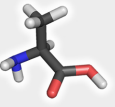
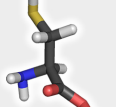
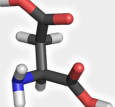
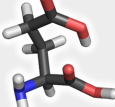
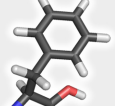
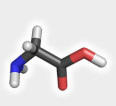
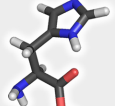
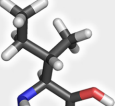
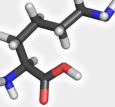
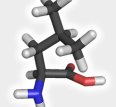
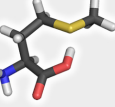
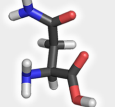
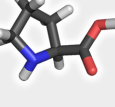
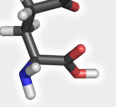
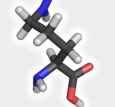
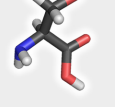
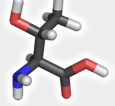
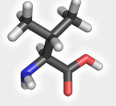
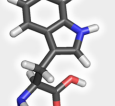
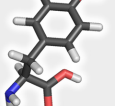


# standard Amino Acids

<b>A</b> L-Alanine <sup>ALA</sup>	<b>C</b> L-Cysteine <sup>CYS</sup>	<b>D</b> L-Aspartic Acid <sup>ASP</sup>	<b>E</b> L-Glutamic Acid <sup>GLU</sup>
 Chemical Formula C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub> Molecular Weight 89.09 Da Polarity Nonpolar Acidity/ Basicity Neutral Hydrophobicity 0.616 Hydrophathy Index 1.8 Isoelectric Point 6.01 pKa (α-COOH) 2.35 pKa (α-NH <sub>2</sub> ) 9.87 Canonical SMILES <chem>CC(N)C(=O)O</chem> PubChem CID 5950	 Chemical Formula C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub> S Molecular Weight 121.16 Da Polarity Polar Acidity/ Basicity Neutral Hydrophobicity 0.680 Hydrophathy Index 2.5 Isoelectric Point 5.05 pKa (α-COOH) 1.92 pKa (α-NH <sub>2</sub> ) 10.70 Canonical SMILES <chem>NC(SC)C(=O)O</chem> PubChem CID 5862	 Chemical Formula C <sub>4</sub> H <sub>7</sub> NO <sub>4</sub> Molecular Weight 133.10 Da Polarity Polar Acidity/ Basicity Acidic Hydrophobicity 0.028 Hydrophathy Index -3.5 Isoelectric Point 2.85 pKa (α-COOH) 1.99 pKa (α-NH <sub>2</sub> ) 9.90 Canonical SMILES <chem>NC(CC(=O)O)C(=O)O</chem> PubChem CID 5960	 Chemical Formula C <sub>5</sub> H <sub>9</sub> NO <sub>4</sub> Molecular Weight 147.13 Da Polarity Polar Acidity/ Basicity Acidic Hydrophobicity 0.043 Hydrophathy Index -3.5 Isoelectric Point 3.15 pKa (α-COOH) 2.10 pKa (α-NH <sub>2</sub> ) 9.47 Canonical SMILES <chem>NC(CCC(=O)O)C(=O)O</chem> PubChem CID 611
<b>F</b> L-Phenylalanine <sup>PHE</sup>	<b>G</b> Glycine <sup>GLY</sup>	<b>H</b> L-Histidine <sup>HIS</sup>	<b>I</b> L-Isoleucine <sup>ILE</sup>
 Chemical Formula C <sub>9</sub> H <sub>9</sub> NO <sub>2</sub> Molecular Weight 165.19 Da Polarity Nonpolar Acidity/ Basicity Neutral Hydrophobicity 1.00 Hydrophathy Index 2.8 Isoelectric Point 5.49 pKa (α-COOH) 2.20 pKa (α-NH <sub>2</sub> ) 9.31 Canonical SMILES <chem>NC(C1=CC=CC=C1)C(=O)O</chem> PubChem CID 994	 Chemical Formula C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub> Molecular Weight 75.07 Da Polarity Nonpolar Acidity/ Basicity Neutral Hydrophobicity 0.501 Hydrophathy Index -0.4 Isoelectric Point 6.06 pKa (α-COOH) 2.35 pKa (α-NH <sub>2</sub> ) 9.78 Canonical SMILES <chem>NCC(=O)O</chem> PubChem CID 750	 Chemical Formula C <sub>6</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub> Molecular Weight 155.15 Da Polarity Polar Acidity/ Basicity Basic (Weak) Hydrophobicity 0.165 Hydrophathy Index -3.2 Isoelectric Point 7.60 pKa (α-COOH) 1.80 pKa (α-NH <sub>2</sub> ) 9.33 Canonical SMILES <chem>NC(Cc1c[nH]c1)C(=O)O</chem> PubChem CID 773	 Chemical Formula C <sub>6</sub> H <sub>13</sub> NO <sub>2</sub> Molecular Weight 131.17 Da Polarity Nonpolar Acidity/ Basicity Neutral Hydrophobicity 0.943 Hydrophathy Index 4.5 Isoelectric Point 6.05 pKa (α-COOH) 2.32 pKa (α-NH <sub>2</sub> ) 9.76 Canonical SMILES <chem>CCC(C)C(N)C(=O)O</chem> PubChem CID 791
<b>K</b> L-Lysine <sup>LYS</sup>	<b>L</b> L-Leucine <sup>LEU</sup>	<b>M</b> L-Methionine <sup>MET</sup>	<b>N</b> L-Asparagine <sup>ASN</sup>
 Chemical Formula C <sub>6</sub> H <sub>11</sub> N <sub>3</sub> O <sub>2</sub> Molecular Weight 146.19 Da Polarity Polar Acidity/ Basicity Basic Hydrophobicity 0.283 Hydrophathy Index -3.9 Isoelectric Point 9.60 pKa (α-COOH) 2.16 pKa (α-NH <sub>2</sub> ) 9.06 Canonical SMILES <chem>NCCCCC(N)C(=O)O</chem> PubChem CID 866	 Chemical Formula C <sub>6</sub> H <sub>13</sub> NO <sub>2</sub> Molecular Weight 131.18 Da Polarity Nonpolar Acidity/ Basicity Neutral Hydrophobicity 0.943 Hydrophathy Index 3.8 Isoelectric Point 6.01 pKa (α-COOH) 2.33 pKa (α-NH <sub>2</sub> ) 9.74 Canonical SMILES <chem>CC(CCC(N)C(=O)O)C(=O)O</chem> PubChem CID 6106	 Chemical Formula C <sub>5</sub> H <sub>11</sub> NO <sub>2</sub> S Molecular Weight 149.21 Da Polarity Nonpolar Acidity/ Basicity Neutral Hydrophobicity 0.738 Hydrophathy Index 1.9 Isoelectric Point 5.74 pKa (α-COOH) 2.13 pKa (α-NH <sub>2</sub> ) 9.28 Canonical SMILES <chem>CSCC(N)C(=O)O</chem> PubChem CID 876	 Chemical Formula C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub> Molecular Weight 132.12 Da Polarity Polar Acidity/ Basicity Neutral Hydrophobicity 0.236 Hydrophathy Index -3.5 Isoelectric Point 5.41 pKa (α-COOH) 2.14 pKa (α-NH <sub>2</sub> ) 8.72 Canonical SMILES <chem>NC(CCC(=O)N)C(=O)O</chem> PubChem CID 236
<b>P</b> L-Proline <sup>PRO</sup>	<b>Q</b> L-Glutamine <sup>GLN</sup>	<b>R</b> L-Arginine <sup>ARG</sup>	<b>S</b> L-Serine <sup>SER</sup>
 Chemical Formula C <sub>5</sub> H <sub>9</sub> NO <sub>2</sub> Molecular Weight 115.13 Da Polarity Nonpolar Acidity/ Basicity Neutral Hydrophobicity 0.711 Hydrophathy Index -1.6 Isoelectric Point 6.30 pKa (α-COOH) 1.95 pKa (α-NH <sub>2</sub> ) 10.64 Canonical SMILES <chem>OC(=O)C1CCCN1</chem> PubChem CID 614	 Chemical Formula C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub> Molecular Weight 146.14 Da Polarity Polar Acidity/ Basicity Neutral Hydrophobicity 0.251 Hydrophathy Index -3.5 Isoelectric Point 5.65 pKa (α-COOH) 2.17 pKa (α-NH <sub>2</sub> ) 9.13 Canonical SMILES <chem>NC(CCC(=O)N)C(=O)O</chem> PubChem CID 5950	 Chemical Formula C <sub>6</sub> H <sub>14</sub> N <sub>4</sub> O <sub>2</sub> Molecular Weight 174.20 Da Polarity Polar Acidity/ Basicity Basic (Strong) Hydrophobicity 0.000 Hydrophathy Index -4.5 Isoelectric Point 10.76 pKa (α-COOH) 1.82 pKa (α-NH <sub>2</sub> ) 8.99 Canonical SMILES <chem>NC(CCCNC(=O)N)C(=O)O</chem> PubChem CID 5950	 Chemical Formula C <sub>3</sub> H <sub>7</sub> NO <sub>3</sub> Molecular Weight 105.09 Da Polarity Polar Acidity/ Basicity Neutral Hydrophobicity 0.359 Hydrophathy Index -0.8 Isoelectric Point 5.68 pKa (α-COOH) 2.19 pKa (α-NH <sub>2</sub> ) 9.21 Canonical SMILES <chem>NC(CO)C(=O)O</chem> PubChem CID 617
<b>T</b> L-Threonine <sup>THR</sup>	<b>V</b> L-Valine <sup>VAL</sup>	<b>W</b> L-Tryptophan <sup>TRP</sup>	<b>Y</b> L-Tyrosine <sup>TYR</sup>
 Chemical Formula C <sub>4</sub> H <sub>9</sub> NO <sub>3</sub> Molecular Weight 119.12 Da Polarity Polar Acidity/ Basicity Neutral Hydrophobicity 0.450 Hydrophathy Index -0.7 Isoelectric Point 5.60 pKa (α-COOH) 2.09 pKa (α-NH <sub>2</sub> ) 9.10 Canonical SMILES <chem>CC(O)C(N)C(=O)O</chem> PubChem CID 6288	 Chemical Formula C <sub>5</sub> H <sub>11</sub> NO <sub>2</sub> Molecular Weight 117.15 Da Polarity Nonpolar Acidity/ Basicity Neutral Hydrophobicity 0.825 Hydrophathy Index 4.2 Isoelectric Point 6.00 pKa (α-COOH) 2.39 pKa (α-NH <sub>2</sub> ) 9.74 Canonical SMILES <chem>CC(C)C(N)C(=O)O</chem> PubChem CID 1182	 Chemical Formula C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> Molecular Weight 204.23 Da Polarity Nonpolar Acidity/ Basicity Neutral Hydrophobicity 0.878 Hydrophathy Index -0.9 Isoelectric Point 5.89 pKa (α-COOH) 2.46 pKa (α-NH <sub>2</sub> ) 9.41 Canonical SMILES <chem>NC(C1=CC=C2C(=C1)C(=CN2)C)C(=O)O</chem> PubChem CID 6305	 Chemical Formula C <sub>9</sub> H <sub>9</sub> NO <sub>3</sub> Molecular Weight 181.19 Da Polarity Nonpolar Acidity/ Basicity Neutral Hydrophobicity 0.880 Hydrophathy Index -1.3 Isoelectric Point 5.64 pKa (α-COOH) 2.20 pKa (α-NH <sub>2</sub> ) 9.21 Canonical SMILES <chem>NC(Cc1ccc(O)cc1)C(=O)O</chem> PubChem CID 1553
<b>B</b> L-Asparagine or L-Aspartic Acid <sup>ASX</sup>	<b>J</b> L-Leucine or L-Isoleucine <sup>XLE</sup>	<b>X</b> Unspecified or Unknown <sup>XAA</sup>	<b>Z</b> L-Glutamine or L-Glutamic Acid <sup>GLX</sup>

Essential amino acids are denoted with yellow spots. Polarity refers to Side Chain Polarity. Acidity/Basicity refer to Side Chain Acidity/Basicity.

2D Structure Generation, 3D optimization: ChemSketch 8.17 (ACD Labs) | 3D Structure Rendering: PyMol 0.99rc6 (DeLano Scientific) | Chemical Formula and Molecular Weight Calculations: ChemSketch 8.17 (ACD Labs) | Hydrophobicity values: Analytical Biochemistry 193:11, 72-82, Elsevier, 1991. | Hydrophathy Index values: J. Mol. Biol. (1982) 157, 105-132. | Canonical SMILES: [www.jmg.ch.cam.ac.uk/data/molecules/smilesindex.html](http://www.jmg.ch.cam.ac.uk/data/molecules/smilesindex.html) | Polarity, Acidity/Basicity, Isoelectric Point, pKa, CAS, PubChem CID data: [en.wikipedia.org/wiki/List\\_of\\_standard\\_amino\\_acids](http://en.wikipedia.org/wiki/List_of_standard_amino_acids) | List of Essential Amino Acids: [en.wikipedia.org/wiki/Amino\\_acid](http://en.wikipedia.org/wiki/Amino_acid) | Typeface: Meta Book

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