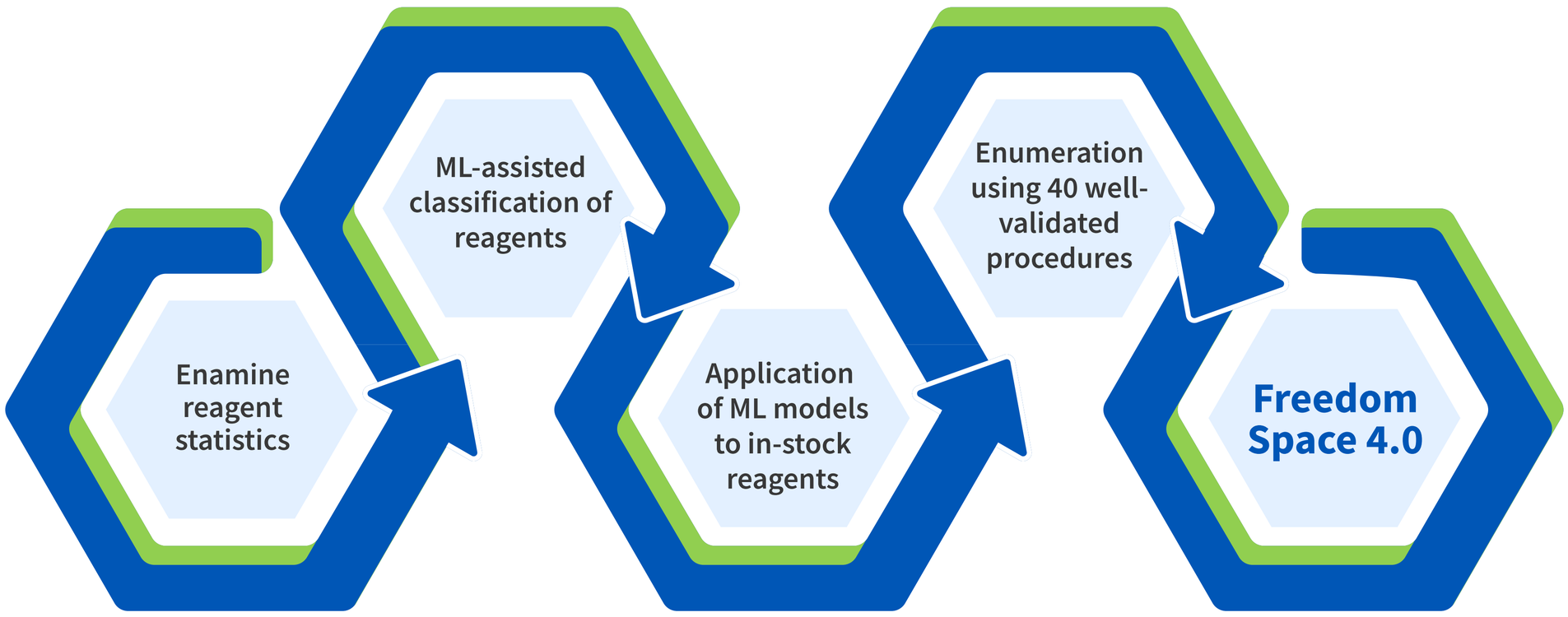
# Freedom Space 4.0

**Freedom to explore.**

CHEM SPACE
Delivering Discovery Solutions®

Freedom Space 4.0 is an ultra-large chemical space designed to facilitate your hit discovery workflows by solving the problem of synthetic accessibility. The specialty of this product is the use of Machine Learning (ML) based filters, that were trained on the reaction success data from Enamine. The latest version – Freedom Space 4.0 includes 142 billion molecules, that can be synthesized in 4-6 weeks with a high success rate.

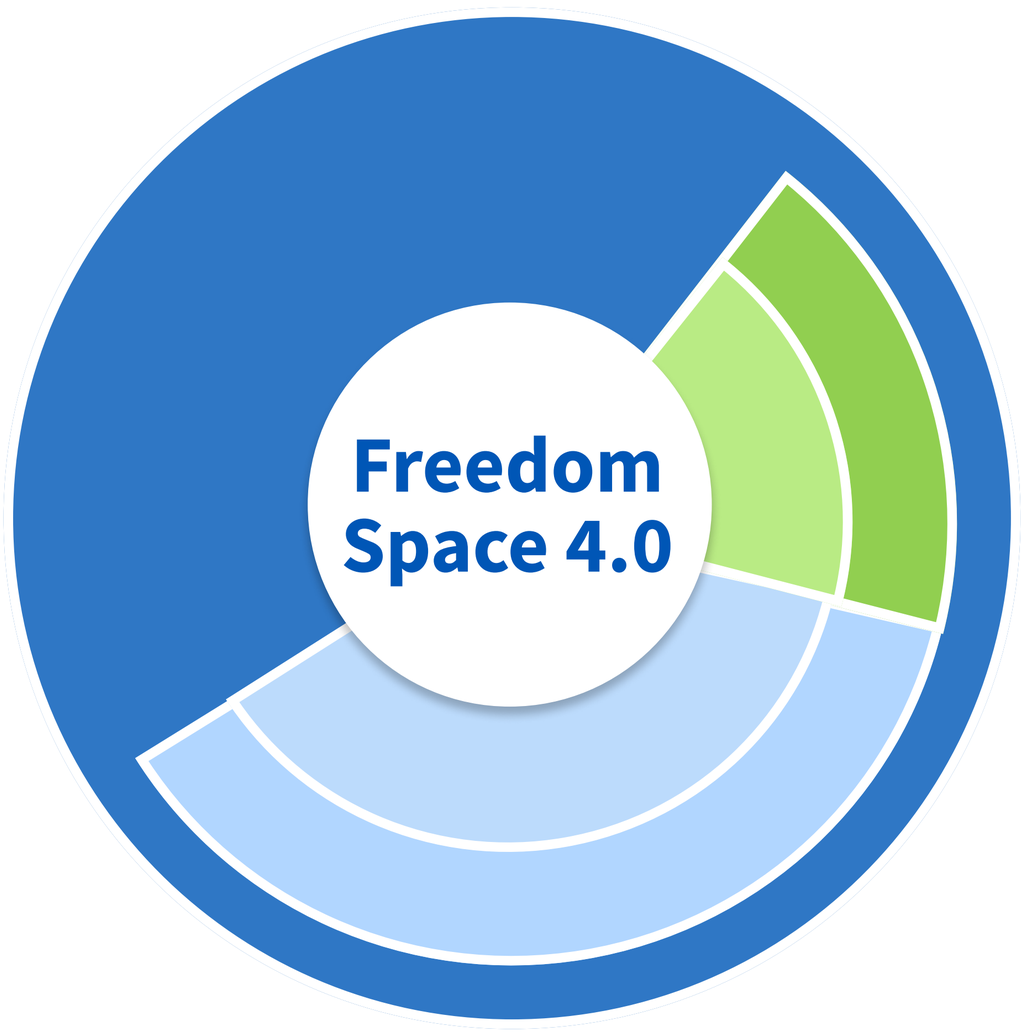
## Space Generation




- ✓ Unique space of 142 billion compounds complementary to Enamine REAL
- ✓ Available as a synthon-based and enumerated spaces
- ✓ Lead time 4-6 weeks
- ✓ Over 80% synthesis success rate
- ✓ Competitive pricing

## What do we offer?

- **Synthon-based space**
  142 billion molecules
- **Rule of Five (Ro5) Enumerated Space**
  20 billion drug-like molecules
- **Beyond Ro5 Enumerated Space**
  68 billion Ro5-extended molecules




**Choose the most suitable subspace according to the specifics of your project!**

# Access Options

## FTP Access

Host: ftp3-rdb-fr.chem-space.com
FTP with TLS
user: user3
password: jG04EACC0yLAdHZM

## Ro5 Space

- ✓ Search for compounds from 5B subset from RO5 space on Chemspace's website (chem-space.com/search)
- ✓ 20 billion molecules from RO5 space can be downloaded using FTP.

## Beyond Ro5 Space

- ✓ 68 billion molecules from Beyond RO5 space can be downloaded using FTP.

## Synthon-based Space

- ✓ The space is available for similarity search through infiniSee by BioSolveIT.
- ✓ You can search for compounds using super-structure or similarity search option through Hyperspace developed by Alipheron.
- ✓ Freedom Space 4.0 is available for synthon-based search via RDKit library.

We also provide raw synthons and reaction files upon request to support synthon-based developments. To request the file, please contact us at sales@chem-space.com.

## Ro5 Enumerated Space

- Molecular Weight: 0-500
- Hydrogen Bond Donors: 0-5
- Hydrogen Bond Acceptors: 0-10
- LogP: ≤ 5

## Beyond Ro5 Enumerated Space

(excluding Rule of 5 molecules)

- Molecular Weight: 0-800
- Hydrogen Bond Donors: 0-8
- Hydrogen Bond Acceptors: 0-15
- LogP: ≤ 6
- Rotatable Bonds: 15