

# MCULE - DNA ENCODED LIBRARY COMPATIBLE BUILDING BLOCK COLLECTION

**The library was created from Mcule full 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_Ester
Amine_N-Cbz-Amino	Amine_N-benzyl-amine
Azide_Aryl-halide	Boronate_Aldehyde
Carboxylic-acid_Aryl-halide	Carboxylic-acid_Isothiocyanate
Carboxylic-acid_Terminal-alkyne	Ester_Isocyanate
N-Boc-Amino_Aldehyde	N-Cbz-Amino_Carboxylic-acid
Amine_Aryl-halide	Amine_N-Boc-Amino Azide_Aldehyde
Amine_N-Fmoc-Amino	Boronate_Carboxylic-acid
Azide_Sulfonyl-halide	Carboxylic-acid_Nitro
Carboxylic-acid_Aryl-pseudohalide	Ester_Sulfonyl-halide
Ester_Aldehyde	Sulfonyl-halide_Aldehyde
N-Boc-Amino_Carboxylic-acid	

**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](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