

The Masses and Compositions of the Twenty Commonly Occurring Amino Acid Residues

Symbols	Name and Composition	Residue Structure	Monoisotopic Mass	Average Mass
Ala A	Alanine C ₃ H ₅ NO	$\begin{array}{c} \text{CH}_3 \\ \\ \text{-NH-CH-CO-} \end{array}$	71.03711	71.0788
Arg R	Arginine C ₆ H ₁₂ N ₄ O	$\begin{array}{c} \text{CH}_2\text{-(CH}_2\text{)}_2\text{-NH-C-NH}_2 \\ \qquad \qquad \qquad \\ \text{-NH-CH-CO-} \qquad \qquad \text{NH} \end{array}$	156.10111	156.1876
Asn N	Asparagine C ₄ H ₆ N ₂ O ₂	$\begin{array}{c} \text{CH}_2\text{-CONH}_2 \\ \\ \text{-NH-CH-CO-} \end{array}$	114.04293	114.1039
Asp D	Aspartic Acid C ₄ H ₅ NO ₃	$\begin{array}{c} \text{CH}_2\text{-COOH} \\ \\ \text{-NH-CH-CO-} \end{array}$	115.02694	115.0886
Cys C	Cysteine C ₃ H ₅ NOS	$\begin{array}{c} \text{CH}_2\text{-SH} \\ \\ \text{-NH-CH-CO-} \end{array}$	103.00919	103.1448
Glu E	Glutamic Acid C ₅ H ₇ NO ₃	$\begin{array}{c} \text{CH}_2\text{-CH}_2\text{-COOH} \\ \\ \text{-NH-CH-CO-} \end{array}$	129.04259	129.1155
Gln Q	Glutamine C ₅ H ₈ N ₂ O ₂	$\begin{array}{c} \text{CH}_2\text{-CH}_2\text{-CONH}_2 \\ \\ \text{-NH-CH-CO-} \end{array}$	128.05858	128.1308
Gly G	Glycine C ₂ H ₃ NO	$\text{-NH-CH}_2\text{-CO-}$	57.02146	57.0520
His H	Histidine C ₆ H ₇ N ₃ O	$\begin{array}{c} \text{CH}_3 \\ \\ \text{-NH-CH-CO-} \\ \\ \text{Imidazole ring} \end{array}$	137.05891	137.1412
Ile I	Isoleucine C ₆ H ₁₁ NO	$\begin{array}{c} \text{CH}(\text{CH}_3)\text{CH}_2\text{-CH}_3 \\ \\ \text{-NH-CH-CO-} \end{array}$	113.08406	113.1595
Leu L	Leucine C ₆ H ₁₁ NO	$\begin{array}{c} \text{CH}_2\text{CH}(\text{CH}_3)_2 \\ \\ \text{-NH-CH-CO-} \end{array}$	113.08406	113.1595
Lys K	Lysine C ₆ H ₁₂ N ₂ O	$\begin{array}{c} \text{CH}_2\text{-(CH}_2\text{)}_4\text{-NH}_2 \\ \\ \text{-NH-CH-CO-} \end{array}$	128.09496	128.1742
Met M	Methionine C ₅ H ₉ NOS	$\begin{array}{c} \text{CH}_2\text{-CH}_2\text{-S-CH}_3 \\ \\ \text{-NH-CH-CO-} \end{array}$	131.04049	131.1986
Phe F	Phenylalanine C ₉ H ₉ NO	$\begin{array}{c} \text{CH}_2\text{-Ph} \\ \\ \text{-NH-CH-CO-} \end{array}$	147.06841	147.1766
Pro P	Proline C ₅ H ₇ NO	$\begin{array}{c} \text{Cyclic secondary amine} \\ \\ \text{-CH-CO-} \end{array}$	97.05276	97.1167
Ser S	Serine C ₃ H ₅ NO ₂	$\begin{array}{c} \text{CH}_2\text{-OH} \\ \\ \text{-NH-CH-CO-} \end{array}$	87.03203	87.0782
Thr T	Threonine C ₄ H ₇ NO ₂	$\begin{array}{c} \text{CH}(\text{OH})\text{CH}_3 \\ \\ \text{-NH-CH-CO-} \end{array}$	101.04768	101.1051
Trp W	Tryptophan C ₁₁ H ₁₀ N ₂ O	$\begin{array}{c} \text{CH}_2 \\ \\ \text{-NH-CH-CO-} \\ \\ \text{Indole ring} \end{array}$	186.07931	186.2133
Tyr Y	Tyrosine C ₉ H ₉ NO ₂	$\begin{array}{c} \text{CH} \\ \\ \text{-NH-CH-CO-} \\ \\ \text{p-Hydroxyphenyl ring} \end{array}$	163.06333	163.1760
Val V	Valine C ₅ H ₉ NO	$\begin{array}{c} \text{CH}(\text{CH}_3)_2 \\ \\ \text{-NH-CH-CO-} \end{array}$	99.06841	99.1326

Data for the Calculation of the Molecular Masses of Peptides and Proteins for use in Mass Spectrometry

The molecular mass of a normally terminated and unmodified peptide or protein may be calculated by summing the masses of the appropriate amino acid residues from the following tables and adding the masses of H and OH for the N and C-termini respectively. The masses of some alternative terminal groups are also listed. In cases where cysteines are linked by disulphide bridges, the mass of 2 hydrogen atoms should be subtracted for each disulphide bridge in the molecule.

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The Masses and Compositions of Some Less Commonly Occurring Amino Acid Residues

Symbols	Name and Composition	Residue Structure	Monoisotopic Mass	Average Mass
Abu	2-Aminobutyric acid C ₄ H ₇ NO	$\begin{array}{c} \text{CH}_2\text{CH}_3 \\ \\ \text{-NH-CH-CO-} \end{array}$	85.05276	85.1057
AECys	Aminoethylcysteine C ₅ H ₁₀ N ₂ OS	$\begin{array}{c} \text{CH}_2\text{-S-(CH}_2\text{)}_2\text{-NH}_2 \\ \\ \text{-NH-CH-CO-} \end{array}$	146.05138	146.2133
Aib	2-Aminoisobutyric acid C ₄ H ₇ NO	$\text{-NH-C(CH}_3\text{)}_2\text{-CO-}$	85.05276	85.1057
Cmc	Carboxymethylcysteine C ₅ H ₇ NO ₃ S	$\begin{array}{c} \text{CH}_2\text{-S-CH}_2\text{-COOH} \\ \\ \text{-NH-CH-CO-} \end{array}$	161.01466	161.1815
Cys(O ₃ H)	Cysteic acid C ₃ H ₅ NO ₄ S	$\begin{array}{c} \text{CH}_2\text{-SO}_3\text{H} \\ \\ \text{-NH-CH-CO-} \end{array}$	150.99393	151.1430
Dha	Dehydroalanine C ₃ H ₃ NO	$\begin{array}{c} \text{CH}_2 \\ \\ \text{-NH-C-CO-} \end{array}$	69.02146	69.0630
Dhb	Dehydroamino-2-butyric acid C ₄ H ₅ NO	$\begin{array}{c} \text{CH-CH}_3 \\ \\ \text{-NH-C-CO-} \end{array}$	83.03711	83.0898
Gla	4-carboxyglutamic acid C ₆ H ₇ NO ₅	$\begin{array}{c} \text{CH}_2\text{-CH(COOH)}_2 \\ \\ \text{-NH-CH-CO-} \end{array}$	173.03242	173.1253
Hse	Homocysteine C ₄ H ₇ NO ₂	$\begin{array}{c} \text{CH}_2\text{-CH}_2\text{OH} \\ \\ \text{-NH-CH-CO-} \end{array}$	101.04768	101.1051
Hyl	Hydroxylysine C ₆ H ₁₂ N ₂ O ₂	$\begin{array}{c} (\text{CH}_2)_4\text{-CH(OH)CH}_2\text{-NH}_2 \\ \\ \text{-NH-CH-CO-} \end{array}$	144.08988	144.1736
Hyp	Hydroxyproline C ₅ H ₇ NO ₂	$\begin{array}{c} \text{Cyclic secondary amine with OH} \\ \\ \text{-CH-CO-} \end{array}$	113.04768	113.1161
Iva	Isovaline C ₅ H ₉ NO	$\begin{array}{c} \text{CH}_2\text{-CH}_3 \\ \\ \text{-NH-C(CH}_3\text{)}_2\text{-CO-} \end{array}$	99.06841	99.1326
Nle	Norleucine C ₆ H ₁₁ NO	$\begin{array}{c} \text{CH}_2(\text{CH}_2)_2\text{-CH}_3 \\ \\ \text{-NH-CH-CO-} \end{array}$	113.08406	113.1595
Orn	Ornithine C ₅ H ₁₀ N ₂ O	$\begin{array}{c} \text{CH}_2\text{-(CH}_2\text{)}_2\text{-NH}_2 \\ \\ \text{-NH-CH-CO-} \end{array}$	114.07931	114.1473
Pip	2-Piperidinecarboxylic acid C ₆ H ₉ NO	$\begin{array}{c} \text{Cyclic secondary amine} \\ \\ \text{-CH-CO-} \end{array}$	111.06841	111.1436
Pyr	Pyroglutamic acid C ₅ H ₅ NO ₂	$\begin{array}{c} \text{Cyclic secondary amine with COOH} \\ \\ \text{-CH-CO-} \end{array}$	111.03203	111.1002
Sar	Sarcosine C ₃ H ₅ NO	$\text{-N(CH}_3\text{)-CH}_2\text{-CO-}$	71.03711	71.0788

The Masses of Some Terminal Groups

N-Terminal Groups	Composition	Monoisotopic Mass	Average Mass
Hydrogen	H	1.00782	1.0079
N-Formyl	HCO	29.00274	29.0183
N-Acetyl	CH ₃ CO	43.01839	43.0452
C-Terminal Groups			
Free acid	OH	17.00274	17.0073
Amide	NH ₂	16.01872	16.0226