

CCS for Primary Metabolites, Secondary Metabolites and Xenobiotics

Compound	CAS Number	Formula	Exact Mass	[M+H] ⁺	Ω Average	Ω RSD %	[M+Na] ⁺	Ω Average	Ω RSD %	[M-H] ⁻	Ω Average	Ω RSD %	
Primary Metabolites													
Amino Acids													
N,N-Dimethylglycine	1118-68-9	C4H9NO2	103.1203	104.1276	123.90	0.12		126.1096	N/A	N/A	102.1131	N/A	N/A
L-Serine	56-45-1	C3H7NO3	105.0419	106.0492	N/A	N/A	128.0311	N/A	N/A	N/A	104.0347	136.66	0.24
L-Proline	147-85-3	C5H9NO2	115.0633	116.0706	129.86	0.19	138.0525	N/A	N/A	N/A	114.0560	133.51	0.27
Betaine	107-43-7	C5H11NO2	117.0783	118.0863	122.15	0.22	140.0681	135.56	0.04	N/A	116.0704	N/A	N/A
L-Valine	72-18-4	C5H11NO2	117.0790	118.0863	134.28	0.57	140.0682	144.07	0.18	N/A	116.0717	132.88	0.22
L-Threonine	72-19-5	C4H9NO3	119.0582	120.0655	N/A	N/A	142.0475	N/A	N/A	N/A	118.0510	141.36	0.28
L-Cysteine	56-89-3	C3H7NO2S	121.0197	122.0276	149.57	0.04	144.0095	151.34	0.04	N/A	120.0119	144.47	0.07
Trans-4-Hydroxy-L-proline	51-35-4	C5H9NO3	131.0576	132.0655	130.23	0.51	154.0473	N/A	N/A	N/A	130.0496	N/A	N/A
N-Acetyl-L-alanine	97-69-8	C5H9NO3	131.0582	132.0655	N/A	N/A	154.0453	138.07	0.08	N/A	130.0510	N/A	N/A
Cis-4-hydroxy-2-proline	618-27-9	C5H9NO3	131.0582	132.0655	N/A	N/A	154.0475	N/A	N/A	N/A	130.0510	130.00	0.67
L-Norleucine	327-57-1	C6H13NO2	131.0946	132.1011	142.63	0.04	154.0844	N/A	N/A	N/A	130.0884	140.07	0.04
L-Allo-isoleucine	1509-34-8	C6H13NO2	131.0946	132.1019	N/A	N/A	154.0838	N/A	N/A	N/A	130.0873	134.45	0.09
L-Leucine	328-38-1	C6H13NO2	131.0946	132.1019	N/A	N/A	154.0838	N/A	N/A	N/A	130.0873	135.76	0.09
L-Leucine	61-90-5	C6H13NO2	131.0946	132.1019	139.65	0.25	154.0838	N/A	N/A	N/A	130.0873	138.71	0.78
Isoleucine	73-32-5	C6H13NO2	131.0946	132.1019	137.70	0.22	154.0837	N/A	N/A	N/A	130.0860	135.59	0.30
L-Asparagine	70-47-3	C4H8N2O3	132.0535	133.0608	131.54	0.39	155.0427	131.94	0.56	N/A	131.0462	127.11	0.88
L-Ornithine	70-26-8	C5H12N2O2	132.0899	133.0971	129.79	0.94	155.0791	N/A	N/A	N/A	131.0826	136.80	0.22
D-Aspartic Acid	617-45-8	C4H7NO4	133.0368	134.0448	N/A	N/A	156.0266	N/A	N/A	N/A	132.0289	121.85	0.79
L-Aspartic Acid	56-84-8	C4H7NO4	133.0375	134.0448	N/A	N/A	156.0267	N/A	N/A	N/A	132.0302	121.92	0.91
Homocysteine	454-29-5	C4H9NO2S	135.0348	136.0432	130.53	0.19	158.0252	N/A	N/A	N/A	134.0276	159.62	0.18
Glutamine	56-85-9	C5H10N2O3	146.0691	147.0764	133.45	0.19	169.0584	138.11	0.92	N/A	145.0619	132.11	0.08
L-Lysine	56-87-1	C6H14N2O2	146.1055	147.1128	133.11	0.13	169.0947	N/A	N/A	N/A	145.0982	141.76	0.80
L-Glutamic Acid	56-86-0	C5H9NO4	147.0532	148.0604	134.59	0.28	170.0424	N/A	N/A	N/A	146.0459	127.72	1.00
L-Methionine	63-68-3	C5H11NO2S	149.0510	150.0583	137.10	0.04	172.0403	N/A	N/A	N/A	148.0438	152.05	0.50
L-Histidine	71-00-1	C6H9N3O2	155.0694	156.0766	133.51	0.15	178.0586	137.00	0.08	N/A	154.0621	131.47	0.09
Tiglyl Glycine	35842-45-6	C7H11NO3	157.0739	158.0812	N/A	N/A	180.0631	146.68	0.07	N/A	156.0666	142.93	0.18
N-Methyl-L-glutamic Acid	35989-16-3	C6H11NO4	161.0681	162.0761	133.71	0.13	184.0579	N/A	N/A	N/A	160.0602	N/A	N/A
L-Phenylalanine	63-91-2	C9H11NO2	165.0790	166.0863	145.24	0.14	188.0682	141.89	0.36	N/A	164.0717	146.52	0.24
N(pil)-Methyl-L-histidine	368-16-1	C7H11N3O2	169.0845	170.0924	134.65	0.23	192.0742	N/A	N/A	N/A	168.0765	141.53	0.20
N-Alpha-Acetyl-L-Asparagine	4033-40-3	C6H10N2O4	174.0634	175.0713	N/A	N/A	197.0532	N/A	N/A	N/A	173.0555	137.87	0.45
L-Arginine	74-79-3	C6H14N4O2	174.1117	175.1189	137.87	0.04	197.1009	N/A	N/A	N/A	173.1044	132.24	0.51
N-Acetyl-L-aspartic Acid	997-55-7	C6H9NO5	175.0474	176.0553	N/A	N/A	198.0372	143.70	0.20	N/A	174.0395	N/A	N/A
L-Citrulline	372-75-8	C6H13N3O3	175.0957	176.1030	N/A	N/A	198.0849	N/A	N/A	N/A	174.1794	139.51	0.30
S-Carboxymethyl-L-cysteine	638-23-3	C5H9NO4S	179.0252	180.0312	141.13	0.11	202.0136	142.13	0.04	N/A	178.0181	N/A	N/A
L-Methionine sulfoximine	15985-39-4	C5H12N2O3S	180.0569	181.0631	139.30	0.12	203.0451	143.10	0.07	N/A	179.0499	141.23	0.41
L-Tyrosine	60-18-4	C9H11NO3	181.0739	182.0812	148.49	0.14	204.0631	N/A	N/A	N/A	180.0666	148.26	0.21
N-Acetyl-L-glutamic Acid	1188-37-0	C7H11NO5	189.0637	190.0699	139.03	0.17	212.0537	149.63	0.10	N/A	188.0566	139.63	0.04
L-Selenomethionine	3211-76-5	C5H11NO2Se	196.9948	198.0028	137.67	0.11	219.9846	N/A	N/A	N/A	195.9869	N/A	N/A
L-Mimosine from Koa Hoale Seeds	500-44-7	C8H11NO4	198.0641	199.0713	143.47	0.35	221.0533	N/A	N/A	N/A	197.0568	N/A	N/A
L-Tryptophan	73-22-3	C11H12N2O2	204.0899	205.0971	154.22	0.07	227.0791	N/A	N/A	N/A	203.0826	158.58	0.59
N-(3-Phenylpropionyl) Glycine	56613-60-6	C11H13NO3	207.0895	208.0968	149.47	0.14	230.0788	150.61	0.73	N/A	206.0823	N/A	N/A
Phosphocreatine	67-07-2	C4H10N3O5P	211.0358	212.0653	153.77	0.15	234.0256	N/A	N/A	N/A	210.0285	N/A	N/A
3-Methoxy-L-Tyrosine	300-48-1	C10H13NO4	211.0845	212.0913	158.73	0.13	234.0727	153.57	0.08	N/A	210.0775	153.27	0.16
O-Succinyl-L-homoserine	1492-23-5	C8H13NO6	219.0736	220.0816	147.46	0.04	242.0634	147.22	0.10	N/A	218.0657	N/A	N/A
L-Cystathionine	535-34-2	C7H14N2O4S	222.0674	223.0747	N/A	N/A	245.0566	N/A	N/A	N/A	221.0601	144.41	0.11
Carnosine	305-84-0	C9H14N4O3	226.1059	227.1139	152.18	0.04	249.0957	N/A	N/A	N/A	225.0980	154.93	0.11
N-Acetyl-D-tryptophan	2280-01-5	C13H14N2O3	246.0998	247.1077	155.67	0.13	269.0896	162.74	0.14	N/A	245.0918	161.97	0.11
Phenylacetyl-L-Glutamine	28047-15-6	C13H16N2O4	264.1110	265.1183	160.93	0.13	287.1002	171.25	0.15	N/A	263.1037	169.17	0.22
S-Adenosyl-L-methionine	29908-03-0	C15H22N6O5S	398.1371	399.1451	186.46	0.25	421.1269	N/A	N/A	N/A	397.1292	N/A	N/A
Sugars													
D-Arabinose	10323-20-3	C5H10O5	150.0528	151.0601	N/A	N/A	173.0420	143.27	0.90	N/A	149.0455	N/A	N/A
L-Arabinose	87-72-9	C5H10O5	150.0528	151.0601	N/A	N/A	173.0420	141.86	0.00	N/A	149.0455	N/A	N/A
D-(-)-Ribose	50-69-1	C5H10O5	150.0528	151.0601	N/A	N/A	173.0420	137.60	0.18	N/A	149.0455	N/A	N/A
L-Ribulose	2042-27-5	C5H10O5	150.0528	151.0601	N/A	N/A	173.0420	132.81	0.67	N/A	149.0455	N/A	N/A
D-Xylulose	551-84-8	C5H10O5	150.0528	151.0601	N/A	N/A	173.0420	141.76	0.31	N/A	149.0455	N/A	N/A
D-(+)-Xylose	58-86-6	C5H10O5	150.0528	151.0601	N/A	N/A	173.0420	132.07	0.16	N/A	149.0455	N/A	N/A
6-Deoxy-L-galactose	2438-80-4	C6H12O5	164.0685	165.0763	N/A	N/A	187.0582	147.32	0.08	N/A	163.0606	N/A	N/A
L-Rhamnose	3615-41-6	C6H12O5	164.0685	165.0763	N/A	N/A	187.0582	146.30	0.07	N/A	163.0606	N/A	N/A
D-Mannosamine	14307-02-9	C6H13NO5	179.0794	180.0872	N/A	N/A	202.0691	146.73	0.52	N/A	178.0715	N/A	N/A
D-Galactose	59-23-4	C6H12O6	180.0634	181.0712	N/A	N/A	203.0532	142.39	0.06	N/A	179.0556	N/A	N/A
D-Glucose	50-99-7	C6H12O6	180.0634	181.0712	N/A	N/A	203.0532	147.32	0.21	N/A	179.0556	N/A	N/A
D-Fructose	57-48-7	C6H12O6	180.0634	181.0712	N/A	N/A	203.0532	141.93	0.12	N/A	179.0556	N/A	N/A
D-Mannose	3458-28-4	C6H12O6	180.0634	181.0712	N/A	N/A	203.0532	141.82	0.12	N/A	179.0556	N/A	N/A
D-Glucuronate	6556-12-3	C6H10O7	194.0420	195.0499	N/A	N/A	217.0318	153.13	0.14	N/A	193.0340	134.23	0.04
D-Erythrose 4-Phosphate	585-18-2	C4H9O7P	200.0086	201.0159	N/A	N/A	222.9978	153.89	0.77	N/A	199.0013	149.16	0.50
D-Sedoheptulose	3019-74-7	C7H14O7	210.0739	211.0812	N/A	N/A	233.0632	150.73	0.10	N/A	209.0667	145.50	0.19
N-Acetyl-D-mannosamine	3615-17-6	C8H15NO6	221.0893	222.0972	N/A	N/A	244.0790	154.76	0.04	N/A	220.0813	N/A	N/A
D-Ribose 5-Phosphate	4300-28-1	C5H10O8P	230.0192	231.0270	N/A	N/A	253.0192	155.80	0.13	N/A	229.0113	141.66	0.07
D-Ribulose 5-Phosphate	4151-19-3	C5H11O8P	230.0192	231.0270	N/A	N/A	253.0089	153.25	0.08	N/A	229.0113	140.85	0.19
D-Xylose 5-Phosphate	4212-65-1	C5H11O8P	230.0192	231.0270	N/A	N/A	253.0089	151.40	0.89	N/A	229.0113	13	

Compound	CAS Number	Formula	Exact Mass	[M+H] ⁺	Q Average	Q RSD %
Cellohexaose	2478-35-5	C36H62O31	990.3275	990.3275	N/A	N/A
Mannoheptaose	70281-36-6	C36H62O31	990.3275	991.3353	N/A	N/A
Maltohexaose	34620-77-4	C36H62O31	990.3275	991.3353	N/A	N/A
Lacto-N-hexaose(LNH)	64003-51-6	C40H68N2O31	1072.3806	1073.3884	N/A	N/A
Lacto-N-neohexaose (LNnH)	64309-00-8	C40H68N2O31	1072.3806	1073.3884	N/A	N/A
Fatty Acids						
Lauric Acid (C12:0)	143-07-7	C12H24O2	200.17706	201.185	N/A	N/A
Myristic Acid (C14:0)	1002-84-2	C14H28O2	242.22396	243.2319	N/A	N/A
Palmitoleic Acid (C16:1)	373-49-9	C16H30O2	254.22396	255.2319	N/A	N/A
Palmitic Acid (C16:0)	57-10-3	C16H32O2	256.23966	257.2476	N/A	N/A
Heptadecanoic Acid (C17:0)	506-12-7	C17H34O2	270.25526	271.2632	N/A	N/A
Linolenic Acid (C18:3)	463-40-1	C18H32O2	278.22396	279.2319	N/A	N/A
Linoleic Acid (C18:2)	60-33-3	C18H32O2	280.23966	281.2476	N/A	N/A
Oleic Acid (C18:1)	112-80-1	C18H34O2	282.25526	283.2632	N/A	N/A
Stearic Acid (C18:0)	57-11-4	C18H36O2	284.27096	285.2789	N/A	N/A
Arachidonic Acid (C20:4)	506-32-1	C20H32O2	304.23956	305.2475	N/A	N/A
Bisomo-gamma-linolenic Acid (C20:3)	1783-84-2	C20H34O2	306.25526	307.2632	N/A	N/A
Icosadienoic Acid (C20:2)	2091-39-6	C20H36O2	308.27086	309.2788	N/A	N/A
Eicosenoic Acid (C20:1)	5561-99-9	C20H38O2	310.28656	311.2945	N/A	N/A
Arachidic Acid (C20:0)	506-30-9	C20H40O2	312.30226	313.3102	N/A	N/A
Docosahexenoic Acid	6217-54-5	C22H38O2	328.2396	329.2468	184.62	0.17
Adrenic Acid	28874-58-0	C22H36O2	332.2709	334.2696	189.41	0.11
Lignoceric Acid (C24:0)	557-59-5	C24H48O2	368.36486	369.3728	N/A	N/A
Lauroyl-L-carnitine (C12-Carnitine)	25518-54-1	C19H37NO4	343.2716	344.2927	201.47	0.12
Palmitoyl-carnitine (C16-Carnitine)	1935-18-8	C23H45NO4	399.3342	400.3539	216.10	0.08
Oleoyl-carnitine (C18:1(Δ9-cis)-Carnitine)	13962-05-5	C25H47NO4	425.3498	426.3692	218.73	0.07
Steroids						
2-Keto-3-deoxy-D-gluconic acid	17510-99-5	C6H10O6	179.0556	180.0629	N/A	N/A
Androstenedione	63-05-8	C19H26O2	286.1933	287.2005	183.95	0.40
Testosterone	58-22-0	C19H28O2	288.2089	289.2162	183.82	0.26
2-Methoxyestrone	362-08-3	C19H24O3	300.1725	301.1798	174.47	0.09
Progesterone	57-83-0	C21H30O2	314.2239	315.2312	186.73	0.35
Pregnenolone	145-13-1	C21H32O2	316.2402	317.2475	177.25	0.56
17α-Hydroxyprogesterone	68-96-2	C21H30O3	330.2194	331.2266	187.57	0.47
17β-Hydroxypregnenolone	387-79-1	C21H32O3	332.2350	333.2430	190.45	0.73
2,1-Hydroxypregnenolone	387-79-1	C21H32O3	332.2351	333.2424	190.52	0.69
Aldosterone	52-39-1	C21H28O5	360.1937	361.2009	196.05	0.14
Cortisol	50-23-7	C21H30O5	362.2093	363.2171	188.88	0.08
B-Cortol	667-65-2	C21H30O5	368.2563	369.2635	N/A	N/A
Lipids						
sn-Glycerol-3-phosphocholine	28319-77-9	C8H20NO6P	257.1028	258.1089	157.17	0.15
Methyl Linoleate	112-63-0	C19H34O2	294.2559	295.2631	187.20	0.19
13-HODE	73804-64-5	C18H32O3	296.2351	297.2424	N/A	N/A
9-HODE	98524-19-7	C18H32O3	296.2351	297.2430	N/A	N/A
5S-HETE	70608-72-9	C20H32O3	320.2345	321.2417	N/A	N/A
12S-HETE	54397-83-0	C20H32O3	320.2345	321.2417	N/A	N/A
11(12)-EET	81276-02-0	C20H32O3	320.2351	321.2424	N/A	N/A
8(9)-EET	81246-85-7	C20H32O3	320.2351	321.2424	N/A	N/A
12R-HETE	82337-46-0	C20H32O3	320.2351	321.2424	N/A	N/A
8S-HETE	98462-03-4	C20H32O3	320.2351	321.2424	N/A	N/A
14(15)-EET	81276-03-1	C20H32O3	320.2351	321.2435	182.43	0.23
Leukotriene B4	71160-24-2	C20H32O4	336.2294	337.2367	N/A	N/A
14(S)-HDHA	119433-37-3	C22H32O3	344.2351	345.2424	N/A	N/A
17(S)-HDHA	92693-03-3	C22H32O3	344.2351	345.2424	N/A	N/A
Carboxylic Thromboxane A2	74034-56-3	C22H36O3	348.2664	349.2737	N/A	N/A
Lipoxin A4	89663-86-5	C20H32O5	352.2250	353.2322	N/A	N/A
Prostaglandin E2	363-24-6	C20H32O5	352.2250	353.2322	N/A	N/A
15R-Prostaglandin F2 alpha	37658-84-7	C20H34O5	354.2399	354.2472	N/A	N/A
11B-Prostaglandin F2 alpha	38432-87-0	C20H34O5	354.2399	355.2472	N/A	N/A
Prostaglandin F2 alpha	551-11-1	C20H34O5	354.2406	355.2479	N/A	N/A
8-iso-Prostaglandin F2 alpha	27415-26-5	C20H34O5	354.2406	355.2479	N/A	N/A
8-iso-15R-Prostaglandin F2 alpha	214748-65-9	C20H34O5	354.2406	355.2479	N/A	N/A
5-IPF2α-Vi	180469-63-0	C20H34O5	354.2406	355.2479	N/A	N/A
Methyl Behenate	929-77-1	C23H46O2	354.3498	355.3570	N/A	N/A
Thromboxane B2	54397-85-2	C20H34O6	370.2349	371.2421	N/A	N/A
Methyl Tetraacanoate	2442-49-1	C25H50O2	382.3811	383.3883	187.54	0.08
LPC 13:0	20559-17-5	C21H44NO7P	453.2849	454.2928	220.71	0.11
DG (12:0/12:0)	60562-15-4	C27H52O5	456.3808	457.3887	N/A	N/A
LPS (16:0/0:0)	143077-66-1	C22H44NP09	497.2752	498.2832	222.79	0.14
LPC 18:1	19420-56-5	C26H52NO7P	521.3475	522.3554	235.59	0.18
PC (11:0/11:0)	27869-47-2	C30H60NO8P	593.4050	594.4129	257.07	0.17
GaCer (d18:1/12:0)	111956-48-0	C36H69NO8	643.5016	644.5096	271.15	0.57
BMP (14:0/14:0)	325466-03-3	C24H67O10P	666.4470	667.4550	270.18	0.62
PS (14:0/14:0)	105405-50-3	C34H66NO10P	679.4423	680.4502	N/A	N/A
SM (d18:1/17:0)	121999-64-2	C40H81N2O6P	716.5825	717.595	290.12	0.24
PC (16:1/16:1) (Δ9-cis)	4724-96-3	C40H76NO8P	729.5376	730.5455	280.16	0.24
PE (18:1/18:1) (Δ9-cis)	4004-05-1	C41H78NO8P	743.5465	744.5543	280.60	0.04
PE (18:1/18:1) (Δ9-trans)	19805-18-6	C41H78NO8P	743.5465	744.5543	284.02	0.57
TG (14:0/16:1/14:0)	875584-25-1	C47H88O6	748.6574	749.6653	302.82	0.28
LaCer (d18:1/8:0)	939036-94-9	C38H71NO13	749.4919	750.4998	280.97	0.29
PG(17:0/17:0)	799268-52-3	C40H79O10P	750.5409	751.5489	N/A	N/A
1,2-Diacyl-sn-glycerol 3-phosphocholine	8002-43-5	C42H80NO8P	711.0769	758.5694	189.57	0.30
PC(18:1/9:1/12:0)	59491-62-2	C42H82NO8P	759.5771	760.5851	291.79	0.31
PG (18:1/18:1) (Δ9-trans)	322647-40-5	C42H79O10P	774.5404	775.5483	294.81	0.09
PG (18:1/18:1) (Δ9-cis)	67254-28-8	C42H79O10P	774.5404	775.5483	294.47	0.09
PC (18:1/18:1) (Δ9-trans)	56782-46-8	C44H84NO8P	785.5928	786.6007	297.29	0.30
PC (18:1/18:1) (Δ9-cis)	56391-91-4	C44H84NO8P	785.5928	786.6007	296.42	0.10
Acetyl coenzyme A	102029-73-2	C23H38N7O17P3S	809.1258	810.1330	249.80	0.10
PG (16:0/16:0) 4Me	474967-73-2	C46H91O10P	834.6343	835.6422	311.40	0.60
Nucleotides						
2'-Deoxycytidine 5'-Monophosphate	1032-65-1	C9H14N3O7P	307.0563	308.0642	165.59	0.34
Thymidine 5'-Monophosphate	33430-62-5	C10H15N2O8P	322.0566	323.0639	163.84	0.04
Cytidine 3'-monophosphate	84-52-6	C9H14N3O8P	323.0512	324.0591	170.98	0.27
Cytidine-5' Monophosphate	63-37-6	C9H14N3O8P	323.0518	324.0591	168.77	0.03
Uridine 5' Monophosphate	58-97-9	C9H13N2O9P	324.0352	325.0431	169.81	0.16
3',5'-Cyclic AMP	60-92-4	C10H12N5O6P	329.0525	330.0589	182.47	0.22
2'-Deoxyadenosine 5'-Monophosphate	653-63-4	C10H14N5O6P	331.0675	332.0754	170.01	0.16
Nicotinamide Mononucleotide	1094-61-7	C11H15N2O8P	334.0560	335.0639	167.13	0.09
Thiamine Monophosphate	10023-48-0	C12H18N4O4P5+	345.0786	345.0815	172.53	0.03
2'-Deoxyguanosine 5'-Monophosphate	902-04-5	C10H14N5O7P	347.0624	348.0704	178.96	0.15
Adenosine 5' Monophosphate	61-19-8	C10H14N5O7P	347.0631	348.0704	173.33	0.57
Inosine 5' Monophosphate	131-99-7	C10H13N4O8P	348.0471	349.0544	177.58	0.28
Guanosine 5' Monophosphate	85-32-5	C9H14N3O8P	363.0580	364.0653	182.21	0.14
Adenosine 5' Diphosphate	58-64-0	C10H15N5O10P2	427.0294	428.0367	188.61	0.21
Riboflavin 5'-Monophosphate	146-17-8	C17H21N4O9P	456.1046	457.1119	201.48	0.28
Thymidine 5' Triphosphate	365-08-2	C10H17N2O14P3	481.9893	482.9971	N/A	N/A
Cytidine 5' Triphosphate	65-47-4	C9H16N3O14P3	482.9845	483.9918	N/A	N/A
Adenosine 5' Triphosphate (ATP)	56-65-5	C10H16N5O13P3	506.9957	508.0030	N/A	N/A
Adenosine-5'-Diphosphoribose	68414-18-6	C15H23N5O14P2	559.0717	560.0789	N/A	N/A
Adenosine 5' Diphosphoglucose	2140-58-1	C16H25N5O15P2	589.0822	590.0895	218.30	0.59
α-Nicotinamide Adenine Dinucleotide (α-NAD+)	7298-93-3	C21H27N7O14P2	663.1091	664.1164	241.93	0.27
β-Nicotinamide Adenine Dinucleotide (β-NAD+)	53-84-9	C21H27N7O14P2	663.1091	664.1164	229.46	0.03
Nicotinamide Hypoxanthine Dinucleotide	1851-07-6	C21H27N6O15P2	665.0997	666.1077	222.79	0.74
Flavin Adenine Dinucleotide	146-14-5	C21H23N9O15P2	785.1571	786.1644	N/A	N/A
Nucleosides						
Uracil	66-22-8	C4H4N2O2	112.0266	113.0346	126.98	0.32
Thymine	65-71-4	C5H6N2O2	126.0423	127.0502	126.14	0.33

[M+Na] ⁺	Q Average	Q RSD %	[M-H] ⁻	Q Average	Q RSD %
1013.3173	283.13	0.14	989.3197	286.20	0.98
1013.3173	281.70	0.56	989.3197	277.27	0.15
1013.3173	279.70	0.26	989.3197	279.97	0.04
1095.3704	301.60	0.49	1071.3728	317.60	0.52
1095.3704	297.57	0.25	1071.3728	320.50	0.60
Fatty Acids			Fatty Acids		
223.1669	N/A	N/A	199.1704	154.96	0.10
265.2138	N/A	N/A	241.2173	165.59	0.11
277.2138	172.62	0.06	253.2173	167.86	0.07
279.2295	185.22	0.13	255.233	169.17	0.03
293.2451	N/A	N/A	269.2486	173.49	0.07
301.2138	172.02	0.00	277.2173	174.53	0.06
303.2295	176.38	0.13	279.233	175.37	0.09
305.2451	181.37	0.10	281.2486	176.07	0.03
307.2608	191.83	0.08	283.2643	177.95	0.15
327.2295	180.97	0.11	303.233	182.21	0.03
329.2451	183.38	0.20	305.2486	182.64	0.11
331.2608	184.05	0.03	307.2643	182.38	0.10
333.2764	188.57	0.06	309.2799	183.95	0.11
335.2921	199.97	0.00	311.2956	186.36	0.12
351.2293	185.06	0.22	327.2316	191.12	0.32
355.2606	192.83	0.60	331.2629	190.92	0.88
391.3547	216.86	0.00	367.3582	200.57	0.05
366.2626	217.50	0.17	342.2643	N/A	N/A
422.3256	230.37	0.07	398.3269	N/A	N/A
448.3412	228.60	0.04	281.2478	N/A	N/A
Steroids			Steroids		
202.0448	N/A	N/A	178.0483	134.32	0.15
309.1825	204.73	0.76	285.1860	N/A	N/A
311.1981	206.07	0.67	287.2016	N/A	N/A
323.1618	201.71	0.12	299.1653	184.55	0.91
337.2131	169.03	0.03	313.2166	N/A	N/A
339.2294	216.16	0.46	315.2329	N/A	N/A
353.2086	210.26	0.68	329.2121	187.64	0.69
355.2242	210.49	0.89	331.2277	N/A	N/A
355.2244	210.63	0.93	331.2279	N/A	N/A
383.1829	204.09	0.05	359.1864	188.31	0.14
385.1991	213.91	0.07	361.2015	N/A	N/A
391.2455	204.59	0.10	367.2490	202.65	0.36
Lipids			Lipids		
280.0912	161.80	0.11	256.0955	N/A	N/A
317.2451	N/A	N/A	293.2486	183.18	0.10
319.2244	191.83	0.69	295.2279	183.11	0.52
319.2249	189.14	0.45	295.2273	180.63	0.09
343.2237	188.21	0.47	319.2272	187.20	0.05
343.2237	193.33	0.43	319.2272	184.82	0.57
343.2244	187.87	0.11	319.2279	185.00	0.19
343.2250	186.83	0.03	319.2253	184.63	0.03
343.2263	194.40	0.00	319.2257	184.10	0.09
343.2244	187.17	0.03	319.2279	185.07	0.14
343.2271	187.07	0.12	319.2256	187.60	0.09
359.2186	196.05	0.15	335.2221	187.44	0.08
367.2255	190.10	0.05	343.2251	190.23	0.03
367.2244	191.52	0.36	343.2279	194.84	0.15
371.2556	203.60	0.05	347.2592	201.10	0.05
375.2142	197.89	0.13	351.2177	194.00	0.67
375.2142	198.53	0.11	351.2177	192.06	0.03
377.2304	207.33	0.03	353.2327	194.60	0.05
377.2373	200.20	0.09	353.2327	194.10	0.00
377.2304	207.33	0.07	353.2356	194.77	0.03
377.2298	199.03	0.06	353.2333	197.25	0.09
377.2298	200.77	0.03	353.2333	197.76	0.10
377.2316	205.53	0.03	353.2315	194.97	0.21
377.3390	N/A	N/A	353.3425	156.13	0.40
393.2241	202.08	0.00	369.2276	194.44	0.05
405.3703	N/A	N/A	381.3738	N/A	N/A
476.2746	225.41	0.16	452.2769	N/A	N/A
479.3706	N/A	N/A	455.3729	211.80	0.03
520.2650	228.69	0.09	496.2673	222.72	0.25
544.3372	237.34	0.09	520.3395	N/A	N/A
616.3947	260.59	0.14	592.3970	N/A	N/A
666.4914	266.83	0.16	642.4937	262.03	0.84
706.4628	N/A	N/A	665.4391	262.00	0.17
702.4321	247.83	0.64	678.4344	N/A	N/A
739.5723	291.89	0.85	715.5746	N/A	N/A
752.5274	286.90	0.20	728.5297	N/A	N/A
766.5362	287.57	0.05	742.5387	274.90	0.11
766.5362	288.54	0.13	742.5387	276.44	0.08
771.6472	301.46	0.50	747.6495	N/A	N/A
772.4816	280.67	0.18	748.4839	270.11	0.24
773.5307	N/A	N/A	749.5330	277.45	0.36
334.0667	189.20	0.29	310.0692	N/A	N/A
782.5669	293.64	0.21	758.5692	N/A	N/A
797.5302	285.26	0.77	773.5325	283.01	0.33
797.5302	289.31	0.30	773.5325	282.68	0.75
808.5825	300.74	0.34	784.5848	N/A	N/A
808.5825	298.03	0.08	784.5848	279.49	0.15
832.1150	263.07	0.10	808.1185	N/A	N/A
857.6241	310.43	0.41	833.6263	294.68	0.33
Nucleotides			Nucleotides		
330.0460	166.62	0.17	306.0483	165.62	0.09
345.0458	169.74	0.09	321.0480	166.26	0.39
346.0410	174.90	0.40	322.0433	170.38	0.03
346.0411	171.53	0.03	322.0446	167.03	0.03
347.0250	175.14	0.15	323.0273	163.88	0.06
352.0399	191.10	0.32	328.0481	175.07	0.28
354.0573	176.68	0.12	330.0596	174.57	0.13
357.0457	N/A	N/A	333.0480	N/A	N/A
367.0611	N/A	N/A	343.0634	N/A	N/A
370.0529	173.87	0.03	346.0545	171.03	0.03
370.0522	180.73	0.58	346.0558	175.33	0.07
371.0363	174.57	0.27	347.0398	173.83	0.48
386.0472	177.95	0.06	362.0507	172.29	0.22
450.0186	196.92	0.19	426.0221	186.87	0.67
479.0938	210.66	0.18	455.0973	200.77	0.26
504.9790	207.41	0.10	480.9814	N/A	N/A
505.9737	204.90	0.32	481.9772	192.16	0.29
529.9850	204.59	0.44	505.9885	198.86	0.32
582.0614	N/A	N/A	558.0639	205.00	0.54
612.0715	177.62	0.62	588.0750	219.14	0.58
686.0983	234.65	0.77	662.1018	227.15	0.20
686.0983	226.24	0.07	662.1018	228.12	0.12
688.0895	232.01	0.13	664.0918	N/A	N/A
808.1463	N/A	N/A	784.1499	259.22	0.63
Nucleosides			Nucleosides		
135.0164	N/A	N/A	111.0187	N/A	N/A
149.0320	N/A	N/A	125.0343	122.42	0.17

Compound	CAS Number	Formula	Exact Mass	[M+H] ⁺	Ω Average	Ω RSD %		[M+Na] ⁺	Ω Average	Ω RSD %		[M-H] ⁻	Ω Average	Ω RSD %
Adenine	73-24-5	C5H5N5	135.0538	136.0619	127.90	0.00		158.043606	N/A	N/A		134.0484	122.30	0.08
5-Hydroxymethyluracil	4433-40-3	C5H6N2O3	142.0372	143.0451	N/A	N/A		165.0269	142.06	0.37		141.0292	124.50	0.09
Guanine	73-40-5	C5H5N5O	151.0487	152.0567	133.55	0.23		174.0385	N/A	N/A		150.0408	N/A	N/A
Deoxycytidine	951-77-9	C9H13N3O4	227.0900	228.0979	N/A	N/A		250.0797	158.41	0.04		226.0820	N/A	N/A
Deoxyuridine	951-78-0	C9H12N2O5	228.0740	229.0819	N/A	N/A		251.0637	159.45	0.22		227.0660	151.64	0.10
Thymidine	50-89-5	C10H14N2O5	242.0896	243.0975	N/A	N/A		265.0794	164.51	0.44		241.0817	157.04	0.17
β-Pseudouridine	1445-07-4	C9H12N2O6	244.0689	245.0761	N/A	N/A		267.0611	164.10	0.00		243.0613	150.77	0.04
Uridine	58-96-8	C9H12N2O6	244.0689	245.0768	N/A	N/A		267.0586	166.00	0.06		243.0609	154.13	0.04
5'-Deoxyadenosine	4754-39-6	C10H13N5O3	251.1018	252.1091	162.10	0.40		274.0911	171.99	0.64		250.0946	160.19	0.32
2'-Deoxyadenosine	958-09-8	C10H13N5O3	251.1018	252.1095	162.73	0.04		274.0902	166.67	0.09		250.0937	160.57	0.10
5-Methylcytidine	2140-61-6	C10H15N3O5	257.1012	258.1084	157.51	0.26		280.0904	168.97	0.60		256.0939	160.46	0.27
Adenosine	58-61-7	C10H13N5O4	267.0961	268.1040	156.97	0.04		290.0859	170.07	0.03		266.0882	162.13	0.07
Inosine	58-63-9	C10H12N4O5	268.0808	269.0880	159.25	0.23		291.0700	175.37	0.47		267.0735	161.70	0.09
Guanosine	118-00-3	C10H13N5O5	283.0910	284.0989	165.02	0.25		306.0808	177.25	0.25		282.0831	164.38	0.44
Xanthosine	146-80-5	C10H12N4O6	284.0757	285.0830	166.49	0.10		307.0649	177.45	0.29		283.0684	161.36	0.11
5'-Methylthioadenosine	2457-80-9	C11H15N5O3S	297.0889	298.0968	173.03	0.00		320.0787	176.54	0.11		296.0810	170.34	0.12
1-Methylguanosine	2140-65-0	C11H15N5O5	297.1073	298.1146	168.80	0.18		320.0965	180.80	0.17		296.1000	166.93	0.09
Vitamins														
Nicotinamide	98-92-0	C6H6N2O	122.0473	123.0553	129.32	0.24		145.0371	137.30	0.36		121.0394	N/A	N/A
Niacinamide	98-92-0	C6H6N2O	122.0479	123.0555	131.67	0.04		145.0075	N/A	N/A		121.0406	N/A	N/A
Nicotinic Acid	59-67-6	C6H5NO2	123.0314	124.0393	128.35	0.09		146.0211	N/A	N/A		122.0234	124.50	0.47
Pyridoxal Hydrochloride	65-22-5	C8H9NO3	167.0582	168.0655	135.42	0.59		190.0475	N/A	N/A		166.0510	132.51	0.72
Pyridoxamine	85-87-0	C8H12N2O2	168.0899	169.0971	135.79	0.17		191.0791	148.49	0.20		167.0826	140.12	0.29
Pyridoxine	65-23-6	C8H11NO3	169.0732	170.0812	135.69	0.04		192.0630	148.49	0.20		168.0653	136.03	0.44
D-Pantothenic Acid	79-83-4	C9H17NO5	219.1107	220.1168	150.17	0.04		242.1012	155.27	0.04		218.1038	149.87	0.02
D-Biotin	58-85-5	C10H16N2O3S	244.0882	245.0954	154.16	0.14		267.0774	164.45	0.55		243.0809	159.72	0.40
Pyridoxal 5'-Phosphate	54-47-7	C8H10NO6P	247.0246	248.0318	154.76	0.48		270.0138	165.05	0.57		246.0173	150.54	0.10
Riboflavin	83-88-5	C17H20N4O6	376.1383	377.1456	192.43	0.14		399.1275	199.40	0.16		375.1310	189.35	0.08
γ + β-Tocopherol	54-28-4	C28H48O2	416.3648	417.3726	212.23	0.00		439.3545	N/A	N/A		415.3569	209.75	0.10
α-Tocopherol	59-02-9	C29H50O2	430.3805	431.3883	215.55	0.16		453.3702	N/A	N/A		429.3726	210.73	0.13
Dihydrofolate	4033-27-6	C19H21N7O6	443.1547	445.1196	193.63	0.03		466.1444	N/A	N/A		440.1342	N/A	N/A
Vitamin K2	863-61-6	C31H40O2	444.3028	445.3101	198.66	0.22		467.2920	N/A	N/A		443.2955	N/A	N/A
5-Methyltetrahydrofolate	68792-52-9	C20H25N7O6	459.1860	460.1938	196.99	0.08		482.1757	200.04	0.13		458.1781	199.57	0.00
Calcium Pantothenate	137-08-6	C18H32CaN2O10	476.1683	477.1756	204.26	0.11		499.1575	N/A	N/A		475.1610	N/A	N/A
Vitamin B12	68-19-9	C63H88CoN14O14P	1354.5674	1355.5746	338.7	0.25		1377.5566	340.1	0.30		1353.5601	338.98	0.49
Bile Acids														
Lithocholic Acid	434-13-9	C24H40O3	376.2977	377.3050	N/A	N/A		399.2894	N/A	N/A		375.2896	200.33	0.14
Ursodeoxycholic Acid (S)	128-13-2	C24H40O7S	392.2920	393.2999	N/A	N/A		415.2818	N/A	N/A		471.2416	208.98	0.43
Cholic Acid	81-25-4	C24H40O5	408.2876	407.2798	N/A	N/A		431.2774	N/A	N/A		407.2797	204.63	0.17
Hyochoic Acid	547-75-1	C24H40O5	408.2876	407.2798	N/A	N/A		431.2774	N/A	N/A		407.2797	206.00	0.13
Urschoic Acid	2955-27-3	C24H40O5	408.2876	407.2798	N/A	N/A		431.2774	N/A	N/A		407.2797	205.10	0.31
α-Muricholic Acid	2393-58-0	C24H40O5	408.2876	407.2798	N/A	N/A		431.2774	N/A	N/A		407.2797	207.44	0.12
β-Muricholic Acid	2393-59-1	C24H40O5	408.2876	407.2798	N/A	N/A		431.2774	N/A	N/A		407.2797	203.02	0.24
Sulfolithocholic Acid	34669-57-3	C24H40O6S	456.6373	457.6453	N/A	N/A		479.6271	N/A	N/A		455.2467	212.20	0.03
Glycocholic Acid Hydrate (S)	1192657-83-2	C26H43NO9S	465.3084	466.3163	N/A	N/A		488.2981	N/A	N/A		454.2580	219.31	0.03
Glycodeoxycholic Acid (S)	16409-34-0	C26H43NO8S	471.2954	472.3033	N/A	N/A		494.2852	N/A	N/A		528.2631	218.94	0.07
Chenodeoxycholic Acid (S)	474-25-9	C24H40O7S	472.2493	473.2573	N/A	N/A		495.2391	N/A	N/A		471.2416	206.57	0.12
Deoxycholic Acid (S)	83-44-3	C24H40O7S	472.2493	473.2573	N/A	N/A		495.2391	N/A	N/A		471.2416	209.86	0.06
Cholic Acid (S)	81-25-4	C24H40O8S	488.2443	489.2522	N/A	N/A		511.2340	N/A	N/A		487.2366	211.06	0.03
Glycolithocholic Acid (S)	24404-83-9	C26H43NO7S	513.2759	514.2838	N/A	N/A		536.2657	N/A	N/A		512.2682	218.90	0.10
Taurochenodeoxycholic Acid (S)	6009-98-9	C26H45NO9S2	521.2780	522.2860	N/A	N/A		544.2678	N/A	N/A		578.2457	221.75	0.37
Taurodeoxycholic Acid (S)	207737-97-1	C26H45NO9S2	521.2780	522.2860	N/A	N/A		544.2678	N/A	N/A		578.2457	221.79	0.24
Glycochenodeoxycholic Acid (S)	16564-43-5	C26H43NO8S	529.2709	530.3219	N/A	N/A		472.3038	N/A	N/A		528.2631	218.80	0.13
Taurocholic Acid (S)	345909-26-4	C26H45NO10S2	537.2729	538.2809	N/A	N/A		560.2627	N/A	N/A		594.2407	221.99	0.23
Other Primary Metabolite														
2-Hydroxybutyric Acid	600-15-7	C4H8O3	104.0473	105.0546	N/A	N/A		127.0366	N/A	N/A		103.0401	124.67	0.24
DL-Beta-Hydroxybutyric Acid	150-83-4	C4H8O3	104.0473	105.0546	N/A	N/A		127.0366	N/A	N/A		103.0401	137.54	0.00
1,2-Phenylethanediamine	95-54-5	C6H8N2	108.0687	109.0760	129.96	0.38		131.0580	N/A	N/A		107.0615	N/A	N/A
3,4-Dihydropyridine	10182-48-6	C5H5NO2	111.0320	112.0393	126.74	0.92		134.0212	N/A	N/A		110.0248	N/A	N/A
Cytosine	71-30-7	C4H5N3O	111.0426	112.0505	121.58	0.05		134.0324	N/A	N/A		110.0347	N/A	N/A
Creatinine	60-27-5	C4H7N3O	113.0583	114.0661	123.93	0.17		136.0480	133.41	0.13		112.0504	120.65	0.17
Fumaric Acid	110-17-8	C4H4O4	116.0110	117.0182	N/A	N/A		139.0002	133.58	0.11		115.0037	N/A	N/A
2-Oxovaleric Acid	1821-02-9	C5H8O3	116.0474	117.0546	N/A	N/A		139.0366	131.64	0.90		115.0401	N/A	N/A
Guanidinoacetic Acid	352-97-6	C3H7N3O2	117.0532	118.0611	126.88	0.29		140.0429	N/A	N/A		116.0452	N/A	N/A
Succinic Acid	110-15-6	C4H6O4	118.0266	119.0339	122.66	0.08		141.0158	N/A	N/A		117.0193	119.84	0.00
Purine	120-73-0	C5H4N4	120.0429	121.0509	125.40	0.09		143.0327	N/A	N/A		119.0350	117.70	0.10
3-Methylhistamine	644-42-8	C6H11N3	125.0953	126.1021	126.53	0.46		148.0851	N/A	N/A		124.0880	N/A	N/A
1-Methylhistamine	501-75-7	C6H11N3	125.0953	126.1026	122.56	0.08		148.0845	N/A	N/A		124.0880	N/A	N/A
Imidazole-4-acetic Acid	645-65-8	C5H6N2O2	126.0429	127.0496	128.23	0.05		149.0229	148.03	0.04		125.0356	N/A	N/A
Mevalonolactone	674-26-0													

Compound	CAS Number	Formula	Exact Mass	[M+H] ⁺	Ω Average	Ω RSD %	[M+Na] ⁺	Ω Average	Ω RSD %	[M-H] ⁻	Ω Average	Ω RSD %
Pyrophosphoric Acid	2466-09-3	H4P2O7	177.9432	178.9505	N/A	N/A	200.9324	145.58	0.48	176.9360	N/A	N/A
Hippuric Acid	495-69-2	C9H9NO2	179.0582	180.0655	146.82	0.34	202.0475	154.06	0.48	178.0510	148.23	0.28
4-Hydroxyphenylpyruvic Acid	156-39-8	C9H8O4	180.0423	181.0495	N/A	N/A	203.0315	N/A	N/A	179.0350	145.75	0.04
Inositol	643-12-9	C6H12O6	180.0627	181.0707	N/A	N/A	203.0519	151.95	0.27	179.0548	144.27	1.01
Homovanillic Acid	60563-13-5	C9H10O4	182.0579	183.0652	N/A	N/A	205.0471	149.57	0.31	181.0506	140.75	0.00
Phosphocholine	107-73-3	C5H15NO4P	183.0654	184.0733	138.54	0.36	206.0551	N/A	N/A	182.0574	N/A	N/A
Epinephrine	51-43-4	C9H13NO3	183.0895	184.0968	N/A	N/A	206.0793	N/A	N/A	182.0831	144.83	0.11
rac 4-hydroxy 3-methoxyphenylethylene glycol	534-82-7	C9H12O4	184.0736	185.0808	N/A	N/A	207.0628	159.05	0.06	183.0663	N/A	N/A
2-Phosphoglyceric Acid	2553-59-5	C3H7O7P	185.9923	187.0002	N/A	N/A	208.9815	N/A	N/A	184.9843	127.65	0.12
3-Phosphoglyceric Acid	3443-58-1	C3H7O7P	185.9923	187.0002	N/A	N/A	208.9815	N/A	N/A	184.9843	125.60	0.12
Kynurenic Acid	492-27-3	C10H7NO3	189.0426	190.0499	140.99	0.11	212.0318	154.12	0.17	188.0353	137.30	0.50
Iso citrate	320-77-4	C6H8O7	192.0263	193.0343	N/A	N/A	215.0156	146.78	0.12	191.0184	130.03	0.59
Citric Acid	77-92-9	C6H8O7	192.0263	193.0343	148.90	0.38	215.0156	146.11	0.75	191.0184	129.49	0.21
Quinic Acid	77-95-2	C7H12O6	192.0634	193.0707	146.35	0.29	215.0526	153.72	0.20	191.0561	138.47	0.04
2-Methylhippuric Acid	42013-20-7	C10H11NO3	193.0739	194.0812	N/A	N/A	216.0631	156.60	0.15	192.0666	153.65	0.26
2-Keto-D-gluconic Acid	669-90-9	C6H10O7	194.0427	195.0499	N/A	N/A	217.0324	N/A	N/A	193.0349	133.43	0.23
2-Hydroxy Hippuric Acid	487-54-7	C9H9NO4	195.0532	196.0604	N/A	N/A	218.0435	154.87	0.07	194.0451	138.02	0.11
Gluconic Acid	526-95-4	C6H12O7	196.0576	197.0656	141.89	0.18	219.0474	149.77	0.31	195.0497	135.16	0.15
2-Chloro-L-Phenylalanine	103616-89-3	C9H10ClNO2	199.0400	200.0473	148.86	0.24	222.0292	N/A	N/A	198.0327	N/A	N/A
Phosphoenol Pyruvic Acid	138-08-9	C3H5O6P	205.9383	206.9455	N/A	N/A	228.9275	N/A	N/A	166.9746	164.28	0.84
Kynurenine	343-65-7	C10H12N2O3	208.0841	209.0921	151.07	0.10	231.0739	N/A	N/A	207.0762	N/A	N/A
D Saccharic Acid	87-73-0	C6H10O8	210.0376	211.0448	N/A	N/A	233.0273	N/A	N/A	209.0303	135.70	0.26
N-Acetyl-D-glucosamine	7512-17-6	C8H15NO6	221.0893	222.0972	N/A	N/A	244.0790	160.36	0.06	220.0813	N/A	N/A
3-Hydroxy-DL-kynurenine	2147-61-7	C10H12N2O4	224.0797	225.0845	157.67	0.10	247.0677	160.83	0.37	223.0719	151.37	0.56
Carnosine	305-84-0	C9H14N4O3	226.1059	227.1142	151.37	0.04	249.0957	N/A	N/A	225.1009	154.10	0.11
Mevalonic Acid 5-Phosphate	1189-94-2	C6H13O7P	228.0399	229.0472	N/A	N/A	251.0291	152.28	0.65	227.0326	140.02	0.27
Tris (2-carboxyethyl) Phosphine	5961-85-3	C9H15O6P	251.0684	252.0757	N/A	N/A	274.0577	N/A	N/A	249.0528	149.63	0.22
3-Deoxy-2-Keto-6-Phosphogluconic Acid	27244-54-8	C6H10O9P	258.0140	259.0219	N/A	N/A	281.0037	N/A	N/A	257.0060	144.13	0.22
6-Phosphogluconic Acid	921-62-0	C6H13O10P	276.0246	277.0319	N/A	N/A	299.0139	167.16	0.07	275.0174	145.75	0.04
Ophthalmic Acid	495-27-2	C11H19N3O6	289.1274	290.1329	167.23	0.58	312.1147	165.70	0.42	288.1207	163.70	0.12
Argininosuccinic Acid	2387-71-5	C10H18N4O6	290.1220	291.1299	167.39	0.06	313.1112	172.22	0.40	289.1140	169.07	0.29
N-Acetyl Sulfamethoxazole	21312-10-7	C12H13N3O4S	295.0627	296.0699	171.45	0.03	318.0519	178.52	0.66	294.0554	172.05	0.03
Glutathione	70-18-8	C10H17N3O6S	307.0838	308.0911	N/A	N/A	330.0730	168.23	0.09	306.0765	164.24	0.13
Mevalonic Acid 5-Pyrophosphate	1492-08-6	C6H14O10P2	308.0062	309.0140	N/A	N/A	330.9960	N/A	N/A	306.9984	153.22	0.11
3,5-Dibromo-1-tyrosine	300-38-9	C9H9Br2NO3	336.8949	337.9022	168.87	0.22	359.8841	162.73	0.18	335.8876	155.60	0.06
Thyrotropin-releasing hormone	24305-27-9	C16H22N6O4	362.1696	363.1775	181.00	0.06	385.1594	184.12	0.03	361.1616	187.07	0.14
5-Hexyl-glutathione	24425-56-7	C16H29N3O6S	391.1777	392.1827	203.20	0.56	414.1675	N/A	N/A	390.1695	191.87	0.15
Cytidine 5'-diphosphocholine	987-78-0	C14H26N4O11P2	488.1072	489.1152	198.86	0.13	511.0970	208.98	0.23	487.0993	208.41	0.22
Biliverdin	114-25-0	C33H34N4O6	582.2478	583.2532	246.50	0.14	605.2356	248.83	0.37	581.2389	249.70	0.17
3-Methylcrotonyl-CoA	793193-48-3	C26H42N7O17P3S	849.1564	850.1649	180.03	0.08	872.1468	N/A	N/A	848.1492	N/A	N/A
Malonyl-CoA	524-14-1	C24H38N7O19P3S	853.1156	854.1229	N/A	N/A	876.1048	N/A	N/A	852.1083	253.05	0.07
Oxytocin	50-56-6	C43H66N12O12S2	1006.4364	1007.4437	N/A	N/A	1029.4257	N/A	N/A	1005.4292	298.97	0.91
Secondary Metabolites												
Alkaloids							Alkaloids			Alkaloids		
Choline ⁺	62-49-7	C5H14NO ⁺	104.1075	105.1154	N/A	N/A	127.0968	N/A	N/A	103.1003	N/A	N/A
Hydroquinone	123-31-9	C6H6O2	110.0368	111.0441	128.79	0.08	133.0260	N/A	N/A	109.0295	119.07	0.27
2-Aminoethylphosphonate	2041-14-7	C2H8NO3P	125.0235	126.0315	132.21	0.15	148.0133	N/A	N/A	124.0156	N/A	N/A
Bis(3-aminopropyl)amine	56-18-8	C6H17N3	131.1416	132.1495	128.52	0.25	154.1314	N/A	N/A	130.1337	N/A	N/A
Trigonelline	535-83-1	C7H7NO2	137.0477	138.0537	126.37	0.20	160.0353	139.87	0.27	136.0404	N/A	N/A
Anabasine	40774-73-0	C10H14N2	162.1157	163.1230	140.18	0.25	185.1049	N/A	N/A	161.1084	N/A	N/A
2,4-Dihydroxypteridine (Lumazine)	487-21-8	C6H4N4O2	164.0334	165.0401	138.90	0.14	187.0224	147.27	0.21	163.0269	128.55	0.20
Theobromine	83-67-0	C7H8N4O2	180.0647	181.0704	134.37	0.11	203.0545	N/A	N/A	179.0576	N/A	N/A
4-Pyridoxate	82-82-6	C8H9NO4	183.0525	184.0604	137.27	0.24	206.0423	151.78	0.17	182.0446	N/A	N/A
Phenolics							Flavonoids			Flavonoids		
Tyrosol	501-94-0	C8H10O2	138.0681	139.0754	N/A	N/A	161.0573	N/A	N/A	137.0608	138.71	0.08
Xylitol	87-99-0	C5H12O5	152.0685	153.0757	N/A	N/A	175.0577	140.79	0.34	151.0612	127.92	0.45
Juglone	481-39-0	C10H6O3	174.0317	175.0390	N/A	N/A	197.0209	N/A	N/A	173.0244	131.20	0.13
Myricitrin	607-91-0	C11H12O3	192.0786	193.0859	141.69	0.08	215.0679	N/A	N/A	191.0714	144.74	0.11
Methyl beta-D-galactoside	1824-94-8	C7H14O6	194.0790	195.0863	N/A	N/A	217.0671	149.97	0.20	193.0718	N/A	N/A
Formononetin	485-72-3	C16H12O4	268.0736	269.0808	N/A	N/A	291.0628	176.14	0.30	267.0663	169.04	0.50
Emodin	518-82-1	C15H10O5	270.0528	271.0601	161.30	0.54	293.0420	N/A	N/A	269.0455	156.91	0.13
Naringenin	480-41-1	C15H12O5	272.0685	273.0757	167.96	0.03	295.0577	N/A	N/A	271.0612	167.33	0.43
Acacetin	480-44-4	C16H12O5	284.0685	285.0757	167.06	0.53	307.0577	N/A	N/A	283.0612	172.92	0.41
Biochanin A	491-80-5	C16H12O5	284.0685	285.0757	N/A	N/A	307.0577	N/A	N/A	283.0612	170.41	0.12
Kaempferol	520-18-3	C15H10O6	286.0477	287.0550	165.99	0.06	309.0370	187.20	0.35	285.0405	165.92	0.40
Cyanidin ⁺	528-58-5	C15H11O6 ⁺	287.0556	288.0634	N/A	N/A	311.0526	N/A	N/A	287.0561	N/A	N/A
Eriodictyol	552-58-9	C15H12O6	288.0634	289.0707	170.48	0.07	311.0526	182.17	0.06	287.0561	N/A	N/A
Catechin	7295-85-4	C15H14O6	290.0790	291.0863	165.18	0.11	313.0683	184.42	0.14	289.0718	159.96	0.06
Hesperetin	520-33-2	C16H14O6	302.0790	303.0863	176.54	0.25	325.0683	184.45	0.17	301.0718	178.49	0.07
Delphinidin ⁺	13270-61-6	C15H11O7 ⁺	303.0505	304.0583	N/A	N/A	326.0397	N/A	N/A	302.0432	N/A	N/A
Isohammetin	480-19-3	C16H12O7	316.0583	317.0656	172.96	0.32	339.0475	195.91	0.18	315.0510	174.60	0.17
Myricitrin	529-44-2	C15H10O8	318.0376	319.0448	174.40	0.46	341.0268	193.90	0.08	317.0303	N/A	

Compound	CAS Number	Formula	Exact Mass	[M+H] ⁺	Ω Average	Ω RSD %	[M+Na] ⁺	Ω Average	Ω RSD %	[M-H] ⁻	Ω Average	Ω RSD %	
Imazapyr	81334-34-1	C13H15N3O3	261.1113	262.1186	157.81	0.42		284.1006	176.07	0.26	260.1041	164.95	0.20
Acetochlor	34256-82-1	C14H20ClNO2	269.1182	270.1255	160.09	0.32		292.1075	174.60	0.12	268.1110	N/A	N/A
Pendimethalin	40487-42-1	C13H19N3O4	281.1375	282.1448	162.60	0.07		304.1268	187.77	0.32	280.1303	167.46	0.59
Metolachlor	51218-45-2	C15H22ClNO2	283.1339	284.1412	161.46	0.19		306.1231	175.84	0.58	282.1266	N/A	N/A
Indaziflam	950782-86-2	C16H20FN5	301.1703	302.1775	169.27	0.09		324.1595	174.60	0.17	300.1630	180.67	0.20
Halosulfuron-methyl	100784-20-1	C13H15ClN6O7S	434.0411	435.0484	196.48	0.30		457.0304	201.41	0.48	433.0339	195.34	0.19
Other Xenobiotics							Other Xenobiotics			Other Xenobiotics			
Diethanolamine	111-42-2	C4H11NO2	105.0783	106.0863	123.33	0.61		128.0681	N/A	N/A	104.0704	N/A	N/A
Sulfanilamide	63-74-1	C6H8N2O2S	172.0300	174.0234	156.07	0.10		195.0200	152.77	0.55	171.0244	141.70	0.07
D-Glucosamine	3416-24-8	C6H13NO5	179.0787	180.0867	135.59	0.24		202.0685	147.19	0.07	178.0708	N/A	N/A
Acetylsalicylic Acid	50-78-2	C9H8O4	180.0416	181.0489	N/A	N/A		203.0334	146.80	0.07	179.0343	N/A	N/A
Paraxanthine	611-59-6	C7H8N4O2	180.0641	181.0720	135.63	0.07		203.0538	N/A	N/A	179.0561	N/A	N/A
Theophylline	58-55-9	C7H8N4O2	180.0641	181.0720	143.06	0.07		203.0538	149.63	0.10	179.0561	135.79	0.15
Caffeine	58-08-2	C8H10N4O2	194.0797	195.0877	145.40	0.07		217.0695	142.93	0.04	193.0718	N/A	N/A
Monoethyl Phthalic Acid	2306-33-4	C10H10O4	194.0579	195.0652	N/A	N/A		217.0471	155.67	0.16	193.0506	148.23	0.58
d-Desthiobiotin	533-48-2	C10H18N2O3	214.1317	215.1390	145.78	0.00		237.1210	159.12	0.29	213.1245	158.01	0.10
Diethyl Phthalic Acid	84-66-2	C12H14O4	222.0891	223.0970	N/A	N/A		245.0789	165.23	0.34	221.0811	N/A	N/A
Naproxen	22204-53-1	C14H14O3	230.0936	231.1023	154.83	0.04		253.0853	163.87	0.04	229.0863	N/A	N/A
Ampicillin	69-53-4	C16H19N3O4S	349.1096	350.1250	193.17	0.03		372.1042	187.93	0.03	348.0996	191.20	0.24
Indomethacin	53-86-1	C19H16ClNO4	357.0768	358.0841	183.55	0.48		380.0660	195.98	0.56	356.0695	N/A	N/A
Tetracycline	60-54-8	C22H24N2O8	444.1533	445.1629	198.48	0.18		467.1482	212.50	0.10	443.1434	200.93	0.03
Leucovorin Calcium	1492-18-8	C20H21CaN7O7	473.1659	474.1737	198.80	0.08		496.1557	N/A	N/A	472.1581	202.35	0.62
Microbial							Microbial			Microbial			
L-Pipecolic Acid	3105-95-1	C6H11NO2	129.0783	130.0863	130.93	0.32		152.0681	N/A	N/A	128.0704	133.82	0.20
Tyramine	51-67-2	C8H11NO	137.0841	121.0653	123.43	0.12		145.0629	139.98	0.83	119.0497	N/A	N/A
Salicylic Acid	54-21-7	C7H6O3	138.0311	139.0390	N/A	N/A		161.0208	N/A	N/A	137.0231	123.36	0.36
Citramalic Acid	2306-22-1	C5H8O5	148.0372	149.1315	N/A	N/A		171.0269	N/A	N/A	147.0306	124.87	0.09
Tryptamine	61-54-1	C10H12N2	160.1004	144.0813	128.42	0.05		168.0789	N/A	N/A	142.0657	N/A	N/A
3-Dehydroshikimic Acid	2922-42-1	C7H8O5	172.0365	173.0445	132.73	0.09		195.0263	N/A	N/A	171.0286	136.77	0.08
Aniline-2-sulfonic Acid	88-21-1	C6H7NO3S	173.0147	174.0219	N/A	N/A		196.0028	153.23	0.10	172.0102	133.90	0.13
Shikimic Acid	138-59-0	C7H10O5	174.0522	175.0601	149.50	0.29		197.0419	N/A	N/A	173.0442	140.55	0.12
LL-2,6-Diaminoheptanedioic Acid	583-93-7	C7H14N2O4	190.0947	191.1026	142.53	0.11		213.0845	N/A	N/A	189.0868	140.02	0.40
3,4-Dihydroxy-L-phenylalanine	59-92-7	C9H11NO4	197.0687	198.0766	154.29	0.15		220.0585	151.11	0.12	196.0607	144.27	0.30
5-Hydroxy-L-Tryptophan	4350-09-8	C11H12N2O3	220.0841	221.0921	157.88	0.10		243.0739	156.47	0.56	219.0762	153.72	0.07

*Compounds as charged molecular ions

Compound	CAS Number	Formula	Exact Mass	[M] ⁺	Ω Average	Ω RSD %
Choline*	62-49-7	C5H14NO+	104.1075	104.1075	119.00	0.10
Cyanidin*	528-58-5	C15H11O6+	287.0556	287.0556	168.33	0.25
Delphinidin*	13270-61-6	C15H11O7+	303.0505	303.0505	171.35	0.03
Malvidin*	10463-84-0	C17H15O7+	331.0818	331.0818	178.55	0.10

Doubly charged ions

Compound	CAS Number	[M+2H] ²⁺	Ω Average	Ω RSD %
Vitamin B12	68-19-9	678.6979	376.55	0.33
Flavin Adenine Dinucleotide	84366-81-4	784.5422	242.23	0.64
Compound	CAS Number	[M+2Na] ²⁺	Ω Average	Ω RSD %
Vitamin B12	68-19-9	689.6889	377.85	0.33

CCS for Polycyclic Aromatic Hydrocarbons (PAHs) and Hydroxy-PAHs

PAHs	CAS	Formula	Exact Mass	[M+H] ⁺	Avg CCS	RSD%	[M] [•] ⁺	Avg CCS	RSD%
Naphthalene	91-20-3	C10H8	128.0626	129.0704	120.28	0.32	128.06	118.84	0.18
1-methylnaphthalene	90-12-0	C11H10	142.0782	143.0861	125.20	0.14	142.08	123.49	0.14
2-methylnaphthalene	91-57-6	C11H10	142.0782	143.0861	124.57	0.11	142.08	123.19	0.04
Acenaphthylene	208-96-8	C12H8	152.0626	153.0704	125.71	0.10	152.06	124.80	0.04
Acenaphthene	83-32-9	C12H10	154.0782	155.0861	N/A	N/A	154.08	128.5	0.11
1, 2-Dimethylnaphthalene	573-98-8	C12H12	156.0939	157.1017	130.93	0.35	156.09	128.35	0.15
1,6-Dimethylnaphthalene	575-43-9	C12H12	156.0939	157.1017	130.13	0.19	156.09	127.82	0.10
2, 7-Dimethylnaphthalene	582-16-1	C12H12	156.0939	157.1017	131.00	0.11	156.09	N/A	N/A
Fluorene	86-73-7	C13H10	166.0782	167.0861	N/A	N/A	166.08	130.9	0.12
Anthracene	120-12-7	C14H10	178.0782	179.0861	N/A	N/A	178.08	133.1	0.14
Perinaphthenon	548-39-0	C13H8O	180.0575	181.0653	134.59	0.55	180.06	N/A	N/A
Acenaphthenequinone	82-86-0	C12H6O2	182.0368	183.0446	145.51	1.50	182.04	N/A	N/A
2-Methylanthracene	613-12-7	C15H12	192.0939	193.1017	138.61	0.30	192.09	137.27	0.28
9-Methylanthracene	779-02-2	C15H12	192.0939	193.1017	N/A	N/A	192.09	136.43	0.06
Pyrene	129-00-0	C16H10	202.0782	203.0861	137.97	0.09	202.08	137.50	0.19
Fluoranthene	206-44-0	C16H10	202.0783	203.0861	138.84	0.00	202.08	138.34	0.06
2, 3-Dimethylanthracene	613-06-9	C16H14	206.1095	207.1174	146.15	0.09	206.11	N/A	N/A
3,6-Dimethylphenanthrene	1576-67-6	C16H14	206.1095	207.1174	145.58	0.06	206.11	144.44	0.09
Anthraquinone	84-65-1	C14H8O2	208.0524	209.0603	141.89	0.13	208.05	N/A	N/A
Triphenylene	217-59-4	C18H12	228.0939	229.1017	N/A	N/A	228.09	144.81	0.03
Benzanthrone	82-05-3	C17H10O	230.0732	231.0810	145.71	0.07	230.07	144.61	0.03
Pyrene-4,5 dione	6217-22-7	C16H8O2	232.0524	233.0603	144.30	0.03	232.05	N/A	N/A
Benz(j)aceanthrylene	202-33-5	C20H12	252.0939	253.1017	155.08	0.03	252.09	152.68	0.08
Benzo(b)fluoranthene	205-99-2	C20H12	252.0939	253.1017	N/A	N/A	252.09	151.95	0.08
Benzo(k)fluoranthene	207-08-9	C20H12	252.0939	253.1017	154.36	0.53	252.09	152.98	0.17
Benzo(a)Pyrene	50-32-8	C20H12	252.0939	253.1017	152.05	0.08	252.09	151.24	0.11
5, 12-naphthacene quinone	1090-13-7	C18H10O2	258.0681	259.0759	157.54	0.88	258.07	N/A	N/A
Benzo(g,h,i)perylene	191-24-2	C22H12	276.0939	277.1017	157.31	0.12	276.09	155.83	0.11
Indeno(1,2,3-cd)pyrene	193-39-5	C22H12	276.0939	277.1017	159.65	0.56	276.09	158.15	0.19
Coronene	191-07-1	C24H12	300.0939	301.1017	N/A	N/A	300.09	161.87	0.12
Dibenzo(a,h)pyrene	189-64-0	C24H14	302.1095	303.1174	166.49	0.10	302.11	165.22	0.08
Dibenzochrysene	191-68-4	C26H16	302.1095	303.1174	166.69	0.05	302.11	165.45	0.06

OH-PAHs	CAS	Formula	Exact Mass	[M-H] ⁻	Avg CCS	RSD%
1, 5 dihydroxynaphthalene	83-56-7	C10H8O2	160.0524	159.0446	134.35	0.35
2, 3-dihydroxynaphthalene	92-44-4	C10H8O2	160.0524	159.0446	132.44	0.16
12-Hydroxybenzo(a)pyrene	56892-33-2	C20H12O	268.0888	267.0810	163.98	0.06
7-hydroxybenzo(a)pyrene	37994-82-4	C20H12O	268.0888	267.0810	164.08	0.00
6-Hydroxychrysene	37515-51-8	C18H12O	244.0888	243.0810	158.68	0.07
1-Hydroxypyrene	5315-79-7	C16H10O	218.0732	217.0653	149.26	0.08

CCS for Peptides

Peptide Name	Sequence	Exact Mass	[M+H] ⁺	Average Ω	RSD%
Substance P	RPKPQQFFGLM	1346.7281	1347.7359	359.66	0.06
Bradykinin	RPPGFSPFR	1059.5614	1060.5701	314.65	0.24
Angiotensin I	DRVYIHPFHL	1295.6775	1296.6853	365.86	1.90
Angiotensin II	DRVYIHPF	1045.5345	1046.5423	315.89	0.15
Kemptide	LRRASLG	771.4715	772.4793	276.28	0.10
Myoglobin Digest	ELGFQG	649.3065	650.3144	241.83	0.02
Cytochrome C Digest	NK	260.1484	261.1557	149.47	0.25
Cytochrome C Digest	ATNE	433.1808	434.1881	201.34	0.06
Cytochrome C Digest	GITWK	603.3380	604.3453	238.31	0.06
Cytochrome C Digest	IFVQK	633.3849	634.3922	250.71	0.09
Cytochrome C Digest	YIPGTK	677.3748	678.3821	256.30	0.06
Cytochrome C Digest	MIFAGIK	778.4411	779.4484	277.01	0.08
Cytochrome C Digest	EDLIAYLK	963.5276	964.5349	308.68	0.02
Cytochrome C Digest	TGPNLHGLFGR	1167.6148	1168.6221	331.37	0.18
Cytochrome C Digest	TGQAPGFTYTDANK	1469.6786	1470.6859	366.96	0.13
Cytochrome C Digest	EETLMEYLENPK	1494.6912	1495.6985	387.44	0.12
Polyalanine	A4	302.2000	303.1658	166.02	0.21
Polyalanine	A5	373.2000	374.2039	180.75	0.17
Polyalanine	A6	444.2000	445.2417	195.08	0.28
Polyalanine	A7	515.3000	516.2786	210.85	0.17
Polyalanine	A8	586.3000	587.3154	227.87	0.12
Polyalanine	A9	657.3000	658.3519	241.61	0.09
Polyalanine	A10	728.4000	729.3892	254.65	0.18
Polyalanine	A11	799.4000	800.427	267.98	0.13
Polyalanine	A12	870.5000	871.4632	281.38	0.16
Polyalanine	A13	941.5000	942.4993	293.92	0.15
Polyalanine	A14	1012.5000	1013.5374	305.33	0.08

Peptide Name	Sequence	[M+2H] ²⁺	Average Ω	RSD%
Substance P	RPKPQQFFGLM	674.3719	385.67	0.46
Substance P	RPKPQQFFGLM	674.3719	398.87	0.12
Bradykinin	RPPGFSPFR	530.7885	343.47	0.19
Fibrinopeptide A	ADSGEGDFLAEGGGVR	768.8504	411.70	0.05
Neurotensin	_{pyro} ELYENKPRRPYIL	836.9626	434.89	0.11
Melittin	GIGAVLKVLTTGLPALISWIKRKRQQ	1423.3849	610.23	0.15
Angiotensin I	DRVYIHPFHL	648.8466	386.50	0.17
Angiotensin II	DRVYIHPF	523.7751	354.43	0.18
Renin	DRVYIHPFHLLVYS	879.9705	461.10	0.12
Kemptide	LRRASLG	386.7436	311.83	0.05
Myoglobin Digest	IPIK	235.6669	282.28	1.03
Myoglobin Digest	TEAEMK	354.6616	299.40	0.61
Myoglobin Digest	HGTVVLTALGGILK	689.9208	399.47	0.05
Myoglobin Digest	HPGDFGADAQGAMTK	751.8346	419.41	0.12
Myoglobin Digest	VEADIAGHGQEVLR	803.9274	439.42	0.09
Myoglobin Digest	GLSDGEWQQVLNVWGK	908.4512	458.89	0.05
Myoglobin Digest	GHHEAELKPLAQSHATK	927.4808	463.55	0.10
Myoglobin Digest	YLEFISDAIIHVLHSK	943.0109	518.41	0.03
Cytochrome C Digest	GITWK	302.6763	276.85	0.23
Cytochrome C Digest	IFVQK	317.6998	290.22	0.25

Peptide Name	Sequence	[M+2H] ²⁺	Average Ω	RSD%
Cytochrome C Digest	YIPGTK	339.6947	294.64	0.05
Cytochrome C Digest	MIFAGIK	390.2278	307.01	0.25
Cytochrome C Digest	EDLIAYLK	482.7711	345.04	0.08
Cytochrome C Digest	TGPNLHGLFGR	584.8147	372.56	0.09
Cytochrome C Digest	TGQAPGFTYTDANK	735.8466	402.95	0.07
Cytochrome C Digest	EETLMEYLENPK	748.3529	418.20	0.08
Polyalanine	A11	801.4337	301.21	0.52
Polyalanine	A12	872.4734	309.75	0.15
Polyalanine	A13	943.5108	321.29	0.02
Polyalanine	A14	1014.546	332.97	0.18
Polyalanine	A15	1085.5851	345.14	0.23
Polyalanine	A16	1156.622	357.58	0.23
Polyalanine	A17	1227.6573	369.45	0.19
Polyalanine	A18	1298.6962	382.02	0.16
Polyalanine	A19	1369.7334	393.66	0.26
Polyalanine	A20	1440.7684	405.00	0.22
Polyalanine	A21	1511.8068	416.71	0.18
Polyalanine	A22	1582.8435	427.95	0.12
Polyalanine	A23	1653.8792	439.95	0.09
Polyalanine	A24	1724.9167	450.50	0.33
Polyalanine	A25	1795.9521	462.87	0.15
Polyalanine	A26	1866.9885	473.84	0.41

Peptide Name	Sequence	[M+3H] ³⁺	Average Ω	RSD%
Bradykinin	RPPGFSPFR	354.1949	424.48	0.43
Bradykinin	RPPGFSPFR	354.1949	448.16	0.09
Substance P	RPKPQQFFGLM	449.9172	497.36	0.23
Neurotensin	_{pyro} ELYENKPRRPYIL	558.3110	495.78	0.18
Neurotensin	_{pyro} ELYENKPRRPYIL	558.3110	525.54	0.19
Fibrinopeptide A	ADSGEGDFLAEGGGVR	512.9029	486.37	0.16
Melittin	GIGAVLKVLTTGLPALISWIKRKRQQ	949.2592	720.95	0.05
Angiotensin I	DRVYIHPFHL	432.9003	476.05	0.08
Angiotensin II	DRVYIHPF	349.5193	435.63	0.13
Renin	DRVYIHPFHLLVYS	586.9829	519.58	0.16
Myoglobin Digest	LFTGHPETLEK	424.5543	499.94	0.64
Myoglobin Digest	HGTVVLTALGGILK	460.2805	502.18	0.40
Myoglobin Digest	HPGDFGADAQGAMTK	501.5564	464.42	0.10
Myoglobin Digest	HPGDFGADAQGAMTK	501.5564	505.90	0.15
Myoglobin Digest	VEADIAGHGQEVLR	536.2849	500.98	0.35
Myoglobin Digest	GLSDGEWQQVNLNVWGK	605.9675	532.85	0.09
Myoglobin Digest	GHHEAELKPLAQSHATK	618.6539	509.69	0.12
Myoglobin Digest	YLEFISDAIIHVLHSK	629.0073	561.30	0.31
Polyalanine	A23	1654.8915	533.80	0.31
Polyalanine	A24	1725.9152	547.54	0.15
Polyalanine	A25	1796.9651	563.04	0.22
Polyalanine	A26	1868.0031	579.07	0.30
Polyalanine	A27	1939.0363	593.67	0.22
Polyalanine	A28	2010.0751	609.33	0.27
Polyalanine	A29	2081.1123	624.59	0.27
Polyalanine	A30	2152.1451	638.93	0.12

Peptide Name	Sequence	[M+3H] ³⁺	Average Ω	RSD%
Polyalanine	A31	2223.1837	654.36	0.33
Polyalanine	A32	2294.2208	667.73	0.27
Polyalanine	A33	2365.2569	680.73	0.14

Peptide Name	Sequence	[M+4H] ⁴⁺	Average Ω	RSD%
Melittin	GIGAVLKVLTTGLPALISWIKRKRQQ	712.1963	757.08	0.01
Angiotensin I	DRVYIHPFHL	324.9272	549.44	0.13
Renin	DRVYIHPFHLLVYS	440.4891	636.34	0.16

Peptide Name	Sequence	[M+5H] ⁵⁺	Average Ω	RSD%
Melittin	GIGAVLKVLTTGLPALISWIKRKRQQ	569.9586	853.16	0.07
Melittin	GIGAVLKVLTTGLPALISWIKRKRQQ	569.9586	815.76	0.23