

Mass Table*

Mass	Sequence	Mass	Sequence	Mass	Sequence	Mass	Sequence
16.0313	CH ₄	198.1004	PT	231.0678	AC(+57), CQ, ACG	256.1171	AAGG
17.0265	NH ₃	198.1368	VV	231.0855	GSS	256.1172	QQ, AAN, AOG
18.0106	H ₂ O	199.0957	AQ, AAG	231.1042	CK	256.1535	QK, AGK
57.0215	G	199.1321	AK	232.0518	CE	256.1899	KK
71.0371	A	200.0620	CP	232.0882	MT	257.0834	PC(+57), CGP
87.0320	S	200.0797	AE	234.0497	CM	257.1012	EQ, AAD, AEG
97.0528	P	200.1161	LS, TV	234.0674	SM(+16)	257.1164	AW
99.0684	V	201.0750	NS, GGS	234.1004	AY, FS	257.1376	EK, ASV, GLS, GTV
101.0477	T	202.0590	DS	234.1117	HP	257.1488	RT
103.0092	C	202.0776	AM, CV	236.1273	HV	258.0852	EE
113.0841	L	202.0954	TT	238.0355	AS(+80), GT(+80)	258.0964	NGS, GGGG
114.0429	N, GG	204.0569	CT, GM(+16)	238.1066	HT	259.0804	DGS
115.0269	D	204.0899	GF	239.1270	AAP	259.0991	QM, VC(+57), AGM, CGV
128.0586	Q, AG	206.0184	CC	240.0681	CH	259.1103	RC
128.0950	K	208.0960	AH	241.1063	GPS	259.1168	AST, GTT
129.0426	E	210.1368	LP	241.1426	QL, AAV, AGL	259.1355	KM
131.0405	M	211.0957	NP, GGP	241.1790	LK	260.0831	EM
137.0589	H	212.0797	DP	242.1015	NQ, ANG, QGG, AGGG	260.1161	PY
142.0742	AA	212.1525	LV	242.1266	EL	260.1195	LM(+16)
144.0535	GS	213.1113	NV, AAA, GGV	242.1379	NK, GKG	260.1525	LF
147.0354	M(+16)	213.1226	RG	243.0297	Y(+80)	261.0783	NM(+16), TC(+57), ACS, CGT, GGM(+16)
147.0684	F	214.0954	DV	243.0855	NE, DQ, ADG, EGG	261.0961	SSS
154.0742	GP	214.1317	LT	243.1008	GW	261.1113	NF, GGF
156.0899	GV	215.0906	NT, QS, AGS, GGT	243.1219	DK, AAT, GSV	262.0623	DM(+16)
156.1011	R	215.1270	KS	243.1331	RS	262.0810	MM
158.0691	AS, GT	216.0746	DT, ES	244.0695	DE	262.0954	DF
160.0307	C(+57), CG	216.0933	CL	244.0882	PM(+16)	262.1317	YV
163.0633	Y	217.0521	NC, GC(+57), CGG	244.1212	FP	263.0398	CC(+57), CCG
166.9984	S(+80)	218.0361	DC	244.1246	LM	264.0511	PS(+80)
168.0899	AP	218.0725	AM(+16), MS	245.0834	NM, AAC, GGM	264.1110	TY
170.1055	AV, GL	218.1055	AF	245.1012	ASS, GST	265.1175	QH, AGH
171.0644	NG, GGG	220.0848	GY	246.0674	DM	265.1426	APP
172.0484	DG	224.0198	GS(+80)	246.1038	VM(+16)	265.1539	HK
172.0848	AT	224.0909	HS	246.1368	FV	266.0668	VS(+80)
174.0463	AC	225.1113	QP, AGP	247.0627	SC(+57), CGS	266.0725	CY
174.0641	SS	225.1477	KP	248.0831	TM(+16)	266.1015	EH
181.0140	T(+80)	226.0954	EP	248.1161	FT	267.1583	APV, GLP
184.0848	PS	226.1681	LL	250.0446	CM(+16)	268.0460	ST(+80), TS(+80)
184.1212	AL	227.1270	NL, QV, AGV, GGL	250.0776	CF	268.0994	HM
185.0800	AN, QG, AGG	227.1382	AR	250.0954	SY	268.1171	GGGP
185.1164	GK	227.1634	KV	250.1430	HL	268.1172	NGP
186.0640	EG	228.0858	GGGG	251.1018	NH, GGH	269.1012	DGP
186.0641	AD	228.0859	NN, NGG	251.1270	GPP	269.1376	APT
186.0793	W	228.0933	MP	252.0511	AT(+80)	269.1739	AVV, GLV
186.1004	SV	228.1110	DL, EV	252.0859	DH	269.1852	RL
188.0620	GM	229.0699	ND, DGG	253.1426	GPV	270.0076	CS(+80)
188.0797	ST	229.1063	QT, AAS, AGT	253.1539	RP	270.1328	AAQ, NGV, AAAG, GGGV
190.0412	CS	229.1426	KT	254.0304	SS(+80)	270.1440	RN, RGG
194.0804	GH	230.0539	DD	255.1219	APS, GPT	270.1692	AAK
194.1055	PP	230.0903	ET	255.1583	AAL, GVV		
196.1212	PV	230.1089	MV	255.1695	RV		

Immonium Ions & Other Fragment Masses*

Amino Acid	Immonium Ion Mass	Other Fragment Masses	Comments
Gly	30		
Ala	44		
Ser	60		High intensity
Pro	70		Proline, if m/z 70 abundant and other arginine fragments are missing
Val	72		
Thr	74		
Cys	76		Low intensity
Ile	86	72	Very low intensity
Leu	86	72	Very low intensity
Asn	87	70	Both ions very low intensity
Asp	88		Ion is absent when C-terminal
Gln	101	84, 129	m/z 129 usually very low intensity
Lys	101	70, 84, 112, 129	m/z 70 an 101 usually very low intensity
Glu	102		Very low intensity when C-terminal
Met	104	61	m/z 104 of very low intensity
His	110	82, 121, 123, 138, 166	Fragment ions of very low intensity; high intensity immonium ion
Phe	120	91	m/z 120 of high intensity and m/z 91 is very low intensity
Arg	129	59, 70, 73, 87, 100, 112	m/z 73 and 129 of very low intensity
Tyr	136	91, 107	High intensity immonium and very low intensity fragment ions
Trp	159	117, 130, 170, 171	High intensity immonium and fragment ions except m/z 117 is low intensity

*A.P. Snyder, Interpreting Protein Mass Spectra, 2000

Ion Type Mass Calculation

Ion Type	Mass	Nominal Mass
a	$\sigma - 26.9871$	$\sigma - 27$
b	$\sigma + 1.0078$	$\sigma + 1$
c	$\sigma + 18.0344$	$\sigma + 18$
x	$\sigma + 44.9977$	$\sigma + 45$
y	$\sigma + 19.0184$	$\sigma + 19$
z	$\sigma + 1.9918$	$\sigma + 2$
z ^o	$\sigma + 2.9997$	$\sigma + 3$

σ = total residue mass or nominal mass
 Example 1: To calculate the b ion nominal mass of GA
 $57 + 71 + 1 = 129$
 Example 2: To calculate the residue sequence of the b ion at 129. First, total residue mass
 $= 129 - 1 = 128$
 Then, look up the mass table to find it. It can be Q, AG (or GA) or K.

*The left column is the monoisotopic mass of the residue and sequences in the right column. Three common PTMs are represented by their nominal mass in the sequence. They are:

- +57 - Carbamidomethyl (57.02146)
- +80 - Phosphorylation (79.96633)
- +16 - Oxidation on M (15.99491)



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Common Amino Acid Residues

Name	3-letter Symbol	1-letter Symbol	Monoisotopic Mass	Average Mass	Residue Composition	Residue Structure
Alanine	Ala	A	71.03711	71.08	C ₃ H ₅ NO	
Arginine	Arg	R	156.10111	156.2	C ₆ H ₁₂ N ₄ O	
Asparagine	Asn	N	114.04293	114.1	C ₄ H ₇ N ₂ O ₂	
Aspartic Acid	Asp	D	115.02694	115.1	C ₄ H ₇ NO ₃	
Cysteine	Cys	C	103.00919	103.1	C ₃ H ₅ NOS	
Glutamic Acid	Glu	E	129.04259	129.1	C ₅ H ₇ NO ₃	
Glutamine	Gln	Q	128.05858	128.1	C ₅ H ₈ N ₂ O ₂	
Glycine	Gly	G	57.02146	57.05	C ₂ H ₃ NO	
Histidine	His	H	137.05891	137.1	C ₆ H ₇ N ₃ O	
Isoleucine	Ile	I	113.08406	113.2	C ₆ H ₁₁ NO	
Leucine	Leu	L	113.08406	113.2	C ₆ H ₁₁ NO	
Lysine	Lys	K	128.09496	128.2	C ₆ H ₁₂ N ₂ O	
Methionine	Met	M	131.04049	131.2	C ₅ H ₉ NOS	
Phenylalanine	Phe	F	147.06841	147.2	C ₉ H ₉ NO	
Proline	Pro	P	97.05276	97.12	C ₅ H ₇ NO	
Serine	Ser	S	87.03203	87.08	C ₃ H ₅ NO ₂	
Threonine	Thr	T	101.04768	101.1	C ₄ H ₇ NO ₂	
Tryptophan	Trp	W	186.07931	186.2	C ₁₁ H ₁₀ N ₂ O	
Tyrosine	Tyr	Y	163.06333	163.2	C ₉ H ₉ NO ₃	
Valine	Val	V	99.06841	99.13	C ₅ H ₉ NO	

Common PTMs

Monoisotopic Mass Δ	Position	Modification
-29.99281	[M]@C-term	Homoserine
-18.01057	Y, T, S, [N, Q]@C-term, [C]@N-term	Dehydration
-17.02655	[Q]@N-term	Pyroglutamic Acid from Gln
-2.01565	C	Disulphide Bond Formation
-0.98402	[X]@C-term	Amidation
0.98402	R	Citrullination
0.98402	R, N, Q	Deamidation
14.01565	T, S, E, D, L, I, [X]@N-term, R, Q, N, K, H, C, [X]@C-term	Methylation
15.99491	W, H, C, M	Oxidation
27.99491	T, K, S, [X]@N-term	Formylation (CHO)
42.01056	C, S, K, [X]@N-term	Acetylation
42.02180	K	Homoarginine
43.98983	W, K, D, E, [M]@N-term	Carboxylation
57.02146	C	Carbamidomethyl
58.00548	C	Carboxymethyl
79.96633	R, C, D, Y, H, T, S	Phosphorylation
79.95682	Y	Sulphation
119.00410	C	Cysteinylation
132.04226		Pentoses (Ara, Rib, Xyl)
146.05791		Deoxyhexoses (Fuc, Rha)
161.06881	K, N, T, W	Hexosamine (GalN, GlcN)
162.05282	Y, R, C, T, W, N, K, [X]@N-term	Hexoses (Fru, Gal, Glc, Man)
188.03296	K	Lipoic Acid (Amide Bond to Lys)
203.07937	S, T, N	N-acetylhexosamine (GalNAc, GlcNAc)
204.18780	C	Farnesylation
210.19836	K, C, [G]@N-term	Myristoylation
226.07760	K, [X]@N-term	Biotinylation (Amide Bond to Lys)
238.22966	C, K, S, T, [X]@N-term	Palmitoylation
272.25040	C	Geranylgeranylation
365.13220		Hex-HexNAc
541.06111	R, C, N, S, E	ADP-Ribosylation (from NAD)

Less Common Amino Acid Residues

Name	3-letter Symbol	Monoisotopic Mass	Average Mass	Residue Composition	Residue Structure	Name	3-letter Symbol	Monoisotopic Mass	Average Mass	Residue Composition	Residue Structure
2-Aminobutyric acid	Abu	85.05276	85.11	C ₄ H ₇ NO		Hydroxyproline	Hyp	113.04768	113.1	C ₅ H ₇ NO ₂	
Carbamidomethyl-cysteine	Cam	160.03065	160.2	C ₅ H ₈ N ₂ O ₂ S		Norleucine	Nle	113.08406	113.2	C ₆ H ₁₁ N	
Carboxymethylcysteine	Cmc	161.01466	161.2	C ₅ H ₈ N ₂ OS		Ornithine	Orn	114.07931	114.1	C ₅ H ₁₀ N ₂ O	
Cysteic acid	Cya	150.99393	151.1	C ₃ H ₅ NO ₃ S		Pyroglutamic acid	Pyr	111.03203	111.1	C ₅ H ₇ NO ₃	
Homoserine	Hse	101.04768	101.1	C ₄ H ₇ NO ₂		Sarcosine	Sar	71.03711	71.08	C ₃ H ₅ NO	
Hydroxylysine	Hyl	144.08988	144.2	C ₆ H ₁₂ N ₂ O ₂							