Molecular Descriptors and Filters

Chemspace Virtual Screening Services

CHEMSPACE
Delivering Discovery Solutions®

Descriptors

Physicochemical descriptors (chem-space.com/search)

- Molecular weight
- Heavy atom count
- LogP
- Number of rotatable bonds
- Number of HB donors
- Number of HB acceptors
- Rings count
- FSP3
- TPSA

Filters

Structure Filters we use

- QED
- PAINS
- BRENK
- NIH
- ZINC
- LILLY
- Other

OUTPUT

What do we offer?

- Generation (prediction) of various physicochemical descriptors for a set of compounds
- Generation (prediction) various medicinally relevant physical chemical properties for your compounds set
- Preparation of libraries with given specific criteria (e.g., compounds that cross BBB)
- Compound libraries, tailored for your needs and complying with the commonly used MedChem filters (i.e., PAINS, LILLY, etc.)

MISSION

Applying Molecular Descriptors and Structure Filters on large datasets makes it faster to search for promising lead compounds and hence facilitates the decision-making process