

Table S1. Most likely chemical formulas of observed features.

Input mass	Adduct	Mass	Dppm	Formula
59.05583	[M+H] ⁺	58.041865	113	C3H6O
99.03254	[M+H-H2O] ⁺	116.0334254	18	C2H4N4O2
109.0671	[M+H] ⁺	108.0575118	21	C7H8O
109.0671	[M+H-H2O] ⁺	126.0680796	16	C7H10O2
111.0324	[M+H-H2O] ⁺	128.0334254	15	C3H4N4O2
112.034	[M+H] ⁺	111.032029	47	C5H5NO2
112.9939	[M+H] ⁺	111.9830293	31	CH4O4S
113.0293	[M+H] ⁺	112.027278	46	C4H4N2O2
113.0293	[M+H-H2O] ⁺	130.0266087	48	C5H6O4
113.0475	[M+H] ⁺	112.0346709	49	C6H8S
113.0475	[M+H] ⁺	112.038511	15	C3H4N4O
113.0475	[M+H-H2O] ⁺	130.0452356	44	C6H10OS
113.0475	[M+H-H2O] ⁺	130.0530982	25	C8H6N2
115.0266	[M+H] ⁺	114.0139355	46	C5H6OS
115.0266	[M+H-H2O] ⁺	132.0245002	42	C5H8O2S
117.0589	[M+H] ⁺	116.047345	36	C5H8O3
117.0589	[M+H-H2O] ⁺	134.0579088	31	C5H10O4
117.0589	[M+H-H2O] ⁺	134.059246	20	C6H6N4
118.0675	[M+H] ⁺	117.057849	20	C8H7N
119.0308	[M+H] ⁺	118.0200835	28	C3H6N2OS
119.0308	[M+H] ⁺	118.02661	25	C4H6O4
119.0308	[M+H-H2O] ⁺	136.0346709	9	C8H8S
119.0308	[M+H-H2O] ⁺	136.037175	30	C4H8O5
119.0308	[M+H-H2O] ⁺	136.0380418	37	C5H12S2
119.0308	[M+H-H2O] ⁺	136.038511	41	C5H4N4O
122.9803	[M+H-H2O] ⁺	139.9779439	41	C2H4O5S
122.9803	[M+H-H2O] ⁺	139.9788123	34	C3H8S3
127.009	[M+H] ⁺	125.998682	23	C2H6O4S
127.009	[M+H-H2O] ⁺	144.0067416	39	C6H8S2
127.026	[M+H] ⁺	126.0139355	37	C6H6OS
129.0419	[M+H] ⁺	128.0334254	9	C3H4N4O2
129.0419	[M+H] ⁺	128.040819	48	C5H8N2S
129.0419	[M+H-H2O] ⁺	146.0401503	34	C6H10O2S
129.0419	[M+H-H2O] ⁺	146.0480128	26	C8H6N2O
131.0321	[M+H] ⁺	130.020085	36	C4H6N2OS
131.0321	[M+H] ⁺	130.0266087	13	C5H6O4
131.0321	[M+H-H2O] ⁺	148.0371734	17	C5H8O5
131.0321	[M+H-H2O] ⁺	148.0380418	24	C6H12S2
136.0234	[M+H] ⁺	135.0142699	13	C7H5NS
136.0234	[M+NH4] ⁺	117.9902232	4	C3H2O5
141.024	[M+H] ⁺	140.0109586	40	C6H4O4
141.024	[M+H] ⁺	140.022192	38	C5H4N2O3
141.024	[M+H-H2O] ⁺	158.0215233	36	C6H6O5
141.024	[M+H-H2O] ⁺	158.032758	42	C5H6N2O4
141.042	[M+H] ⁺	140.0295856	36	C7H8OS
141.042	[M+H] ⁺	140.040819	43	C6H8N2S
141.042	[M+NH4] ⁺	123.0142699	43	C6H5NS
141.042	[M+H-H2O] ⁺	158.0401503	32	C7H10O2S
141.042	[M+H-H2O] ⁺	158.0439901	5	C4H6N4O3
149.0979	[M+H] ⁺	148.088815	12	C10H12O

Input mass	Adduct	Mass	Dppm	Formula
149.0979	[M+H] ⁺	148.0921858	10	C7H16OS
149.0979	[M+NH ₄] ⁺	131.058226	39	C5H9NO3
149.0979	[M+NH ₄] ⁺	131.0694765	36	C4H9N3O2
149.0979	[M+H-H ₂ O] ⁺	166.0966944	26	C6H10N6
149.0979	[M+H-H ₂ O] ⁺	166.099371	8	C10H14O2
150.9758	[M+H-H ₂ O] ⁺	167.982378	25	C3H5O6P
151.0254	[M+H] ⁺	150.0139355	27	C8H6OS
151.0254	[M+H-H ₂ O] ⁺	168.0245005	24	C8H8O2S
151.0254	[M+H-H ₂ O] ⁺	168.028341	1	C5H4N4O3
152.0636	[M+H] ⁺	151.04941	45	C5H5N5O
152.0636	[M+H] ⁺	151.063284	45	C8H9NO2
152.0636	[M+NH ₄] ⁺	134.032758	19	C3H6N2O4
152.0636	[M+NH ₄] ⁺	134.0367794	46	C8H6O2
152.0636	[M+H-H ₂ O] ⁺	169.073894	49	C8H11NO3
152.9904	[M+H] ⁺	151.9779439	33	C3H4O5S
152.9904	[M+H] ⁺	151.9874598	28	C3H5O5P
152.9904	[M+H-H ₂ O] ⁺	169.9885086	30	C3H6O6S
152.9904	[M+H-H ₂ O] ⁺	169.9980245	31	C3H7O6P
154.9869	[M+H] ⁺	153.9758354	24	C3H6O3S2
155.0573	[M+H] ⁺	154.0452356	30	C8H10OS
155.0573	[M+NH ₄] ⁺	137.0299199	41	C7H7NS
155.0573	[M+H-H ₂ O] ⁺	172.0524268	49	C11H8O2
155.0573	[M+H-H ₂ O] ⁺	172.0636629	23	C10H8N2O
157.0368	[M+H] ⁺	156.0245002	31	C7H8O2S
157.0368	[M+H] ⁺	156.034193	29	C8H9ClO
157.0368	[M+H] ⁺	156.0357336	39	C6H8N2OS
157.0368	[M+H-H ₂ O] ⁺	174.0316941	49	C10H6O3
157.0368	[M+H-H ₂ O] ⁺	174.0429274	21	C9H6N2O2
158.1563	[M+NH ₄] ⁺	140.1201151	14	C9H16O
159.0327	[M+H] ⁺	158.0215233	24	C6H6O5
159.0327	[M+H] ⁺	158.0327567	46	C5H6N2O4
159.0327	[M+NH ₄] ⁺	141.0062076	46	C5H3NO4
159.0327	[M+H-H ₂ O] ⁺	176.032088	21	C6H8O6
159.0327	[M+H-H ₂ O] ⁺	176.040819	33	C9H8N2S
159.0327	[M+H-H ₂ O] ⁺	176.0433214	49	C5H8N2O5
166.9713	[M+H-H ₂ O] ⁺	183.977293	19	C3H5O7P
168.9858	[M+H] ⁺	167.9728586	33	C3H4O6S
168.9858	[M+H] ⁺	167.9823744	22	C3H5O6P
168.9858	[M+H-H ₂ O] ⁺	185.992943	26	C3H7O7P
168.9858	[M+H-H ₂ O] ⁺	185.9944531	34	C5H3ClN4O2
170.9648	[M+H-H ₂ O] ⁺	187.9635562	23	C3H8O3S3
171.052	[M+H] ⁺	170.0401503	26	C8H10O2S
171.052	[M+H] ⁺	170.0439901	4	C5H6N4O3
171.052	[M+H] ⁺	170.051385	38	C7H10N2OS
171.052	[M+NH ₄] ⁺	153.0190943	5	C3H8NO4P
171.052	[M+H-H ₂ O] ⁺	188.0473441	43	C11H8O3
171.052	[M+H-H ₂ O] ⁺	188.0585775	22	C10H8N2O2
172.99	[M+H-H ₂ O] ⁺	189.993594	4	C6H6O5S
173.0139	[M+H] ⁺	172.0007878	33	C6H4O6
173.0139	[M+H] ⁺	172.0136745	40	C3H9O6P
173.0139	[M+H-H ₂ O] ⁺	190.011355	30	C6H6O7
180.9854	[M+H-H ₂ O] ⁺	197.9834232	26	C4H6O7S

Input mass	Adduct	Mass	Dppm	Formula
180.9854	[M+H-H ₂ O] ⁺	197.9929391	26	C ₄ H ₇ O ₇ P
185.068	[M+H] ⁺	184.0524295	44	C ₁₂ H ₈ O ₂
185.068	[M+H] ⁺	184.0558003	26	C ₉ H ₁₂ O ₂ S
185.068	[M+H] ⁺	184.0636629	15	C ₁₁ H ₈ N ₂ O
185.068	[M+NH ₄] ⁺	167.0252285	48	C ₄ H ₉ NO ₄ S
185.068	[M+NH ₄] ⁺	167.026567	41	C ₅ H ₅ N ₅ S
185.068	[M+NH ₄] ⁺	167.0347443	3	C ₄ H ₁₀ NO ₄ P
185.068	[M+NH ₄] ⁺	167.036464	12	C ₃ H ₉ N ₃ O ₃ S
185.068	[M+NH ₄] ⁺	167.0404846	34	C ₈ H ₉ NOS
185.068	[M+H-H ₂ O] ⁺	202.0629942	41	C ₁₂ H ₁₀ O ₃
185.068	[M+H-H ₂ O] ⁺	202.0718581	6	C ₄ H ₁₅ N ₂ O ₅ P
185.068	[M+H-H ₂ O] ⁺	202.0742276	18	C ₁₁ H ₁₀ N ₂ O ₂
185.068	[M+H-H ₂ O] ⁺	202.0782503	40	C ₁₆ H ₁₀
187.009	[M+H-H ₂ O] ⁺	204.0189365	38	C ₈ H ₉ ClO ₄
187.0284	[M+H] ⁺	186.0164379	25	C ₇ H ₆ O ₆
187.0284	[M+H-H ₂ O] ⁺	204.0270026	22	C ₇ H ₈ O ₇
187.0284	[M+H-H ₂ O] ⁺	204.0357336	24	C ₁₀ H ₈ N ₂ OS
189.0601	[M+H] ⁺	188.0473441	28	C ₁₁ H ₈ O ₃
189.0601	[M+H] ⁺	188.0585775	30	C ₁₀ H ₈ N ₂ O ₂
189.0601	[M+NH ₄] ⁺	171.0217694	23	C ₅ H ₁₁ Cl ₂ NO
189.0601	[M+NH ₄] ⁺	171.0353992	48	C ₇ H ₉ NO ₂ S
189.0601	[M+H-H ₂ O] ⁺	206.0579088	26	C ₁₁ H ₁₀ O ₄
189.0601	[M+H-H ₂ O] ⁺	206.069143	33	C ₁₀ H ₁₀ N ₂ O ₃
194.9997	[M+H-H ₂ O] ⁺	212.0004107	10	C ₆ H ₄ N ₄ O ₃ S
196.9806	[M+H-H ₂ O] ⁺	213.9870688	18	C ₇ H ₆ N ₂ O ₂ S ₂
196.9806	[M+H-H ₂ O] ⁺	213.987858	22	C ₄ H ₇ O ₈ P
197.0401	[M+H] ⁺	196.0232546	48	C ₆ H ₄ N ₄ O ₄
197.0401	[M+H] ⁺	196.0371734	22	C ₉ H ₈ O ₅
197.0401	[M+H-H ₂ O] ⁺	214.0412129	8	C ₈ H ₁₀ N ₂ O ₃ S
197.0401	[M+H-H ₂ O] ⁺	214.0477381	24	C ₉ H ₁₀ O ₆
197.0401	[M+H-H ₂ O] ⁺	214.0490755	31	C ₁₀ H ₆ N ₄ O ₂
197.0401	[M+H-H ₂ O] ⁺	214.052444	48	C ₇ H ₁₀ N ₄ O ₂ S
197.0671	[M+H] ⁺	196.0524295	37	C ₁₃ H ₈ O ₂
197.0671	[M+H] ⁺	196.059641	0	C ₇ H ₈ N ₄ O ₃
197.0671	[M+H] ⁺	196.067035	36	C ₉ H ₁₂ N ₂ OS
197.0671	[M+NH ₄] ⁺	179.0252285	40	C ₅ H ₉ NO ₄ S
197.0671	[M+NH ₄] ⁺	179.0404846	36	C ₉ H ₉ NOS
197.0671	[M+NH ₄] ⁺	179.042987	49	C ₅ H ₉ NO ₆
197.0671	[M+H-H ₂ O] ⁺	214.0629942	34	C ₁₃ H ₁₀ O ₃
197.0671	[M+H-H ₂ O] ⁺	214.066365	17	C ₁₀ H ₁₄ O ₃ S
197.0671	[M+H-H ₂ O] ⁺	214.0702048	1	C ₇ H ₁₀ N ₄ O ₄
197.0671	[M+H-H ₂ O] ⁺	214.0776	39	C ₉ H ₁₄ N ₂ O ₂ S
197.9826	[M+H-H ₂ O] ⁺	214.9807768	23	C ₈ H ₆ ClNO ₂ S
198.038	[M+H] ⁺	197.0324223	8	C ₈ H ₇ NO ₅
198.038	[M+H] ⁺	197.0357932	25	C ₅ H ₁₁ NO ₅ S
198.038	[M+H-H ₂ O] ⁺	215.033091	38	C ₁₀ H ₅ N ₃ O ₃
203.0035	[M+H] ⁺	201.993594	12	C ₇ H ₆ O ₅ S
203.0236	[M+H] ⁺	202.0113525	24	C ₇ H ₆ O ₇
203.0236	[M+NH ₄] ⁺	184.9994077	47	C ₃ H ₇ NO ₆ S
203.0236	[M+H-H ₂ O] ⁺	220.0219172	21	C ₇ H ₈ O ₈
205.0289	[M+H] ⁺	204.027005	26	C ₇ H ₈ O ₇
205.0289	[M+H-H ₂ O] ⁺	222.0350649	16	C ₁₁ H ₁₀ O ₃ S

Input mass	Adduct	Mass	Dppm	Formula
206.9989	[M+H-H ₂ O] ⁺	224.0078043	29	C ₉ H ₈ N ₂ O ₅ S ₂
213.0452	[M+H] ⁺	212.032088	27	C ₉ H ₈ O ₆
213.0452	[M+H] ⁺	212.0473441	44	C ₁₃ H ₈ O ₃
213.0452	[M+NH ₄] ⁺	195.020146	41	C ₅ H ₉ N ₁ O ₅ S
213.0452	[M+H-H ₂ O] ⁺	230.057891	46	C ₁₃ H ₁₀ O ₄
214.9911	[M+H] ⁺	213.9870688	15	C ₇ H ₆ N ₂ O ₂ S ₂
214.9911	[M+H-H ₂ O] ⁺	232.0041587	47	C ₈ H ₈ O ₆ S
219.0858	[M+H] ⁺	218.0691422	42	C ₁₁ H ₁₀ N ₂ O ₃
219.0858	[M+H] ⁺	218.072513	27	C ₈ H ₁₄ N ₂ O ₃ S
219.0858	[M+H] ⁺	218.072515	27	C ₈ H ₁₄ N ₂ O ₃ S ₁
219.0858	[M+H] ⁺	218.073161	24	C ₁₆ H ₁₀ O
219.0858	[M+H] ⁺	218.0790382	2	C ₉ H ₁₄ O ₆
219.0858	[M+H-H ₂ O] ⁺	236.079708	40	C ₁₁ H ₁₂ N ₂ O ₄
219.0858	[M+H-H ₂ O] ⁺	236.0830777	24	C ₈ H ₁₆ N ₂ O ₄ S
219.0858	[M+H-H ₂ O] ⁺	236.0837296	21	C ₁₆ H ₁₂ O ₂
219.0858	[M+H-H ₂ O] ⁺	236.090941	10	C ₁₀ H ₁₂ N ₄ O ₃
219.0858	[M+H-H ₂ O] ⁺	236.094963	29	C ₁₅ H ₁₂ N ₂ O
225.0123	[M+H] ⁺	224.0078043	12	C ₉ H ₈ N ₂ O ₅ S ₂
239.024	[M+H-H ₂ O] ⁺	256.0371734	43	C ₁₄ H ₈ O ₅