

## H+ ADDUCT

## Compound search (+/- 0.01da)

0.2Da BINS	Likely Mass (0.005Binning)	H+ adduct	Exact mass	Formula
71	70.98			
78	77.99			
79	78.9725			
82	81.9725	Bisulfite	80.9646398907	HSO3
82.4	82.495			
83	82.995			
85	84.995	Sodium bicarbonate	83.9823381716	NaHCO3
87	87.0025			
88	87.9825			
89.6	89.5			
90	90.005			
90.4	90.4875			
94	94.005			
94.6	94.505			
95	95.005			
97.4	97.4975			
98.6	98.5075			
99.4	99.495			
100	99.99			
103	103.0125			
104	104.07	2-aminobutyrate	103.063328533	C4H9NO2
		Dimethylglycine	103.063328533	C4H9NO2
		(R)-3-Amino-2-methylpropanoate	103.063328533	C4H9NO2
		(R)-2-Aminobutanoic acid	103.063328533	C4H9NO2
		(S)-2-Aminobutanoate	103.063328533	C4H9NO2
		N-Methyl-L-alanine	103.063328533	C4H9NO2
		(S)-3-Amino-2-methylpropanoate	103.063328533	C4H9NO2
		2-Amino-2-methylpropanoate	103.063328533	C4H9NO2
		3-Amino-2-methylpropanoate	103.063328533	C4H9NO2
		N-Ethylglycine	103.063328533	C4H9NO2
105	105.08			
105.6	105.5175			
106.6	106.505			
110	109.0225			
110.6	110.5225			
111	111.005			
112.8	112.8625			
113.6	113.51			
114	114.005			
114.6	114.5225			
114.8	114.8625			
115	115.0225			
115.6	115.52			
116	116.035	maleamate	115.026943024	C4H5NO3
118	118.01	3-Nitroacrylate	117.006207579	C3H3NO4
122.6	122.5125			
123	123.01			
123.6	123.525			
126.6	126.5275			
127	126.95			
129	129.0175			
130	130.0175			
130.2	130.1275			
130.6	130.535			

131	131.0325	2,5-Dioxopentanoate	130.026608671	C5H6O4
		2-Methylfumarate	130.026608671	C5H6O4
		Acetylpyruvate	130.026608671	C5H6O4
		(E)-Glutaconate	130.026608671	C5H6O4
134	134.02	4,5-Dioxopentanoate	130.026608671	C5H6O4
134.6	134.515			
135	135.035			
135.6	135.535			
136	136.0375			
138.6	138.525			
139	139.02	acetylphosphonate	138.008195333	C3H7O4P
		Fosfomicin	138.008195333	C3H7O4P
139.8	139.885			
141	140.975			
141.8	141.885			
142	142.04			
143	143.025	4-Chloro-3-methylphenol	142.018542524	C7H7ClO
143.6	143.53			
144	144.0275			
145	144.9775	2-chloroethylphosphonate	143.974308361	C2H6O3PCl
146.2	146.1325	L-Lysinamide	145.121512115	C6H15N3O
146.6	146.5325			
147	147.05	2-Tetrahydrothiopheneacetic acid	146.04015056	C6H10O2S
150	150.025			
151	151.02	(-)-Tartaric acid	150.01643791	C4H6O6
152	152	3-mercapto-2-mercaptomethylpropanoate	150.988746464	C4H7O2S2
154.6	154.52			
155	155.03	4-Chloroacetophenone	154.018542524	C8H7ClO
		3,4-Dihydroxybenzoate	154.0266087	C7H6O4
		2,5-Dihydroxybenzoate	154.0266087	C7H6O4
156	156.0475	N-Methylethanolamine phosphate	155.034744434	C3H10NO4P
		(R)-1-Aminopropan-2-yl phosphate	155.034744434	C3H10NO4P
158	158.065	1-Nitrosonaphthalene	157.052763849	C10H7NO
159	158.995			
160	160.045			
161	160.96			
165	165.0325			
167	166.995			
168	167.995	2-Mercaptobenzothiazole	166.986341165	C7H5NS2
169	169			
170	169.9875			
171	170.9875			
173	173.01	Benzenamine sulfate	172.006839056	C6H6NO3S
174.8	174.87			
175	175.0925	L-Citrulline ester	174.087866258	C6H12N3O3R
		1,6-Hexanedicarboxylic acid	174.089208927	C8H14O4
		Dimethyl adipate	174.089208927	C8H14O4
176	176.0925	2-Benzimidazolylguanidine	175.085795313	C8H9N5
180	179.9975	5-Methyl-3-isoxazolyl sulfate	178.988843263	C4H5NO5S

182	182.005	2-Methylthiobenzothiazole	181.001991229	C8H7NS2
185	185.005	2-Pyrone-4,6-dicarboxylate	184.000787846	C7H4O6
		4-Oxo-4H-pyran-2,6-dicarboxylic acid	184.000787846	C7H4O6
186	186.005	L-serine O-sulfate	184.999407947	C3H7NO6S
187	187.0025	3-Phosphoglycerate	185.992939191	C3H7O7P
		4-Formylbenzenesulfonate	185.998679671	C7H6O4S
188	188.005			
192	192.0275			
196.8	196.8475			
198	197.9925	1-Acyl-glycerone 3-phosphate	196.985114159	C4H6O7PR
200	200.02	2-(S)-hydroxypropyl-CoM	199.009875831	C5H11O4S2
201	201.02	D-Threose 4-phosphate	200.008589256	C4H9O7P
		Erythrulose 1-phosphate	200.008589256	C4H9O7P
		D-Erythrulose 4-phosphate	200.008589256	C4H9O7P
202	201.99			
204	204.03	(E)-4-oxobut-1-ene-1,2,4-tricarboxylate	203.019177561	C7H7O7
		trifluoromethionine	203.019177561	C5H8NO2F3S
205	205.0275	Carbonyl cyanide m-chlorophenyl hydrazone	204.02027386	C9H5ClN4
207	206.9875			
209	209.025	1-Naphthalenesulfonic acid	208.019415115	C10H8O3S
210	210.025			
211	211.025	fluoro-citrate	210.017580781	C6H7O7F
212	212.02			
212.8	212.82			
213	213.045	beta-Hydroxy-L-tyrosyl-[pcp]	212.038139184	C9H10NO3SR
214.8	214.815			
219	218.9975	5-Sulfosalicylate	217.98850891	C7H6O6S
221	221.0125			
222	222.0075			
223	222.965			
224	223.9475	N(omega)-Phosphohypotaurocyamine	232.015703095	C3H11N3O5PS
225	225.0025			
230.8	230.855			
232	232.015			
233	233.02			
234	234.01			
236	235.95			
240.8	240.8425			
241	241.04	2-Hydroxy-3-methyl-beta-keto-L-tyrosyl-[pcp]	240.033053804	C10H10NO4SR
248	247.995			
258	258.0825	2-Amino-6-(benzylthio)purine	257.073516377	C12H11N5S
		6-Chloro-3,5-diaminopyrazine-3-carboxamide	257.079185718	C8H12ClN7O
262	262.035			
263	262.9925			
270	269.965			
273	273.0375	dinitro-4-hydroxyphenylpyruvate	272.028065223	C9H8N2O8
277	277.005			
280	280.065			
288.2	288.26			
289	289.015			
296	296.375			
307	307.475			

313.8	313.7675			
341.8	341.7825			
365	365.0825			
381	381.0475			
382	382.0575			
383	383.045			
425	425.05	Sinabin	424.037212778	C14H18NO10S2
425.2	425.115			
500	499.9			
502	501.915			
514	513.93			
515	514.935			
516	515.93			
561.2	561.135			
570	569.99			
577.2	577.13	Epicatechin-(2beta->7,4beta->8)-epicatechin	576.126776204	C30H24O12
591.2	591.11			
617	617.0925			

## Na<sup>+</sup> ADDUCT

0.2Da BINS	Likely Mass (0.005Binning)	Na <sup>+</sup> adduct	Exact mass	Formula
71	70.98			
78	77.99			
79	78.9725			
82	81.9725			
82.4	82.495			
83	82.995			
85	84.995			
87	87.0025			
88	87.9825			
89.6	89.5			
90	90.005			
90.4	90.4875			
94	94.005			
94.6	94.505			
95	95.005	Methylglyoxal	72.02112937	C3H4O2
97.4	97.4975			
98.6	98.5075			
99.4	99.495			
100	99.99			
103	103.0125			
104	104.07			
105	105.08			
105.6	105.5175			
106.6	106.505			
110	109.0225			
110.6	110.5225			
111	111.005	Pyruvic Acid	88.01604399	C3H4O3
112.8	112.8625			
113.6	113.51			
114	114.005			
114.6	114.5225			
114.8	114.8625			
115	115.0225			
115.6	115.52			
116	116.035			
118	118.01			

122.6	122.5125			
123	123.01			
123.6	123.525			
126.6	126.5275			
127	126.95			
129	129.0175	D-Glyceric acid	106.0266087	C3H6O4
130	130.0175			
130.2	130.1275			
130.6	130.535			
131	131.0325			
134	134.02			
134.6	134.515			
135	135.035	Parasorbic acid	112.052495	C6H8O2
135.6	135.535			
136	136.0375	L-delta1-Pyrroline-5-carboxylate	113.0476785	C5H7NO2
138.6	138.525			
139	139.02			
139.8	139.885			
141	140.975			
141.8	141.885			
142	142.04	L-Homoserine	119.0582432	C4H9NO3
		L-Threonine	119.0582432	C4H9NO3
143	143.025	Erythrose	120.0422587	C4H8O4
143.6	143.53			
144	144.0275			
145	144.9775			
146.2	146.1325			
146.6	146.5325			
147	147.05	p-Hydrobenzyl alcohol	124.0524295	C7H8O2
		4-Methylcatechol	124.0524295	C7H8O2
150	150.025			
151	151.02			
152	152			
154.6	154.52			
155	155.03	Glutaric acid	132.0422587	C5H8O4
156	156.0475			
158	158.065	Phenylacetaldoxime	135.0684139	C8H9NO
159	158.995			
160	160.045	Anthranilic acid	137.0476785	C7H7NO2
		p-Aminobenzoic acid	137.0476785	C7H7NO2
		Trigonelline	137.0476785	C7H7NO2
161	160.96			
165	165.0325			
167	166.995			
168	167.995			
169	169			
170	169.9875			
171	170.9875			
173	173.01	L-(+)-Tartaric acid	150.0164379	C4H6O6
174.8	174.87			
175	175.0925			
176	176.0925			
180	179.9975			
182	182.005			
185	185.005			
186	186.005			
187	187.0025			
188	188.005			

192	192.0275	Dihydrodipicolinic acid	169.0375077	C7H7NO4
196.8	196.8475			
198	197.9925			
200	200.02			
201	201.02	Esculetin	178.0266087	C9H6)4
202	201.99			
204	204.03			
205	205.0275			
207	206.9875			
209	209.025			
210	210.025			
211	211.025			
212	212.02			
212.8	212.82			
213	213.045			
214.8	214.815			
219	218.9975			
221	221.0125			
222	222.0075	)-Phospho-L-homoserine	199.0245736	C4H10NO6P
223	222.965			
224	223.9475			
225	225.0025			
230.8	230.855			
232	232.015	4-Chloroindole-3-acetic acid	209.0243562	C10H8ClNO2
233	233.02			
234	234.01			
236	235.95			
240.8	240.8425			
241	241.04			
248	247.995			
258	258.0825			
262	262.035			
263	262.9925			
270	269.965			
273	273.0375			
277	277.005	Shikimic acid 3-phosphate	254.0191538	C7H11O8P
280	280.065			
288.2	288.26			
289	289.015			
296	296.375			
307	307.475			
313.8	313.7675			
341.8	341.7825			
365	365.0825	Caffeic acid 3-glucoside	342.0950822	C15H18O9
381	381.0475			
382	382.0575			
383	383.045			
425	425.05			
425.2	425.115	Nobiletin	402.1314677	C21H22O8
500	499.9			
502	501.915			
514	513.93			
515	514.935			
516	515.93			
561.2	561.135			
570	569.99			
577.2	577.13			
591.2	591.11			
617	617.0925	Catechin 5,7-di-O-gallate	594.1009554	C29H22O14

## K+ ADDUCT

0.2Da BINS	Likely Mass (0.005Binning)	K+ adduct	Exact mass	Formula
71	70.98			
78	77.99			
79	78.9725			
82	81.9725			
82.4	82.495			
83	82.995	Acetaldehyde	44.02621475	C2H4O
85	84.995			
87	87.0025			
88	87.9825			
89.6	89.5			
90	90.005			
90.4	90.4875			
94	94.005			
94.6	94.505			
95	95.005			
97.4	97.4975			
98.6	98.5075			
99.4	99.495			
100	99.99			
103	103.0125			
104	104.07			
105	105.08			
105.6	105.5175			
106.6	106.505			
110	109.0225			
110.6	110.5225			
111	111.005			
112.8	112.8625			
113.6	113.51			
114	114.005	Glycine	75.03202841	C2H5NO2
114.6	114.5225			
114.8	114.8625			
115	115.0225	(+)-Propylene glycol	76.0524295	C3H8O2
115.6	115.52			
116	116.035			
118	118.01			
122.6	122.5125			
123	123.01			
123.6	123.525			
126.6	126.5275			
127	126.95			
129	129.0175			
130	130.0175			
130.2	130.1275			
130.6	130.535			
131	131.0325			
134	134.02			
134.6	134.515			
135	135.035			
135.6	135.535			
136	136.0375			
138.6	138.525			
139	139.02	Tiglic acid	100.0524295	C5H8O2
139.8	139.885			

141	140.975		
141.8	141.885		
142	142.04		
143	143.025		
143.6	143.53		
144	144.0275		
145	144.9775		
146.2	146.1325		
146.6	146.5325		
147	147.05	Fucoserratene	108.0939004 C8H12
150	150.025		
151	151.02	Parasorbic acid	112.0524295 C6H8O2
152	152		
154.6	154.52		
155	155.03		
156	156.0475	L-Valine	117.0789786 C5H11NO2
158	158.065		
159	158.995		
160	160.045		
161	160.96		
165	165.0325		
167	166.995		
168	167.995		
169	169		
170	169.9875		
171	170.9875		
173	173.01		
174.8	174.87		
175	175.0925		
176	176.0925		
180	179.9975		
182	182.005		
185	185.005		
186	186.005		
187	187.0025	Citramalic acid	148.0371734 C5H8O5
188	188.005	L-Methionine	149.0510493 C5H11NO2S
192	192.0275		
196.8	196.8475		
198	197.9925		
200	200.02	Indole-3-carboxylic acid	161.0476785 C9H7NO2
201	201.02	1,6-Anhydroglucose	162.0528234 C6H10O5
202	201.99		
204	204.03		
205	205.0275	Caffeyl alcohol	166.0629942 C9H10O3
207	206.9875		
209	209.025		
210	210.025		
211	211.025	2,3,4,5-Tetrahydrodipicolinate	171.5315778 C7H9NO4
212	212.02		
212.8	212.82		
213	213.045	Indole-3-acetamide	174.7931296 C10H10N2O
214.8	214.815		
219	218.9975	Caffeic acid	180.0422587 C9H8O4
221	221.0125	4-Hydroxy-3,5-dimethoxybenzaldehyde	182.0579088 C9H10O4
222	222.0075		
223	222.965		
224	223.9475		
225	225.0025		
230.8	230.855		



232	232.015		
233	233.02	Ferulic acid	194.0579909 C10H10O4
234	234.01		
236	235.95		
240.8	240.8425		
241	241.04		
248	247.995		
258	258.0825	Pantothenic acid	219.1106727 C9H17NO5
262	262.035		
263	262.9925		
270	269.965		
273	273.0375		
277	277.005	D-erythro-Imidazolylglycerol phosphate	238.0354726 C6H11N2O6P
280	280.065		
288.2	288.26		
289	289.015		
296	296.375		
307	307.475		
313.8	313.7675		
341.8	341.7825		
365	365.0825		
381	381.0475		
382	382.0575		
383	383.045		
425	425.05		
425.2	425.115		
500	499.9		
502	501.915		
514	513.93		
515	514.935		
516	515.93		
561.2	561.135		
570	569.99		
577.2	577.13		
591.2	591.11		
617	617.0925		