

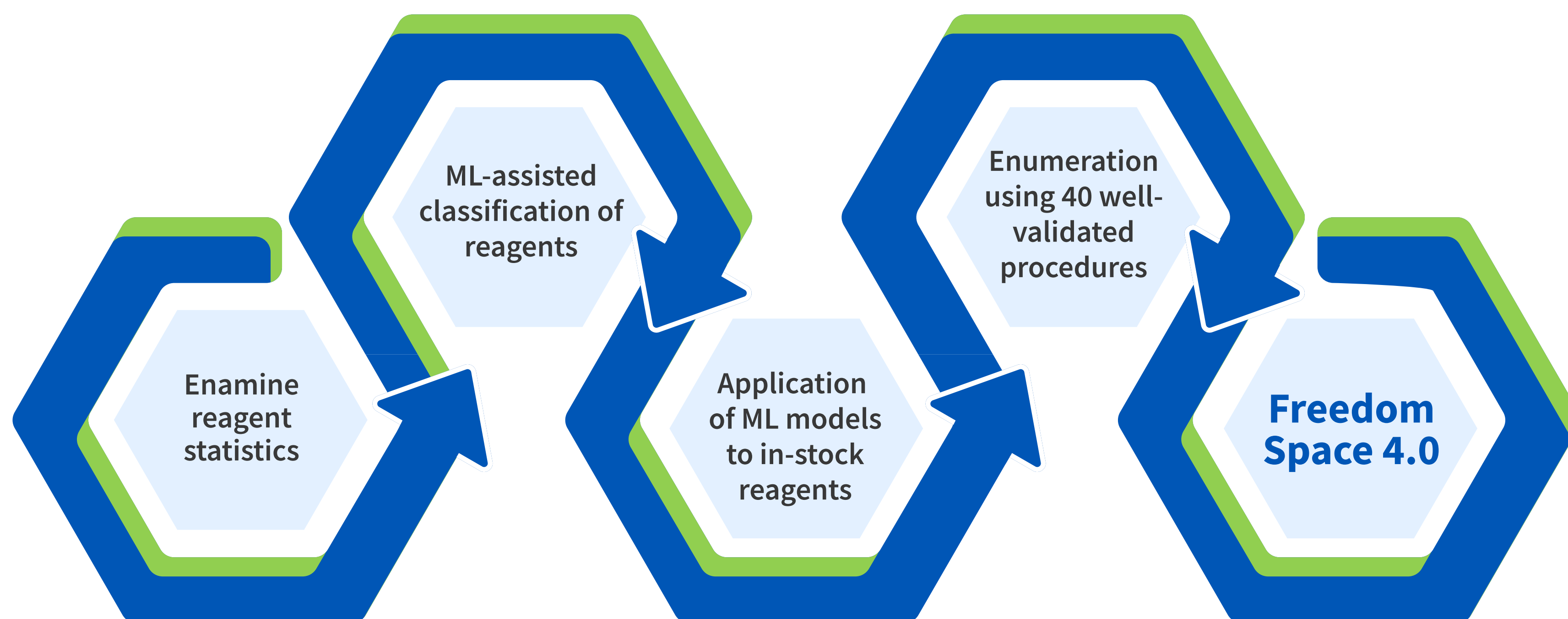
Freedom Space 4.0

Freedom to explore.

CHEM
S P A C E
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 4-5 weeks with a high success rate.

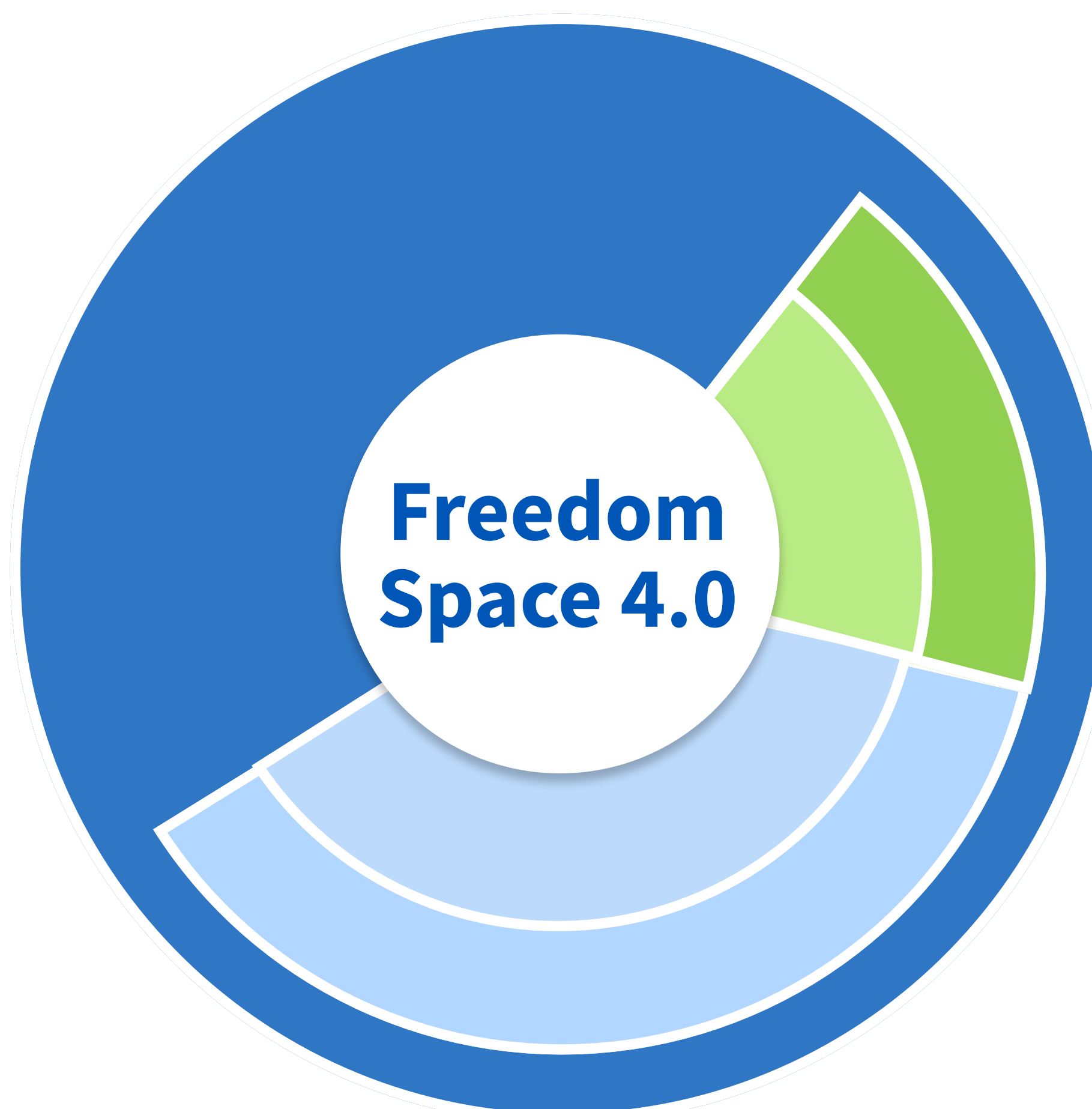
Space Generation



- ✓ Unique space of 142 billion compounds complementary to Enamine REAL
- ✓ Available as a synthon-based and enumerated spaces
- ✓ Lead time 4-5 weeks
- ✓ Over 75% synthesis success rate
- ✓ Competitive pricing

What do we offer?

- **Synthon-based space**
142 billion molecules
- **Rule of Five (Ro5)**
20 billion drug-like molecules
- **Beyond Ro5**
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)
- ✓ RO5 space can be downloaded using FTP.

Beyond Ro5 Space

- ✓ Beyond RO5 space can be downloaded using FTP.

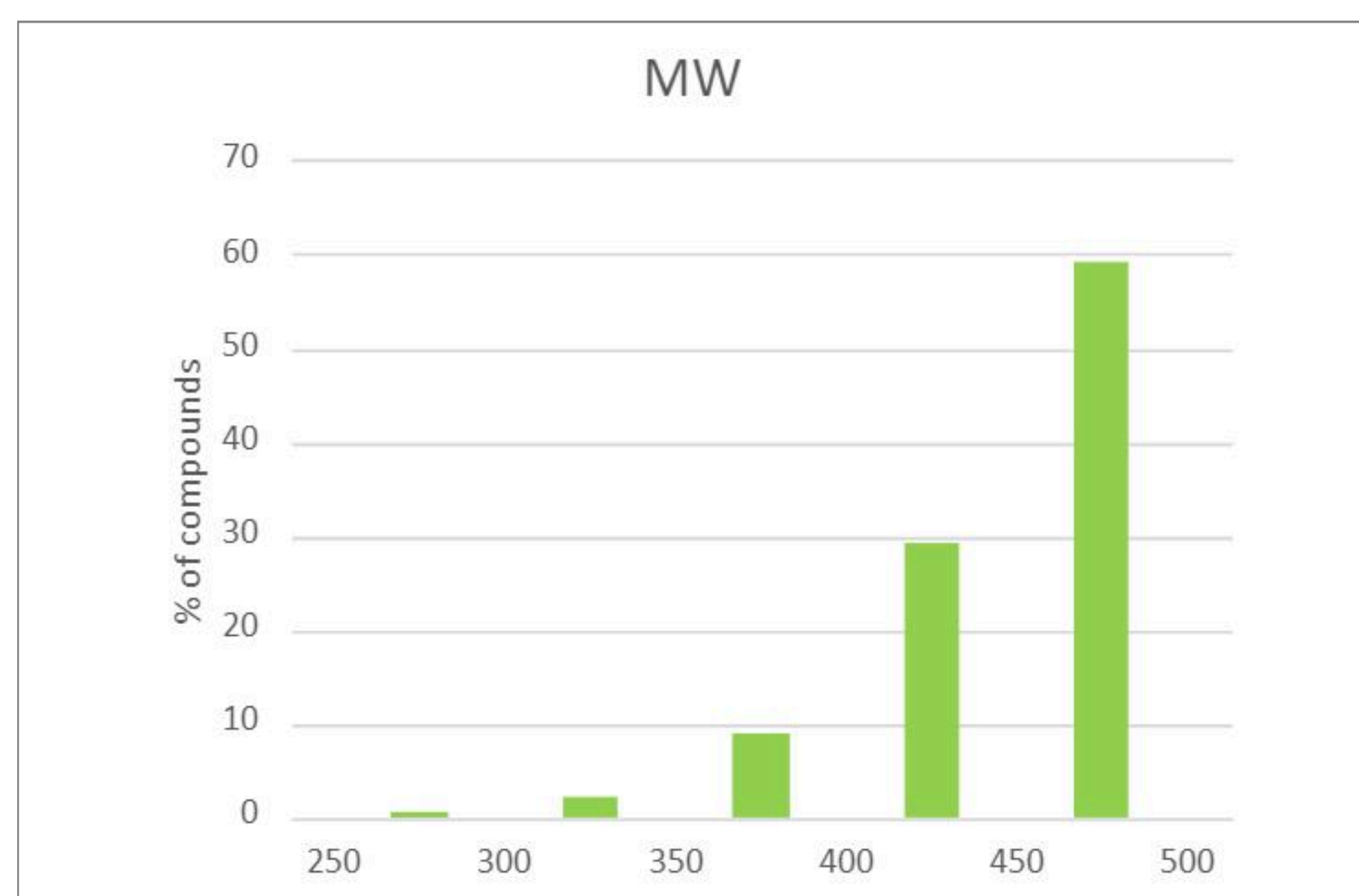
Synthon-based Space

- ✓ 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.

Rule of Five Space

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



Beyond Ro5 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

