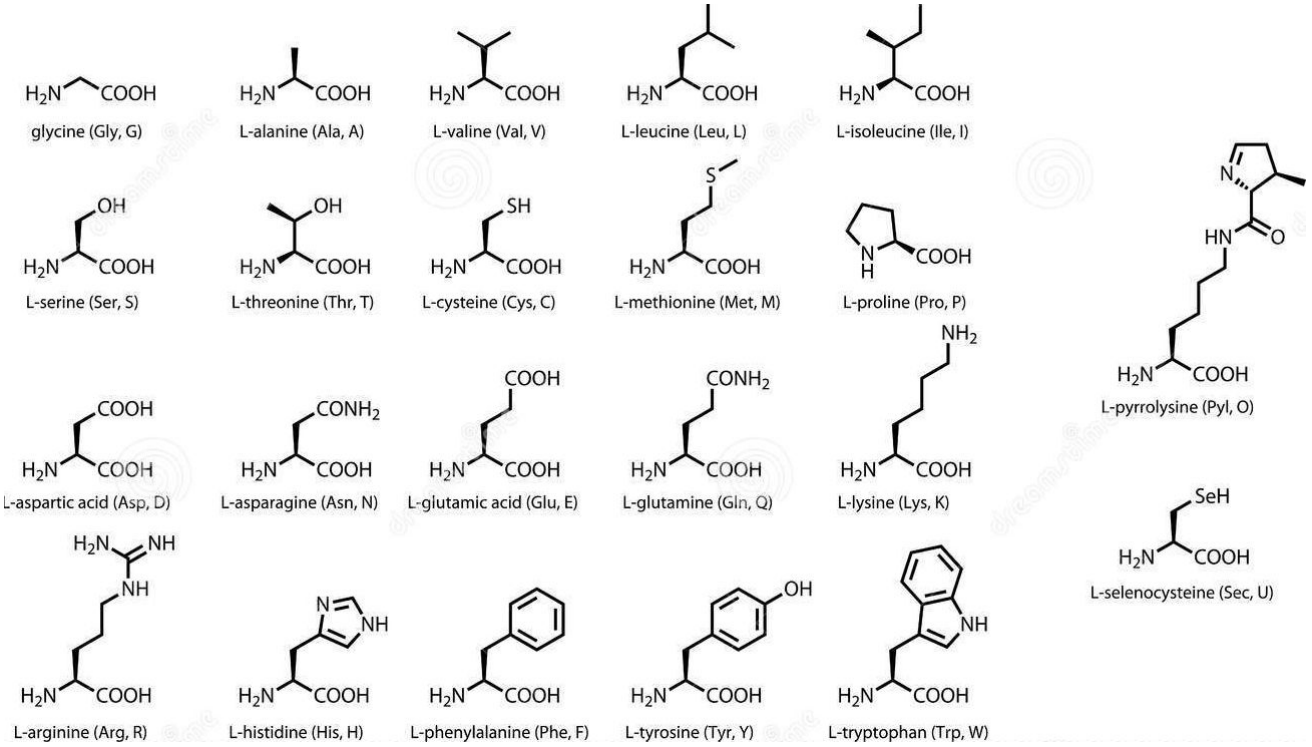
MCULE - AMINO ACID LIBRARY

The library contains the derivatives of the following 22 amino acids in separate files referenced by their 3-character codes.



https://www.dreamstime.com/royalty-free-stock-image-22-standard-amino-acids-chemical-structures-image25479916

The derivatives were defined as follows:

The NH and COOH ends may be substituted.

The heteroatoms of the side chains may be substituted

The carbon atoms cannot be substituted if they form a chain.

Sidechain rings (Pro, Phe, Tyr, Trp, His, Pyl) are allowed to be substituted on any ring atoms, including the carbons.

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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] rules.

The tar file contains a file for each of the amino acid derivatives in SMILES (SMILES ID) format.

If you would prefer other molecular format or further filtering - feel free to contact us at support@mcule.com.

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

1, Baell, J. B. & Holloway, G. A. New Substructure Filters for Removal of Pan Assay Interference Compounds (PAINS) from Screening Libraries and for Their Exclusion in Bioassays. J. Med. Chem. 2719–2740 (2010).
2, Saubern, S., Guha, R. & Baell, J. B. KNIME Workflow to Assess PAINS Filters in SMARTS Format . Comparison of RDKit and Indigo Cheminformatics Libraries. Mol. Inform. 30, 847–850 (2011).
3, Pearce, B. C., Sofia, M. J., Good, A. C., Drexler, D. M. & Stock, D. A. An Empirical Process for the Design of High-Throughput Screening Deck Filters. 1060–1068 (2006).