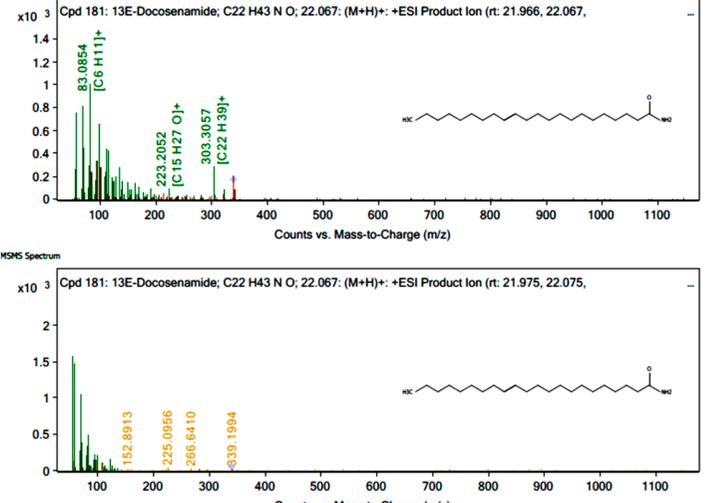
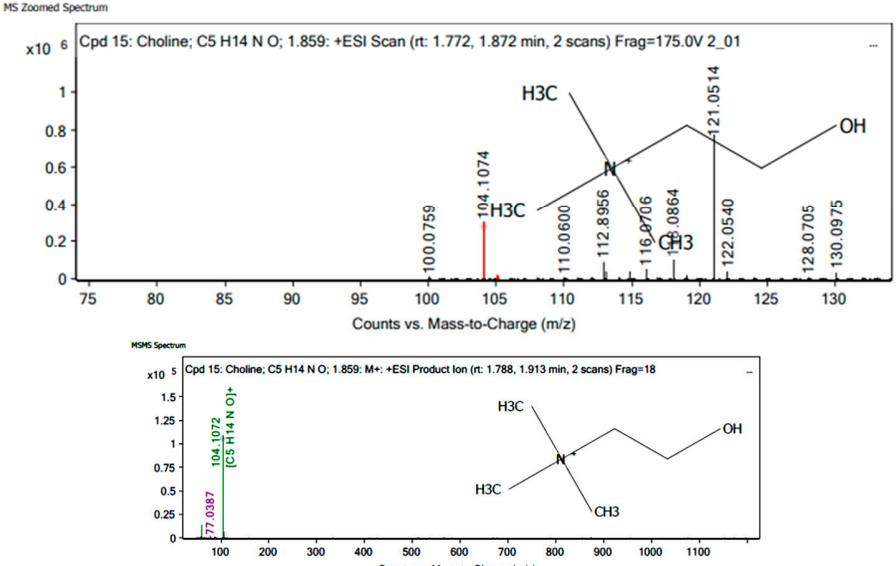
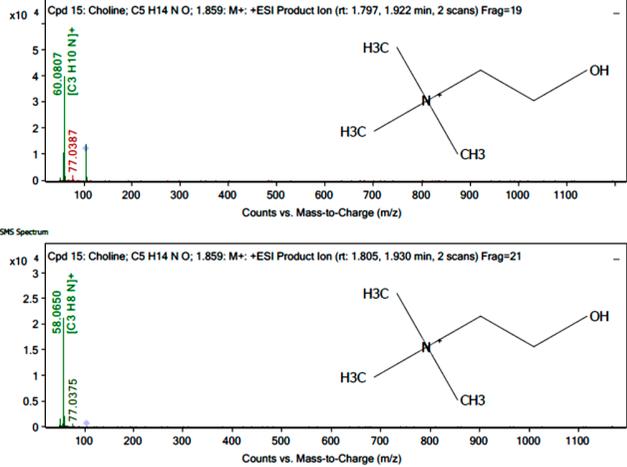
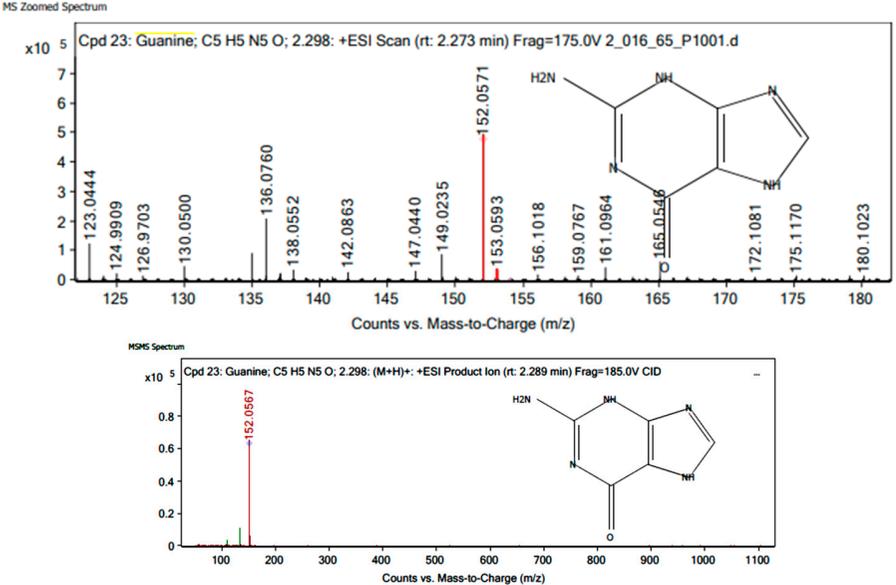
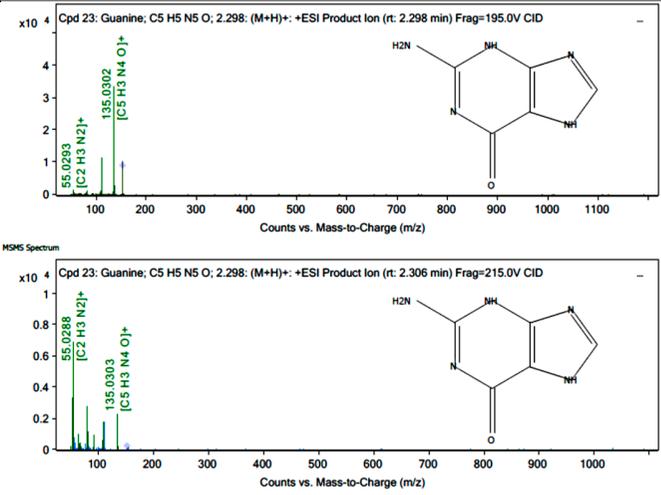
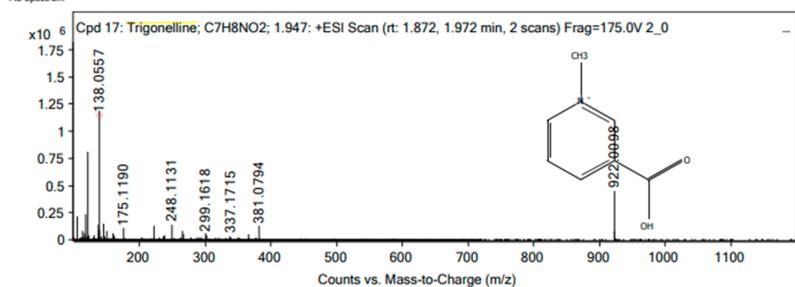
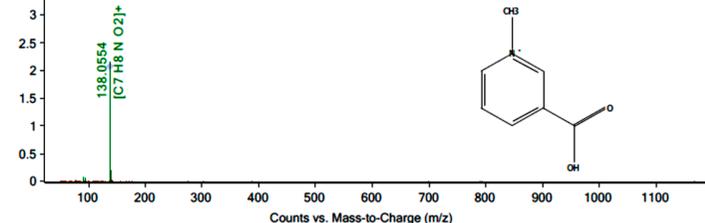
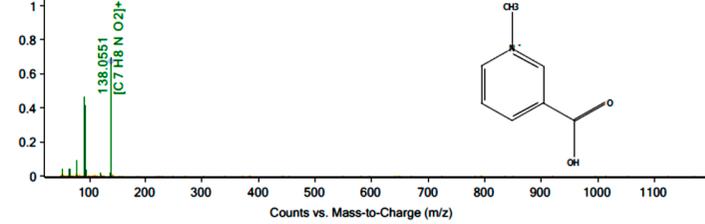
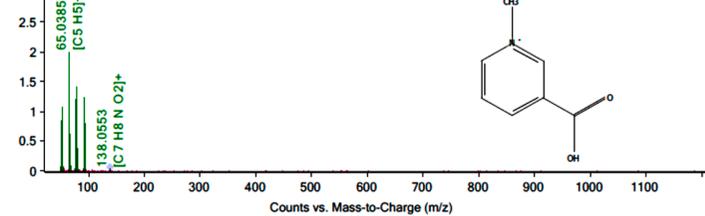


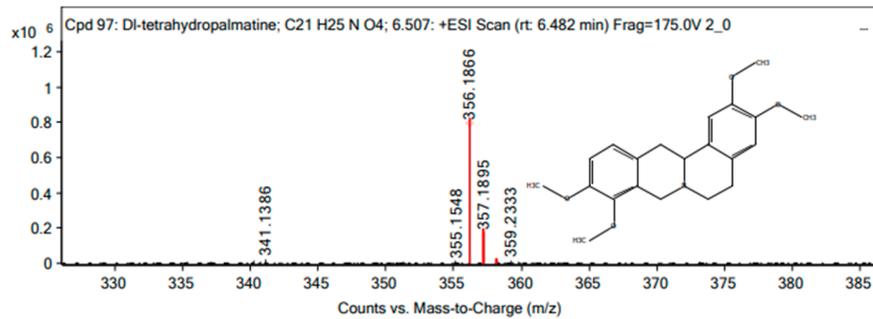
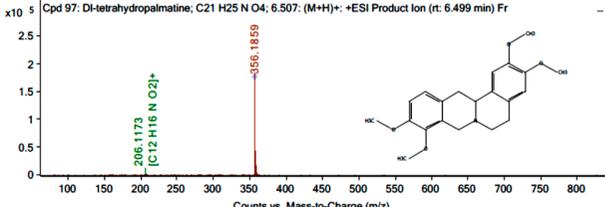
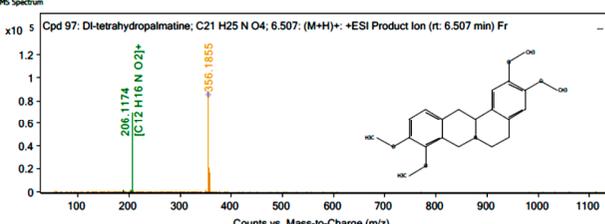
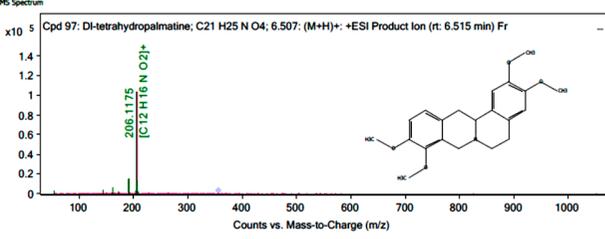


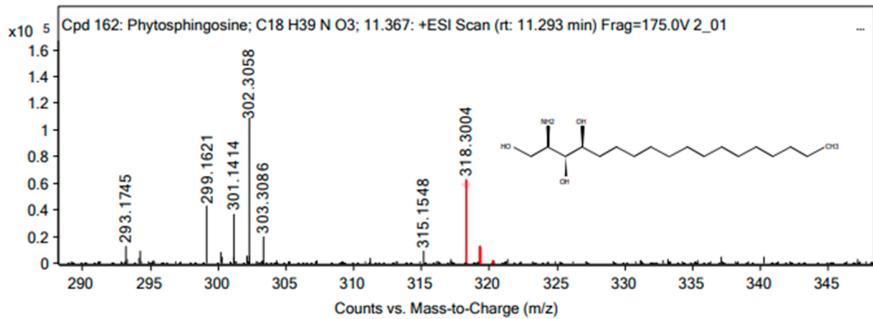
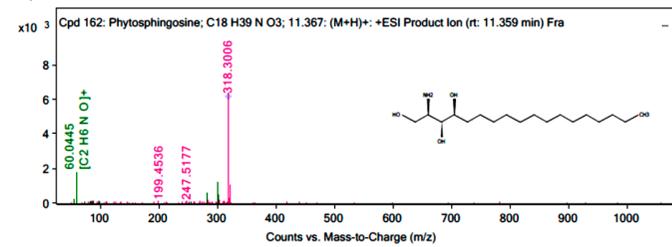
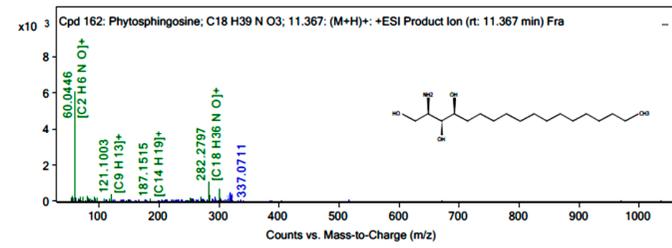
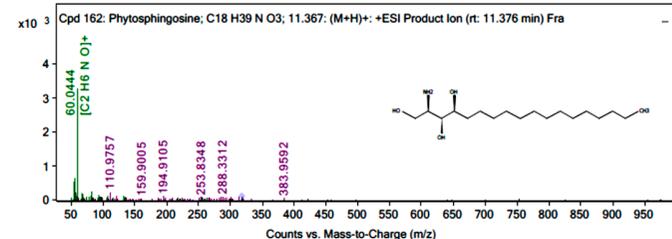
No.	Polarity	Name of compound identification	Mass spectra
			 <p>Cpd 181: 13E-Docosenamide; C22 H43 N O; 22.067; (M+H)+; +ESI Product Ion (rt: 21.966, 22.067, ...)</p> <p>MSMS Spectrum</p> <p>Cpd 181: 13E-Docosenamide; C22 H43 N O; 22.067; (M+H)+; +ESI Product Ion (rt: 21.975, 22.075, ...)</p>
2		Choline	 <p>MS Zoomed Spectrum</p> <p>Cpd 15: Choline; C5 H14 N O; 1.859; +ESI Scan (rt: 1.772, 1.872 min, 2 scans) Frag=175.0V 2_01</p> <p>MSMS Spectrum</p> <p>Cpd 15: Choline; C5 H14 N O; 1.859; M+; +ESI Product Ion (rt: 1.788, 1.913 min, 2 scans) Frag=18</p>

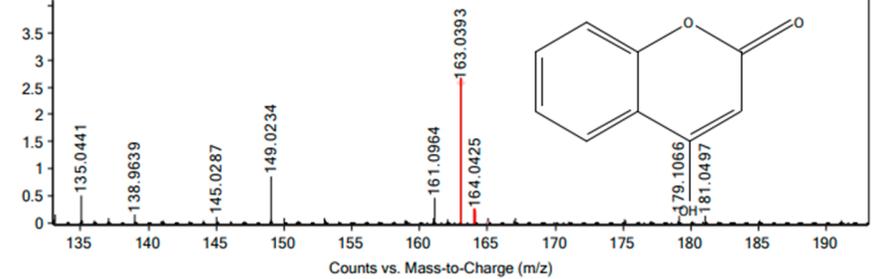
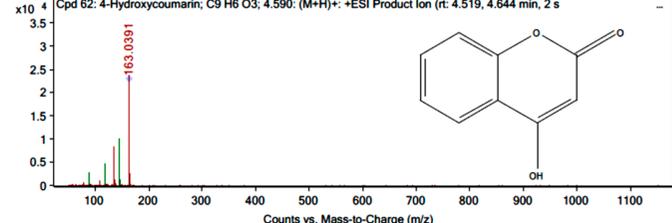
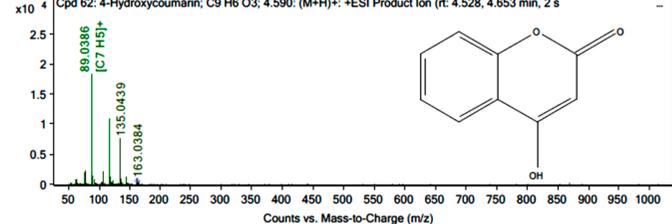
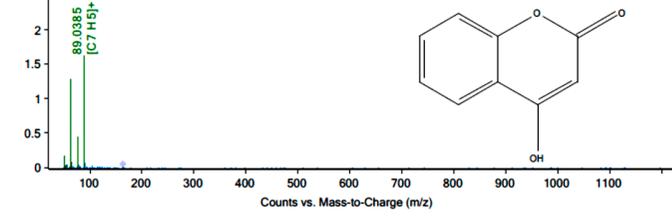
No.	Polarity	Name of compound identification	Mass spectra
			 <p>Cpd 15: Choline, C5 H14 N O; 1.859: M<sup>+</sup>; +ESI Product Ion (rt: 1.797, 1.922 min, 2 scans) Frag=19</p> <p>Cpd 15: Choline, C5 H14 N O; 1.859: M<sup>+</sup>; +ESI Product Ion (rt: 1.805, 1.930 min, 2 scans) Frag=21</p>
3		Guanine	 <p>Cpd 23: Guanine, C5 H5 N5 O; 2.298: +ESI Scan (rt: 2.273 min) Frag=175.0V_2_016_65_P1001.d</p> <p>Cpd 23: Guanine, C5 H5 N5 O; 2.298: (M+H)<sup>+</sup>; +ESI Product Ion (rt: 2.289 min) Frag=185.0V CID</p>

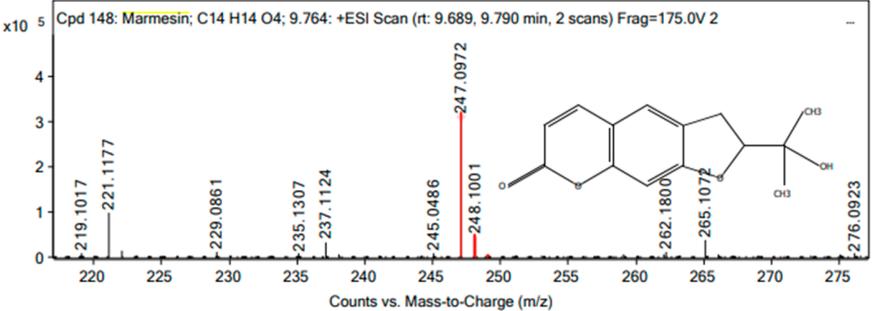
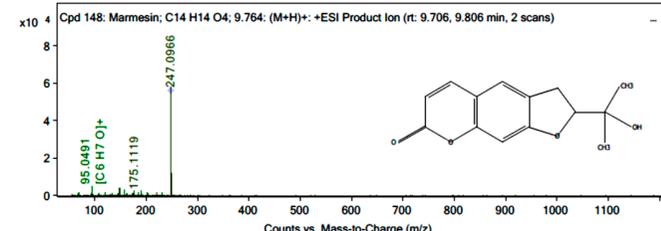
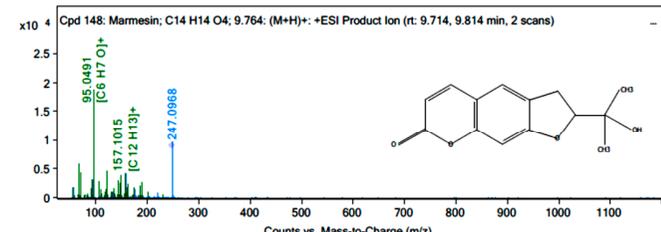
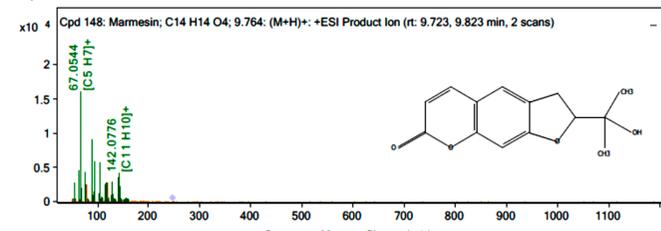
No.	Polarity	Name of compound identification	Mass spectra
			 <p>Cpd 23: Guanine, C5 H5 N5 O, 2.298: (M+H)+. +ESI Product Ion (rt: 2.298 min) Frag=195.0V CID</p> <p>Cpd 23: Guanine, C5 H5 N5 O, 2.298: (M+H)+. +ESI Product Ion (rt: 2.306 min) Frag=215.0V CID</p>
4		Trigonelline	 <p>Cpd 17: Trigonelline, C7H8NO2, 1.947: +ESI Scan (rt: 1.872, 1.972 min, 2 scans) Frag=175.0V 2_0</p>

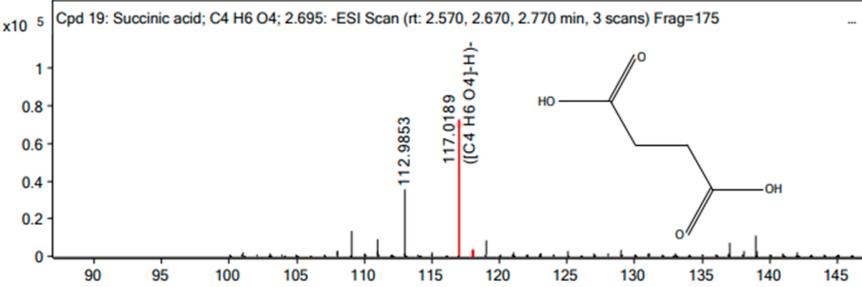
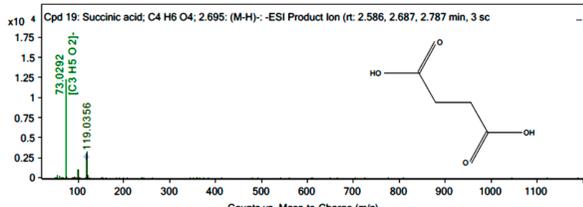
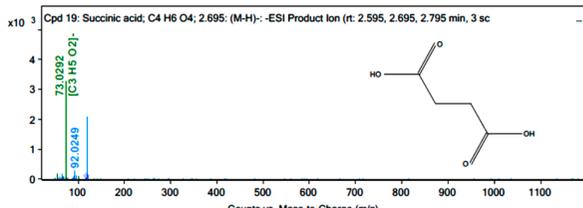
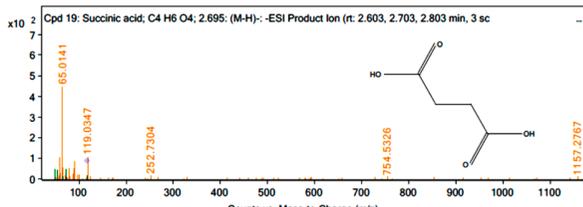
No.	Polarity	Name of compound identification	Mass spectra
			<p data-bbox="1064 263 1769 287">Cpd 17: Trigonelline; C7H8NO2; 1.947: M+: +ESI Product Ion (rt: 1.889, 1.989 min, 2 scans) Frag=</p>  <p data-bbox="1064 518 1769 542">MS/MS Spectrum</p> <p data-bbox="1064 550 1769 574">Cpd 17: Trigonelline; C7H8NO2; 1.947: M+: +ESI Product Ion (rt: 1.897, 1.997 min, 2 scans) Frag=</p>  <p data-bbox="1064 805 1769 829">MS/MS Spectrum</p> <p data-bbox="1064 837 1769 861">Cpd 17: Trigonelline; C7H8NO2; 1.947: M+: +ESI Product Ion (rt: 1.905, 2.005 min, 2 scans) Frag=</p> 

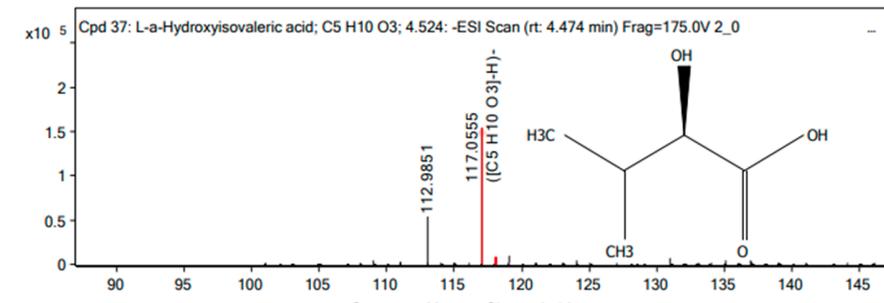
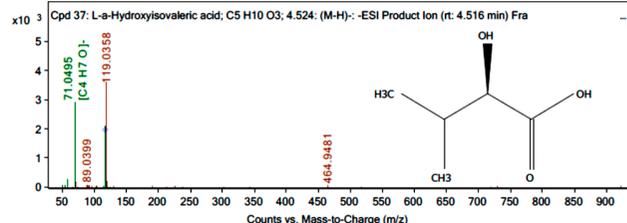
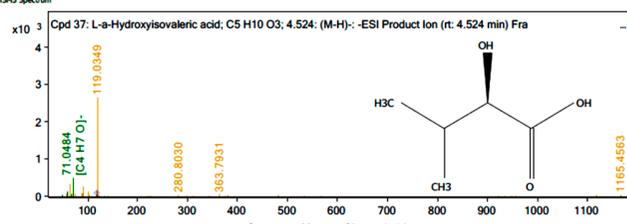
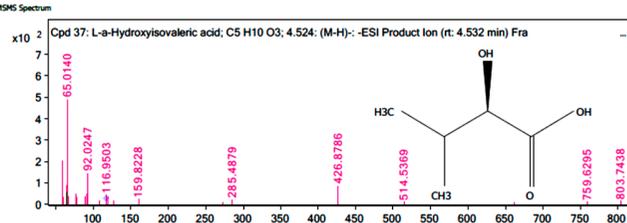
No.	Polarity	Name of compound identification	Mass spectra
5		DI-tetrahydropalmatine	<p>MS Zoomed Spectrum</p>  <p>Cpd 97: DI-tetrahydropalmatine; C21 H25 N O4; 6.507: +ESI Scan (rt: 6.482 min) Frag=175.0V_2_0</p> <p>Counts vs. Mass-to-Charge (m/z)</p> <p>MS/MS Spectrum</p>  <p>Cpd 97: DI-tetrahydropalmatine; C21 H25 N O4; 6.507: (M+H)+: +ESI Product Ion (rt: 6.499 min) Fr</p> <p>Counts vs. Mass-to-Charge (m/z)</p> <p>MS/MS Spectrum</p>  <p>Cpd 97: DI-tetrahydropalmatine; C21 H25 N O4; 6.507: (M+H)+: +ESI Product Ion (rt: 6.507 min) Fr</p> <p>Counts vs. Mass-to-Charge (m/z)</p> <p>MS/MS Spectrum</p>  <p>Cpd 97: DI-tetrahydropalmatine; C21 H25 N O4; 6.507: (M+H)+: +ESI Product Ion (rt: 6.515 min) Fr</p> <p>Counts vs. Mass-to-Charge (m/z)</p>

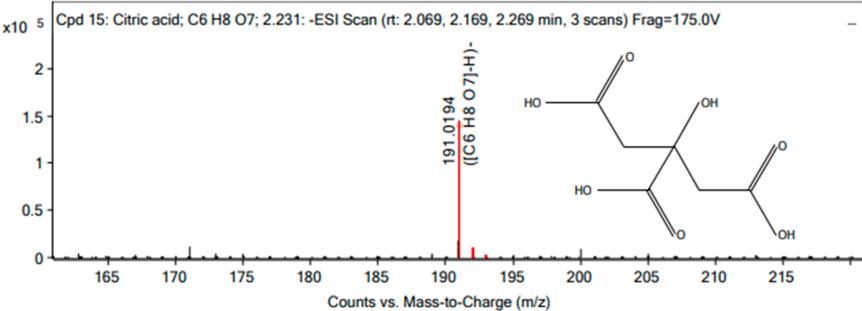
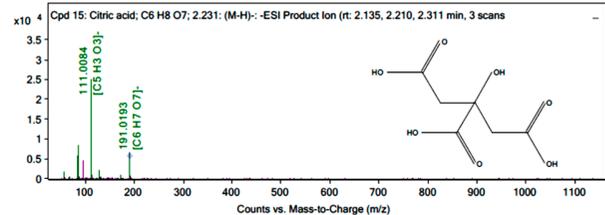
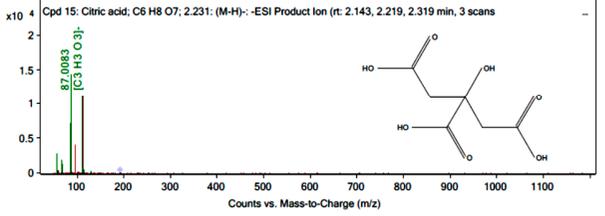
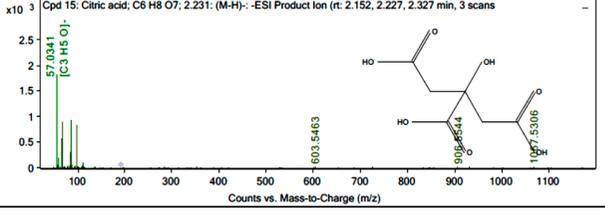
No.	Polarity	Name of compound identification	Mass spectra
6		Phytosphingosine	<p>MS Zoomed Spectrum</p>  <p>Cpd 162: Phytosphingosine; C18 H39 N O3; 11.367: +ESI Scan (rt: 11.293 min) Frag=175.0V 2_01</p> <p>MSMS Spectrum</p>  <p>Cpd 162: Phytosphingosine; C18 H39 N O3; 11.367: (M+H)+: +ESI Product Ion (rt: 11.359 min) Fra</p> <p>MSMS Spectrum</p>  <p>Cpd 162: Phytosphingosine; C18 H39 N O3; 11.367: (M+H)+: +ESI Product Ion (rt: 11.367 min) Fra</p> <p>MSMS Spectrum</p>  <p>Cpd 162: Phytosphingosine; C18 H39 N O3; 11.367: (M+H)+: +ESI Product Ion (rt: 11.376 min) Fra</p>

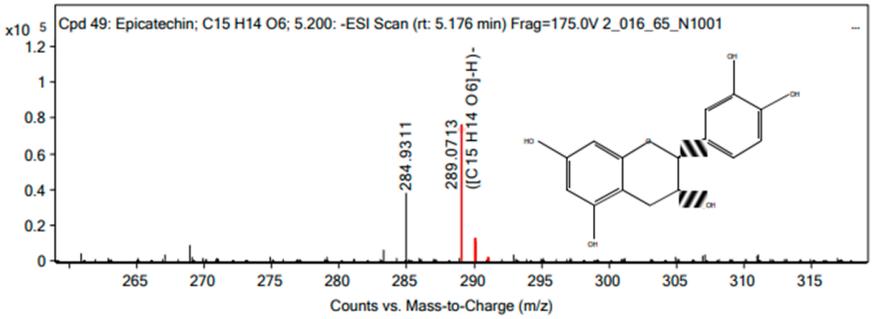
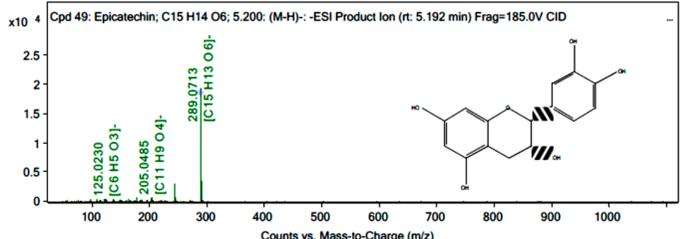
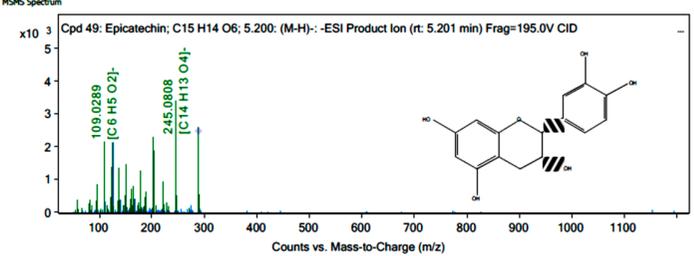
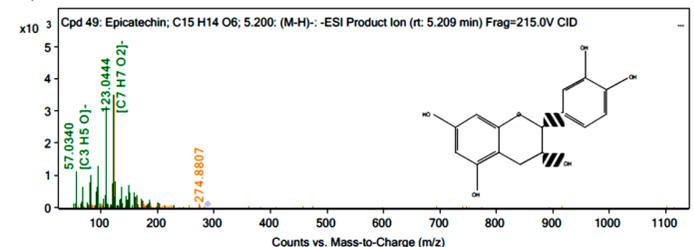
No.	Polarity	Name of compound identification	Mass spectra
7		4-Hydroxycoumarin	<p data-bbox="884 263 1758 287">Cpd 62: 4-Hydroxycoumarin; C<sub>9</sub>H<sub>6</sub>O<sub>3</sub>; 4.590: +ESI Scan (rt: 4.478, 4.578 min, 2 scans) Frag=175</p>  <p data-bbox="1064 582 1736 606">MS/MS Spectrum Cpd 62: 4-Hydroxycoumarin; C<sub>9</sub>H<sub>6</sub>O<sub>3</sub>; 4.590: (M+H)<sup>+</sup>: +ESI Product Ion (rt: 4.519, 4.644 min, 2 s)</p>  <p data-bbox="1064 845 1736 869">MS/MS Spectrum Cpd 62: 4-Hydroxycoumarin; C<sub>9</sub>H<sub>6</sub>O<sub>3</sub>; 4.590: (M+H)<sup>+</sup>: +ESI Product Ion (rt: 4.528, 4.653 min, 2 s)</p>  <p data-bbox="1064 1109 1736 1133">MS/MS Spectrum Cpd 62: 4-Hydroxycoumarin; C<sub>9</sub>H<sub>6</sub>O<sub>3</sub>; 4.590: (M+H)<sup>+</sup>: +ESI Product Ion (rt: 4.536, 4.661 min, 2 s)</p> 

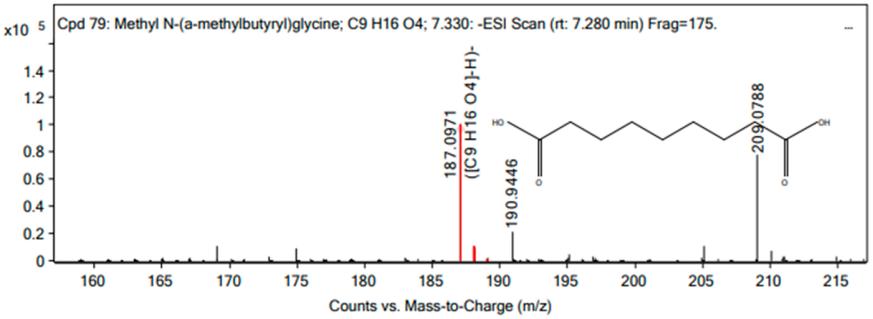
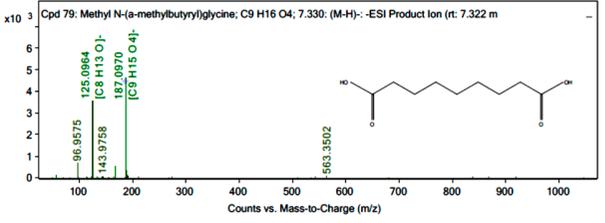
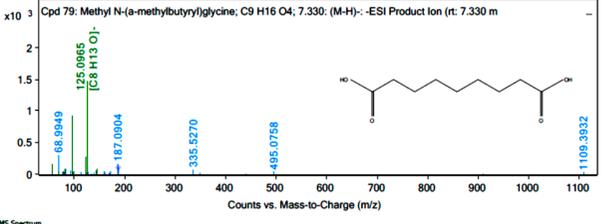
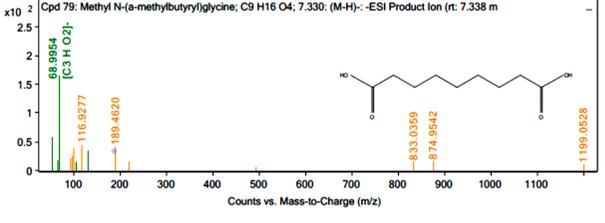
No.	Polarity	Name of compound identification	Mass spectra
8		Marmesin	<p>MS Zoomed Spectrum</p>  <p>Cpd 148: Marmesin; C<sub>14</sub>H<sub>14</sub>O<sub>4</sub>; 9.764: +ESI Scan (rt: 9.689, 9.790 min, 2 scans) Frag=175.0V 2</p> <p>Counts vs. Mass-to-Charge (m/z)</p> <p>MSMS Spectrum</p>  <p>Cpd 148: Marmesin; C<sub>14</sub>H<sub>14</sub>O<sub>4</sub>; 9.764: (M+H)+: +ESI Product Ion (rt: 9.706, 9.806 min, 2 scans)</p> <p>Counts vs. Mass-to-Charge (m/z)</p> <p>MSMS Spectrum</p>  <p>Cpd 148: Marmesin; C<sub>14</sub>H<sub>14</sub>O<sub>4</sub>; 9.764: (M+H)+: +ESI Product Ion (rt: 9.714, 9.814 min, 2 scans)</p> <p>Counts vs. Mass-to-Charge (m/z)</p> <p>MSMS Spectrum</p>  <p>Cpd 148: Marmesin; C<sub>14</sub>H<sub>14</sub>O<sub>4</sub>; 9.764: (M+H)+: +ESI Product Ion (rt: 9.723, 9.823 min, 2 scans)</p> <p>Counts vs. Mass-to-Charge (m/z)</p>

No.	Polarity	Name of compound identification	Mass spectra
1	Negative	Succinic acid	<p>MS Zoomed Spectrum</p>  <p>Cpd 19: Succinic acid; C4 H6 O4; 2.695: -ESI Scan (rt: 2.570, 2.670, 2.770 min, 3 scans) Frag=175</p> <p>Counts vs. Mass-to-Charge (m/z)</p> <p>19MS Spectrum</p>  <p>Cpd 19: Succinic acid; C4 H6 O4; 2.695: (M-H)-: -ESI Product Ion (rt: 2.586, 2.687, 2.787 min, 3 sc)</p> <p>Counts vs. Mass-to-Charge (m/z)</p> <p>19MS Spectrum</p>  <p>Cpd 19: Succinic acid; C4 H6 O4; 2.695: (M-H)-: -ESI Product Ion (rt: 2.595, 2.695, 2.795 min, 3 sc)</p> <p>Counts vs. Mass-to-Charge (m/z)</p> <p>19MS Spectrum</p>  <p>Cpd 19: Succinic acid; C4 H6 O4; 2.695: (M-H)-: -ESI Product Ion (rt: 2.603, 2.703, 2.803 min, 3 sc)</p> <p>Counts vs. Mass-to-Charge (m/z)</p>

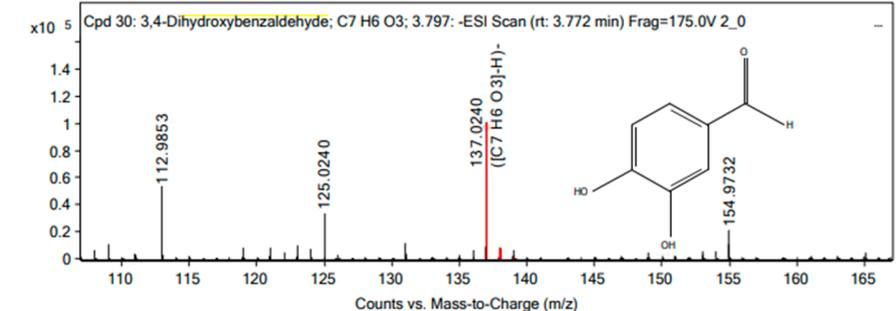
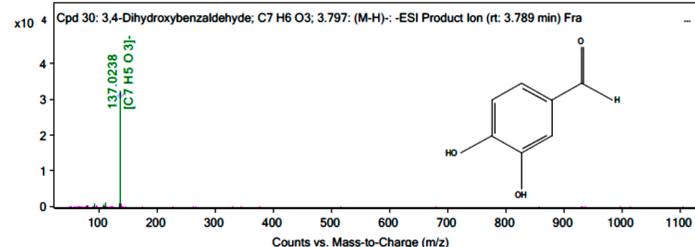
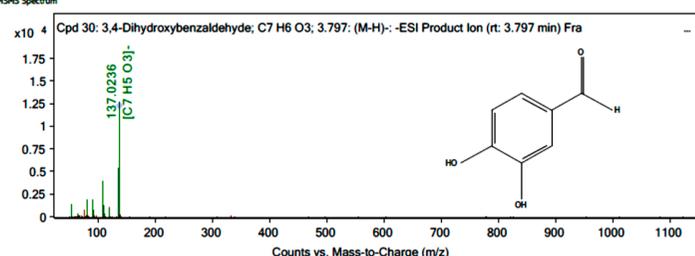
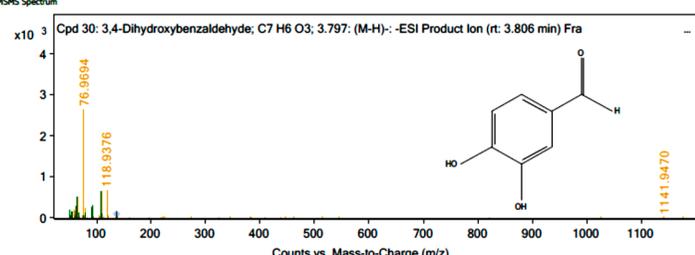
No.	Polarity	Name of compound identification	Mass spectra
2		L- $\alpha$ -Hydroxyisovaleric acid	<p>MS Zoomed Spectrum</p>  <p>Cpd 37: L-<math>\alpha</math>-Hydroxyisovaleric acid; C<sub>5</sub>H<sub>10</sub>O<sub>3</sub>; 4.524: -ESI Scan (rt: 4.474 min) Frag=175.0V_2_0</p> <p>Counts vs. Mass-to-Charge (m/z)</p> <p>MSMS Spectrum</p>  <p>Cpd 37: L-<math>\alpha</math>-Hydroxyisovaleric acid; C<sub>5</sub>H<sub>10</sub>O<sub>3</sub>; 4.524: (M-H)<sup>-</sup> -ESI Product Ion (rt: 4.516 min) Fra</p> <p>Counts vs. Mass-to-Charge (m/z)</p> <p>MSMS Spectrum</p>  <p>Cpd 37: L-<math>\alpha</math>-Hydroxyisovaleric acid; C<sub>5</sub>H<sub>10</sub>O<sub>3</sub>; 4.524: (M-H)<sup>-</sup> -ESI Product Ion (rt: 4.524 min) Fra</p> <p>Counts vs. Mass-to-Charge (m/z)</p> <p>MSMS Spectrum</p>  <p>Cpd 37: L-<math>\alpha</math>-Hydroxyisovaleric acid; C<sub>5</sub>H<sub>10</sub>O<sub>3</sub>; 4.524: (M-H)<sup>-</sup> -ESI Product Ion (rt: 4.532 min) Fra</p> <p>Counts vs. Mass-to-Charge (m/z)</p>

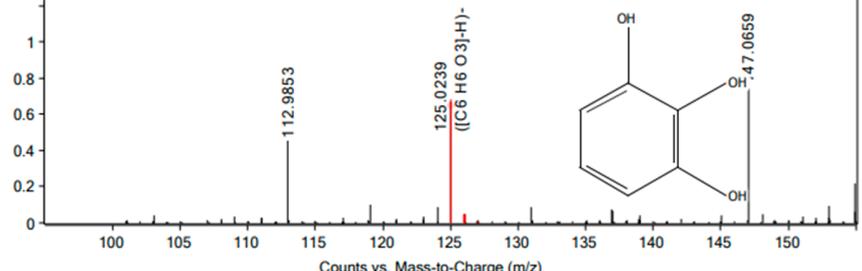
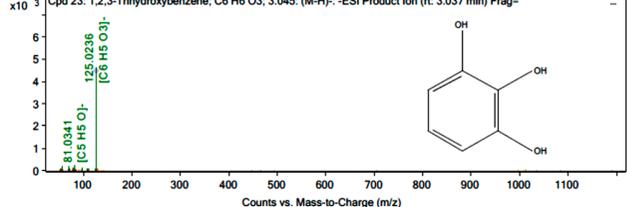
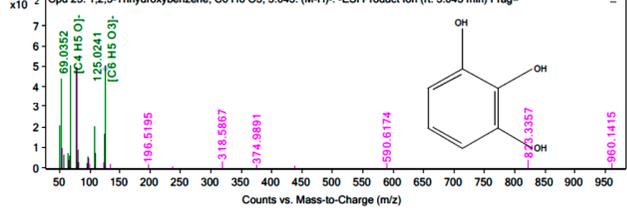
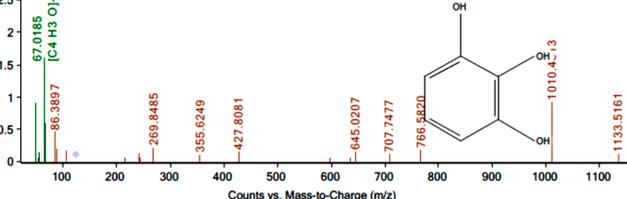
No.	Polarity	Name of compound identification	Mass spectra
3		Citric acid	<p>MS Zoomed Spectrum</p>  <p>Cpd 15: Citric acid; C6 H8 O7; 2.231: -ESI Scan (rt: 2.069, 2.169, 2.269 min, 3 scans) Frag=175.0V</p> <p>MSMS Spectrum</p>  <p>Cpd 15: Citric acid; C6 H8 O7; 2.231: (M-H)-: -ESI Product Ion (rt: 2.135, 2.210, 2.311 min, 3 scans)</p>  <p>Cpd 15: Citric acid; C6 H8 O7; 2.231: (M-H)-: -ESI Product Ion (rt: 2.143, 2.219, 2.319 min, 3 scans)</p>  <p>Cpd 15: Citric acid; C6 H8 O7; 2.231: (M-H)-: -ESI Product Ion (rt: 2.152, 2.227, 2.327 min, 3 scans)</p>

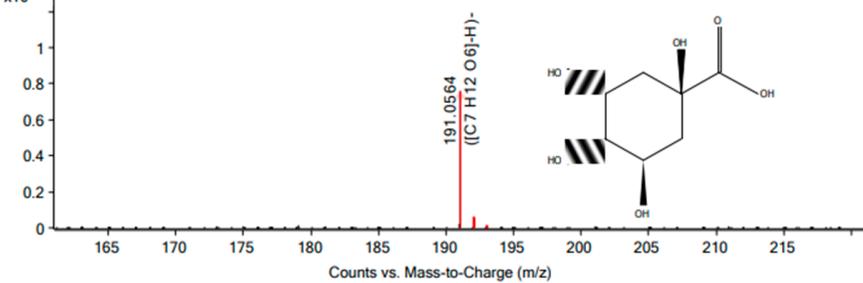
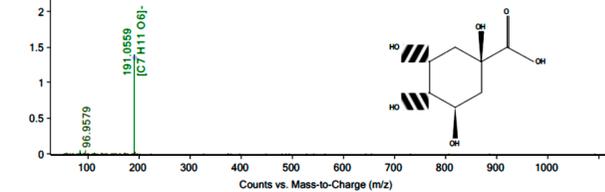
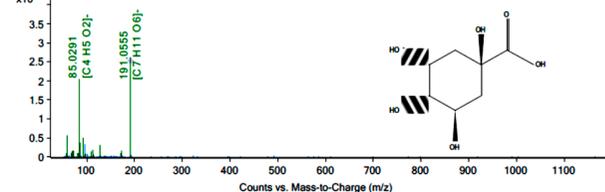
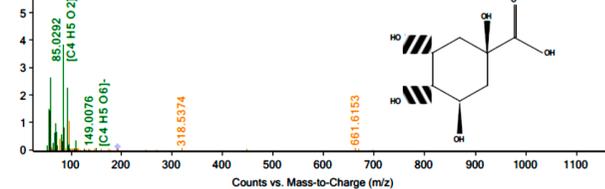
No.	Polarity	Name of compound identification	Mass spectra
4		Epicatechin	<p>MS Zoomed Spectrum</p>  <p>Cpd 49: Epicatechin; C15 H14 O6; 5.200: -ESI Scan (rt: 5.176 min) Frag=175.0V 2_016_65_N1001</p> <p>Counts vs. Mass-to-Charge (m/z)</p> <p>MSMS Spectrum</p>  <p>Cpd 49: Epicatechin; C15 H14 O6; 5.200: (M-H)-: -ESI Product Ion (rt: 5.192 min) Frag=185.0V CID</p> <p>Counts vs. Mass-to-Charge (m/z)</p> <p>MSMS Spectrum</p>  <p>Cpd 49: Epicatechin; C15 H14 O6; 5.200: (M-H)-: -ESI Product Ion (rt: 5.201 min) Frag=195.0V CID</p> <p>Counts vs. Mass-to-Charge (m/z)</p> <p>MSMS Spectrum</p>  <p>Cpd 49: Epicatechin; C15 H14 O6; 5.200: (M-H)-: -ESI Product Ion (rt: 5.209 min) Frag=215.0V CID</p> <p>Counts vs. Mass-to-Charge (m/z)</p>

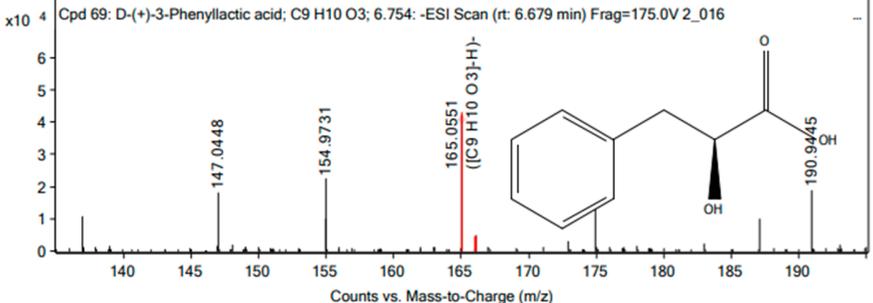
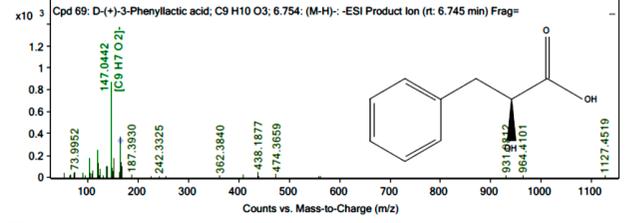
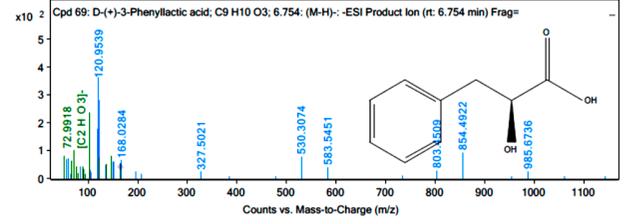
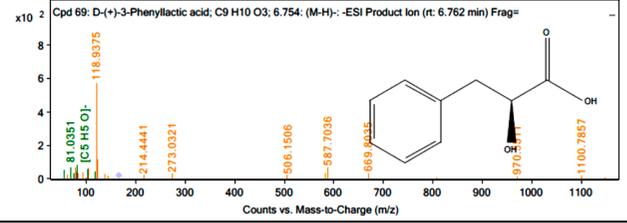
No.	Polarity	Name of compound identification	Mass spectra
5		Methyl N-( $\alpha$ -methylbutyryl) glycine	<p>MS Zoomed Spectrum</p>  <p>Cpd 79: Methyl N-(<math>\alpha</math>-methylbutyryl)glycine; C<sub>9</sub> H<sub>16</sub> O<sub>4</sub>; 7.330; -ESI Scan (rt: 7.280 min) Frag=175.</p> <p>Counts vs. Mass-to-Charge (m/z)</p> <p>MSMS Spectrum</p>  <p>Cpd 79: Methyl N-(<math>\alpha</math>-methylbutyryl)glycine; C<sub>9</sub> H<sub>16</sub> O<sub>4</sub>; 7.330; (M-H)<sup>-</sup>; -ESI Product Ion (rt: 7.322 m)</p> <p>Counts vs. Mass-to-Charge (m/z)</p> <p>MSMS Spectrum</p>  <p>Cpd 79: Methyl N-(<math>\alpha</math>-methylbutyryl)glycine; C<sub>9</sub> H<sub>16</sub> O<sub>4</sub>; 7.330; (M-H)<sup>-</sup>; -ESI Product Ion (rt: 7.330 m)</p> <p>Counts vs. Mass-to-Charge (m/z)</p> <p>MSMS Spectrum</p>  <p>Cpd 79: Methyl N-(<math>\alpha</math>-methylbutyryl)glycine; C<sub>9</sub> H<sub>16</sub> O<sub>4</sub>; 7.330; (M-H)<sup>-</sup>; -ESI Product Ion (rt: 7.338 m)</p> <p>Counts vs. Mass-to-Charge (m/z)</p>

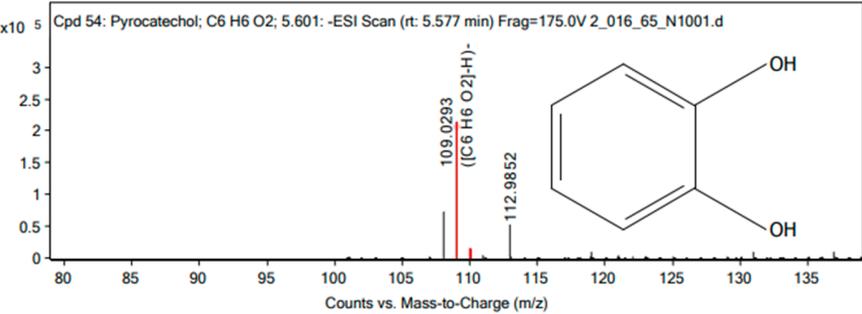
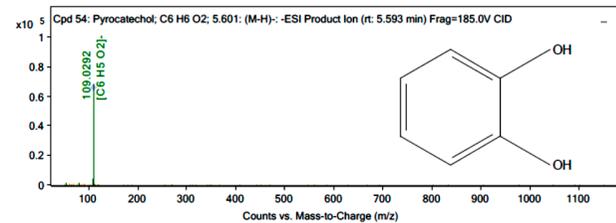
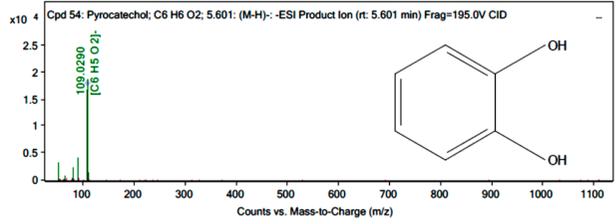
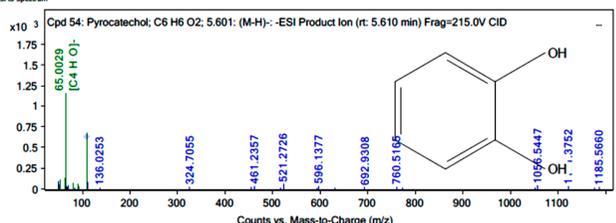
No.	Polarity	Name of compound identification	Mass spectra
6		3-Dehydroshikimic acid	<p>MS Zoomed Spectrum</p> <p>Cpd 12: 3-Dehydroshikimic acid; C7 H8 O5; 1.968: -ESI Scan (rt: 1.868, 1.969 min, 2 scans) Frag=</p> <p>Counts vs. Mass-to-Charge (m/z)</p> <p>MS/MS Spectrum</p> <p>Cpd 12: 3-Dehydroshikimic acid; C7 H8 O5; 1.968: (M-H)-: -ESI Product Ion (rt: 1.935, 1.985 min, 2</p> <p>Counts vs. Mass-to-Charge (m/z)</p> <p>MS/MS Spectrum</p> <p>Cpd 12: 3-Dehydroshikimic acid; C7 H8 O5; 1.968: (M-H)-: -ESI Product Ion (rt: 1.943, 1.993 min, 2</p> <p>Counts vs. Mass-to-Charge (m/z)</p> <p>MS/MS Spectrum</p> <p>Cpd 12: 3-Dehydroshikimic acid; C7 H8 O5; 1.968: (M-H)-: -ESI Product Ion (rt: 1.951, 2.002 min, 2</p> <p>Counts vs. Mass-to-Charge (m/z)</p>

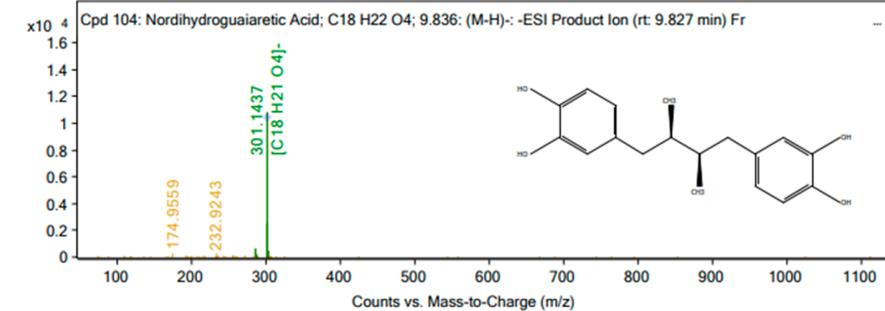
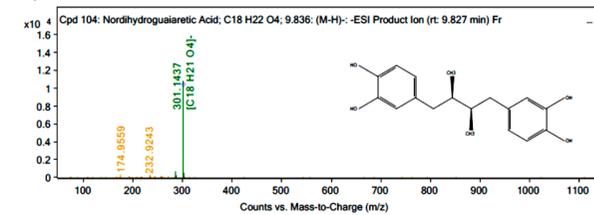
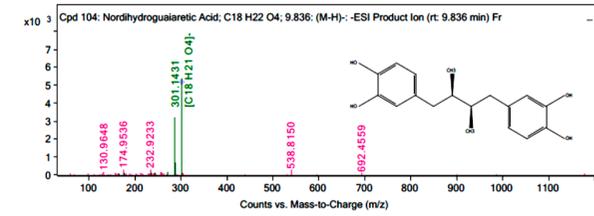
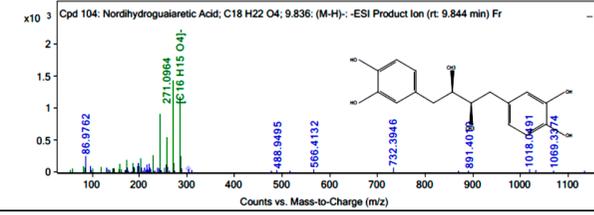
No.	Polarity	Name of compound identification	Mass spectra
7		3,4-Dihydroxybenzaldehyde	<p>MS Zoomed Spectrum</p> <p>Cpd 30: 3,4-Dihydroxybenzaldehyde; C7 H6 O3; 3.797: -ESI Scan (rt: 3.772 min) Frag=175.0V 2_0</p>  <p>MSMS Spectrum</p> <p>Cpd 30: 3,4-Dihydroxybenzaldehyde; C7 H6 O3; 3.797: (M-H)-: -ESI Product Ion (rt: 3.789 min) Fra</p>  <p>MSMS Spectrum</p> <p>Cpd 30: 3,4-Dihydroxybenzaldehyde; C7 H6 O3; 3.797: (M-H)-: -ESI Product Ion (rt: 3.797 min) Fra</p>  <p>MSMS Spectrum</p> <p>Cpd 30: 3,4-Dihydroxybenzaldehyde; C7 H6 O3; 3.797: (M-H)-: -ESI Product Ion (rt: 3.806 min) Fra</p> 

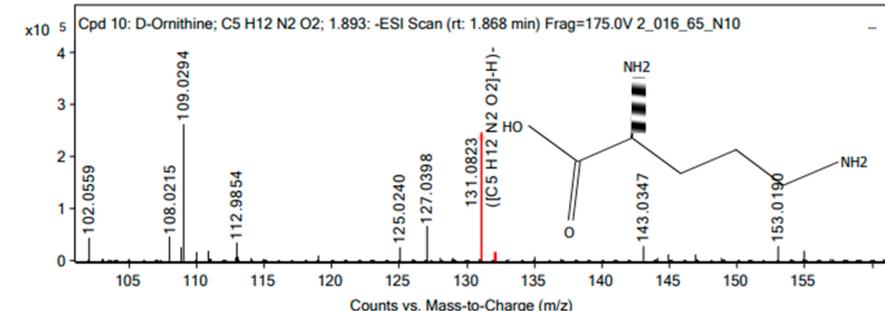
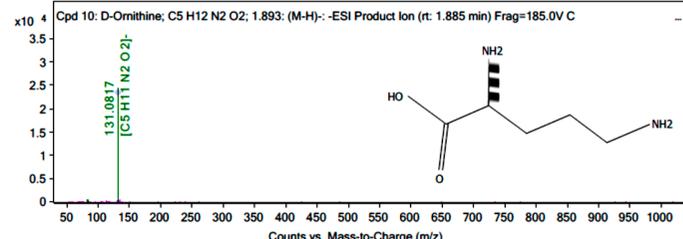
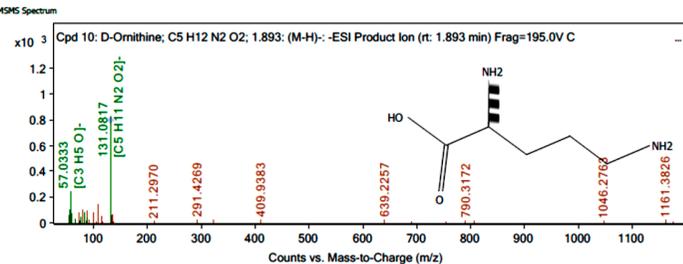
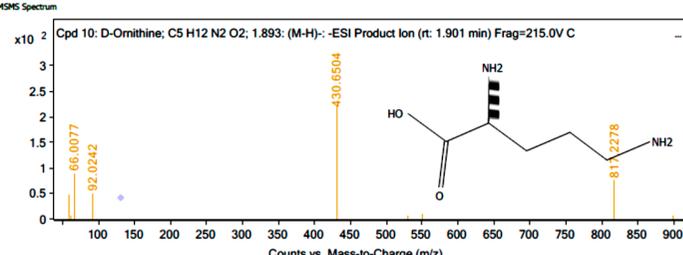
No.	Polarity	Name of compound identification	Mass spectra
8		1,2,3-Trihydroxybenzene	<p data-bbox="884 263 1758 295">Cpd 23: 1,2,3-Trihydroxybenzene; C6 H6 O3; 3.045: -ESI Scan (rt: 2.971 min) Frag=175.0V 2_016</p>  <p data-bbox="1086 574 1724 606">MS/MS Spectrum Cpd 23: 1,2,3-Trihydroxybenzene; C6 H6 O3; 3.045: (M-H)<sup>-</sup>-ESI Product Ion (rt: 3.037 min) Frag=</p>  <p data-bbox="1086 821 1724 853">MS/MS Spectrum Cpd 23: 1,2,3-Trihydroxybenzene; C6 H6 O3; 3.045: (M-H)<sup>-</sup>-ESI Product Ion (rt: 3.045 min) Frag=</p>  <p data-bbox="1086 1069 1724 1101">Cpd 23: 1,2,3-Trihydroxybenzene; C6 H6 O3; 3.045: (M-H)<sup>-</sup>-ESI Product Ion (rt: 3.054 min) Frag=</p> 

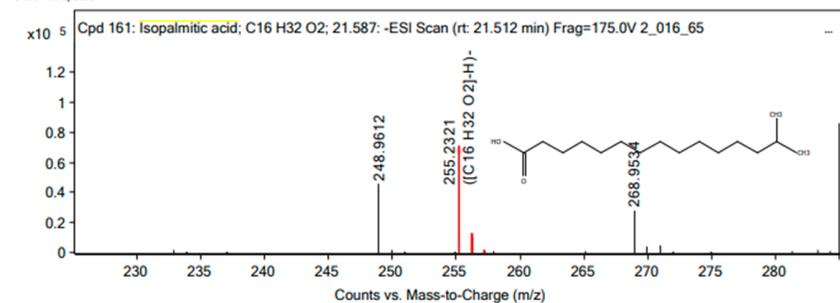
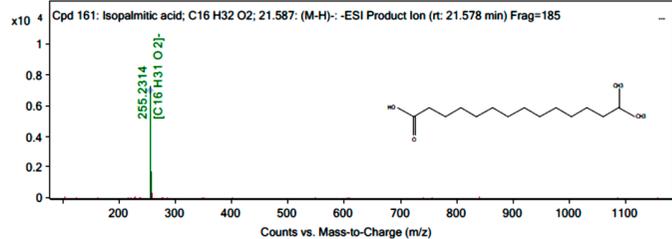
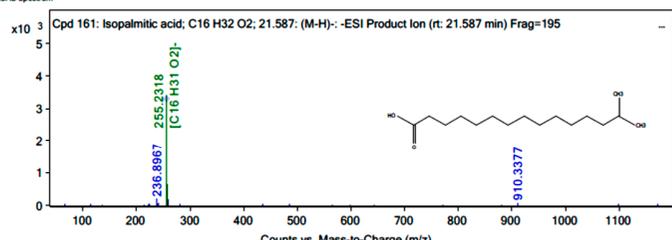
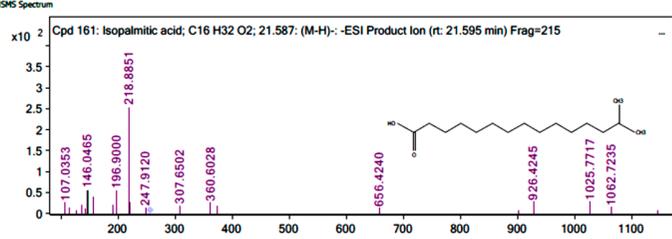
No.	Polarity	Name of compound identification	Mass spectra
9		Quinic acid	<p data-bbox="969 268 1832 288">Cpd 39: Quinic acid; C7 H12 O6; 4.599: -ESI Scan (rt: 4.574 min) Frag=175.0V 2_016_65_N1001.d</p>  <p data-bbox="1104 571 1709 592">MS/MS Spectrum</p> <p data-bbox="1104 592 1709 612">Cpd 39: Quinic acid; C7 H12 O6; 4.599: (M-H)<sup>-</sup>-ESI Product Ion (rt: 4.591 min) Frag=185.0V CID</p>  <p data-bbox="1104 804 1709 825">MS/MS Spectrum</p> <p data-bbox="1104 825 1709 845">Cpd 39: Quinic acid; C7 H12 O6; 4.599: (M-H)<sup>-</sup>-ESI Product Ion (rt: 4.599 min) Frag=195.0V CID</p>  <p data-bbox="1104 1037 1709 1058">MS/MS Spectrum</p> <p data-bbox="1104 1058 1709 1078">Cpd 39: Quinic acid; C7 H12 O6; 4.599: (M-H)<sup>-</sup>-ESI Product Ion (rt: 4.607 min) Frag=215.0V CID</p> 

No.	Polarity	Name of compound identification	Mass spectra
10		D-(+)-3-Phenyllactic acid	<p>MS Zoomed Spectrum</p>  <p>Cpd 69: D-(+)-3-Phenyllactic acid; C9 H10 O3; 6.754: -ESI Scan (rt: 6.679 min) Frag=175.0V 2_016</p> <p>Counts vs. Mass-to-Charge (m/z)</p> <p>MS Spectrum</p>  <p>Cpd 69: D-(+)-3-Phenyllactic acid; C9 H10 O3; 6.754: (M-H)- -ESI Product Ion (rt: 6.745 min) Frag=</p> <p>Counts vs. Mass-to-Charge (m/z)</p> <p>MS Spectrum</p>  <p>Cpd 69: D-(+)-3-Phenyllactic acid; C9 H10 O3; 6.754: (M-H)- -ESI Product Ion (rt: 6.754 min) Frag=</p> <p>Counts vs. Mass-to-Charge (m/z)</p> <p>MS Spectrum</p>  <p>Cpd 69: D-(+)-3-Phenyllactic acid; C9 H10 O3; 6.754: (M-H)- -ESI Product Ion (rt: 6.762 min) Frag=</p> <p>Counts vs. Mass-to-Charge (m/z)</p>

No.	Polarity	Name of compound identification	Mass spectra
11		Pyrocatechol	<p>MS Zoomed Spectrum</p>  <p>Cpd 54: Pyrocatechol; C6 H6 O2; 5.601: -ESI Scan (rt: 5.577 min) Frag=175.0V 2_016_65_N1001.d</p> <p>MSMS Spectrum</p>  <p>Cpd 54: Pyrocatechol; C6 H6 O2; 5.601: (M-H)-: -ESI Product Ion (rt: 5.593 min) Frag=185.0V CID</p>  <p>Cpd 54: Pyrocatechol; C6 H6 O2; 5.601: (M-H)-: -ESI Product Ion (rt: 5.601 min) Frag=195.0V CID</p>  <p>Cpd 54: Pyrocatechol; C6 H6 O2; 5.601: (M-H)-: -ESI Product Ion (rt: 5.610 min) Frag=215.0V CID</p>

No.	Polarity	Name of compound identification	Mass spectra
12		Nordihydroguaiaretic Acid	<p>MS/MS Spectrum</p> <p>Cpd 104: Nordihydroguaiaretic Acid; C<sub>18</sub>H<sub>22</sub>O<sub>4</sub>; 9.836: (M-H)<sup>-</sup>-ESI Product Ion (rt: 9.827 min) Fr</p>  <p>MS/MS Spectrum</p> <p>Cpd 104: Nordihydroguaiaretic Acid; C<sub>18</sub>H<sub>22</sub>O<sub>4</sub>; 9.836: (M-H)<sup>-</sup>-ESI Product Ion (rt: 9.827 min) Fr</p>  <p>MS/MS Spectrum</p> <p>Cpd 104: Nordihydroguaiaretic Acid; C<sub>18</sub>H<sub>22</sub>O<sub>4</sub>; 9.836: (M-H)<sup>-</sup>-ESI Product Ion (rt: 9.836 min) Fr</p>  <p>MS/MS Spectrum</p> <p>Cpd 104: Nordihydroguaiaretic Acid; C<sub>18</sub>H<sub>22</sub>O<sub>4</sub>; 9.836: (M-H)<sup>-</sup>-ESI Product Ion (rt: 9.844 min) Fr</p> 

No.	Polarity	Name of compound identification	Mass spectra
13		D-Ornithine	<p>MS Zoomed Spectrum</p> <p>Cpd 10: D-Ornithine; C5 H12 N2 O2; 1.893: -ESI Scan (rt: 1.868 min) Frag=175.0V 2_016_65_N10</p>  <p>Counts vs. Mass-to-Charge (m/z)</p> <p>MSMS Spectrum</p> <p>Cpd 10: D-Ornithine; C5 H12 N2 O2; 1.893: (M-H)-: -ESI Product Ion (rt: 1.885 min) Frag=185.0V C</p>  <p>Counts vs. Mass-to-Charge (m/z)</p> <p>MSMS Spectrum</p> <p>Cpd 10: D-Ornithine; C5 H12 N2 O2; 1.893: (M-H)-: -ESI Product Ion (rt: 1.893 min) Frag=195.0V C</p>  <p>Counts vs. Mass-to-Charge (m/z)</p> <p>MSMS Spectrum</p> <p>Cpd 10: D-Ornithine; C5 H12 N2 O2; 1.893: (M-H)-: -ESI Product Ion (rt: 1.901 min) Frag=215.0V C</p>  <p>Counts vs. Mass-to-Charge (m/z)</p>

No.	Polarity	Name of compound identification	Mass spectra
14		Isopalmitic acid	<p>MS Zoomed Spectrum</p>  <p>Cpd 161: Isopalmitic acid; C16 H32 O2; 21.587: -ESI Scan (rt: 21.512 min) Frag=175.0V 2_016_65</p> <p>Counts vs. Mass-to-Charge (m/z)</p> <p>MSMS Spectrum</p>  <p>Cpd 161: Isopalmitic acid; C16 H32 O2; 21.587: (M-H)-: -ESI Product Ion (rt: 21.578 min) Frag=185</p> <p>Counts vs. Mass-to-Charge (m/z)</p> <p>MSMS Spectrum</p>  <p>Cpd 161: Isopalmitic acid; C16 H32 O2; 21.587: (M-H)-: -ESI Product Ion (rt: 21.587 min) Frag=195</p> <p>Counts vs. Mass-to-Charge (m/z)</p> <p>MSMS Spectrum</p>  <p>Cpd 161: Isopalmitic acid; C16 H32 O2; 21.587: (M-H)-: -ESI Product Ion (rt: 21.595 min) Frag=215</p> <p>Counts vs. Mass-to-Charge (m/z)</p>