# MCULE **DNA-ENCODED LIBRARY** COMPATIBLE INSTOCK BUILDING BLOCK COLLECTION

**The library was created from Mcule Instock database by selecting BB's that have reactive sites suitable for DEL synthesis.**

**In the '2RS' files you can find BB's with two reactive sites of the functional groups listed below. Each combination is in a separate file.**

Aldehyde_Nitro

Amine_N-Cbz-Amino

Azide_Aryl-halide

Carboxylic-acid_Aryl-halide

Carboxylic-acid_Terminal-alkyne

N-Boc-Amino_Aldehyde

Amine_Aryl-halide

Amine_N-Fmoc-Amino

Azide_Sulfonyl-halide

Carboxylic-acid_Aryl-pseudohalide

Ester_Aldehyde

N-Boc-Amino_Carboxylic-acid

Amine_Ester

Amine_N-benzyl-amine

Boronate_Aldehyde

Carboxylic-acid_Isothiocyanate

Ester_Isocyanate

N-Cbz-Amino_Carboxylic-acid

Amine_N-Boc-Amino  Azide_Aldehyde

Boronate_Carboxylic-acid

Carboxylic-acid_Nitro

Ester_Sulfonyl-halide

Sulfonyl-halide_Aldehyde

**In the '3RS' files you can find BB's with three reactive sites of the functional groups listed below. Each combination is in a separate file.**

Amine_Aryl-halide_N-Boc-Amino

Aryl-halide_N-Fmoc-Amino_Carboxylic-acid

Carboxylic-acid_Aryl-halide_Nitro

N-Boc-Amino_N-Cbz-Amino_Carboxylic-acid

Terminal-alkyne_N-Boc-Amino_Carboxylic-acid

Amine_Aryl-halide_Nitro

Carboxylic-acid_Aldehyde_Nitro

Carboxylic-acid_Ester_Nitro

Nitro_N-Boc-Amino_Carboxylic-acid

Aryl-halide_N-Boc-Amino_Carboxylic-acid

Carboxylic-acid_Aryl-halide_Ester

Ester_N-Fmoc-Amino_Carboxylic-acid

Nitro_N-Fmoc-Amino_Carboxylic-acid

**The 'Ro3' folder contains fragments that furthermore fulfill the Ro3 criterias (see below).**

| Property | Min | Max |
|---|---|---|
| Molar mass | - | 300 |
| H-bond acceptors | - | 3 |
| H-bond donors | - | 3 |
| Rotatable bonds | - | 3 |

All the files contain the molecules 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