Common Background Contamination Ions in Mass Spectrometry

Common background contamination ions encountered in mass spectrometers are polyethylene glycol, polypropylene glycol, phthalates, organic solvent clusters, solvent modifiers, fatty acids, metal ions, triflons, tweens and siloxanes. Metal ions form adducts with varying numbers of substrates to give characteristic ESI+ ions. In this poster, the accurate mass of elements, organic solvents and all potential contaminant ions observed in mass spectrometry are listed in the tables below to help troubleshoot potential contamination in LC-MS systems.

**Table 1. Accurate Mass of Organic Solvents**

<table>
<thead>
<tr>
<th>Solvents</th>
<th>Formula</th>
<th>Accurate Mass</th>
</tr>
</thead>
<tbody>
<tr>
<td>Silver-107</td>
<td>Ag-107</td>
<td>106.905094</td>
</tr>
<tr>
<td>Copper-65</td>
<td>Cu-65</td>
<td>64.927794</td>
</tr>
<tr>
<td>Copper-63</td>
<td>Cu-63</td>
<td>62.929601</td>
</tr>
<tr>
<td>Boron-11</td>
<td>B-11</td>
<td>11.009305</td>
</tr>
<tr>
<td>Iodine</td>
<td>I</td>
<td>126.904473</td>
</tr>
<tr>
<td>Bromine-81</td>
<td>Br-81</td>
<td>80.916291</td>
</tr>
<tr>
<td>Sulfur-32</td>
<td>S-32</td>
<td>31.972071</td>
</tr>
<tr>
<td>Nitrogen-14</td>
<td>N-14</td>
<td>14.003074</td>
</tr>
<tr>
<td>Water H2O</td>
<td></td>
<td>18.0106</td>
</tr>
<tr>
<td>Triethylamine C6H15N</td>
<td></td>
<td>101.1204</td>
</tr>
<tr>
<td>Butanone 2-</td>
<td>C4H8O</td>
<td>72.0575</td>
</tr>
<tr>
<td>Tetrachlorocarbon</td>
<td>CCl4</td>
<td>151.8754</td>
</tr>
<tr>
<td>Methanol CH4O</td>
<td></td>
<td>32.0262</td>
</tr>
<tr>
<td>Ethyl acetate C4H8O2</td>
<td></td>
<td>88.0524</td>
</tr>
<tr>
<td>DMSO</td>
<td></td>
<td>(M+DMSO+H)+ 1.007276</td>
</tr>
<tr>
<td>(M+CH3OH+H)+</td>
<td></td>
<td>33.03349</td>
</tr>
<tr>
<td>(M+NH4)+</td>
<td></td>
<td>18.03383</td>
</tr>
<tr>
<td>Propanol C3H8O</td>
<td></td>
<td>60.0575</td>
</tr>
<tr>
<td>Tripropylamine C9H21N</td>
<td></td>
<td>144.1747 161.2012 166.1566 182.1306</td>
</tr>
<tr>
<td>DMSO</td>
<td></td>
<td>(C2H6OS)3 235.0491 252.0756 257.0310 273.0050</td>
</tr>
<tr>
<td>Oleamide C18H35NO</td>
<td></td>
<td>304.2611 321.2876 326.2430 342.2170</td>
</tr>
<tr>
<td>Tributylamine C12H27N</td>
<td></td>
<td>186.2216 203.2482 208.2036 224.1775</td>
</tr>
<tr>
<td>NaTFA</td>
<td></td>
<td>C2F3O2Na 158.9640</td>
</tr>
<tr>
<td>Diisopropylethylamine C8H19N</td>
<td></td>
<td>130.1590 147.1856 152.1410 168.1149</td>
</tr>
<tr>
<td>Dimethylaminopyridine C7H10N2</td>
<td></td>
<td>123.0917 140.1182 145.0736 161.0476</td>
</tr>
<tr>
<td>Dimethylformamide C3H7NO</td>
<td></td>
<td>74.0600 91.0866 96.0420 112.0159</td>
</tr>
<tr>
<td>Acetonitrile + Methanol clusters (CH3CN)(CH3OH)</td>
<td></td>
<td>74.0600 91.0866 96.0420 112.0159</td>
</tr>
<tr>
<td>Acetonitrile/Acetic acid (CH3CN)(CH3COOH)</td>
<td></td>
<td>102.0550 119.0815 124.0369 140.0108</td>
</tr>
<tr>
<td>Stearyl-palmityldimethylammonium chloride C36H76NCl</td>
<td></td>
<td>522.5972</td>
</tr>
<tr>
<td>Erucamide C22H43NO</td>
<td></td>
<td>338.3417 355.3683 360.3237 376.2976</td>
</tr>
<tr>
<td>Monomethoxytrityl cation C20H17O</td>
<td></td>
<td>273.1274</td>
</tr>
<tr>
<td>Acetic acid-Fe-O- complex (C2H4O2)6-6H+3Fe+O</td>
<td></td>
<td>537.8790 554.9056 559.8610 575.8349</td>
</tr>
<tr>
<td>Acetic acid-Fe-O- complex (C2H4O2)6-6H+H2O+3Fe+O</td>
<td></td>
<td>555.8896</td>
</tr>
<tr>
<td>-thiodipropionate oxidized to sulfone C30H58O6S</td>
<td></td>
<td>547.4027 564.4292 569.3846 585.3586</td>
</tr>
<tr>
<td>-thiodipropionate C30H58O4S</td>
<td></td>
<td>515.4129 532.4394 537.3948 553.3687</td>
</tr>
<tr>
<td>C2H6OS</td>
<td>79.0212 96.0478 101.0032 116.9771</td>
<td></td>
</tr>
<tr>
<td>CH3CN</td>
<td>42.0338 59.0604 64.0158 79.9897</td>
<td></td>
</tr>
<tr>
<td>(CH3OH)(H2O)</td>
<td>51.0446 68.0712 73.0265 89.0005</td>
<td></td>
</tr>
<tr>
<td>CH3OH</td>
<td>33.0335 50.0600 55.0154 70.9894</td>
<td></td>
</tr>
<tr>
<td>(C2H6OS)3</td>
<td>235.0491 252.0756 257.0310 273.0050</td>
<td></td>
</tr>
<tr>
<td>(CH3CN)3</td>
<td>124.0869 141.1135 146.0689 162.0428</td>
<td></td>
</tr>
<tr>
<td>(CH3OH)3</td>
<td>97.0859 114.1125 119.0679 135.0418</td>
<td></td>
</tr>
</tbody>
</table>

Visit eu.fishersci.com/go/fisher-chemical