

**Table 1: List of peaks observed in positive APCI**

M/Z	Relative Abundance (%)	Fragment Formula	Attribution
51.02308	0.2	C <sub>4</sub> H <sub>3</sub> <sup>+</sup>	
53.03872	2.3	C <sub>4</sub> H <sub>5</sub> <sup>+</sup>	
53.52256	5.0	C <sub>2</sub> H <sub>7</sub> N <sub>2</sub> O <sub>3</sub> <sup>2+</sup>	
53.77340	0.6	n.i.	
54.02150	0.2	C <sub>2</sub> H <sub>2</sub> N <sub>2</sub> <sup>+</sup>	
55.05438	1.7	C <sub>4</sub> H <sub>7</sub> <sup>+</sup>	Butadiene
55.76609	1.1	n.i.	
56.26091	1.7	n.i.	
57.07005	1.5	C <sub>4</sub> H <sub>9</sub> <sup>+</sup>	Butene
59.04933	10.0	C <sub>3</sub> H <sub>7</sub> O <sup>+</sup>	Acetone, Propenol, Propanal
60.05268	0.4	n.i.	
61.03983	0.3	CH <sub>5</sub> ON <sub>2</sub> <sup>+</sup>	Urea
65.03880	0.3	C <sub>5</sub> H <sub>5</sub> <sup>+</sup>	
67.05446	0.4	C <sub>5</sub> H <sub>7</sub> <sup>+</sup>	
69.07011	0.8	C <sub>5</sub> H <sub>9</sub> <sup>+</sup>	Pentadiene
70.26302	0.6	n.i.	
71.08577	0.6	C <sub>5</sub> H <sub>11</sub> <sup>+</sup>	Pentene
72.08102	2.3	C <sub>4</sub> H <sub>10</sub> N <sup>+</sup>	Pyrrolidine, Butenamine
73.02866	0.7	C <sub>3</sub> H <sub>5</sub> O <sub>2</sub> <sup>+</sup>	
73.04705	3.0	C <sub>3</sub> H <sub>9</sub> Si <sup>+</sup>	Trimethylsilyle
73.06503	2.2	C <sub>4</sub> H <sub>9</sub> O <sup>+</sup>	Butenol, Butanone
75.02631	9.0	C <sub>3</sub> H <sub>7</sub> S <sup>+</sup>	Thioacetone
76.02590	0.4	n.i.	
<b>77.03879</b>	<b>40.0</b>	<b>C<sub>6</sub>H<sub>5</sub><sup>+</sup></b>	<b>Phenyl</b>
78.04214	0.7	n.i.	
79.05447	1.5	C <sub>6</sub> H <sub>7</sub> <sup>+</sup>	Benzene
81.07011	5.0	C <sub>6</sub> H <sub>9</sub> <sup>+</sup>	Cyclohexadiene
83.08575	0.7	C <sub>6</sub> H <sub>11</sub> <sup>+</sup>	Cyclohexene
85.10143	0.4	C <sub>6</sub> H <sub>13</sub> <sup>+</sup>	Cyclohexane
87.04430	1.1	C <sub>4</sub> H <sub>7</sub> O <sub>2</sub> <sup>+</sup>	Butanedione...
89.05997	1.5	C <sub>4</sub> H <sub>9</sub> O <sub>2</sub> <sup>+</sup>	Isopropylformate, Dioxane, Hydroxybutanone...
91.05448	1.8	C <sub>7</sub> H <sub>7</sub> <sup>+</sup>	Tropylium
91.05761	0.8	C <sub>4</sub> H <sub>11</sub> S <sup>+</sup>	
93.03688	2.7	n.i.	
93.07015	0.5	C <sub>7</sub> H <sub>9</sub> <sup>+</sup>	Toluene
<b>95.04935</b>	<b>59.0</b>	<b>C<sub>6</sub>H<sub>7</sub>O<sup>+</sup></b>	<b>Phenol</b>
96.05269	3.5	n.i.	
97.06501	0.3	C <sub>6</sub> H <sub>9</sub> O <sup>+</sup>	Cyclohexadienol
97.10139	0.5	C <sub>7</sub> H <sub>13</sub> <sup>+</sup>	Methylcyclohexene
99.08067	1.2	C <sub>6</sub> H <sub>11</sub> O <sup>+</sup>	Cyclohexenol
105.04498	4.5	C <sub>6</sub> H <sub>5</sub> N <sub>2</sub> <sup>+</sup>	Benzenediazonium
107.08578	1.0	C <sub>8</sub> H <sub>11</sub> <sup>+</sup>	Xylenes, Ethylbenzene
109.10144	0.8	C <sub>8</sub> H <sub>13</sub> <sup>+</sup>	Dimethylcyclohexadiene
111.11710	0.7	C <sub>8</sub> H <sub>15</sub> <sup>+</sup>	Dimethylcyclohexene
119.08584	0.6	C <sub>9</sub> H <sub>11</sub> <sup>+</sup>	Trimethylbenzyne
121.02869	0.3	C <sub>7</sub> H <sub>5</sub> O <sub>2</sub> <sup>+</sup>	

121.10149	0.3	$C_9H_{13}^+$	Trimethylbenzenes, Ethylmethylbenzenes
123.11713	0.4	$C_9H_{15}^+$	Trimethylcyclohexadienes, Ethylmethylcyclohexadienes
133.08627	0.6	$C_6H_{13}O_3^+$	
133.10156	0.3	$C_{10}H_{13}^+$	
135.11719	0.3	$C_{10}H_{15}^+$	Tetramethylbenzenes, Diethylbenzenes, Methylpropylbenzenes, Butylbenzene
137.13286	0.7	$C_{10}H_{17}^+$	Tetramethylcyclohexadienes, Diethylcyclohexadienes, Methylpropylcyclohexadienes, Butylcyclohexadienes
<b>141.00079</b>	<b>100.0</b>	$C_6H_5(SO_2)^+$	<b>Sulfobenzene (-H<sub>2</sub>O)</b>
142.00409	6.0	n.i.	
142.99655	4.2	n.i.	
149.02370	6.0	$C_8H_5O_3^+$	
149.04518	2.2	n.i.	
153.02019	4.2	$Al(NO_2)_2(NH_3)_2^+$	
<b>158.02740</b>	<b>74.0</b>	$C_6H_4(SO_2H)(NH_3)^+$	<b>Sulfoaniline</b>
159.03065	5.5	n.i.	
160.02310	3.7	n.i.	
169.05151	2.1	$C_9H_5N_4^+$	
171.03072	0.8	n.i.	
196.16962	2.0	$C_{12}H_{22}NO^+$	
198.18578	4.0	$C_{12}H_{24}NO^+$	
207.03288	1.2	n.i.	
209.01222	5.5	$C_6H_9O_6S^+$	
210.01193	0.8	n.i.	

n.i.: not identified

**Table 2: List of peaks observed in negative APCI**

M/Z	Relative Abundance (%)	Fragment Formula	Attribution
53.01849	16.0	n.i.	
53.26928	1.6	n.i.	
59.01363	27.0	C <sub>2</sub> H <sub>3</sub> O <sub>2</sub> <sup>-</sup>	Acetic acid
60.99289	40.0	HCO <sub>3</sub> <sup>-</sup>	Carbonate
61.98812	18.0	NO <sub>3</sub> <sup>-</sup>	Nitrate
63.96221	1.2	SO <sub>2</sub> <sup>-</sup>	Sulfur dioxide
71.01358	0.8	C <sub>3</sub> H <sub>3</sub> O <sub>2</sub> <sup>-</sup>	Lactic Acid (-H <sub>2</sub> O)
73.02924	0.2	C <sub>3</sub> H <sub>5</sub> O <sub>2</sub> <sup>-</sup>	Propionic acid, Glycerol (-H <sub>2</sub> O)
74.99051	2.0	C <sub>2</sub> H <sub>3</sub> OS <sup>-</sup>	Thioacetic acid
75.00849	0.4	C <sub>2</sub> H <sub>3</sub> O <sub>3</sub> <sup>-</sup>	Glycolic acid
78.91861	9.5	Br <sup>-</sup>	Bromide
80.91656	10.0	Br <sup>-</sup>	Bromide
80.96487	2.5	HSO <sub>3</sub> <sup>-</sup>	Sulfite
87.04484	3.0	C <sub>4</sub> H <sub>7</sub> O <sub>2</sub> <sup>-</sup>	Butyric acid
89.02411	3.0	C <sub>3</sub> H <sub>5</sub> O <sub>3</sub> <sup>-</sup>	Lactic acid
89.04250	2.1	n.i.	
91.02171	100.0	n.i.	
91.03959	6.0	C <sub>3</sub> H <sub>7</sub> O <sub>3</sub> <sup>-</sup>	Glycerol
92.02126	5.0	n.i.	
93.00095	8.6	C <sub>2</sub> H <sub>5</sub> O <sub>2</sub> S <sup>-</sup>	
93.01733	16.5	n.i.	
93.03411	1.6	C <sub>6</sub> H <sub>5</sub> O <sup>-</sup>	Phenol
94.91336	1.9	n.i.	
94.98017	6.5	H <sub>3</sub> SiO <sub>4</sub> <sup>-</sup>	Silicic acid
94.99657	2.2	n.i.	
95.95184	0.6	SO <sub>4</sub> <sup>-</sup>	Sulfate
96.91132	2.0	n.i.	
96.95970	0.6	HSO <sub>4</sub> <sup>-</sup>	Hydrogenosulfate
101.06035	2.0	C <sub>5</sub> H <sub>9</sub> O <sub>2</sub> <sup>-</sup>	Valeric acid
103.07598	0.5	C <sub>5</sub> H <sub>11</sub> O <sub>2</sub> <sup>-</sup>	
108.02116	0.5	C <sub>6</sub> H <sub>4</sub> O <sub>2</sub> <sup>-</sup>	
109.96718	0.5	n.i.	
114.92177	0.4	n.i.	
115.03953	0.5	C <sub>5</sub> H <sub>7</sub> O <sub>3</sub> <sup>-</sup>	
115.05073	0.3	C <sub>4</sub> H <sub>7</sub> N <sub>2</sub> O <sub>2</sub> <sup>-</sup>	
115.07591	0.5	C <sub>6</sub> H <sub>11</sub> O <sub>2</sub> <sup>-</sup>	Caproic acid
120.04492	1.0	C <sub>7</sub> H <sub>6</sub> NO <sup>-</sup>	
121.02894	1.8	C <sub>7</sub> H <sub>5</sub> O <sub>2</sub> <sup>-</sup>	Benzoic acid
124.01917	7.1	n.i.	
124.03712	1.4	n.i.	
125.99840	1.5	n.i.	
127.97763	4.9	H <sub>4</sub> O <sub>6</sub> Si <sup>-</sup>	
141.00093	2.9	C <sub>6</sub> H <sub>5</sub> (SO <sub>2</sub> ) <sup>-</sup>	Sulfobenzene (-H <sub>2</sub> O)
143.10706	0.9	C <sub>8</sub> H <sub>15</sub> O <sub>2</sub> <sup>-</sup>	Caprylic acid
148.03970	1.5	C <sub>8</sub> H <sub>6</sub> (NO <sub>2</sub> ) <sup>-</sup>	Nitrostyrene
156.01172	25.0	C <sub>6</sub> H <sub>4</sub> (NH <sub>2</sub> )(SO <sub>2</sub> ) <sup>-</sup>	Sulfoaniline (-H <sub>2</sub> O)
156.99573	0.6	n.i.	

157.01508	1.4	n.i.	
157.12260	0.7	$C_9H_{17}O_2^-$	Pelargonic acid
157.83643	3.6	$Br_2^-$	Dibromine
159.83440	8.0	$Br_2^-$	Dibromine
161.83232	3.6	$Br_2^-$	Dibromine
165.04005	4.8	n.i.	
167.03563	1.5	n.i.	
171.13817	0.9	$C_{10}H_{19}O_2^-$	Capric acid
182.02722	0.8	$C_8H_6(NH_2)(SO_2)^-$	Aminosulfofostyrene (-H <sub>2</sub> O)
193.00838	0.5	n.i.	
194.00365	0.7	n.i.	
196.16972	1.2	$C_{12}H_{22}NO^-$	
198.81718	1.1	n.i.	
205.15891	2.3	$C_{14}H_{21}O^-$	
208.04306	0.5	n.i.	

---

n.i.: not identified