

MASS SPECTROMETRY AID

INTRODUCTION

The following tables are designed to aid with the interpretation of mass spectrometry data.

- Common mass differences
- Amino acid residue masses
- Masses of selected elements

COMMON MASS DIFFERENCES

Modification	Monoisotopic Mass Change	Average Mass Change
Homeserine 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
Deamidation of Asn or Gln	0.98402	0.9847
Methylation	14.01565	14.0269
Hydroxylation	15.99491	15.9994
Oxidation of Met to Met sulphoxide	15.99491	15.9994
Loss of water e.g. by cleavage of a single peptide bond	18.0106	18.0153
Formylation	27.99491	28.0104
Oxidation of Met to Met sulphone	31.98982	31.9988
Acetylation	42.01056	42.0373
Carbamylation	43.00582	
Carboxylation of Asp and Glu	43.98983	44.0098
Carboxyamidomethylcysteine (Cam) from Cys (iodoacetamide)	57.02146	57.0520
Carboxymethylcysteine (Cme) from Cys (iodoacetic acid)	58.00548	58.0367
Phosphorylation	79.96633	79.9799
Sulphation	79.95682	80.0624
S-B-(4-pyridyl-ethyl) cysteine from 4-Vinyl pyridine treatment	104.058	
Farnesylation	204.18780	204.3556
Myristoylation	210.19836	210.3598
Biotinylation	226.07760	226.2994
Gluthathione	305.06816	305.3117

AMINO ACID RESIDUE MASSES

Note the masses given in this table are for the residue mass as it is within a peptide chain and not for the full stand alone amino acid.

Full name	3 letter code	Single letter code	Chemical composition	Average Mass (Da)	Monoisotopic Mass (Da)	Sidechain Mass (Da)
Alanine	Ala	A	C ₃ H ₅ NO	71.03711	71.08	15
Arginine	Arg	R	C ₆ H ₁₂ N ₄ O	156.10111	156.2	100
Asparagine	Asn	N	C ₄ H ₆ N ₂ O ₂	114.04293	114.1	58
Aspartic Acid	Asp	D	C ₄ H ₅ NO ₃	115.02694	115.1	59
Cysteine	Cys	C	C ₃ H ₅ NOS	103.00919	103.1	47
Glutamic Acid	Glu	E	CH ₇ NO ₃	129.04259	129.1	73
Glutamine	Gln	Q	C ₅ H ₈ N ₂ O ₂	128.05858	128.1	72
Glycine	Gly	G	C ₂ H ₃ NO	57.02146	57.05	1
Histidine	His	H	C ₆ H ₇ N ₃ O	137.05891	137.1	81
Isoleucine	Ile	I	C ₆ H ₁₁ NO	113.08406	113.2	57
Leucine	Leu	L	C ₆ H ₁₁ NO	113.08406	113.2	57
Lysine	Lys	K	C ₆ H ₁₂ N ₂ O	128.09496	128.2	72
Methionine	Met	M	C ₅ H ₉ NOS	131.04049	131.2	75
Phenylalanine	Phe	F	C ₉ H ₉ NO	147.06841	147.2	91
Proline	Pro	P	C ₅ H ₇ NO	97.05276	97.12	41
Serine	Ser	S	C ₃ H ₅ NO ₂	87.03203	87.08	31
Threonine	Thr	T	C ₄ H ₇ NO ₂	101.04768	101.1	45
Tryptophan	Trp	W	C ₁₁ H ₁₀ N ₂ O	186.07931	186.2	130
Tyrosine	Tyr	Y	C ₉ H ₉ NO ₂	163.06333	163.2	107
Valine	Val	V	C ₅ H ₉ NO	99.06841	99.13	43

MASSES OF SELECTED ELEMENTS

Element	Mass (Da)
H	1.007825
C	12.000000
N	14.003074
O	15.994915
Na	22.989768
Mg	23.985142
P	30.973762
S	31.972071
Cl	34.968853
K	38.963707
Ca	39.962591

N.B. Mass given is for the most abundant isotope