

## Amino acid residue and fragment ion mass values

Residue	3-letter	1-letter	Mass	b1 ion	y1 ion	bn-1 ion
Alanine	Ala	A	71.0371	72.0444	90.055	54.0338
Cysteine	Cys	C	102.0014	103.0086	121.0192	84.9981
Asp. acid	Asp	D	115.0269	116.0342	134.0448	98.0237
Glu. acid	Glu	E	129.0426	130.0499	148.0604	112.0393
Phenylalanine	Phe	F	147.0684	148.0757	166.0863	130.0651
Glycine	Gly	G	57.0215	58.0287	76.0393	40.0182
Histidine	His	H	137.0589	138.0662	156.0768	120.0556
Isoleucine	Ile	I	113.0841	114.0913	132.1019	96.0808
Lysine	Lys	K	128.095	129.1022	147.1128	111.0917
Leucine	Leu	L	113.0841	114.0913	132.1019	96.0808
Methionine	Met	M	131.0405	132.0478	150.0583	114.0372
Asparagine	Asn	N	114.0429	115.0502	133.0608	97.0396
Proline	Pro	P	97.0528	98.06	116.0706	80.0495
Glutamine	Gln	Q	128.0586	129.0659	147.0764	111.0553
Arginine	Arg	R	156.1011	157.1084	175.119	139.0978
Serine	Ser	S	87.032	88.0393	106.0499	70.0287
Threonine	Thr	T	101.0477	102.055	120.0655	84.0444
Valine	Val	V	99.0684	100.0757	118.0863	82.0651
Tryptophan	Trp	W	186.0793	187.0866	205.0972	169.076
Tyrosine	Tyr	Y	163.0633	164.0706	182.0812	146.06