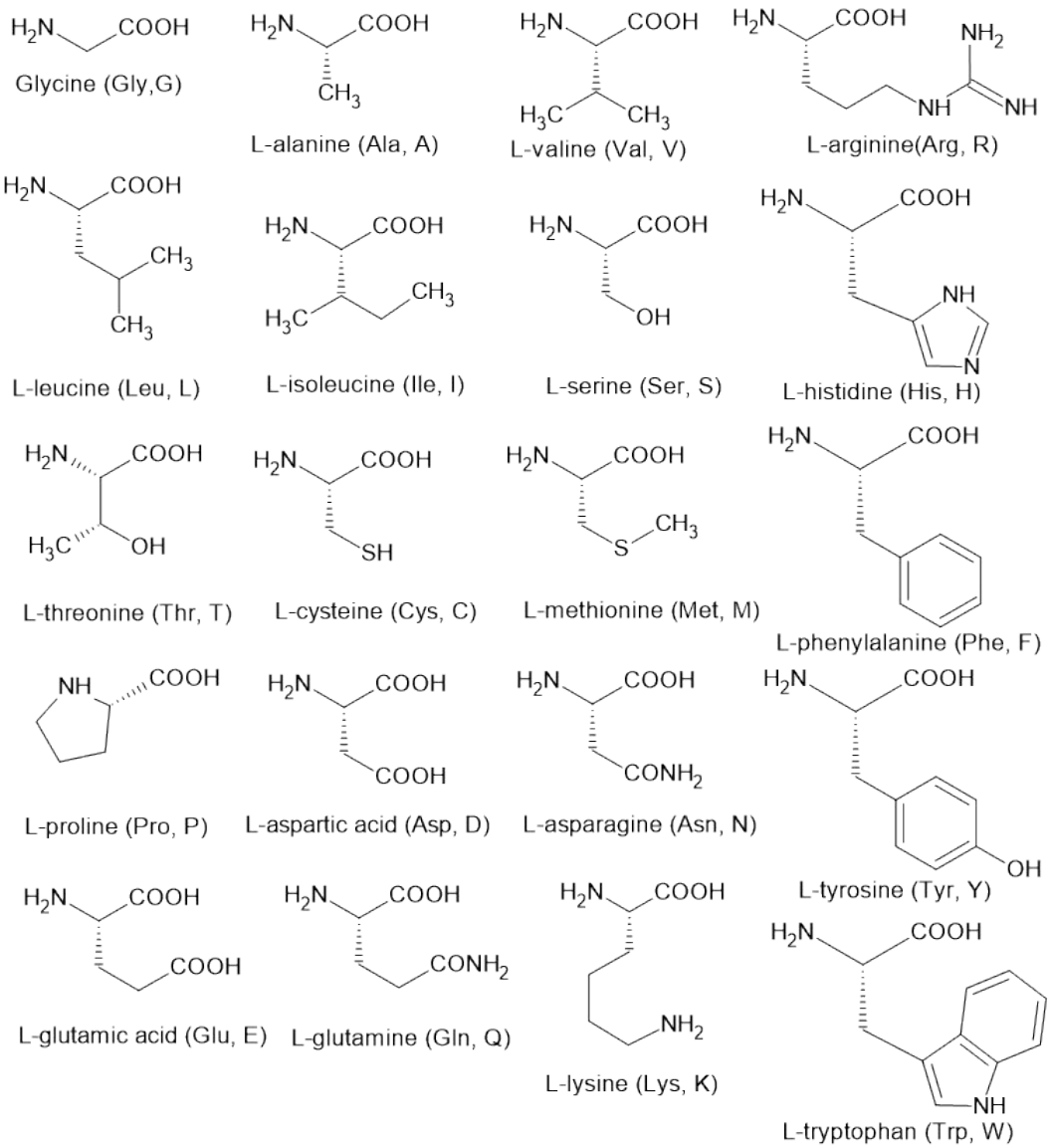
MCULE AMINO ACID LIBRARY

THE MCULE AMINO ACID LIBRARY WAS ESTABLISHED TO AID PEPTIDE SYNTHESIS PROJECTS BY COLLECTING THE DERIVATIVES OF 22 AMINO ACIDS ILLUSTRATED BELOW.

To define the derivatives, we applied the following methodology:

- The NH and COOH ends can be substituted.
- The heteroatoms of the side chains may be substituted.
- Chain member carbon atoms cannot be substituted.
- Sidechain rings (Pro, Phe, Tyr, Trp, Hisl) are allowed to be substituted on any ring atoms, including the carbons.

FILTERED AMINO ACIDS WITH ABBREVIATIONS:



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The molecules were further filtered against more than 600 SMARTS-based structural filters, including PAINS[1,2], and other MedChem filters[3] to eliminate chemical functions enhancing true positive hits during screening.

Click **here** to access the downloadable data file of Mcule Amino Acid Library. This ZIP file contains a file for each of the amino acid derivatives in SMILES format (*SMILES ID*). If you would prefer other molecular format or further filtering contact us at support@mcule.com.

Additionally, our professional laboratory services include:

- Transferring samples to plates/vials as solid or DMSO solution,
- Solubility characterization,
- Temperature controlled shipping,
- Quality control via LC-MS & NMR (on demand).

Please also reach out to our cheminformatics experts with projects related to:

- Screening library building/expansion,
- Generation of synthetically feasible chemical spaces based on your building blocks,
- Filtering the Mcule database based on your criteria.

Mcule's Custom Solution Experts are ready to guide you through the selection and ordering process free of charge! If you have any questions or need any help, please feel free to contact us at **support@mcule.com.**

REFERENCES

[1] New Substructure Filters for Removal of Pan Assay Interference Compounds (PAINS) from Screening Libraries and for Their Exclusion in Bioassays, Baell, J. B. & Holloway, G. A., *J. Med. Chem.* **2010**, 53 (7) 2719–2740.

[2] KNIME Workflow to Assess PAINS Filters in SMARTS Format . Comparison of RDKit and Indigo Cheminformatics Libraries., Saubern, S., Guha, R. & Baell, J. B., *Mol. Inform.* **2011**, 30 (10) 847–850.

[3] An Empirical Process for the Design of High-Throughput Screening Deck Filters, Pearce, B. C., Sofia, M. J., Good, A. C., Drexler, D. M. & Stock, D. A., *J. Chem. Inf. Model.* **2006,** 46 (3) 1060–1068.