

Chemical composition	Tentative metabolite name	Theoretical signal	Observed Signal	Error (Da)	Error (PPM)	Minimum signal (au)	Average signal (au)	Maximum signal (au)
[C ₃ H ₄ O ₃ - H] ⁻	Pyruvic acid	87.0088	87.0101	0.001	14.787	0.003	557.920	3260.224
[C ₄ H ₆ O ₄ - H] ⁻	Fumaric acid	115.0037	115.0065	0.003	24.359	23.708	2016.507	9899.783
[C ₄ H ₈ O ₄ - H] ⁻	Butanedioic acid	117.0193	117.0192	0.000	0.919	6.503	136.877	749.570
[C ₄ H ₄ O ₅ - H] ⁻	Oxaloacetate	130.9986	131.0046	0.006	45.762	0.004	70.391	708.388
[C ₄ H ₇ NO ₃ - H] ⁻	Aspartate	132.0302	132.0372	0.007	53.124	0.055	94.852	1881.964
[C ₄ H ₆ O ₅ - H] ⁻	Malic acid	133.0142	133.0172	0.003	22.395	15.712	246.326	1358.739
[C ₄ H ₈ NO ₃ - H] ⁻	Glutamate	146.0459	146.0480	0.002	14.212	0.024	46.402	966.109
[C ₃ H ₅ O ₇ P + Cl] ⁻	Phosphoenolpyruvate	166.9751	166.9731	0.020	11.970	*	*	*
[C ₇ H ₁₀ O ₆ - H] ⁻	3-Dehydroquinic acid	189.0405	189.0385	0.002	10.637	4.052	150.295	1934.285
[C ₆ H ₈ O ₇ - H] ⁻	Citrate / Isocitrate	191.0197	191.0279	0.008	42.987	47.885	963.434	3906.750
[C ₃ H ₅ O ₇ P - H] ⁻	Erythrose-4-phosphate	199.0013	199.0206	0.019	96.756	6.315	237.013	1281.142
[C ₃ H ₅ O ₇ P + Cl] ⁻	Phosphoenolpyruvate + Cl	202.9518	202.9389	0.013	63.479	0.085	64.973	1108.480
[C ₆ H ₈ O ₈ P - H] ⁻	6-Phosphogluconolactone - H ₂ O	238.9962	238.9934	0.003	11.994	2.226	183.411	1210.830
[C ₆ H ₁₀ O ₈ P - H] ⁻	Glucose-6-Phosphate	259.0224	259.0294	0.007	27.047	4.687	285.093	2516.319
[C ₆ H ₁₀ O ₁₀ P - H] ⁻	Phosphogluconic acid	275.0174	275.0335	0.016	58.724	62.774	321.854	915.276
[C ₇ H ₁₂ O ₁₀ P - H] ⁻	3-Deoxy-D-arabino-heptulosonic acid 7-phosphate	287.0167	287.0174	0.001	2.424	4.999	137.302	996.279
[C ₇ H ₁₄ O ₁₀ P - H] ⁻	Sedoheptulose-7-phosphate	289.0330	289.0371	0.004	14.189	155.191	1291.139	7586.075
[C ₉ H ₁₃ N ₅ O ₁₀ P - H] ⁻	Uridine monophosphate	323.0286	323.0364	0.008	24.101	88.436	553.213	5694.636
[C ₆ H ₁₄ O ₁₂ P ₂ - H] ⁻	Fructose-1,6-bisphosphate	338.9888	338.9824	0.006	18.829	4.442	237.169	1360.370
[C ₁₀ H ₁₄ N ₅ O ₁₀ P - H] ⁻	Guanosine monophosphate	362.0507	362.0642	0.013	37.246	0.115	34.588	140.204
[C ₁₀ H ₁₄ N ₅ O ₁₂ P ₂ - H] ⁻	Uridine diphosphate	402.9949	402.9952	0.000	0.635	25.481	404.551	2978.756
[C ₁₀ H ₁₅ N ₅ O ₁₀ P ₂ - H] ⁻	Adenosine diphosphate	426.0221	426.0248	0.003	6.198	70.859	1295.376	7013.796
[C ₁₀ H ₁₅ N ₅ O ₁₁ P ₂ - H] ⁻	Guanosine diphosphate	442.0171	442.0101	0.007	15.662	4.713	344.961	2817.733
[C ₉ H ₁₃ N ₅ O ₁₅ P ₃ - H] ⁻	Uridine triphosphate	482.9613	482.9503	0.011	22.705	9.860	543.594	3174.335
[C ₁₀ H ₁₆ N ₅ O ₁₃ P ₃ - H] ⁻	Adenosine triphosphate	505.9885	505.9792	0.009	18.227	56.672	1960.527	11192.315
[C ₁₀ H ₁₆ N ₅ O ₁₄ P ₃ - H] ⁻	Guanosine triphosphate	521.9834	521.9785	0.005	9.329	11.485	436.935	3946.622
[C ₁₂ H ₂₄ N ₅ O ₁₇ P ₂ - H] ⁻	Uridine diphosphate glucose	565.0477	565.0422	0.006	9.858	0.087	31.211	684.231
[C ₁₇ H ₂₇ N ₅ O ₁₇ P ₂ - H] ⁻	Uridine diphosphate N-acetylglucosamine	606.0743	606.0566	0.018	29.128	0.024	70.635	3258.626
[C ₂₁ H ₂₉ N ₇ O ₁₆ P ₂ - H] ⁻	Nicotinamide adenine dinucleotide	664.1175	664.1193	0.002	2.751	0.002	17.213	727.649
[C ₂₁ H ₃₅ N ₇ O ₁₆ P ₃ S - H] ⁻	Coenzyme A	766.1079	766.1054	0.003	3.298	0.004	10.432	52.650
[C ₂₃ H ₃₅ N ₇ O ₁₇ P ₃ S - H] ⁻	Acetyl coenzyme A	808.1185	808.1243	0.006	7.139	0.001	34.118	542.709