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## Metabolomics

## Amino Acids Reference Chart

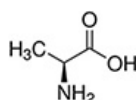


Hydrophobic - aliphatic  
Hydrophobic - aromatic  
Neutral - polar side chains  
Acidic

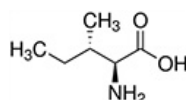
Basic  
Unique  
Properties of Common Amino Acids  
Hydrophobicity Index

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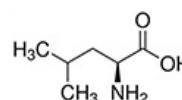
## Amino Acids with Hydrophobic Side Chain – Aliphatic



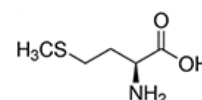
**Alanine, Ala, A**



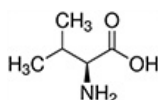
**Isoleucine, Ile, I**



**Leucine, Leu, L**

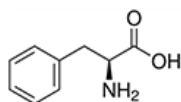


**Methionine, Met, M**

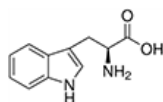


**Valine, Val, V**

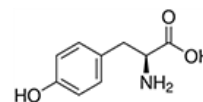
## Amino Acids with Hydrophobic Side Chain – Aromatic



**Phenylalanine, Phe, F**

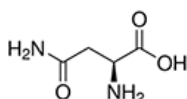


**Tryptophan, Trp, W**

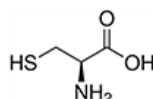


**Tyrosine, Tyr, Y**

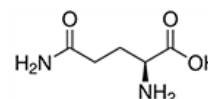
## Amino Acids with Polar Neutral Side Chains



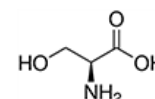
**Asparagine, Asn, N**



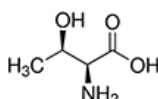
**Cysteine, Cys, C**



**Glutamine, Gln, Q**

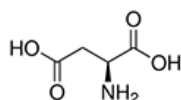


**Serine, Ser, S**

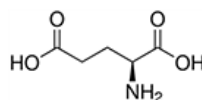


**Threonine, Thr, T**

## Amino Acids with Electrically Charged Side Chains – Acidic



**Aspartic acid, Asp, D**



**Glutamic acid, Glu, E**

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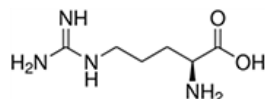
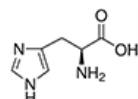
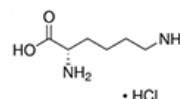
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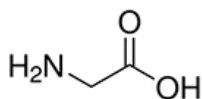
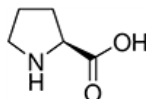
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## Amino Acids with Electrically Charged Side Chains – Basic

**Arginine, Arg, R****Histidine, His, H****Lysine, Lys, K**

## Unique Amino Acids

**Glycine, Gly, G****Proline, Pro, P**

## Properties of Common Amino Acids

Name	3-Letter Symbol	1-Letter Symbol	Molecular Weight	Molecular Formula	Residue Formula	Residue Weight (-H <sub>2</sub> O)	pKa <sup>1</sup>	pKb <sup>2</sup>	pKx <sup>3</sup>	pI <sup>4</sup>
Alanine	Ala	A	89.10	C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub>	C <sub>3</sub> H <sub>5</sub> NO	71.08	2.34	9.69	–	6.00
Arginine	Arg	R	174.20	C <sub>6</sub> H <sub>14</sub> N <sub>4</sub> O <sub>2</sub>	C <sub>6</sub> H <sub>12</sub> N <sub>4</sub> O	156.19	2.17	9.04	12.48	10.76
Asparagine	Asn	N	132.12	C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub>	C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>	114.11	2.02	8.80	–	5.41
Aspartic acid	Asp	D	133.11	C <sub>4</sub> H <sub>7</sub> NO <sub>4</sub>	C <sub>4</sub> H <sub>5</sub> NO <sub>3</sub>	115.09	1.88	9.60	3.65	2.77
Cysteine	Cys	C	121.16	C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub> S	C <sub>3</sub> H <sub>5</sub> NOS	103.15	1.96	10.28	8.18	5.07
Glutamic acid	Glu	E	147.13	C <sub>5</sub> H <sub>9</sub> NO <sub>4</sub>	C <sub>5</sub> H <sub>7</sub> NO <sub>3</sub>	129.12	2.19	9.67	4.25	3.22
Glutamine	Gln	Q	146.15	C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub>	C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub>	128.13	2.17	9.13	–	5.65
Glycine	Gly	G	75.07	C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub>	C <sub>2</sub> H <sub>3</sub> NO	57.05	2.34	9.60	–	5.97
Histidine	His	H	155.16	C <sub>6</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub>	C <sub>6</sub> H <sub>7</sub> N <sub>3</sub> O	137.14	1.82	9.17	6.00	7.59
Hydroxyproline	Hyp	O	131.13	C <sub>5</sub> H <sub>9</sub> NO <sub>3</sub>	C <sub>5</sub> H <sub>7</sub> NO <sub>2</sub>	113.11	1.82	9.65	–	–
Isoleucine	Ile	I	131.18	C <sub>6</sub> H <sub>13</sub> NO <sub>2</sub>	C <sub>6</sub> H <sub>11</sub> NO	113.16	2.36	9.60	–	6.02
Leucine	Leu	L	131.18	C <sub>6</sub> H <sub>13</sub> NO <sub>2</sub>	C <sub>6</sub> H <sub>11</sub> NO	113.16	2.36	9.60	–	5.98
Lysine	Lys	K	146.19	C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>	C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> O	128.18	2.18	8.95	10.53	9.74
Methionine	Met	M	149.21	C <sub>5</sub> H <sub>11</sub> NO <sub>2</sub> S	C <sub>5</sub> H <sub>9</sub> NOS	131.20	2.28	9.21	–	5.74
Phenylalanine	Phe	F	165.19	C <sub>9</sub> H <sub>11</sub> NO <sub>2</sub>	C <sub>9</sub> H <sub>9</sub> NO	147.18	1.83	9.13	–	5.48
Proline	Pro	P	115.13	C <sub>5</sub> H <sub>9</sub> NO <sub>2</sub>	C <sub>5</sub> H <sub>7</sub> NO	97.12	1.99	10.60	–	6.30
Pyroglutamic	Glp	U	139.11	C <sub>5</sub> H <sub>7</sub> NO <sub>3</sub>	C <sub>5</sub> H <sub>5</sub> NO <sub>2</sub>	121.09	–	–	–	5.68
Serine	Ser	S	105.09	C <sub>3</sub> H <sub>7</sub> NO <sub>3</sub>	C <sub>3</sub> H <sub>5</sub> NO <sub>2</sub>	87.08	2.21	9.15	–	5.68
Threonine	Thr	T	119.12	C <sub>4</sub> H <sub>9</sub> NO <sub>3</sub>	C <sub>4</sub> H <sub>7</sub> NO <sub>2</sub>	101.11	2.09	9.10	–	5.60
Tryptophan	Trp	W	204.23	C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>	C <sub>11</sub> H <sub>10</sub> N <sub>2</sub> O	186.22	2.83	9.39	–	5.89
Tyrosine	Tyr	Y	181.19	C <sub>9</sub> H <sub>11</sub> NO <sub>3</sub>	C <sub>9</sub> H <sub>9</sub> NO <sub>2</sub>	163.18	2.20	9.11	10.07	5.66
Valine	Val	V	117.15	C <sub>5</sub> H <sub>11</sub> NO <sub>2</sub>	C <sub>5</sub> H <sub>9</sub> NO	99.13	2.32	9.62	–	5.96

<sup>1</sup> pKa is the negative of the logarithm of the dissociation constant for the -COOH group.<sup>2</sup> pKb is the negative of the logarithm of the dissociation constant for the -NH<sub>3</sub> group.<sup>3</sup> pKx is the negative of the logarithm of the dissociation constant for any other group in the molecule.<sup>4</sup> pI is the pH at the isoelectric point.Reference: D.R. Lide, *Handbook of Chemistry and Physics, 72nd Edition*, CRC Press, Boca Raton, FL, 1991.

Hydrophobicity Index for Common Amino Acids

The hydrophobicity index is a measure of the relative hydrophobicity, or how soluble an amino acid is in water. In a protein, hydrophobic amino acids are likely to be found in the interior, whereas hydrophilic amino acids are likely to be in contact with the aqueous environment.

The values in the table below are normalized so that the most hydrophobic residue is given a value of 100 relative to glycine, which is considered neutral (0 value). The scales were extrapolated to residues which are more hydrophilic than glycine.

At pH 2 <sup>A</sup>		At pH 7 <sup>B</sup>	
Very Hydrophobic			
Leu	100	Phe	100
Ile	100	Ile	99
Phe	92	Trp	97
Trp	84	Leu	97
Val	79	Val	76
Met	74	Met	74
Hydrophobic			
Cys	52	Tyr	63
Tyr	49	Cys	49
Ala	47	Ala	41
Neutral			
Thr	13	Thr	13
Glu	8	His	8
Gly	0	Gly	0
Ser	-7	Ser	-5
Gln	-18	Gln	-10
Asp	-18		
Hydrophilic			
Arg	-26	Arg	-14
Lys	-37	Lys	-23
Asn	-41	Asn	-28
His	-42	Glu	-31
Pro	-46	Pro	-46 (used pH 2)
		Asp	-55

<sup>A</sup>pH 2 values: Normalized from Sereda et al., *J. Chrom.* 676: 139-153 (1994).

<sup>B</sup>pH 7 values: Monera et al., *J. Protein Sci.* 1: 319-329 (1995).

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[Growth of human stem cell-derived neurons on solid three-dimensional polymers.](#)  
Hayman MW1, Smith KH, Cameron NR, Przyborski SA.  
2005 Mar 31;62(3):231-40. Epub 2004 Dec 30.  
Understanding neural differentiation and the development of complex neurite networks in three-dimensional matrices is critical for neural tissue engineering in vitro. In this study we describe for the first time the growth of human stem cell-derived neurons on solid polystyrene matrices coated with bioactive molecules. Highly  
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[read abstract](#)[Resveratrol attenuates the expression of HMG-CoA reductase mRNA in hamsters.](#)

Cho JJ, Ahn JY, Kim S, Choi MS, Ha TY.

2008 Feb 29;367(1):190-4. doi: 10.1016/j.bbrc.2007.12.140. Epub 2007 Dec 31.

We investigated the hypolipidemic effect of resveratrol focused on the mRNA expression and hepatic HMG-CoA reductase (HMGR) activity in hamsters fed a high-fat diet. Male Syrian Golden hamsters were fed a high-fat diet containing 0.025% fenofibrate or 0.025% resveratrol for 8 weeks. The concentrations of serum total cholesterol [Read More](#)

[read abstract](#)[The slice overlay assay: a versatile tool to study the influence of extracellular signals on neuronal development.](#)

Polleux F1, Ghosh A.

2002 Jun 11;2002(136):p19.

We have developed a technique that allows characterization and identification of extracellular signals that regulate various aspects of neuronal differentiation. In this in vitro assay, dissociated cells isolated from the developing cerebral wall are labeled and cultured over organotypic cortical slices. We have used this slice [Read More](#)

[read abstract](#)[Brain edema in acute liver failure: inhibition by L-histidine.](#)

Rama Rao KV1, Reddy PV, Tong X, Norenberg MD.

2010 Mar;176(3):1400-8. doi: 10.2353/ajpath.2010.090756. Epub 2010 Jan 14.

Brain edema and the associated increase in intracranial pressure are potentially lethal complications of acute liver failure (ALF). Astrocyte swelling (cytotoxic edema) represents a significant component of the brain edema in ALF, and elevated blood and brain ammonia levels have been strongly implicated in its formation. We earl[Read More](#)

[read abstract](#)[Improved biocytin labeling and neuronal 3D reconstruction.](#)

Marx M1, Günter RH, Hucko W, Radnikow G, Feldmeyer D.

2012 Feb 2;7(2):394-407. doi: 10.1038/nprot.2011.449.


In this report, we describe a reliable protocol for biocytin labeling of neuronal tissue and diaminobenzidine (DAB)-based processing of brain slices. We describe how to embed tissues in different media and how to subsequently histochemically label the tissues for light or electron microscopic examination. We provide a detailed [Read More](#)

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