

## Supplementary information

Measured m/z	Calculated m/z	Sum formula	Analyte	Adduct	Mass error (ppm)
115.0026	115.0037	C <sub>4</sub> H <sub>4</sub> O <sub>4</sub>	Fumarate	[M-H] <sup>-</sup>	-9.4
124.0064	124.0074	C <sub>2</sub> H <sub>7</sub> NO <sub>3</sub> S	Taurine	[M-H] <sup>-</sup>	-7.7
134.0461	134.0472	C <sub>5</sub> H <sub>5</sub> N <sub>5</sub>	Adenine	[M-H] <sup>-</sup>	-8.2
136.0061	-	-	-	-	-
138.0221	-	-	-	-	-
146.0450	146.0459	C <sub>5</sub> H <sub>9</sub> NO <sub>4</sub>	Glutamate	[M-H] <sup>-</sup>	-5.9
150.0413	150.0421	C <sub>5</sub> H <sub>5</sub> N <sub>5</sub> O	Guanine	[M-H] <sup>-</sup>	-5.3
159.9831	159.9841	C <sub>2</sub> H <sub>7</sub> NO <sub>3</sub> S	Taurine	[M+Cl] <sup>-</sup>	-6.3
161.9801	-	-	-	-	-
170.0231	170.0239	C <sub>5</sub> H <sub>5</sub> N <sub>5</sub>	Adenine	[M+Cl] <sup>-</sup>	-4.7
172.0201	-	-	-	-	-
175.9881	-	-	-	-	-
186.0181	186.0188	C <sub>5</sub> H <sub>5</sub> N <sub>5</sub> O	Guanine	[M+Cl] <sup>-</sup>	-3.8
192.0662	-	-	-	-	-
193.0352	193.0354	C <sub>6</sub> H <sub>10</sub> O <sub>7</sub>	-	[M-H] <sup>-</sup>	-1
195.0506	195.0510	C <sub>6</sub> H <sub>12</sub> O <sub>7</sub>	-	[M-H] <sup>-</sup>	-2.1
197.0032	-	-	-	-	-
207.9972	-	-	-	-	-
212.9722	-	-	-	-	-
214.9692	-	-	-	-	-
221.9952	-	-	-	-	-
232.0829	-	-	-	-	-

238.0485	238.0488	C <sub>8</sub> H <sub>13</sub> NO <sub>5</sub>	N-acetyl-L-2-aminoadipate	[M+Cl] <sup>-</sup>	-1.1
263.0963	-	-	-	-	-
282.0753	-	-	-	-	-
419.2569	419.2569	C <sub>21</sub> H <sub>41</sub> O <sub>6</sub> P	Cyclic Phosphatidic acid (18:0)	[M-H] <sup>-</sup>	0
885.5495	885.5498	C <sub>47</sub> H <sub>83</sub> O <sub>13</sub> P	Phosphatidylinositol (38:4)	[M-H] <sup>-</sup>	-0.3