FREEDOM SPACE 3.0

Freedom to explore.

Access data

Freedom Space 3.0

Database in SMILES format sorted by Heavy Atom Count.

Access options:

Protocol: FTPS/sFTP

Host: ftp2-rdb-fr.chem-space.com

User user3

Password 5P29cK73cDgre9DK

Folder FreedomSpace_3_HAC

Virtual screening of ultra-large databases is a very challenging process. Besides that, the synthesis of hit compounds is usually expensive or even impossible due to the complexity of the molecules.
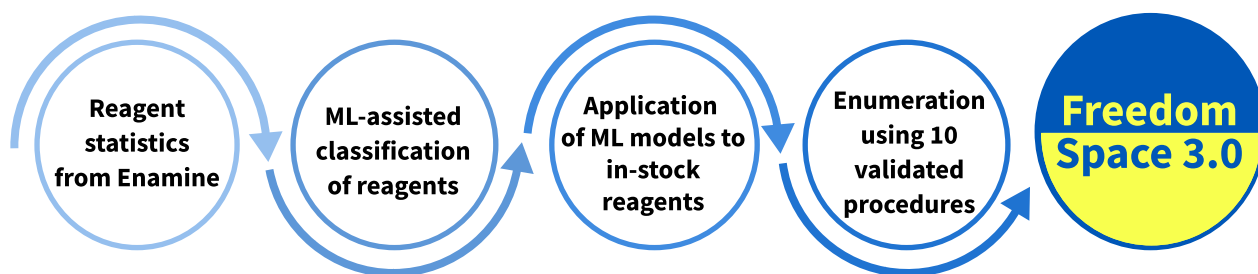
To address this issue, we introduce **Freedom Space 3.0** – a diverse collection of 5B molecules, that can be synthesized for you on-demand within 4-5 weeks. It is a valuable addition to Enamine REAL Space.

Space generation

Freedom Space 3.0 is unique space that was created using machine learning (ML) based filters, that were trained on the reaction success data from Enamine.

First, a collection of in-stock building blocks from several suppliers was created, the blocks were filtered using ML models and combined utilizing 10 well-validated chemical transformations. The process is visualized in the graphic below.

ML-Assisted Space Generation

Reagent statistics from Enamine → ML-assisted classification of reagents → Application of ML models to in-stock reagents → Enumeration using 10 validated procedures → **Freedom Space 3.0**

Benefits of Freedom Space 3.0:

- Unique space of molecules
- Competitive compound pricing
- High synthesis success rate
- Lead time 4-5 weeks.

Space application

PRODUCT WORKFLOW

Freedom Space

SAR

Virtual Screening 50-200 hits

Delivery of reagents required for the hit molecules to CRO(s)

Wet screening

Synthesis of the hits by CRO(s)