

# Mcule Functional Group Annotated Library

Mcule Functional Group Annotated Library is a unique subset of the Mcule Full Database containing molecules possessing specific functional groups. We have **annotated 23 reaction sites** and **counted the occurrence of these functions** in the molecules.

## List of the annotated reaction sites:

- Carboxylic acid
  - Aldehyde
  - Aryl halide
  - Alkyne
  - Amine
  - Methyl-ester
  - Ethyl-ester
  - N-Boc
- N-FMoc
  - Aromatic alcohol
  - Boronate
  - Isocyanate
  - Primary aliphatic amine
  - Primary aromatic amine
  - Secondary aliphatic amine
  - Secondary aromatic amine
- Sulfinyl-chloride
  - Sulfinyl-halide
  - N-Cbz
  - N-Benzyl-amine
  - Aryl-pseudohalide
  - Nitro
  - Azide

The Mcule Functional Group Annotated Library is accessible in a CSV file. The molecules are represented in the following format: each row belongs to one molecule, the columns contain SMILES, Mcule ID, and the number of the specific functional group in the given molecule, separated by “,” characters respectively.

SMILES	Mcule_ID	No. <i>Carboxylic acid</i> site	No. <i>Aldehyde</i> sites	...
--------	----------	---------------------------------	---------------------------	-----

If you prefer another molecular format or further filtering, please contact us at [support@mcule.com](mailto: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