

BACHEM'S PEPTIDE CALCULATOR

Calculation of the Molecular Weight

The following formula is used for the calculation of the molecular weight of an amino acid sequence:

$$M = M_n + M_c + \sum_i N_i M_i$$

- M Molecular weight of the amino acid sequence
- M_n Molecular weight of the N-terminus
- M_c Molecular weight of the C-terminus
- N_i Number of the amino acid residues
- M_i Molecular weight of the amino acid residues

Amino Acid		Molecular Weight
One Letter Code	Three Letter Code	
A	Ala	71.07884
C	Cys	103.1448
D	Asp	115.0886
E	Glu	129.1155
F	Phe	147.1766
G	Gly	57.05196
H	His	137.1412
I	Ile	113.1595
K	Lys	128.1742
L	Leu	113.1591
M	Met	131.1986
N	Asn	114.1039
P	Pro	97.11671
Q	Gln	128.1308
R	Arg	156.1876
S	Ser	87.07824
T	Thr	101.1051
V	Val	99.13259
W	Trp	186.2133
Y	Tyr	163.176

N-Terminus	Molecular Weight
H	1.00794
Ac	43.04522
Biotinyl	227.3074
Pyr	112.1082

C-Terminus	Molecular Weight
OH	17.00734
NH ₂	16.02262

Calculation of the Net Charge

The following formula is used for the calculation of the net charge of a peptide sequence at a given pH:

$$Z = \sum_i N_i \frac{10^{pK_{a_i}}}{10^{pH} + 10^{pK_{a_i}}} - \sum_j N_j \frac{10^{pH}}{10^{pH} + 10^{pK_{a_j}}}$$

Z Net charge of the peptide sequence

N_i Number of arginine, lysine, and histidine residues and the N-terminus

pK_{a_i} pKa values of the N-terminus and the arginine, lysine, and histidine residues

N_j Number of of aspartic acid, glutamic acid, cysteine, and tyrosine residues and the C-terminus

pK_{a_j} pKa values of the C-terminus and the aspartic acid, glutamic acid, cysteine, and tyrosine residues

pH pH value

Amino Acid		pKa Value*
One Letter Code	Three Letter Code	
C	Cys	8.33
D	Asp	3.86
E	Glu	4.25
H	His	6.0
K	Lys	10.53
R	Arg	12.48
Y	Tyr	10.07

N-Terminus	pKa Value*
H	9.69

C-Terminus	pKa Value*
OH	2.34

*Lehninger (1982) Principles of Biochemistry

Calculation of the Isoelectric Point

The isoelectric point, pI, is the pH at which the net charge of the peptide is zero. The isoelectric point is calculated by approximation (accuracy ± 0.01).

Calculation of the Average Hydrophilicity

Amino Acid		Hydrophilicity Value*
One Letter Code	Three Letter Code	
A	Ala	-0.5
C	Cys	-1.0
D	Asp	3.0
E	Glu	3.0
F	Phe	-2.5
G	Gly	0.0
H	His	-0.5
I	Ile	-1.8
K	Lys	3.0
L	Leu	-1.8
M	Met	-1.3
N	Asn	0.2
P	Pro	0.0
Q	Gln	0.2
R	Arg	3.0
S	Ser	0.3
T	Thr	-0.4
V	Val	-1.5
W	Trp	-3.4
Y	Tyr	-2.3

The following values are used for the calculation of the average hydrophilicity:

*Hopp & Woods

The hydrophilicity value for each amino acid in the peptide sequence is indicated in a bar graph. The ratio of hydrophilic residues to total number of amino acids is reported in %.