

FREEDOM SPACE 4.0

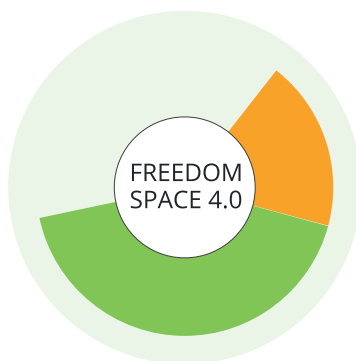
FREEDOM TO EXPLORE

Freedom Space 4.0 is an ultra-large chemical space designed to accelerate hit discovery while ensuring synthetic accessibility. The space generation workflow utilizes Machine Learning (ML) based filters trained in synthesis success data from Enamine REAL. Freedom Space 4.0 includes 142 billion molecules that can be synthesized in just 4-6 weeks with high success rate.

Synthon Space

142 billion molecules

No constraints



Ro5 Enumerated Subset

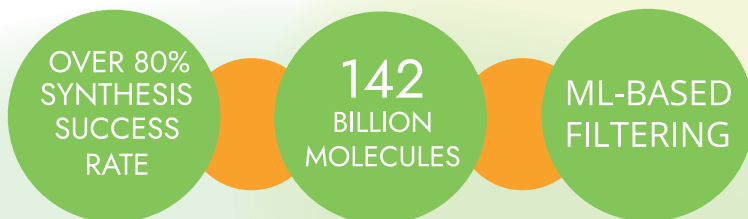
20 billion molecules

- Molecular weight: 0-500
- Hydrogen bond donors: 0-5
- Hydrogen bond acceptors: 0-10
- $\text{LogP} \leq 5$

Beyond Ro5 Enumerated Subset

68 billion molecules

- Molecular weight: 0-800 (Excluding Ro5 subset)
- Hydrogen bond donors: 0-8
- Hydrogen bond acceptors: 0-15
- $\text{LogP} \leq 6$
- Rotatable bonds: 0-15



VIRTUAL SREENING

Explore vast chemical diversity to identify hits with high success rate.

HIT EXPANSION

Search for molecules with improved properties using Freedom Space 4.0 and Chemspace's discovery services.

GROW FRAGMENTS

Identify and grow the fragments of interest into the direction of choice.

