1.16% (18)</td>
</tr>
<tr>
<td>m183.083</td>
<td>183.083</td>
<td>C_{12}H_{22}OH^+ (-1.1)</td>
<td>150</td>
<td>1.50, (-0.04, 1.04, 3.63)</td>
<td>0.057</td>
<td>0.134% (134)</td>
</tr>
<tr>
<td>m183.173</td>
<td>183.173</td>
<td>C_{12}H_{22}OH^+ (-1.1)</td>
<td>150</td>
<td>1.50, (-0.04, 1.04, 3.63)</td>
<td>0.057</td>
<td>0.134% (134)</td>
</tr>
<tr>
<td>m184.001</td>
<td>184.001</td>
<td>C\textsubscript{10}HNO\textsubscript{3}H\textsuperscript{+} (-1.7), C\textsubscript{2}HNNO\textsubscript{3}H\textsuperscript{+} (2.3)</td>
<td>150</td>
<td>0.37, (0.00, 0.26, 0.80)</td>
<td>0.012</td>
<td>0.033% (325)</td>
</tr>
<tr>
<td>m184.086</td>
<td>184.086</td>
<td>C\textsubscript{13}H\textsubscript{16}OH\textsuperscript{+} (2.4), C\textsubscript{11}H\textsubscript{9}N\textsubscript{3}H\textsuperscript{+} (-0.7)</td>
<td>150</td>
<td>2.3, (0.02, 1.3, 5.2)</td>
<td>0.019</td>
<td>0.20% (100)</td>
</tr>
<tr>
<td>m184.935</td>
<td>184.935</td>
<td></td>
<td>150</td>
<td>0.022, (0.001, 0.017, 0.046)</td>
<td>0.005</td>
<td>0.0020% (589)</td>
</tr>
<tr>
<td>m184.986</td>
<td>184.986</td>
<td></td>
<td>150</td>
<td>0.47, (0.00, 0.39, 0.90)</td>
<td>0.009</td>
<td>0.042% (294)</td>
</tr>
<tr>
<td>m185.082</td>
<td>185.082</td>
<td>C\textsubscript{2}H\textsubscript{12}O\textsubscript{4}H\textsuperscript{+} (1.4)</td>
<td>150</td>
<td>11.1, (-0.02, 7.3, 26.6)</td>
<td>0.298</td>
<td>0.99% (22)</td>
</tr>
<tr>
<td>m185.151</td>
<td>185.151</td>
<td>C\textsubscript{11}H\textsubscript{20}O\textsubscript{2}H\textsuperscript{+} (-2.4)</td>
<td>150</td>
<td>2.2, (-0.04, 1.6, 5.2)</td>
<td>0.136</td>
<td>0.20% (104)</td>
</tr>
<tr>
<td>m185.938</td>
<td>185.938</td>
<td></td>
<td>150</td>
<td>0.030, (0.000, 0.019, 0.073)</td>
<td>0.003</td>
<td>0.0027% (564)</td>
</tr>
<tr>
<td>m186.083</td>
<td>186.083</td>
<td>C\textsubscript{2}H\textsubscript{12}O\textsubscript{4}H\textsuperscript{+} (-0.9)</td>
<td>150</td>
<td>1.79, (0.00, 1.15, 4.14)</td>
<td>0.065</td>
<td>0.161% (115)</td>
</tr>
<tr>
<td>m186.192</td>
<td>186.192</td>
<td>C\textsubscript{12}H\textsubscript{24}OH\textsuperscript{+} (-1.1)</td>
<td>150</td>
<td>0.080, (-0.004, 0.054, 0.206)</td>
<td>0.020</td>
<td>0.0071% (486)</td>
</tr>
<tr>
<td>m186.934</td>
<td>186.934</td>
<td></td>
<td>150</td>
<td>0.060, (0.000, 0.038, 0.137)</td>
<td>0.005</td>
<td>0.0054% (504)</td>
</tr>
<tr>
<td>m187.062</td>
<td>187.062</td>
<td>C\textsubscript{5}H\textsubscript{10}O\textsubscript{5}H\textsuperscript{+} (2.2), C\textsubscript{9}H\textsubscript{14}S\textsubscript{2}H\textsuperscript{+} (1.3)</td>
<td>150</td>
<td>4.9, (-0.01, 2.4, 12.9)</td>
<td>0.079</td>
<td>0.44% (50)</td>
</tr>
<tr>
<td>m187.151</td>
<td>187.151</td>
<td>C\textsubscript{10}H\textsubscript{19}NO\textsubscript{2}H\textsuperscript{+} (-0.9), C\textsubscript{11}H\textsubscript{22}SH\textsuperscript{+} (-0.2)</td>
<td>150</td>
<td>1.13, (-0.03, 0.70, 2.62)</td>
<td>0.067</td>
<td>0.102% (176)</td>
</tr>
<tr>
<td>m187.971</td>
<td>187.971</td>
<td></td>
<td>150</td>
<td>0.059, (0.001, 0.043, 0.125)</td>
<td>0.005</td>
<td>0.0053% (505)</td>
</tr>
<tr>
<td>m188.063</td>
<td>188.063</td>
<td>C\textsubscript{8}H\textsubscript{10}O\textsubscript{5}H\textsuperscript{+} (-0.1)</td>
<td>150</td>
<td>1.21, (0.00, 0.62, 2.95)</td>
<td>0.038</td>
<td>0.108% (166)</td>
</tr>
<tr>
<td>m189.024</td>
<td>189.024</td>
<td></td>
<td>150</td>
<td>0.74, (0.02, 0.69, 1.55)</td>
<td>0.012</td>
<td>0.066% (234)</td>
</tr>
<tr>
<td>m189.076</td>
<td>189.076</td>
<td>C\textsubscript{2}H\textsubscript{12}O\textsubscript{5}H\textsuperscript{+} (0.6), C\textsubscript{11}H\textsubscript{9}NO\textsubscript{2}H\textsuperscript{+} (2.4), C\textsubscript{9}H\textsubscript{16}S\textsubscript{2}H\textsuperscript{+} (-0.3)</td>
<td>150</td>
<td>2.7, (0.00, 2.1, 6.6)</td>
<td>0.040</td>
<td>0.24% (89)</td>
</tr>
<tr>
<td>m189.126</td>
<td>189.126</td>
<td>C\textsubscript{13}H\textsubscript{16}OH\textsuperscript{+} (-1.1), C\textsubscript{8}H\textsubscript{16}N\textsubscript{2}O\textsubscript{3}H\textsuperscript{+} (3.0)</td>
<td>150</td>
<td>0.42, (-0.01, 0.29, 1.00)</td>
<td>0.028</td>
<td>0.037% (314)</td>
</tr>
<tr>
<td>m189.979</td>
<td>189.979</td>
<td></td>
<td>150</td>
<td>0.080, (0.003, 0.069, 0.164)</td>
<td>0.007</td>
<td>0.0071% (487)</td>
</tr>
<tr>
<td>m190.055</td>
<td>C_{11}H_{8}O_{3}H^{+} (-2.6)</td>
<td>250</td>
<td>0.159, (0.002, 0.153, 0.326)</td>
<td>0.008</td>
<td>0.0142% (425)</td>
<td></td>
</tr>
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<td></td>
</tr>
<tr>
<td>m190.083</td>
<td>C_{11}H_{11}NO_{2}H^{+} (-2.9)</td>
<td>150</td>
<td>0.62, (0.00, 0.39, 1.40)</td>
<td>0.008</td>
<td>0.055% (260)</td>
<td></td>
</tr>
<tr>
<td>m190.166</td>
<td>C_{14}H_{20}H^{+} (-0.8)</td>
<td>150</td>
<td>0.117, (-0.006, 0.075, 0.263)</td>
<td>0.022</td>
<td>0.0105% (450)</td>
<td></td>
</tr>
<tr>
<td>m190.968</td>
<td>C_{11}H_{10}O_{3}H^{+} (-0.9)</td>
<td>150</td>
<td>1.57, (-0.01, 0.88, 4.50)</td>
<td>0.213</td>
<td>0.140% (450)</td>
<td></td>
</tr>
<tr>
<td>m191.069</td>
<td>C_{11}H_{10}O_{3}H^{+} (-0.9)</td>
<td>150</td>
<td>1.61, (0.00, 1.33, 3.35)</td>
<td>0.132</td>
<td>0.144% (127)</td>
<td></td>
</tr>
<tr>
<td>m191.102</td>
<td>C_{7}H_{14}O_{4}H^{+} (-0.2)</td>
<td>150</td>
<td>1.06, (-0.02, 0.76, 2.52)</td>
<td>0.057</td>
<td>0.095% (181)</td>
<td></td>
</tr>
<tr>
<td>m191.972</td>
<td>C_{10}H_{8}O_{4}H^{+} (2.9), C_{7}H_{12}O_{4}H^{+} (-0.5)</td>
<td>150</td>
<td>0.88, (0.00, 0.70, 1.80)</td>
<td>0.026</td>
<td>0.078% (212)</td>
<td></td>
</tr>
<tr>
<td>m193.088</td>
<td>C_{7}H_{16}O_{4}H^{+} (2.5), C_{7}H_{16}O_{3}SH^{+} (-0.9)</td>
<td>200</td>
<td>0.84, (0.00, 0.63, 1.86)</td>
<td>0.018</td>
<td>0.075% (218)</td>
<td></td>
</tr>
<tr>
<td>m193.118</td>
<td>C_{10}H_{16}N_{2}O_{4}H^{+} (0.2), C_{10}H_{13}N_{3}OH^{+} (2.0)</td>
<td>150</td>
<td>1.19, (-0.04, 0.87, 2.83)</td>
<td>0.061</td>
<td>0.106% (169)</td>
<td></td>
</tr>
<tr>
<td>m193.969</td>
<td>C_{11}H_{12}O_{3}H^{+} (2.5), C_{10}H_{13}N_{3}OH^{+} (2.0)</td>
<td>150</td>
<td>0.133, (0.001, 0.088, 0.348)</td>
<td>0.024</td>
<td>0.0119% (438)</td>
<td></td>
</tr>
<tr>
<td>m194.095</td>
<td>C_{14}H_{11}NH^{+} (-1.0)</td>
<td>200</td>
<td>0.60, (0.02, 0.45, 1.32)</td>
<td>0.004</td>
<td>0.054% (263)</td>
<td></td>
</tr>
<tr>
<td>m194.121</td>
<td>C_{7}H_{16}N_{2}O_{4}H^{+} (-0.2)</td>
<td>150</td>
<td>0.195, (0.001, 0.123, 0.484)</td>
<td>0.010</td>
<td>0.0175% (402)</td>
<td></td>
</tr>
<tr>
<td>m194.961</td>
<td>C_{8}H_{16}N_{2}O_{4}H^{+} (-2.9), C_{12}H_{7}N_{3}H^{+} (-1.1)</td>
<td>150</td>
<td>0.34, (0.00, 0.22, 0.88)</td>
<td>0.048</td>
<td>0.030% (336)</td>
<td></td>
</tr>
<tr>
<td>m195.073</td>
<td>C_{10}H_{10}N_{2}O_{3}H^{+} (-2.9), C_{12}H_{7}N_{3}H^{+} (-1.1)</td>
<td>150</td>
<td>1.79, (-0.01, 1.27, 3.85)</td>
<td>0.045</td>
<td>0.161% (114)</td>
<td></td>
</tr>
<tr>
<td>m</td>
<td>m-1</td>
<td>C_{11}H_{17}O_{3}H^{+} (-0.1), C_{10}H_{11}NH^{+} (1.7)</td>
<td>150</td>
<td>2.3, (0.05, 1.6, 5.5)</td>
<td>0.072</td>
<td>0.21% (98)</td>
</tr>
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</tr>
<tr>
<td>m195.101</td>
<td>195.101</td>
<td>C_{14}H_{11}O_{3}H^{+} (1.8), C_{3}H_{13}N_{3}O_{5}H^{+} (-1.3)</td>
<td>150</td>
<td>0.058, (0.000, 0.041, 0.134)</td>
<td>0.007</td>
<td>0.0052% (508)</td>
</tr>
<tr>
<td>m196.091</td>
<td>196.092</td>
<td>C_{10}H_{13}NO_{2}H^{+} (2.7), C_{8}H_{14}N_{2}O_{5}H^{+} (-1.4)</td>
<td>150</td>
<td>0.52, (0.00, 0.31, 1.22)</td>
<td>0.029</td>
<td>0.047% (274)</td>
</tr>
<tr>
<td>m196.958</td>
<td>196.959</td>
<td>C_{14}H_{11}O_{3}H^{+} (1.8), C_{3}H_{13}N_{3}O_{5}H^{+} (-1.3)</td>
<td>150</td>
<td>0.126, (0.005, 0.086, 0.296)</td>
<td>0.010</td>
<td>0.0035% (442)</td>
</tr>
<tr>
<td>m197.095</td>
<td>197.096</td>
<td>C_{14}H_{12}OH^{+} (-0.5), C_{3}H_{13}N_{3}O_{5}H^{+} (-0.6)</td>
<td>150</td>
<td>3.1, (0.10, 1.7, 7.7)</td>
<td>0.810</td>
<td>0.28% (79)</td>
</tr>
<tr>
<td>m199.052</td>
<td>199.053</td>
<td>C_{16}H_{15}H^{+} (-1.6), C_{11}H_{6}N_{2}O_{2}H^{+} (2.4), C_{3}H_{7}N_{3}O_{4}H^{+} (-1.7)</td>
<td>150</td>
<td>2.6, (0.01, 1.9, 5.9)</td>
<td>0.038</td>
<td>0.23% (93)</td>
</tr>
<tr>
<td>m199.095</td>
<td>199.096</td>
<td>C_{10}H_{14}O_{4}H^{+} (-0.9), C_{13}H_{11}NOH^{+} (0.9)</td>
<td>150</td>
<td>6.7, (0.00, 3.9, 16.2)</td>
<td>0.055</td>
<td>0.60% (41)</td>
</tr>
<tr>
<td>m200.062</td>
<td>200.063</td>
<td>C_{3}H_{10}O_{5}H^{+} (-0.8)</td>
<td>150</td>
<td>0.025, (-0.001, 0.015, 0.061)</td>
<td>0.008</td>
<td>0.0022% (580)</td>
</tr>
<tr>
<td>m200.097</td>
<td>200.098</td>
<td>C_{10}H_{14}O_{3}H^{+} (-2.2), C_{3}H_{13}N_{3}SH^{+} (1.2)</td>
<td>150</td>
<td>1.32, (0.00, 0.67, 3.16)</td>
<td>0.010</td>
<td>0.118% (148)</td>
</tr>
<tr>
<td>m201.170</td>
<td>201.171</td>
<td>C_{11}H_{21}NO_{2}H^{+} (2.8)</td>
<td>150</td>
<td>0.73, (0.00, 0.49, 1.64)</td>
<td>0.024</td>
<td>0.066% (236)</td>
</tr>
<tr>
<td>m201.935</td>
<td>201.936</td>
<td>C_{11}H_{21}NO_{2}H^{+} (2.8)</td>
<td>150</td>
<td>0.022, (-0.001, 0.014, 0.054)</td>
<td>0.006</td>
<td>0.00195% (590)</td>
</tr>
<tr>
<td>m</td>
<td>m</td>
<td>Formula</td>
<td>m/z</td>
<td>Intensity</td>
<td>M/z</td>
<td>Width</td>
</tr>
<tr>
<td>-----</td>
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</tr>
<tr>
<td>202.084</td>
<td>202.085</td>
<td>C_{12}H_{11}NO_{2}H^{+} (-1.6), C_{7}H_{11}N_{3}O_{4}H^{+} (2.4)</td>
<td>150</td>
<td>0.79, (-0.01, 0.47, 1.87)</td>
<td>0.012</td>
<td>0.071% (224)</td>
</tr>
<tr>
<td>202.171</td>
<td>202.172</td>
<td></td>
<td>150</td>
<td>0.29, (-0.01, 0.19, 0.73)</td>
<td>0.034</td>
<td>0.026% (357)</td>
</tr>
<tr>
<td>203.092</td>
<td>203.093</td>
<td>C_{9}H_{14}O_{5}H^{+} (1.3), C_{10}H_{18}S_{2}H^{+} (0.4)</td>
<td>150</td>
<td>1.66, (0.00, 1.24, 3.77)</td>
<td>0.054</td>
<td>0.149% (121)</td>
</tr>
<tr>
<td>204.095</td>
<td>204.096</td>
<td>C_{9}H_{14}O_{5}H^{+} (1.0), C_{7}H_{13}N_{3}O_{4}H^{+} (-2.2)</td>
<td>150</td>
<td>0.48, (0.00, 0.28, 1.10)</td>
<td>0.010</td>
<td>0.043% (285)</td>
</tr>
<tr>
<td>204.181</td>
<td>204.182</td>
<td>C_{15}H_{22}H^{+} (-1.1), C_{10}H_{22}N_{2}O_{2}H^{+} (3.0)</td>
<td>150</td>
<td>0.073, (-0.002, 0.045, 0.176)</td>
<td>0.026</td>
<td>0.0065% (495)</td>
</tr>
<tr>
<td>204.988</td>
<td>204.989</td>
<td>C_{5}H_{4}N_{2}O_{5}SH^{+} (-2.6)</td>
<td>150</td>
<td>0.33, (0.00, 0.30, 0.67)</td>
<td>0.017</td>
<td>0.030% (341)</td>
</tr>
<tr>
<td>205.084</td>
<td>205.085</td>
<td>C_{12}H_{12}O_{3}H^{+} (-1.2), C_{15}H_{9}NH^{+} (0.6), C_{7}H_{12}N_{2}O_{5}H^{+} (2.8)</td>
<td>150</td>
<td>1.74, (-0.03, 1.36, 4.07)</td>
<td>0.065</td>
<td>0.156% (117)</td>
</tr>
<tr>
<td>205.936</td>
<td>205.937</td>
<td></td>
<td>150</td>
<td>0.017, (0.000, 0.012, 0.039)</td>
<td>0.006</td>
<td>0.00157% (604)</td>
</tr>
<tr>
<td>206.086</td>
<td>206.087</td>
<td>C_{12}H_{12}O_{3}H^{+} (-2.5), C_{7}H_{12}N_{2}O_{5}H^{+} (1.5)</td>
<td>150</td>
<td>0.46, (0.00, 0.33, 1.02)</td>
<td>0.013</td>
<td>0.042% (296)</td>
</tr>
<tr>
<td>207.032</td>
<td>207.033</td>
<td>C_{7}H_{10}O_{5}SH^{+} (0.6)</td>
<td>150</td>
<td>0.53, (-0.01, 0.41, 1.12)</td>
<td>0.019</td>
<td>0.048% (272)</td>
</tr>
<tr>
<td>207.101</td>
<td>207.102</td>
<td>C_{12}H_{14}O_{3}H^{+} (0.2), C_{15}H_{11}NH^{+} (2.0)</td>
<td>150</td>
<td>1.38, (0.00, 0.95, 3.17)</td>
<td>0.032</td>
<td>0.124% (144)</td>
</tr>
<tr>
<td>207.132</td>
<td>207.133</td>
<td>C_{9}H_{18}N_{2}O_{4}H^{+} (-1.1), C_{11}H_{15}N_{3}OH^{+} (0.7)</td>
<td>150</td>
<td>0.54, (-0.02, 0.34, 1.30)</td>
<td>0.068</td>
<td>0.048% (271)</td>
</tr>
<tr>
<td>207.934</td>
<td>207.935</td>
<td></td>
<td>150</td>
<td>0.018, (0.000, 0.013, 0.044)</td>
<td>0.006</td>
<td>0.00165% (601)</td>
</tr>
<tr>
<td>208.076</td>
<td>208.077</td>
<td>C_{14}H_{9}NOH^{+} (1.1), C_{10}H_{10}N_{2}O_{2}H^{+} (-2.9), C_{11}H_{13}NOSH^{+} (-2.2)</td>
<td>150</td>
<td>0.56, (0.01, 0.46, 1.19)</td>
<td>0.021</td>
<td>0.050% (269)</td>
</tr>
<tr>
<td>208.936</td>
<td>208.937</td>
<td></td>
<td>150</td>
<td>0.036, (0.000, 0.022, 0.095)</td>
<td>0.016</td>
<td>0.0033% (548)</td>
</tr>
<tr>
<td>m209.062</td>
<td>209.063</td>
<td>C_{12}H_{21}O_{2}H^{+} (-2.7), C_{10}H_{3}NO_{4}H^{+} (-0.9), C_{11}H_{12}OSH^{+} (-0.2)</td>
<td>150</td>
<td>1.23, (0.09, 0.92, 2.63)</td>
<td>0.068</td>
<td>0.110% (159)</td>
</tr>
<tr>
<td>m209.151</td>
<td>209.152</td>
<td>C_{13}H_{26}O_{2}H^{+} (-1.8), C_{8}H_{20}N_{2}O_{4}H^{+} (2.3)</td>
<td>150</td>
<td>1.65, (-0.11, 1.13, 4.18)</td>
<td>0.129</td>
<td>0.148% (122)</td>
</tr>
<tr>
<td>m209.936</td>
<td>209.937</td>
<td>C_{13}H_{21}O_{2}H^{+} (-1.1), C_{12}H_{7}N_{3}OH^{+} (1.7)</td>
<td>150</td>
<td>0.41, (0.01, 0.23, 1.01)</td>
<td>0.015</td>
<td>0.036% (316)</td>
</tr>
<tr>
<td>m210.067</td>
<td>210.068</td>
<td>C_{14}H_{10}O_{2}H^{+} (2.5), C_{10}H_{11}NO_{3}H^{+} (-1.5), C_{11}H_{14}OSH^{+} (-0.8)</td>
<td>150</td>
<td>1.44, (0.02, 1.20, 2.90)</td>
<td>0.230</td>
<td>0.129% (139)</td>
</tr>
<tr>
<td>m210.153</td>
<td>210.154</td>
<td>C_{14}H_{26}OH^{+} (-0.7)</td>
<td>150</td>
<td>0.35, (0.00, 0.25, 0.84)</td>
<td>0.072</td>
<td>0.032% (331)</td>
</tr>
<tr>
<td>m211.077</td>
<td>211.078</td>
<td>C_{14}H_{10}O_{2}H^{+} (-2.7), C_{12}H_{6}NO_{3}H^{+} (0.1)</td>
<td>150</td>
<td>0.66, (0.03, 0.46, 1.44)</td>
<td>0.040</td>
<td>0.059% (253)</td>
</tr>
<tr>
<td>m211.204</td>
<td>211.205</td>
<td>150</td>
<td>0.35, (0.00, 0.25, 0.84)</td>
<td>0.072</td>
<td>0.032% (331)</td>
<td></td>
</tr>
<tr>
<td>m211.967</td>
<td>211.968</td>
<td>C_{13}H_{11}O_{2}H^{+} (1.7), C_{9}H_{12}N_{2}O_{4}H^{+} (-1.3), C_{10}H_{15}NO_{2}SH^{+} (-1.6)</td>
<td>150</td>
<td>0.77, (-0.01, 0.54, 1.75)</td>
<td>0.010</td>
<td>0.069% (228)</td>
</tr>
<tr>
<td>m213.079</td>
<td>213.080</td>
<td>C_{12}H_{21}NO_{2}H^{+} (2.1)</td>
<td>150</td>
<td>3.3, (0.00, 2.1, 8.2)</td>
<td>0.044</td>
<td>0.30% (73)</td>
</tr>
<tr>
<td>m213.169</td>
<td>213.170</td>
<td>C_{12}H_{21}NO_{2}H^{+} (2.1)</td>
<td>150</td>
<td>0.70, (-0.02, 0.47, 1.76)</td>
<td>0.141</td>
<td>0.063% (242)</td>
</tr>
<tr>
<td>m213.936</td>
<td>213.937</td>
<td>0.020, (-0.001, 0.014, 0.045)</td>
<td>0.007</td>
<td>0.00179% (598)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>m214.087</td>
<td>214.088</td>
<td>C_{13}H_{12}NO_{2}H^{+} (1.7), C_{9}H_{12}N_{2}O_{4}H^{+} (-2.4), C_{10}H_{15}NO_{2}SH^{+} (-1.6)</td>
<td>150</td>
<td>0.77, (-0.01, 0.54, 1.75)</td>
<td>0.010</td>
<td>0.069% (228)</td>
</tr>
<tr>
<td>m214.170</td>
<td>214.171</td>
<td>0.165, (-0.003, 0.106, 0.392)</td>
<td>0.025</td>
<td>0.0147% (422)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>m214.924</td>
<td>214.925</td>
<td>0.031, (-0.001, 0.020, 0.069)</td>
<td>0.007</td>
<td>0.0027% (562)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>m215.035</td>
<td>215.036</td>
<td>C_{12}H_{6}O_{4}H^{+} (2.1), C_{9}H_{10}O_{4}SH^{+} (-1.3)</td>
<td>150</td>
<td>0.38, (0.00, 0.27, 0.85)</td>
<td>0.013</td>
<td>0.034% (321)</td>
</tr>
<tr>
<td>m</td>
<td>m</td>
<td>C_{10}H_{14}O_{5}H^+ (2.6), C_{11}H_{18}S_{2}H^+ (1.7)</td>
<td>150</td>
<td>1.98, (-0.01, 1.10, 4.99)</td>
<td>0.047</td>
<td>0.178% (106)</td>
</tr>
<tr>
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</tr>
<tr>
<td>m215.093</td>
<td>m215.094</td>
<td>C_{13}H_{15}NO_{2}H^+ (-2.9), C_{8}H_{13}N_{3}O_{4}H^+ (1.1)</td>
<td>150</td>
<td>0.61, (0.00, 0.34, 1.46)</td>
<td>0.006</td>
<td>0.055% (262)</td>
</tr>
<tr>
<td>m215.964</td>
<td>m215.965</td>
<td>C_{15}H_{15}NOH^+ (-2.7), C_{10}H_{5}N_{3}O_{3}H^+ (1.3)</td>
<td>150</td>
<td>0.32, (0.00, 0.22, 0.72)</td>
<td>0.016</td>
<td>0.029% (345)</td>
</tr>
<tr>
<td>m216.098</td>
<td>m216.099</td>
<td>C_{10}H_{16}O_{5}H^+ (2.0)</td>
<td>150</td>
<td>1.19, (-0.03, 0.99, 2.69)</td>
<td>0.048</td>
<td>0.106% (170)</td>
</tr>
<tr>
<td>m217.108</td>
<td>m217.109</td>
<td>C_{10}H_{16}O_{5}H^+ (2.7), C_{8}H_{15}N_{3}O_{4}H^+ (-0.5)</td>
<td>150</td>
<td>0.37, (-0.01, 0.25, 0.83)</td>
<td>0.010</td>
<td>0.033% (326)</td>
</tr>
<tr>
<td>m218.112</td>
<td>m218.113</td>
<td>C_{10}H_{16}O_{5}H^+ (2.7), C_{8}H_{15}N_{3}O_{4}H^+ (-0.5)</td>
<td>150</td>
<td>0.37, (-0.01, 0.25, 0.83)</td>
<td>0.010</td>
<td>0.033% (326)</td>
</tr>
<tr>
<td>m219.049</td>
<td>m219.050</td>
<td>C_{13}H_{14}O_{5}H^+ (-2.5), C_{16}H_{11}NH^+ (-0.7), C_{8}H_{14}O_{2}S_{2}H^+ (0.2)</td>
<td>150</td>
<td>0.29, (0.00, 0.20, 0.66)</td>
<td>0.043</td>
<td>0.026% (358)</td>
</tr>
<tr>
<td>m219.098</td>
<td>m219.099</td>
<td>C_{13}H_{14}O_{5}H^+ (-2.5), C_{16}H_{11}NH^+ (-0.7), C_{8}H_{14}O_{2}S_{2}H^+ (0.2)</td>
<td>150</td>
<td>0.50, (-0.01, 0.35, 1.14)</td>
<td>0.010</td>
<td>0.044% (282)</td>
</tr>
<tr>
<td>m219.135</td>
<td>m219.136</td>
<td>C_{14}H_{18}O_{2}H^+ (0.9), C_{10}H_{9}N_{3}O_{2}H^+ (2.2)</td>
<td>150</td>
<td>0.85, (-0.02, 0.64, 1.89)</td>
<td>0.082</td>
<td>0.076% (216)</td>
</tr>
<tr>
<td>m219.947</td>
<td>m219.948</td>
<td>C_{14}H_{18}O_{2}H^+ (0.9), C_{10}H_{9}N_{3}O_{2}H^+ (2.2)</td>
<td>150</td>
<td>0.85, (-0.02, 0.64, 1.89)</td>
<td>0.082</td>
<td>0.076% (216)</td>
</tr>
<tr>
<td>m220.053</td>
<td>m220.054</td>
<td>C_{8}H_{10}O_{7}H^+ (0.2), C_{10}H_{9}N_{3}OSH^+ (0.2)</td>
<td>150</td>
<td>0.195, (0.000, 0.122, 0.474)</td>
<td>0.009</td>
<td>0.0175% (403)</td>
</tr>
<tr>
<td>m221.080</td>
<td>m221.081</td>
<td>C_{12}H_{12}O_{2}H^+ (0.3), C_{15}H_{5}NOH^+ (2.1)</td>
<td>150</td>
<td>0.93, (0.00, 0.62, 2.15)</td>
<td>0.033</td>
<td>0.083% (196)</td>
</tr>
<tr>
<td>m221.153</td>
<td>m221.154</td>
<td>C_{14}H_{20}O_{2}H^+ (0.6), C_{11}H_{24}O_{2}SH^+ (-2.8)</td>
<td>150</td>
<td>1.03, (-0.03, 0.62, 2.58)</td>
<td>0.197</td>
<td>0.093% (183)</td>
</tr>
<tr>
<td>m222.156</td>
<td>m222.157</td>
<td>C_{14}H_{20}O_{2}H^+ (0.2), C_{12}H_{19}N_{3}OH^+ (2.9)</td>
<td>150</td>
<td>0.30, (-0.01, 0.18, 0.78)</td>
<td>0.039</td>
<td>0.027% (355)</td>
</tr>
<tr>
<td>Mass (m)</td>
<td>ppm (m)</td>
<td>Formula</td>
<td>Charge</td>
<td>Retention Time (min)</td>
<td>RT Error (min)</td>
<td>EIMS (eV)</td>
</tr>
<tr>
<td>---------</td>
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</tr>
<tr>
<td>222.938</td>
<td>222.939</td>
<td>C_{12}H_{14}O_{2}H^+ (-1.3), C_{15}H_{11}NOH^+ (0.5)</td>
<td>150</td>
<td>0.045, (0.000, 0.033, 0.104)</td>
<td>0.010</td>
<td>0.0040% (526)</td>
</tr>
<tr>
<td>223.094</td>
<td>223.095</td>
<td>C_{14}H_{22}O_{3}H^+ (-2.0), C_{14}H_{22}N_{2}O_{4}H^+ (2.0)</td>
<td>150</td>
<td>1.38, (-0.08, 0.92, 3.36)</td>
<td>0.149</td>
<td>0.123% (145)</td>
</tr>
<tr>
<td>223.166</td>
<td>223.167</td>
<td>C_{14}H_{22}O_{2}H^+ (-0.4), C_{15}H_{17}N_{3}SH^+ (-1.0)</td>
<td>150</td>
<td>0.49, (-0.01, 0.30, 1.25)</td>
<td>0.119</td>
<td>0.044% (284)</td>
</tr>
<tr>
<td>224.069</td>
<td>224.070</td>
<td>C_{14}H_{22}O_{2}H^+ (-2.0), C_{12}H_{17}N_{3}O_{4}H^+ (2.0)</td>
<td>150</td>
<td>0.28, (-0.01, 0.16, 0.72)</td>
<td>0.027</td>
<td>0.025% (362)</td>
</tr>
<tr>
<td>225.047</td>
<td>225.048</td>
<td>C_{14}H_{22}O_{3}H^+ (-2.3), C_{12}H_{19}N_{3}O_{5}H^+ (-0.5)</td>
<td>150</td>
<td>0.22, (-0.02, 0.12, 0.53)</td>
<td>0.059</td>
<td>0.020% (392)</td>
</tr>
<tr>
<td>225.113</td>
<td>225.114</td>
<td>C_{12}H_{16}O_{4}H^+ (2.1), C_{12}H_{20}O_{6}H^+ (-1.2)</td>
<td>150</td>
<td>1.29, (0.00, 0.76, 3.12)</td>
<td>0.021</td>
<td>0.116% (151)</td>
</tr>
<tr>
<td>225.148</td>
<td>225.149</td>
<td>C_{13}H_{20}O_{5}H^+ (0.8), C_{16}H_{17}NH^+ (2.5)</td>
<td>150</td>
<td>0.50, (-0.01, 0.37, 1.17)</td>
<td>0.261</td>
<td>0.045% (281)</td>
</tr>
<tr>
<td>226.152</td>
<td>226.153</td>
<td>C_{13}H_{20}O_{3}H^+ (1.4), C_{11}H_{19}N_{3}O_{4}H^+ (-1.7)</td>
<td>150</td>
<td>0.083, (-0.010, 0.051, 0.193)</td>
<td>0.014</td>
<td>0.0074% (480)</td>
</tr>
<tr>
<td>226.942</td>
<td>226.943</td>
<td>C_{11}H_{14}O_{3}H^+ (-2.1), C_{14}H_{11}NO_{3}H^+ (0.4), C_{16}H_{14}NH^+ (0.4)</td>
<td>200</td>
<td>0.33, (0.00, 0.18, 0.79)</td>
<td>0.011</td>
<td>0.029% (343)</td>
</tr>
<tr>
<td>227.088</td>
<td>227.089</td>
<td>C_{11}H_{14}O_{3}H^+ (-2.1), C_{14}H_{11}NO_{3}H^+ (0.3), C_{15}H_{14}SH^+ (0.4)</td>
<td>150</td>
<td>1.46, (-0.01, 0.83, 3.62)</td>
<td>0.079</td>
<td>0.131% (138)</td>
</tr>
<tr>
<td>228.042</td>
<td>228.043</td>
<td>C_{14}H_{15}NOH^+ (-1.0), C_{11}H_{5}N_{3}O_{3}H^+ (3.0)</td>
<td>150</td>
<td>0.029, (0.000, 0.020, 0.066)</td>
<td>0.007</td>
<td>0.0026% (567)</td>
</tr>
<tr>
<td>228.094</td>
<td>228.095</td>
<td>C_{11}H_{12}O_{3}H^+ (0.6), C_{12}H_{13}N_{3}O_{4}H^+ (-2.5)</td>
<td>150</td>
<td>0.38, (0.00, 0.22, 0.90)</td>
<td>0.019</td>
<td>0.034% (323)</td>
</tr>
<tr>
<td>229.081</td>
<td>229.082</td>
<td>C_{17}H_{9}NH^+ (-1.7), C_{10}H_{12}N_{2}O_{3}H^+ (0.5), C_{12}H_{9}N_{3}O_{2}H^+ (2.3), C_{13}H_{12}N_{3}SH^+ (3.0)</td>
<td>200</td>
<td>0.45, (0.01, 0.26, 1.07)</td>
<td>0.006</td>
<td>0.041% (300)</td>
</tr>
<tr>
<td>m</td>
<td>m/z</td>
<td>Formula</td>
<td>Charge</td>
<td>Retention Time (min)</td>
<td>RSD (%)</td>
<td>Ions (ppm)</td>
</tr>
<tr>
<td>-------</td>
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<td>--------------------------</td>
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</tr>
<tr>
<td>m229.099</td>
<td>229.100</td>
<td>C_{18}H_{12}H^+ (-0.8), C_{9}H_{13}N_{3}O_{4}H^+ (-0.8), C_{10}H_{16}N_{2}O_{3}SH^+ (-0.1)</td>
<td>150</td>
<td>0.83, (-0.06, 0.45, 2.20)</td>
<td>0.062</td>
<td>0.074% (220)</td>
</tr>
<tr>
<td>m230.105</td>
<td>230.106</td>
<td>C_{18}H_{12}H^+ (1.9)</td>
<td>150</td>
<td>0.37, (0.00, 0.20, 0.88)</td>
<td>0.015</td>
<td>0.033% (324)</td>
</tr>
<tr>
<td>m230.201</td>
<td>230.202</td>
<td>C_{12}H_{6}O_{5}H^+ (-2.4), C_{15}H_{3}NO_{2}H^+ (-0.6)</td>
<td>150</td>
<td>0.190, (0.002, 0.147, 0.418)</td>
<td>0.018</td>
<td>0.0170% (405)</td>
</tr>
<tr>
<td>m231.025</td>
<td>231.026</td>
<td>C_{16}H_{10}N_{3}H^+ (2.8), C_{12}H_{11}N_{3}O_{2}H^+ (-1.3), C_{13}H_{14}N_{3}SH^+ (-0.6)</td>
<td>150</td>
<td>0.64, (0.00, 0.44, 1.47)</td>
<td>0.015</td>
<td>0.058% (256)</td>
</tr>
<tr>
<td>m231.135</td>
<td>231.136</td>
<td>C_{15}H_{18}O_{2}H^+ (-1.5), C_{10}H_{18}N_{2}O_{4}H^+ (2.5)</td>
<td>150</td>
<td>0.142, (-0.003, 0.082, 0.375)</td>
<td>0.067</td>
<td>0.0127% (434)</td>
</tr>
<tr>
<td>m233.153</td>
<td>233.155</td>
<td>C_{15}H_{20}O_{2}H^+ (0.9), C_{12}H_{24}O_{2}SH^+ (-2.5)</td>
<td>150</td>
<td>0.83, (-0.05, 0.53, 2.08)</td>
<td>0.069</td>
<td>0.074% (221)</td>
</tr>
<tr>
<td>m234.158</td>
<td>234.160</td>
<td>C_{15}H_{20}O_{2}H^+ (2.6), C_{13}H_{19}N_{3}OH^+ (-0.6)</td>
<td>150</td>
<td>0.22, (-0.01, 0.14, 0.55)</td>
<td>0.015</td>
<td>0.020% (391)</td>
</tr>
<tr>
<td>m236.171</td>
<td>236.173</td>
<td>C_{15}H_{22}O_{2}H^+ (0.0)</td>
<td>150</td>
<td>0.25, (-0.01, 0.15, 0.63)</td>
<td>0.024</td>
<td>0.023% (378)</td>
</tr>
<tr>
<td>m237.144</td>
<td>237.146</td>
<td>C_{14}H_{20}O_{2}H^+ (-2.9), C_{17}H_{22}NH^+ (-1.1), C_{9}H_{20}N_{2}O_{3}H^+ (1.1), C_{12}H_{17}N_{3}O_{2}H^+ (2.9)</td>
<td>150</td>
<td>1.21, (-0.01, 0.64, 2.98)</td>
<td>0.113</td>
<td>0.109% (164)</td>
</tr>
<tr>
<td>m238.113</td>
<td>238.115</td>
<td>C_{13}H_{16}O_{3}H^+ (-0.8), C_{10}H_{15}N_{3}SH^+ (2.6)</td>
<td>150</td>
<td>0.32, (-0.01, 0.18, 0.83)</td>
<td>0.025</td>
<td>0.028% (348)</td>
</tr>
<tr>
<td>m239.064</td>
<td>239.066</td>
<td>C_{18}H_{7}NH^+ (-2.8), C_{10}H_{10}N_{2}O_{2}H^+ (-0.6), C_{13}H_{2}N_{3}O_{2}H^+ (1.2), C_{6}H_{14}N_{4}O_{2}S_{2}H^+ (2.6)</td>
<td>150</td>
<td>0.39, (0.00, 0.25, 0.87)</td>
<td>0.037</td>
<td>0.035% (318)</td>
</tr>
<tr>
<td>m</td>
<td>m/z</td>
<td>Formula</td>
<td>m/z</td>
<td>Intensity (amu)</td>
<td>Intensity (ppm)</td>
<td>Relative Abundance (%)</td>
</tr>
<tr>
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</tr>
<tr>
<td>m239.128</td>
<td>239.130</td>
<td>C_{13}H_{18}O_4H^+ (1.9), C_{10}H_{22}O_4SH^+ (-1.5)</td>
<td>150</td>
<td>0.39, (0.00, 0.16, 1.05)</td>
<td>0.007</td>
<td>0.035% (320)</td>
</tr>
<tr>
<td>m241.103</td>
<td>241.105</td>
<td>C_{12}H_{16}O_3H^+ (-2.3), C_{15}H_{13}NO_3H^+ (-0.5), C_{16}H_{16}SH^+ (0.2)</td>
<td>150</td>
<td>1.05, (-0.02, 0.60, 2.76)</td>
<td>0.064</td>
<td>0.094% (182)</td>
</tr>
<tr>
<td>m242.087</td>
<td>242.089</td>
<td>C_{15}H_{12}O_3H^+ (-0.5)</td>
<td>150</td>
<td>0.24, (0.00, 0.14, 0.60)</td>
<td>0.011</td>
<td>0.022% (383)</td>
</tr>
<tr>
<td>m243.116</td>
<td>243.118</td>
<td>C_{19}H_{14}H^+ (1.0), C_{10}H_{15}N_2O_4H^+ (0.9), C_{11}H_{18}N_2O_2SH^+ (1.6)</td>
<td>150</td>
<td>0.63, (-0.03, 0.36, 1.64)</td>
<td>0.056</td>
<td>0.056% (257)</td>
</tr>
<tr>
<td>m246.118</td>
<td>246.119</td>
<td>C_{15}H_{16}O_3H^+ (-0.7)</td>
<td>150</td>
<td>0.174, (-0.005, 0.098, 0.422)</td>
<td>0.011</td>
<td>0.0156% (416)</td>
</tr>
<tr>
<td>m246.957</td>
<td>246.959</td>
<td>C_{16}H_{22}O_2H^+ (2.7), C_{12}H_{23}NO_4H^+ (-1.4), C_{13}H_{26}O_2SH^+ (-0.7)</td>
<td>150</td>
<td>0.48, (-0.04, 0.30, 1.22)</td>
<td>0.061</td>
<td>0.043% (289)</td>
</tr>
<tr>
<td>m247.170</td>
<td>247.172</td>
<td>C_{16}H_{22}O_2H^+ (2.3), C_{14}H_{21}N_2OH^+ (-0.8)</td>
<td>150</td>
<td>0.095, (-0.003, 0.054, 0.244)</td>
<td>0.013</td>
<td>0.0085% (465)</td>
</tr>
<tr>
<td>m248.173</td>
<td>248.175</td>
<td>C_{16}H_{20}O_2H^+ (1.1), C_{13}H_{25}O_2SH^+ (-2.3)</td>
<td>150</td>
<td>0.77, (-0.04, 0.48, 2.02)</td>
<td>0.069</td>
<td>0.069% (227)</td>
</tr>
<tr>
<td>m250.123</td>
<td>250.125</td>
<td>C_{17}H_{15}NOH^+ (2.4), C_{13}H_{16}N_2O_3H^+ (-1.7)</td>
<td>150</td>
<td>0.123, (-0.001, 0.070, 0.264)</td>
<td>0.014</td>
<td>0.0110% (444)</td>
</tr>
<tr>
<td>m250.186</td>
<td>250.188</td>
<td>C_{16}H_{24}O_2H^+ (-0.3)</td>
<td>150</td>
<td>0.081, (-0.004, 0.050, 0.212)</td>
<td>0.013</td>
<td>0.0073% (484)</td>
</tr>
<tr>
<td>m251.003</td>
<td>251.005</td>
<td>C_{16}H_{24}O_2H^+ (-0.3)</td>
<td>150</td>
<td>0.069, (-0.002, 0.043, 0.161)</td>
<td>0.013</td>
<td>0.0062% (500)</td>
</tr>
<tr>
<td>m251.172</td>
<td>251.174</td>
<td>C_{14}H_{22}N_2O_2H^+ (-1.4)</td>
<td>150</td>
<td>0.93, (-0.06, 0.53, 2.44)</td>
<td>0.093</td>
<td>0.083% (197)</td>
</tr>
<tr>
<td>m252.160</td>
<td>252.162</td>
<td>C_{14}H_{21}NO_3H^+ (2.6), C_{10}H_{22}N_2O_3H^+ (-1.4)</td>
<td>150</td>
<td>0.25, (-0.01, 0.14, 0.66)</td>
<td>0.029</td>
<td>0.022% (381)</td>
</tr>
<tr>
<td>m253.002</td>
<td>253.004</td>
<td>C_{14}H_{20}O_2H^+ (-1.4), C_{17}H_{17}NOH^+ (0.4)</td>
<td>150</td>
<td>0.069, (-0.004, 0.048, 0.169)</td>
<td>0.019</td>
<td>0.0062% (501)</td>
</tr>
<tr>
<td>m253.140</td>
<td>253.142</td>
<td>C_{14}H_{20}O_2H^+ (-1.4), C_{17}H_{17}NOH^+ (0.4)</td>
<td>150</td>
<td>0.86, (-0.01, 0.42, 2.15)</td>
<td>0.042</td>
<td>0.077% (215)</td>
</tr>
<tr>
<td>m254.005</td>
<td>254.007</td>
<td>C_{13}H_{3}NO_{5}H^{+} (-1.3)</td>
<td>150</td>
<td>0.021, (-0.001, 0.014, 0.051)</td>
<td>0.008</td>
<td>0.00186% (596)</td>
</tr>
<tr>
<td>m254.999</td>
<td>255.001</td>
<td>C_{12}H_{2}N_{2}O_{5}H^{+} (-2.5)</td>
<td>150</td>
<td>0.035, (-0.001, 0.022, 0.090)</td>
<td>0.018</td>
<td>0.0032% (549)</td>
</tr>
<tr>
<td>m255.121</td>
<td>255.123</td>
<td>C_{13}H_{18}O_{5}H^{+} (0.4), C_{16}H_{15}NO_{2}H^{+} (2.2)</td>
<td>150</td>
<td>0.67, (-0.02, 0.33, 1.76)</td>
<td>0.049</td>
<td>0.060% (249)</td>
</tr>
<tr>
<td>m255.230</td>
<td>255.232</td>
<td>C_{16}H_{30}O_{2}H^{+} (0.3)</td>
<td>150</td>
<td>0.38, (0.01, 0.21, 0.95)</td>
<td>0.065</td>
<td>0.034% (322)</td>
</tr>
<tr>
<td>m256.122</td>
<td>256.124</td>
<td>C_{13}H_{18}O_{5}H^{+} (-1.9)</td>
<td>150</td>
<td>0.171, (-0.005, 0.084, 0.426)</td>
<td>0.014</td>
<td>0.0153% (418)</td>
</tr>
<tr>
<td>m257.026</td>
<td>257.028</td>
<td>C_{10}H_{8}O_{5}H^{+} (-1.0), C_{13}H_{5}NO_{3}H^{+} (0.8), C_{6}H_{12}N_{2}O_{5}S_{2}H^{+} (2.2)</td>
<td>150</td>
<td>0.051, (-0.002, 0.036, 0.123)</td>
<td>0.011</td>
<td>0.0045% (518)</td>
</tr>
<tr>
<td>m257.107</td>
<td>257.109</td>
<td>C_{18}H_{12}N_{2}H^{+} (1.9), C_{14}H_{13}N_{2}O_{2}H^{+} (-2.2), C_{15}H_{16}N_{2}SH^{+} (-1.5)</td>
<td>150</td>
<td>0.43, (-0.02, 0.22, 1.10)</td>
<td>0.042</td>
<td>0.039% (307)</td>
</tr>
<tr>
<td>m259.019</td>
<td>259.021</td>
<td>C_{13}H_{6}O_{6}H^{+} (-2.4), C_{16}H_{3}NO_{3}H^{+} (-0.6), C_{6}H_{10}N_{2}O_{3}S_{2}H^{+} (0.7)</td>
<td>150</td>
<td>0.054, (-0.003, 0.043, 0.118)</td>
<td>0.010</td>
<td>0.0048% (512)</td>
</tr>
<tr>
<td>m259.107</td>
<td>259.109</td>
<td>C_{19}H_{14}OH^{+} (-2.5), C_{14}H_{14}N_{2}O_{2}H^{+} (1.6), C_{10}H_{15}N_{2}O_{2}H^{+} (-2.5), C_{11}H_{18}N_{2}O_{3}SH^{+} (-1.8)</td>
<td>200</td>
<td>0.24, (-0.01, 0.17, 0.59)</td>
<td>0.084</td>
<td>0.022% (384)</td>
</tr>
<tr>
<td>m260.109</td>
<td>260.111</td>
<td>C_{14}H_{14}N_{2}O_{2}H^{+} (0.2), C_{15}H_{17}NOSH^{+} (0.9)</td>
<td>150</td>
<td>0.104, (-0.003, 0.057, 0.260)</td>
<td>0.017</td>
<td>0.0093% (456)</td>
</tr>
<tr>
<td>m261.116</td>
<td>261.118</td>
<td>0.34, (-0.01, 0.22, 0.87)</td>
<td>200</td>
<td>0.999</td>
<td>0.030% (338)</td>
<td></td>
</tr>
<tr>
<td>m262.118</td>
<td>262.120</td>
<td>C_{18}H_{15}NOH^{+} (-2.3), C_{13}H_{15}N_{2}O_{3}H^{+} (1.7)</td>
<td>200</td>
<td>0.092, (-0.004, 0.052, 0.212)</td>
<td>0.022</td>
<td>0.0082% (468)</td>
</tr>
<tr>
<td>m263.123</td>
<td>263.125</td>
<td>C_{15}H_{18}O_{3}H^{+} (-2.4), C_{18}H_{15}NOH^{+} (-0.6)</td>
<td>200</td>
<td>0.36, (-0.02, 0.20, 0.86)</td>
<td>0.082</td>
<td>0.032% (329)</td>
</tr>
<tr>
<td>m264.127</td>
<td>264.129</td>
<td>C_{15}H_{18}O_{3}H^{+} (-1.7)</td>
<td>150</td>
<td>0.138, (-0.006, 0.068, 0.327)</td>
<td>0.028</td>
<td>0.0124% (436)</td>
</tr>
<tr>
<td>m</td>
<td>m265.142</td>
<td>265.144</td>
<td>( \text{C}<em>{15}\text{H}</em>{20}\text{O}<em>{4}\text{H}^+ ) (1.0), ( \text{C}</em>{18}\text{H}_{17}\text{NOH}^+ ) (2.8)</td>
<td>150</td>
<td>0.65, (-0.03, 0.34, 1.57)</td>
<td>0.067</td>
</tr>
<tr>
<td>-------</td>
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<td>-------------------------------------------------</td>
<td>-----</td>
<td>--------------------------</td>
<td>-------</td>
</tr>
<tr>
<td>m266.174</td>
<td>266.176</td>
<td>( \text{C}<em>{15}\text{H}</em>{23}\text{NO}<em>{2}\text{H}^+ ) (1.4), ( \text{C}</em>{11}\text{H}<em>{24}\text{N}</em>{2}\text{O}_{3}\text{H}^+ ) (-2.7)</td>
<td>150</td>
<td>0.083, (0.000, 0.048, 0.186)</td>
<td>0.037</td>
<td>0.0075% (479)</td>
</tr>
<tr>
<td>m267.155</td>
<td>267.158</td>
<td>( \text{C}<em>{15}\text{H}</em>{22}\text{O}<em>{4}\text{H}^+ ) (-1.6), ( \text{C}</em>{18}\text{H}_{19}\text{NOH}^+ ) (0.2)</td>
<td>150</td>
<td>0.69, (-0.04, 0.33, 1.79)</td>
<td>0.070</td>
<td>0.062% (244)</td>
</tr>
<tr>
<td>m269.136</td>
<td>269.139</td>
<td>( \text{C}<em>{14}\text{H}</em>{20}\text{O}<em>{5}\text{H}^+ ) (0.2), ( \text{C}</em>{17}\text{H}<em>{17}\text{NO}</em>{2}\text{H}^+ ) (2.0)</td>
<td>150</td>
<td>0.51, (-0.02, 0.24, 1.44)</td>
<td>0.041</td>
<td>0.046% (279)</td>
</tr>
<tr>
<td>m270.139</td>
<td>270.142</td>
<td>( \text{C}<em>{14}\text{H}</em>{20}\text{O}_{4}\text{H}^+ ) (-0.1)</td>
<td>150</td>
<td>0.044, (-0.003, 0.020, 0.136)</td>
<td>0.023</td>
<td>0.0039% (529)</td>
</tr>
<tr>
<td>m270.236</td>
<td>270.239</td>
<td>( \text{C}<em>{14}\text{H}</em>{22}\text{O}<em>{5}\text{H}^+ ) (-1.4), ( \text{C}</em>{17}\text{H}<em>{19}\text{NO}</em>{2}\text{H}^+ ) (0.4)</td>
<td>150</td>
<td>0.178, (0.001, 0.115, 0.368)</td>
<td>0.057</td>
<td>0.0160% (413)</td>
</tr>
<tr>
<td>m271.150</td>
<td>271.153</td>
<td>( \text{C}<em>{20}\text{H}</em>{16}\text{OH}^+ ) (2.3), ( \text{C}<em>{16}\text{H}</em>{12}\text{NO}<em>{3}\text{H}^+ ) (-1.8), ( \text{C}</em>{11}\text{H}<em>{17}\text{N}</em>{2}\text{O}<em>{3}\text{H}^+ ) (2.3), ( \text{C}</em>{17}\text{H}_{20}\text{OH}^+ ) (-1.1)</td>
<td>150</td>
<td>0.26, (0.00, 0.16, 0.68)</td>
<td>0.067</td>
<td>0.024% (372)</td>
</tr>
<tr>
<td>m274.130</td>
<td>274.133</td>
<td>( \text{C}<em>{20}\text{H}</em>{16}\text{OH}^+ ) (2.0), ( \text{C}<em>{18}\text{H}</em>{15}\text{N}_{3}\text{H}^+ ) (-1.1)</td>
<td>150</td>
<td>0.075, (-0.001, 0.039, 0.188)</td>
<td>0.016</td>
<td>0.0068% (490)</td>
</tr>
<tr>
<td>m275.135</td>
<td>275.139</td>
<td>( \text{C}<em>{18}\text{H}</em>{15}\text{N}_{3}\text{H}^+ ) (-2.5)</td>
<td>200</td>
<td>0.172, (0.001, 0.105, 0.392)</td>
<td>0.034</td>
<td>0.0154% (417)</td>
</tr>
<tr>
<td>m275.163</td>
<td>275.166</td>
<td>( \text{C}<em>{17}\text{H}</em>{22}\text{O}<em>{5}\text{H}^+ ) (1.6), ( \text{C}</em>{13}\text{H}<em>{23}\text{NO}</em>{3}\text{H}^+ ) (-2.5), ( \text{C}<em>{14}\text{H}</em>{26}\text{O}_{3}\text{SH}^+ ) (-1.8)</td>
<td>150</td>
<td>0.078, (-0.010, 0.044, 0.194)</td>
<td>0.040</td>
<td>0.0070% (489)</td>
</tr>
<tr>
<td>m276.140</td>
<td>276.143</td>
<td>( \text{C}<em>{15}\text{H}</em>{18}\text{N}<em>{2}\text{O}</em>{3}\text{H}^+ ) (0.4)</td>
<td>150</td>
<td>0.085, (-0.002, 0.052, 0.190)</td>
<td>0.024</td>
<td>0.0077% (475)</td>
</tr>
<tr>
<td>m277.137</td>
<td>277.140</td>
<td>( \text{C}<em>{19}\text{H}</em>{17}\text{NOH}^+ ) (-1.8), ( \text{C}<em>{14}\text{H}</em>{17}\text{N}<em>{2}\text{O}</em>{2}\text{H}^+ ) (2.2), ( \text{C}<em>{15}\text{H}</em>{20}\text{N}<em>{2}\text{O}</em>{3}\text{H}^+ ) (2.9)</td>
<td>150</td>
<td>0.32, (-0.01, 0.19, 0.76)</td>
<td>0.077</td>
<td>0.029% (347)</td>
</tr>
<tr>
<td>m278.137</td>
<td>278.140</td>
<td>( \text{C}<em>{15}\text{H}</em>{19}\text{NO}<em>{4}\text{H}^+ ) (1.2), ( \text{C}</em>{18}\text{H}<em>{16}\text{N}</em>{2}\text{OH}^+ ) (3.0)</td>
<td>150</td>
<td>0.064, (-0.001, 0.032, 0.137)</td>
<td>0.015</td>
<td>0.0058% (502)</td>
</tr>
<tr>
<td>m</td>
<td>mW</td>
<td>Formula</td>
<td>m/z</td>
<td>RF (ppm)</td>
<td>Retention Time (min)</td>
<td>p/n (ppm)</td>
</tr>
<tr>
<td>---------</td>
<td>----------</td>
<td>------------------------</td>
<td>---------</td>
<td>------------</td>
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<td>-----------</td>
</tr>
<tr>
<td>m278.186</td>
<td>278.189</td>
<td>C\textsubscript{20}H\textsubscript{22}NH\textsuperscript{+} (-1.5), C\textsubscript{15}H\textsubscript{23}N\textsubscript{2}O\textsubscript{2}H\textsuperscript{+} (2.6)</td>
<td>150</td>
<td>0.023, (-0.002, 0.014, 0.062)</td>
<td>0.012</td>
<td>0.0021% (587)</td>
</tr>
<tr>
<td>m279.159</td>
<td>279.162</td>
<td>C\textsubscript{16}H\textsubscript{22}O\textsubscript{2}H\textsuperscript{+} (2.8)</td>
<td>150</td>
<td>0.31, (-0.02, 0.23, 0.73)</td>
<td>0.095</td>
<td>0.028% (354)</td>
</tr>
<tr>
<td>m280.162</td>
<td>280.165</td>
<td>C\textsubscript{16}H\textsubscript{22}O\textsubscript{2}H\textsuperscript{+} (2.5), C\textsubscript{14}H\textsubscript{21}N\textsubscript{2}O\textsubscript{3}H\textsuperscript{+} (-0.6)</td>
<td>150</td>
<td>0.074, (-0.004, 0.055, 0.167)</td>
<td>0.022</td>
<td>0.0066% (494)</td>
</tr>
<tr>
<td>m283.043</td>
<td>283.046</td>
<td>C\textsubscript{12}H\textsubscript{10}O\textsubscript{8}H\textsuperscript{+} (1.2), C\textsubscript{15}H\textsubscript{11}NO\textsubscript{5}H\textsuperscript{+} (-0.6)</td>
<td>150</td>
<td>0.126, (-0.001, 0.101, 0.279)</td>
<td>0.030</td>
<td>0.0113% (443)</td>
</tr>
<tr>
<td>m284.042</td>
<td>284.045</td>
<td>C\textsubscript{19}H\textsubscript{6}O\textsubscript{3}H\textsuperscript{+} (2.7), C\textsubscript{17}H\textsubscript{7}NO\textsubscript{3}H\textsuperscript{+} (-0.4)</td>
<td>200</td>
<td>0.201, (-0.001, 0.017, 0.045)</td>
<td>0.111</td>
<td>0.00192% (594)</td>
</tr>
<tr>
<td>m285.026</td>
<td>285.029</td>
<td>C\textsubscript{17}H\textsubscript{4}N\textsubscript{2}O\textsubscript{3}H\textsuperscript{+} (-0.4), C\textsubscript{20}HN\textsubscript{4}H\textsuperscript{+} (1.4)</td>
<td>150</td>
<td>0.040, (0.000, 0.026, 0.091)</td>
<td>0.015</td>
<td>0.0036% (539)</td>
</tr>
<tr>
<td>m285.259</td>
<td>285.262</td>
<td>C\textsubscript{17}H\textsubscript{3}NO\textsubscript{3}H\textsuperscript{+} (0.3), C\textsubscript{18}H\textsubscript{3}SH\textsuperscript{+} (1.0)</td>
<td>200</td>
<td>0.114, (0.014, 0.089, 0.264)</td>
<td>0.055</td>
<td>0.0102% (453)</td>
</tr>
<tr>
<td>m287.142</td>
<td>287.145</td>
<td>C\textsubscript{21}H\textsubscript{18}OH\textsuperscript{+} (2.1), C\textsubscript{17}H\textsubscript{19}NO\textsubscript{3}H\textsuperscript{+} (-2.0), C\textsubscript{12}H\textsubscript{19}N\textsubscript{2}O\textsubscript{3}H\textsuperscript{+} (2.1), C\textsubscript{18}H\textsubscript{22}OSH\textsuperscript{+} (-1.3)</td>
<td>150</td>
<td>0.178, (-0.009, 0.097, 0.460)</td>
<td>0.035</td>
<td>0.0160% (412)</td>
</tr>
<tr>
<td>m288.146</td>
<td>288.149</td>
<td>C\textsubscript{21}H\textsubscript{18}OH\textsuperscript{+} (2.8), C\textsubscript{19}H\textsubscript{17}N\textsubscript{3}H\textsuperscript{+} (-0.3)</td>
<td>150</td>
<td>0.070, (-0.002, 0.030, 0.162)</td>
<td>0.012</td>
<td>0.0063% (498)</td>
</tr>
<tr>
<td>m295.078</td>
<td>295.081</td>
<td>C\textsubscript{14}H\textsubscript{14}O\textsubscript{7}H\textsuperscript{+} (0.2), C\textsubscript{17}H\textsubscript{11}NO\textsubscript{3}H\textsuperscript{+} (2.0), C\textsubscript{18}H\textsubscript{14}O\textsubscript{2}SH\textsuperscript{+} (2.7)</td>
<td>200</td>
<td>0.177, (-0.004, 0.134, 0.413)</td>
<td>0.063</td>
<td>0.0158% (414)</td>
</tr>
<tr>
<td>m300.065</td>
<td>300.069</td>
<td>C\textsubscript{15}H\textsubscript{10}N\textsubscript{2}O\textsubscript{3}H\textsuperscript{+} (-1.0)</td>
<td>150</td>
<td>0.047, (0.003, 0.035, 0.106)</td>
<td>0.022</td>
<td>0.0042% (524)</td>
</tr>
<tr>
<td>m301.059</td>
<td>301.063</td>
<td>C\textsubscript{23}H\textsubscript{8}OH\textsuperscript{+} (-2.2), C\textsubscript{18}H\textsubscript{8}N\textsubscript{2}O\textsubscript{3}H\textsuperscript{+} (1.8), C\textsubscript{14}H\textsubscript{9}N\textsubscript{3}O\textsubscript{3}H\textsuperscript{+} (-2.2)</td>
<td>150</td>
<td>0.057, (0.005, 0.040, 0.128)</td>
<td>0.025</td>
<td>0.0051% (510)</td>
</tr>
<tr>
<td>m306.187</td>
<td>306.191</td>
<td>C\textsubscript{22}H\textsubscript{24}OH\textsuperscript{+} (-2.6), C\textsubscript{17}H\textsubscript{24}N\textsubscript{2}O\textsubscript{3}H\textsuperscript{+} (1.5)</td>
<td>150</td>
<td>0.054, (-0.003, 0.031, 0.141)</td>
<td>0.015</td>
<td>0.0048% (513)</td>
</tr>
<tr>
<td>m306.924</td>
<td>306.928</td>
<td>C\textsubscript{22}H\textsubscript{24}OH\textsuperscript{+} (-2.6), C\textsubscript{17}H\textsubscript{24}N\textsubscript{2}O\textsubscript{3}H\textsuperscript{+} (1.5)</td>
<td>150</td>
<td>0.019, (-0.003, 0.018, 0.045)</td>
<td>0.008</td>
<td>0.00172% (599)</td>
</tr>
<tr>
<td>m</td>
<td>m</td>
<td>Compositions</td>
<td>Delta</td>
<td>Intensity</td>
<td>M / Z</td>
<td>Ionization Percentage</td>
</tr>
<tr>
<td>-------</td>
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<td>-------------------------------------------</td>
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</tr>
<tr>
<td>308.923</td>
<td>308.927</td>
<td>C_{15}H_{16}O_{2}H^+ (1.0), C_{18}H_{13}NO_{4}H^+ (2.8)</td>
<td>0.025, (-0.003, 0.024, 0.054)</td>
<td>0.012</td>
<td>0.0022% (581)</td>
<td></td>
</tr>
<tr>
<td>309.094</td>
<td>309.098</td>
<td>C_{16}H_{10}O_{3}H^+ (-1.2), C_{19}H_{7}NO_{4}H^+ (0.6)</td>
<td>0.052, (-0.001, 0.029, 0.140)</td>
<td>0.017</td>
<td>0.0046% (516)</td>
<td></td>
</tr>
<tr>
<td>311.094</td>
<td>311.098</td>
<td>C_{20}H_{11}N_{3}OH^+ (-2.9)</td>
<td>0.110, (-0.002, 0.079, 0.271)</td>
<td>0.037</td>
<td>0.0099% (454)</td>
<td></td>
</tr>
<tr>
<td>311.094</td>
<td>311.098</td>
<td>C_{20}H_{11}N_{3}OH^+ (-2.9)</td>
<td>0.110, (-0.002, 0.079, 0.271)</td>
<td>0.037</td>
<td>0.0099% (454)</td>
<td></td>
</tr>
<tr>
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<td></td>
</tr>
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<td>311.094</td>
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<td>C_{20}H_{11}N_{3}OH^+ (-2.9)</td>
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<td>0.037</td>
<td>0.0099% (454)</td>
<td></td>
</tr>
<tr>
<td>311.094</td>
<td>311.098</td>
<td>C_{20}H_{11}N_{3}OH^+ (-2.9)</td>
<td>0.110, (-0.002, 0.079, 0.271)</td>
<td>0.037</td>
<td>0.0099% (454)</td>
<td></td>
</tr>
<tr>
<td>311.094</td>
<td>311.098</td>
<td>C_{20}H_{11}N_{3}OH^+ (-2.9)</td>
<td>0.110, (-0.002, 0.079, 0.271)</td>
<td>0.037</td>
<td>0.0099% (454)</td>
<td></td>
</tr>
</tbody>
</table>

**Notes:**
- m = Measured Mass
- m = Calculated Mass
- Delta = Mass Error
- Intensity = Peak Height
- Ionization Percentage = Ionization Efficiency