| 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

|  |  |
| --- | --- |
| 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 | 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.