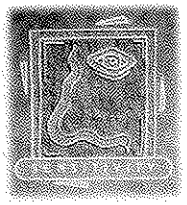
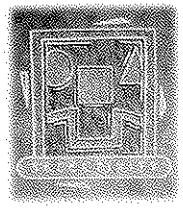
Data for the calculation of the molecular masses of peptides and proteins for use in mass spectrometry

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- terminii respectively.

The masses of some alternative terminal groups are also listed. In cases where cysteines are linked by disulphide bonds, the mass of two hydrogen atoms should be subtracted for each disulphide bond in the molecule.





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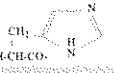
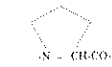
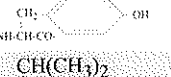
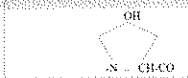
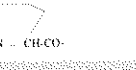
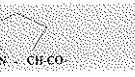
The masses and compositions of the twenty commonly occurring amino acid residues

Symbols	Name and Composition	Residue Structure	Monoisotopic Mass	Average Mass
Ala A	Alanine C_3H_5NO	CH_3 -NH-CH-CO-	71.03711	71.0788
Arg R	Arginine $C_6H_{12}N_4O$	CH_2-$(CH_2)_2$-NH-C-NH_2 -NH-CH-CO- NH	156.10111	156.1876
Asn N	Asparagine $C_4H_6N_2O_2$	CH_2-$CONH_2$ -NH-CH-CO-	114.04293	114.1039
Asp D	Aspartic Acid $C_4H_5NO_3$	CH_2-$COOH$ -NH-CH-CO-	115.02694	115.0886
Cys C	Cysteine C_3H_5NOS	CH_2-SH -NH-CH-CO-	103.00919	103.1448
Gln Q	Glutamine $C_5H_8N_2O_2$	CH_2-CH_2-$CONH_2$ -NH-CH-CO-	128.05858	128.1308
Glu E	Glutamic Acid $C_5H_7NO_3$	CH_2-CH_2-$COOH$ -NH-CH-CO-	129.04259	129.1155
Gly G	Glycine C_2H_3NO	-NH-CH_2-CO-	57.02146	57.0520
His H	Histidine $C_6H_7N_3O$		137.05891	137.1412
Ile I	Isoleucine $C_6H_{11}NO$	$CH(CH_3)$-CH_2-CH_3 -NH-CH-CO-	113.08406	113.1595
Leu L	Leucine $C_6H_{11}NO$	CH_2-$CH(CH_3)_2$ -NH-CH-CO-	113.08406	113.1595
Lys K	Lysine $C_6H_{12}N_2O$	CH_2-$(CH_2)_3$-NH_2 -NH-CH-CO-	128.09496	128.1742
Met M	Methionine C_5H_9NOS	CH_2-CH_2-S-CH_3 -NH-CH-CO-	131.04049	131.1986
Phe F	Phenylalanine C_9H_9NO	CH_2-Ph -NH-CH-CO-	147.06841	147.1766
Pro P	Proline C_5H_7NO		97.05276	97.1167
Ser S	Serine $C_3H_5NO_2$	CH_2-OH -NH-CH-CO-	87.03203	87.0782
Thr T	Threonine $C_4H_7NO_2$	$CH(OH)$-CH_3 -NH-CH-CO-	101.04768	101.1051
Trp W	Tryptophan $C_{11}H_{10}N_2O$		186.07931	186.2133
Tyr Y	Tyrosine $C_9H_9NO_2$		163.06333	163.1760
Val V	Valine C_5H_9NO	$CH(CH_3)_2$ -NH-CH-CO-	99.06841	99.1326

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_4H_7NO	CH_2-CH_3 -NH-CH-CO-	85.05276	85.1057
AE-Cys	Aminoethylcysteine $C_5H_{10}N_2OS$	CH_2-S-$(CH_2)_2$-NH_2 -NH-CH-CO-	146.05138	146.2133
Cam	Carboxyamidomethyl cysteine $C_5H_8N_2O_2S$	CH_2-S-CH_2-$CONH_2$ -NH-CH-CO-	160.03065	160.1968
Cmc	Carboxymethylcysteine $C_5H_7NO_3S$	CH_2-S-CH_2-$COOH$ -NH-CH-CO-	161.01466	161.1815
Cys(O_3H)	Cysteic acid $C_3H_5NO_4S$	CH_2-SO_3H -NH-CH-CO-	150.99393	151.1430
Dha	Dehydroalanine C_3H_3NO	CH_2 -NH-C-CO-	69.02146	69.0630
Dhb	Dehydroamino-2-butyric acid C_4H_5NO	CH-CH_3 -NH-C-CO-	83.03711	83.0898
Gla	4-carboxyglutamic acid $C_6H_7NO_5$	CH_2-$CH(COOH)_2$ -NH-CH-CO-	173.03242	173.1253
Hse	Homoserine $C_4H_7NO_2$	CH_2-CH_2OH -NH-CH-CO-	101.04768	101.1051
Hyl	Hydroxylysine $C_6H_{12}N_2O_2$	$(CH_2)_2$-$CH(OH)CH_2$-NH_2 -NH-CH-CO-	144.08988	144.1736
Hyp	Hydroxyproline $C_5H_7NO_2$		113.04768	113.1161
Iva	Isovaline C_5H_9NO	CH_2-CH_3 -NH-C(CH_3)-CO-	99.06841	99.1326
Nle	Norleucine $C_6H_{11}NO$	CH_2-$(CH_2)_2$-CH_3 -NH-CH-CO-	113.08406	113.1595
Orn	Ornithine $C_5H_{10}N_2O$	CH_2-$(CH_2)_2$-NH_2 -NH-CH-CO-	114.07931	114.1473
Pip	2-Piperidinecarboxylic acid C_6H_9NO		111.06841	111.1436
Pyr	Pyroglutamic acid $C_5H_5NO_2$		111.03203	111.1002
Sar	Sarcosine C_3H_5NO	-N(CH_3)-CH_2-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_3CO	43.01839	43.0452
C-Terminal Groups			
Free acid	OH	17.00274	17.0073
Amide	NH_2	16.01872	16.0226

Post-translational modifications of peptides and proteins

For peptides and proteins which have undergone post-translational modification, a table of the mass change produced by the modification is given below. A second table details some of the mass changes produced by protecting groups and side reactions encountered with synthetic peptides. To obtain the molecular mass of a modified peptide or protein the appropriate mass changes listed in the tables should be algebraically added directly to the molecular mass calculated for the unmodified molecule.

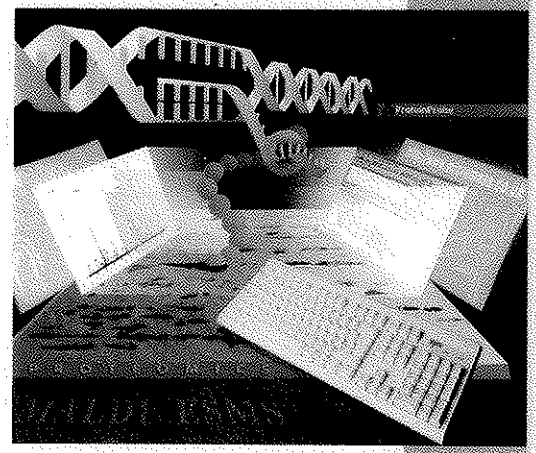
Mass changes due to some post-translational modifications of peptides and proteins

Modification	Monoisotopic Mass Change	Average Mass Change
Homoserine formed from Met by CNBr treatment	-29.99281	-30.0935
Pyroglutamic acid formed from Gln	-17.02655	-17.0306
Disulphide bond formation	- 2.01565	- 2.0159
C-terminal amide formed from Gly	- 0.98402	- 0.9847
Deamidation of Asn and Gln	0.98402	0.9847
Methylation	14.01565	14.0269
Hydroxylation	15.99491	15.9994
Oxidation of Met	15.99491	15.9994
Formylation	27.99491	28.0104
Acetylation	42.01056	42.0373
Carboxylation of Asp and Glu	43.98983	44.0098
Carboxyamidomethylcysteine (Cam) from Cys (iodoacetamide)	57.02146	57.0520
Carboxymethylcysteine (Cmc) from Cys (iodoacetic acid)	58.00548	58.0367
Phosphorylation	79.96633	79.9799
Sulphation	79.95682	80.0642
Pyridylethylcysteine (PE-Cys) from Cys (4-vinylpyridine)	105.05785	105.1393
Cysteinylation	119.00410	119.1442
Pentoses (Ara, Rib, Xyl)	132.04226	132.1161
Deoxyhexoses (Fuc, Rha)	146.05791	146.1430
Hexosamines (GalN, GlcN)	161.06881	161.1577
Hexoses (Fru, Gal, Glc, Man)	162.05282	162.1424
Lipoic acid (amide bond to lysine)	188.03296	188.3147
N-acetylhexosamines (GalNAc, GlcNAc)	203.07937	203.1950
Farnesylation	204.18780	204.3556
Myristoylation	210.19836	210.3598
Biotinylation (amide bond to lysine)	226.07760	226.2994
Pyridoxal phosphate (Schiff Base formed to lysine)	231.02966	231.1449
Palmitoylation	238.22966	238.4136
Stearoylation	266.26096	266.4674
Geranylgeranlylation	272.25040	272.4741
N-acetylneuraminic acid (Sialic acid, NeuAc, NANA, SA)	291.09542	291.2579
Glutathionylation	305.06816	305.3117
N-glycolylneuraminic acid (NeuGc)	307.09033	307.2573
5'-Adenosylation	329.05252	329.2091
4'-Phosphopantetheine	339.07797	339.3294
ADP-ribosylation (from NAD)	541.06111	541.3052

Mass changes due to some protecting groups and side reactions encountered in synthetic peptide analysis

Modification	Monoisotopic Mass Change	Average Mass Change
Methyl (Me)	14.01565	14.0269
Formyl (CHO)	27.99491	28.0104
Ethyl (Et)	28.03130	28.0538
Acetyl (Ac)	42.01056	42.0373
t-Butyl (t-Bu)	56.06260	56.1075
Anisyl	90.04695	90.1246
Benzyl (Bzl)	90.04695	90.1246
Trifluoroacetyl (Tfa)	95.98230	96.0087
N-hydroxysuccinimide (ONSu, OSu)	97.01638	97.0734
t-Butyloxycarbonyl (Boc)	100.05243	100.1173
Benzoyl (Bz)	104.02621	104.1082
4-Methylbenzyl (Meb)	104.06260	104.1515
Thioanisyl	106.02411	106.1912
Thiocresyl	106.02411	106.1912
Benzyloxymethyl (Bom)	120.05751	120.1509
4-Nitrophenyl (ONp)	121.01638	121.0954
Benzyloxycarbonyl (Z)	134.03678	134.1344
2-Nitrobenzoyl (NBz)	149.01129	149.1058
2-Nitrophenylsulphenyl (Nps)	152.98845	153.1614
4-Toluenesulphonyl (Tosyl, Tos)	154.00885	154.1894
Pentafluorophenyl (Pfp)	165.98419	166.0501
Diphenylmethyl (Dpm)	166.07825	166.2224
2-Chlorobenzyloxycarbonyl (Cl-Z)	167.99781	168.5792
2, 4, 5-Trichlorophenyl	177.91438	179.4320
2-Bromobenzyloxycarbonyl (Br-Z)	211.94729	213.0305
9-Fluorenylmethyloxycarbonyl (Fmoc)	222.06808	222.2432
Triphenylmethyl (Trityl, Trt)	242.10955	242.3202
2, 2, 5, 7, 8-pentamethylchroman-6-sulphonyl (Pmc)	266.09767	266.3611

The monoisotopic masses were calculated using the following atomic masses of the most abundant isotope of the elements:
C=12.0000000, H=1.0078250, N=14.0030740, O=15.9949146, F=18.9984033, P=30.9737634, S=31.9720718, Cl=34.9688527, Br=78.9183361.
The average masses were calculated using the following atomic weights of the elements:
C=12.011, H=1.00794, N=14.00674, O=15.9994, F=18.99840, P=30.97376, S=32.066, Cl=35.4527, Br=79.904.



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Protein Sequencing