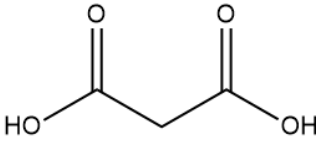
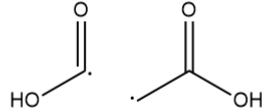
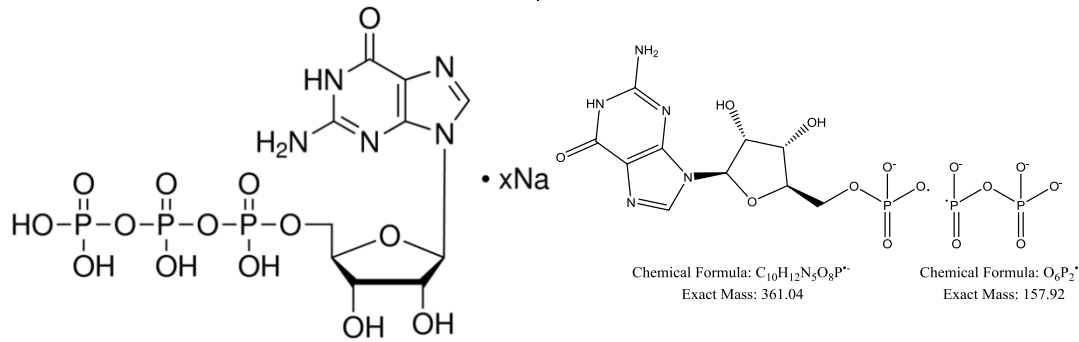
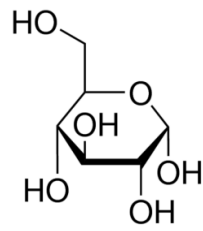
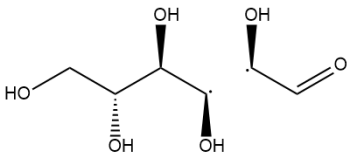
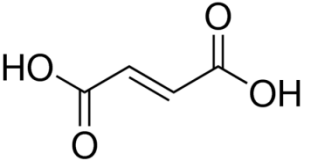
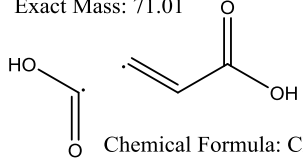
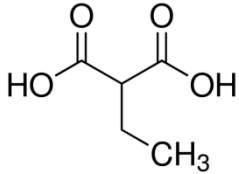
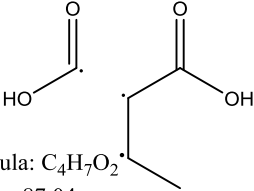
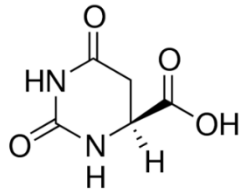
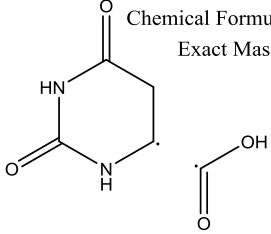
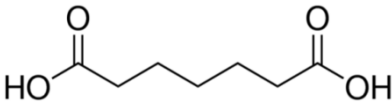
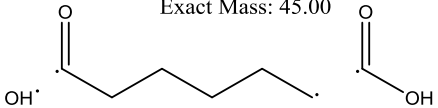
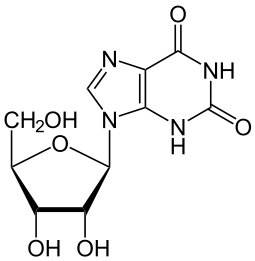
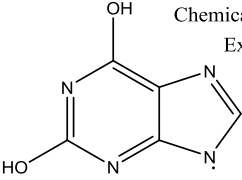
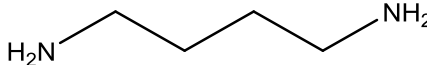
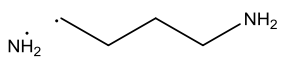
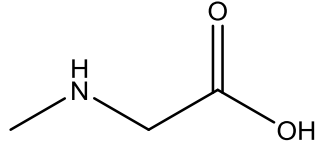
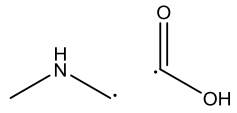
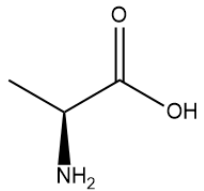
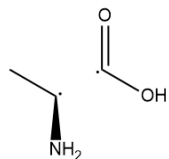
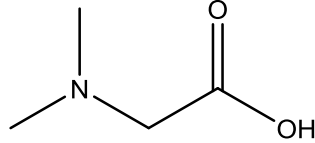
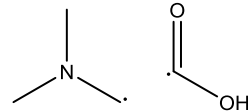


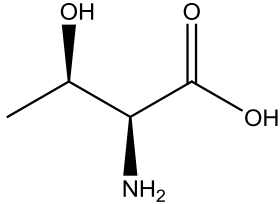
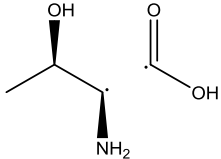
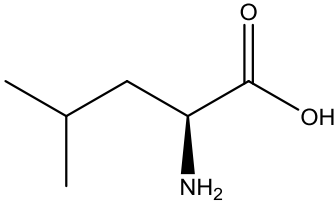
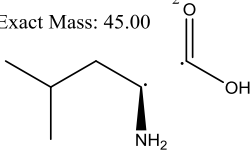
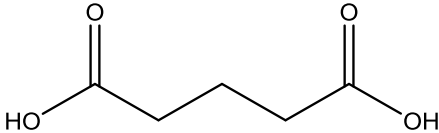
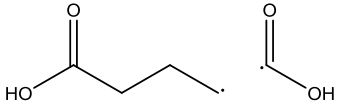
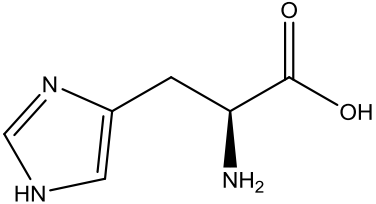
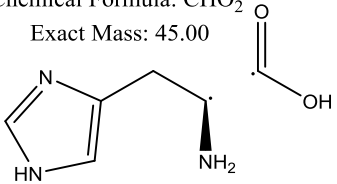
Supplemental Table 2. MRM transitions for light/heavy metabolites pairs.

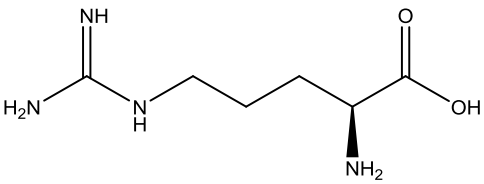
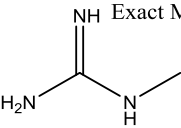
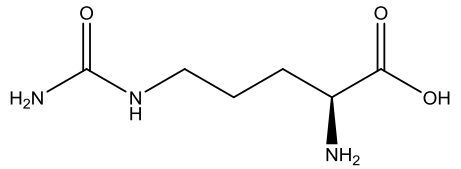
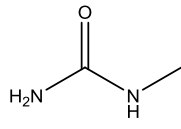
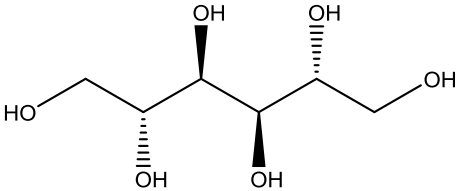
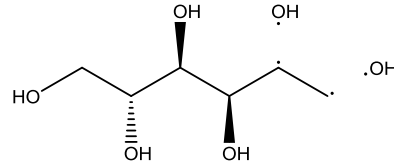
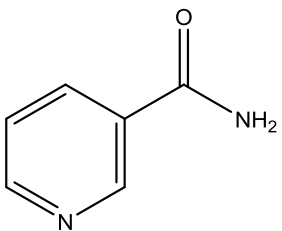
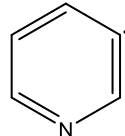
No.	Name	Formula	MW	Q1	Q3	Structure	Fragmentation
Negative mode							
1	Malonic acid	C ₃ H ₄ O ₄	104.06	103	59.2		Chemical Formula: C ₂ H ₃ O ₂ ⁻ Exact Mass: 59.01
				106	61.2		 Chemical Formula: CHO ₂ ⁻ Exact Mass: 45.00
2	GTP (Guanosine 5'-triphosphate sodium salt hydrate)	C ₁₀ H ₁₆ N ₅ O ₁₄ P ₃ · xNa ⁺	523.18	522.3	158.9		Chemical Formula: C ₁₀ H ₁₂ N ₅ O ₈ P ⁻ Exact Mass: 361.04 Chemical Formula: O ₆ P ₂ ⁻³ Exact Mass: 157.92
				537.3	158.9		
3	Glucose	C ₆ H ₁₂ O ₆	180.16	179.0	59.1		Chemical Formula: C ₂ H ₃ O ₂ ⁻ Exact Mass: 59.01
				185.0	61.1		 Chemical Formula: C ₄ H ₉ O ₄ ⁻ Exact Mass: 121.05
4	Fumaric acid	C ₄ H ₄ O ₄	116.07	115.1	70.9		Chemical Formula: C ₃ H ₃ O ₂ ⁻ Exact Mass: 71.01
				119.1	73.9		 Chemical Formula: CHO ₂ ⁻ Exact Mass: 45.00

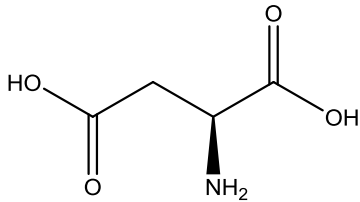
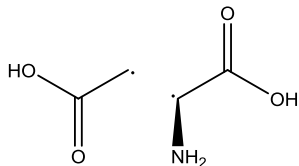
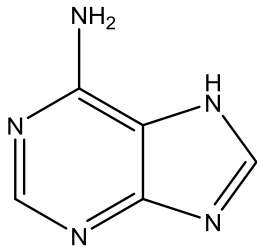
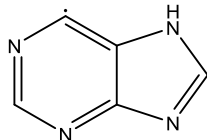
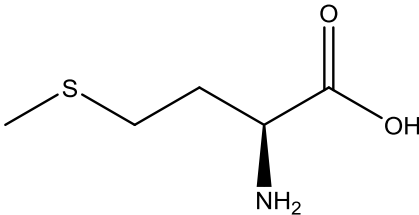
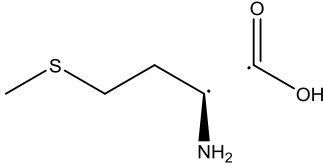
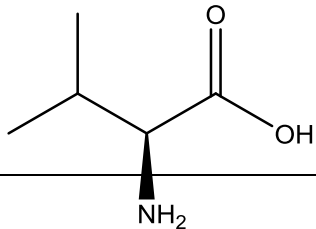
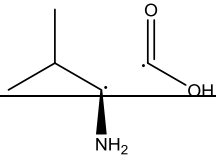
5	Ethylmalonic acid	$C_5H_8O_4$	132.11	131.1	87.1		<p>Chemical Formula: CHO_2^* Exact Mass: 45.00</p>  <p>Chemical Formula: $C_4H_7O_2^*$ Exact Mass: 87.04</p>
				136.1	91.1		
6	L-Dihydroorotic acid	$C_5H_6N_2O_4$	158.11	157.1	112.9		<p>Chemical Formula: $C_4H_5N_2O_2^*$ Exact Mass: 113.04</p>  <p>Chemical Formula: CHO_2^* Exact Mass: 45.00</p>
				164.1	118.9		
7	Pimelic acid	$C_7H_{12}O_4$	160.17	159.1	96.8		<p>Chemical Formula: CHO_2^* Exact Mass: 45.00</p>  <p>Chemical Formula: $C_6H_{10}O_2^*$ Exact Mass: 98.07</p>
				166.1	102.8		
8	Xanthosine	$C_{10}H_{12}N_4O_6$	284.23	283	150.9		<p>Chemical Formula: $C_5H_3N_4O_2^*$ Exact Mass: 151.03</p>  <p>Chemical Formula: $C_5H_3O_4^*$ Exact Mass: 133.05</p>
				297	159.9		

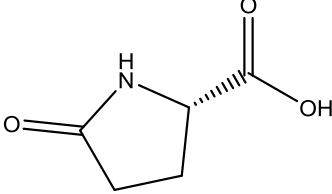
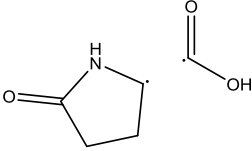
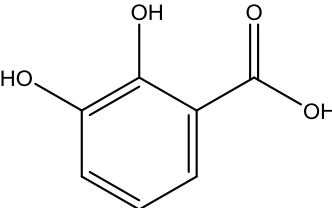
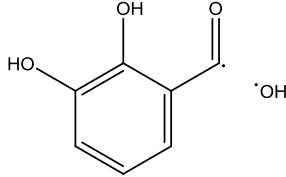
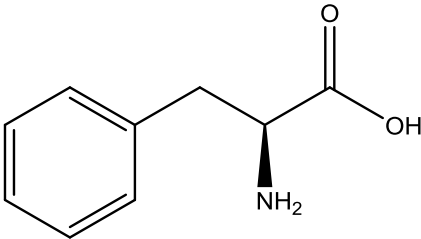
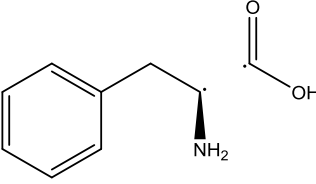
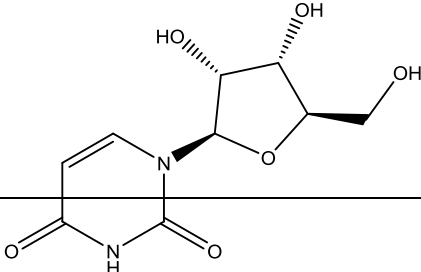
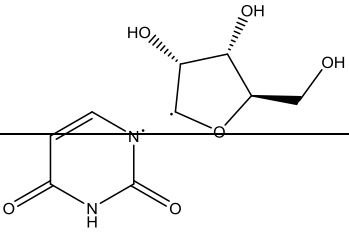
Positive mode

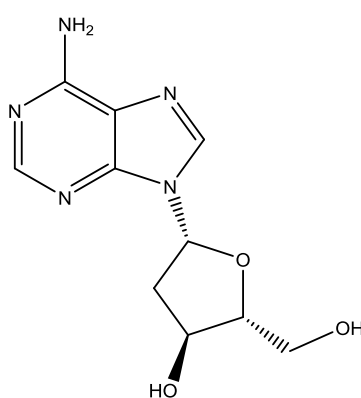
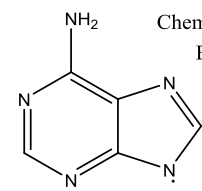
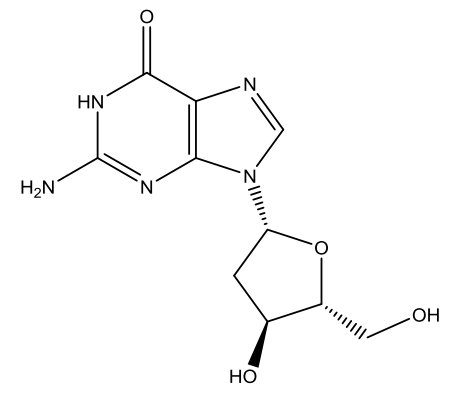
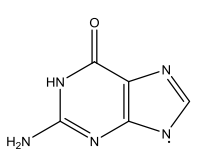
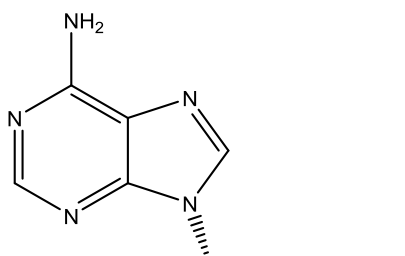
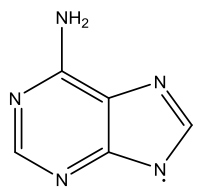
9	1,4-Diaminobutane	$C_4H_{12}N_2$	88.15	89.1	72		Chemical Formula: $C_4H_{10}N^+$ Exact Mass: 72.08  Chemical Formula: H_2N^+ Exact Mass: 16.02
				95.1	77		
10	Sarcosine	$C_3H_7NO_2$	89.09	89.9	44.1		Chemical Formula: CHO_2^+ Exact Mass: 45.00  Chemical Formula: $C_2H_6N^+$ Exact Mass: 44.05
				93.9	47.1		
11	Alanine	$C_3H_7NO_2$	89.09	90	44		Chemical Formula: CHO_2^+ Exact Mass: 45.00  Chemical Formula: $C_2H_6N^+$ Exact Mass: 44.05
				94	47		
12	N,N-Dimethylglycine	$C_4H_9NO_2$	103.12	104	58.1		Chemical Formula: CHO_2^+ Exact Mass: 45.00  Chemical Formula: $C_3H_8N^+$ Exact Mass: 58.07
				109	62.1		

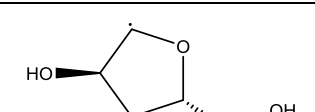
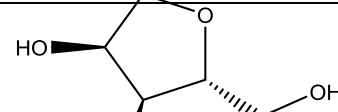
13	Threonine	$C_4H_9NO_3$	119.12	120	74		<p>Chemical Formula: CHO_2^* Exact Mass: 45.00</p>  <p>Chemical Formula: $C_3H_8NO^*$ Exact Mass: 74.06</p>
				125	78		
14	Leucine	$C_6H_{13}NO_2$	131.17	132	86		<p>Chemical Formula: CHO_2^* Exact Mass: 45.00</p>  <p>Chemical Formula: $C_5H_{12}N^*$ Exact Mass: 86.10</p>
				139	92		
15	Glutaric acid	$C_5H_8O_4$	132.12	133.1	87		<p>Chemical Formula: $C_4H_7O_2^*$ Exact Mass: 87.04</p>  <p>Chemical Formula: CHO_2^* Exact Mass: 45.00</p>
				138.1	91		
16	Histidine	$C_6H_9N_3O_2$	155.15	156	110		<p>Chemical Formula: CHO_2^* Exact Mass: 45.00</p>  <p>Chemical Formula: $C_5H_8N_3^*$ Exact Mass: 110.07</p>
				165	118		

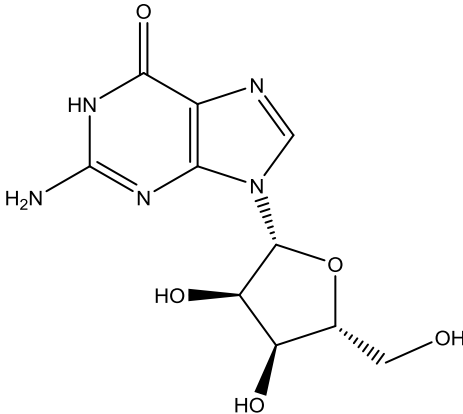
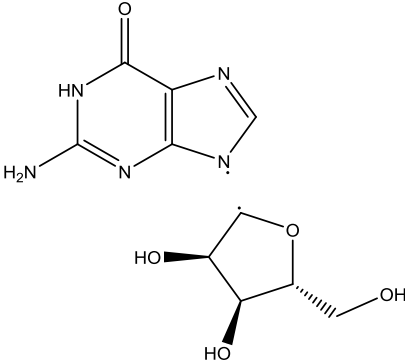
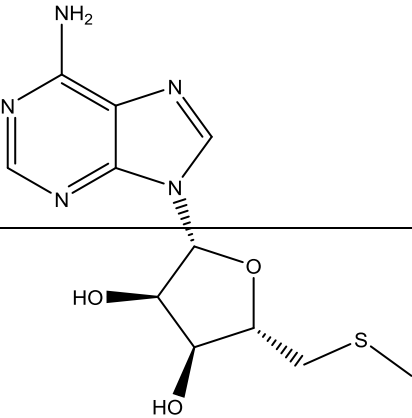
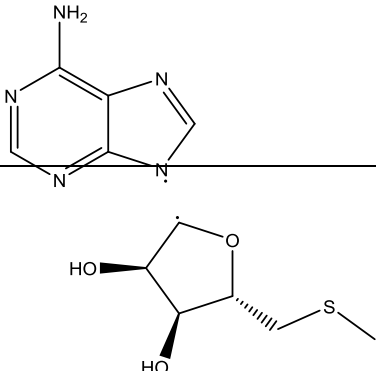
17	Arginine	$C_6H_{14}N_4O_2$	174.20	175	70		<p>Chemical Formula: $C_2H_6N_3^+$ Exact Mass: 72.06</p>  <p>Chemical Formula: $C_4H_8NO_2^+$ Exact Mass: 102.06</p>
				185	75		
18	L-Citrulline	$C_6H_{13}N_3O_3$	175.19	176.1	70		<p>Chemical Formula: $C_4H_8NO_2^+$ Exact Mass: 102.06</p>  <p>Chemical Formula: $C_2H_5N_2O^+$ Exact Mass: 73.04</p>
				185.1	74		
19	D-Mannitol	$C_6H_{14}O_6$	182.17	183.1	147.1		<p>Chemical Formula: HO Exact Mass: 17.00</p>  <p>Chemical Formula: $C_6H_{12}O_4^{2-}$ Exact Mass: 148.07</p>
				189.1	153.1		
20	Nicotinamide	$C_6H_6N_2O$	122.13	123.1	79.8		<p>Chemical Formula: CH_2NO^+ Exact Mass: 44.01</p>  <p>Chemical Formula: $C_5H_4N^+$ Exact Mass: 78.03</p>
				131.1	85.8		

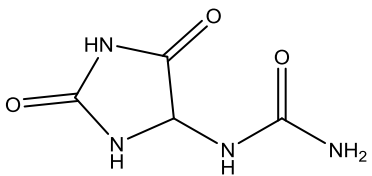
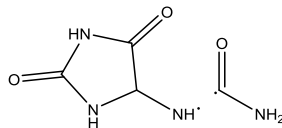
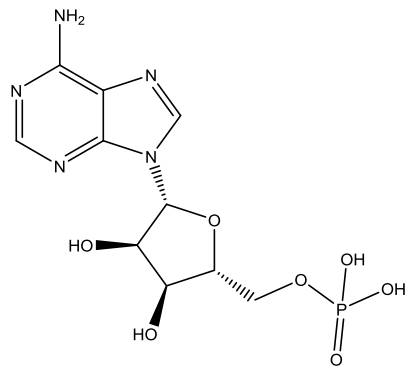
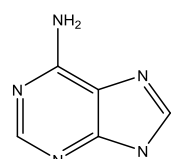
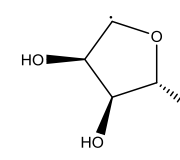
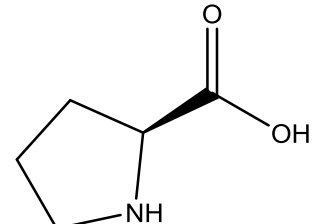
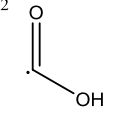
21	Aspartic Acid	$C_4H_7NO_4$	133.10	134	74		Chemical Formula: $C_2H_4NO_2^+$ Exact Mass: 74.02  Chemical Formula: $C_2H_3O_2^+$ Exact Mass: 59.01
				139	77		
22	Adenine	$C_5H_5N_5$	135.13	135.88	119		Chemical Formula: H_2N^+ Exact Mass: 16.02  Chemical Formula: $C_3H_3N_4^+$ Exact Mass: 119.04
				145.88	128		
23	Methionine	$C_5H_{11}NO_2S$	149.05	150	104		Chemical Formula: CHO_2^+ Exact Mass: 45.00  Chemical Formula: $C_4H_{10}NS^+$ Exact Mass: 104.05
				156	109		
24	Valine	$C_5H_{11}NO_2$	117.15	118	71.9		Chemical Formula: CHO_2^+ Exact Mass: 45.00  Chemical Formula: $C_4H_{10}N^+$ Exact Mass: 73.08

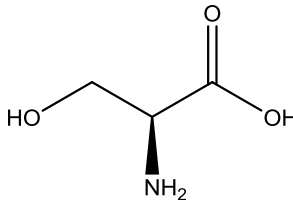
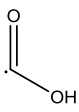
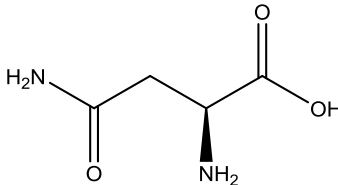
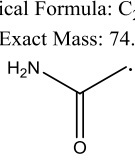
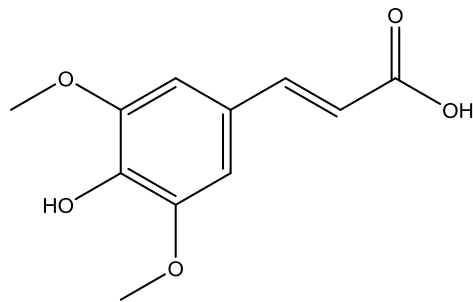

				124	76.9		
25	Pyroglutamic acid	$C_5H_7NO_3$	129.12	129.8	84		Chemical Formula: CHO_2^* Exact Mass: 45.00
				135.8	89		 Chemical Formula: $C_4H_6NO^*$ Exact Mass: 84.04
26	2,3-Dihydroxybenzoic Acid	$C_7H_6O_4$	154.12	155.04	137.04		 Chemical Formula: HO^* Exact Mass: 17.00
				162.04	144.04		Chemical Formula: $C_7H_5O_3^*$ Exact Mass: 137.02
27	Phenylalanine	$C_9H_{11}NO_2$	165.19	166	120		Chemical Formula: CHO_2^* Exact Mass: 45.00
				176	129		 Chemical Formula: $C_8H_{10}N^*$ Exact Mass: 120.08
28	Uridine	$C_9H_{12}N_2O_6$	244.2	245.06 9	113		Chemical Formula: $C_5H_6O_4^*$ Exact Mass: 133.05
						 Chemical Formula: $C_4H_3N_2O_2^*$ Exact Mass: 111.02	

				256.069	119		
29	2-Deoxyadenosine	$C_{10}H_{13}N_5O_3$	251.25	252.1	136.1		 Chemical Formula: $C_5H_4N_5^+$ Exact Mass: 134.05
				267.1	146.1		
30	2-Deoxyguanosine monohydrate	$C_{10}H_{13}N_5O_4$	267.25	268.2	152.1		 Chemical Formula: $C_5H_4N_5O^+$ Exact Mass: 150.04
				283.2	162.1		
31	Adenosine	$C_{10}H_{13}N_5O_4$	267.25	268.24	136		 Chemical Formula: $C_5H_4N_5^+$ Exact Mass: 134.05



				283.24	146		
32	Guanosine	$C_{10}H_{13}N_5O_5$	283.24	284	152	 <p>Chemical structure of Guanosine: A guanine base (a fused pyrimidine and imidazole ring system with a carbonyl group and an amino group) attached to a ribose sugar (a five-membered ring with hydroxyl groups at the 2' and 3' positions and a hydroxymethyl group at the 4' position).</p>	<p>Chemical Formula: $C_5H_4N_5O^+$ Exact Mass: 150.04</p>  <p>Chemical structure of Guanosine cation: Similar to Guanosine, but with a positive charge on the nitrogen atom in the imidazole ring.</p> <p>Chemical Formula: $C_5H_9O_4^+$ Exact Mass: 133.05</p>
				299	162		
33	5-Deoxy-5-methylthio-adenosine	$C_{11}H_{15}N_5O_3S$	297.33	298.1	136.1	 <p>Chemical structure of 5-Deoxy-5-methylthio-adenosine: An adenine base (a fused pyrimidine and imidazole ring system with an amino group) attached to a ribose sugar that has a methylthio group (-S-CH₃) at the 5' position instead of a hydroxyl group.</p>	<p>Chemical Formula: $C_5H_4N_5^+$ Exact Mass: 134.05</p>  <p>Chemical structure of 5-Deoxy-5-methylthio-adenosine cation: Similar to 5-Deoxy-5-methylthio-adenosine, but with a positive charge on the nitrogen atom in the imidazole ring.</p> <p>Chemical Formula: $C_6H_{11}O_3S^+$ Exact Mass: 163.04</p>

				314.1	146.1		
34	Allantoin	$C_4H_6N_4O_3$	158.12	159.1	116.2		 Chemical Formula: $C_3H_4N_3O_2^*$ Exact Mass: 114.03
				167.1	122.2		
35	AMP	$C_{10}H_{14}N_5O_7P$	347.22	348.4	135.9		Chemical Formula: $C_5H_4N_5^*$ Exact Mass: 134.05   Chemical Formula: $C_5H_{10}O_7P^*$ Exact Mass: 213.02
				363.4	145.9		
36	Proline	$C_5H_9NO_2$	115.13	116	70		Chemical Formula: CHO_2^* Exact Mass: 45.00  Chemical Formula: $C_4H_8N^*$ Exact Mass: 70.07
				122	75		

37	Serine	$C_3H_7NO_3$	105.09	105.9	59.8		<p>Chemical Formula: CHO_2^* Exact Mass: 45.00</p>  <p>Chemical Formula: $C_2H_6NO^*$ Exact Mass: 60.04</p>
				109.9	62.8		
38	Asparagine	$C_4H_8N_2O_3$	132.12	133	74		<p>Chemical Formula: $C_2H_4NO_2^*$ Exact Mass: 74.02</p>  <p>Chemical Formula: $C_2H_4NO^*$ Exact Mass: 58.03</p>
				139	77		
39	Sinapinic acid	$C_{11}H_{12}O_5$	224.21	225.2	206.9		<p>Chemical Formula: HO^* Exact Mass: 17.00</p>  <p>Chemical Formula: $C_{11}H_{11}O_4^*$ Exact Mass: 207.07</p>
				236.2	217.9		