

Elemental mass values, amino acids and immonium ions

H-1	1.007825035
H-2	2.014101787
C-12	12.000000000
N-14	14.003074002
O-16	15.994914630
P-31	30.973762000
S-32	31.972070700
C-13	13.003354826
N-15	15.000108970
O-18	17.999160300
Electron	0.000548580

Elemental mass values of the most commonly occurring elements

Amino Acid	Abbr	Code	Monomer composition	Monoisotopic mass
Glycine	Gly	G	C2H3NO	57.021464
Alanine	Ala	A	C3H5NO	71.037114
Serine	Ser	S	C3H5NO2	87.032028
Proline	Pro	P	C5H7NO	97.052764
Valine	Val	V	C5H9NO	99.068414
Threonine	Thr	T	C4H7NO2	101.047679
Cysteine	Cys	C	C3H5NOS	103.009185
Isoleucine	Ile	I	C6H11NO	113.084064
Leucine	Leu	L	C6H11NO	113.084064
Asparagine	Asn	N	C4H6N2O2	114.042927
Aspartic acid	Asp	D	C4H5NO3	115.026943
Glutamine	Gln	Q	C5H8N2O2	128.058578
Lysine	Lys	K	C6H12N2O	128.094963
Glutamic acid	Glu	E	C5H7NO3	129.042593
Methionine	Met	M	C5H9NOS	131.040485
Histidine	His	H	C6H7N3O	137.058912
Phenylalanine	Phe	F	C9H9NO	147.068414
Arginine	Arg	R	C6H12N4O	156.101111
Tyrosine	Tyr	Y	C9H9NO2	163.063329
Tryptophan	Trp	W	C11H10N2O	186.079313

Names and mass values of the 20 commonly occurring amino acid residues

Amino Acid	Code	Immonium and fragment ions	Neutral loss
Glycine	G	30.03	
Alanine	A	44.05	
Serine	S	60.04	18.01 (H2O)
Proline	P	70.07	
Valine	V	72.08	
Threonine	T	74.06	18.01 (H2O)
Isoleucine	I	86.10	
Leucine	L	86.10	
Asparagine	N	87.06, 70.03	17.03 (NH3)
Aspartic acid	D	88.04, 70.03	18.01 (H2O)
Glutamine	Q	129.10, 101.07, 84.04, 56.05	17.03 (NH3)
Lysine	K	129.11, 101.11, 84.08, 56.05	17.03 (NH3)
Glutamic acid	E	102.05, 84.04	18.01 (H2O)
Methionine	M	104.06	48.00 (CH4S)
Histidine	H	110.07	
Phenylalanine	F	120.08	
Arginine	R	129.11, 115.09, 112.09, 87.09, 70.07, 60.06	17.03 (NH3)
Cysteine-cbm	C	133.04	91.01 (C2H5NOS)
Tyrosine	Y	136.08	
Tryptophan	W	159.09, 132.08, 130.07	

Low mass fragment ions and neutral losses from the common 20 amino acid residues. Cysteines are derivatized with iodoacetamide to form carbamidomethylcysteine.