

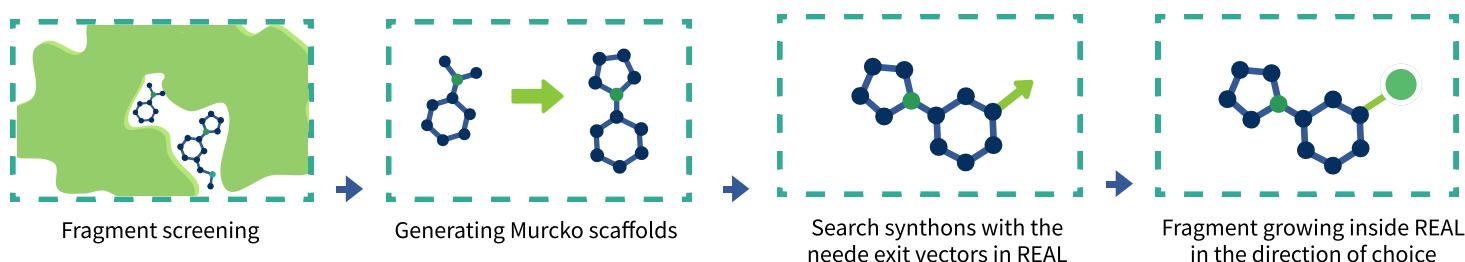
REAL Fragment Pre-Plated Library

Efficient fragment growing inside Enamine REAL space

Fragment-based drug discovery is a powerful method for identifying promising starting points for new drugs, but growing fragments into lead compounds is often challenging. This problem can be solved using commercially accessible combinatorial chemical spaces like Enamine REAL, which offers **2.7T molecules** at a competitive price. Due to the modular nature of this space, all its structural elements can be annotated in terms of the growth vectors they contain, thus enabling the creation of focused chemical spaces.

Approach Overview

For this library, we grouped all synthons by their scaffolds and superimposed each group in 2D space. This enabled us to select scaffolds with exit vectors in more than two quadrants, allowing for growth in multiple directions. Consequently, we mapped scaffolds to synthons and chose those that produced the most chemically diverse compounds.



REAL Fragment Pre-Plated Library

We offer a final set of 4,960 compounds that are pre-plated and can be ordered from Chemspace, though we support any kind of customization. The final set of fragments represents the whole Enamine REAL Space including the chemical diversity and variety of chemical transformations.

- ✓ Pre-plated library;
- ✓ Contains sociable scaffolds;
- ✓ High coverage of REAL scaffolds;
- ✓ Available for cherry-picking.

Have questions?
Contact us at:

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