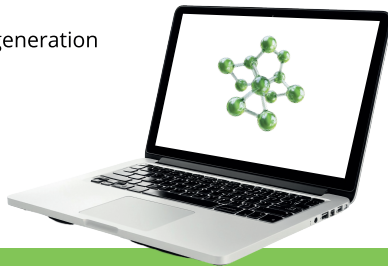


# ML-ASSISTED CUSTOM SPACE GENERATION

Explore the previously unannotated regions of chemical universe!

Our solution is ML-based filtering of building blocks for space generation

- ✓ Does not require full enumeration
- ✓ Cheap inference
- ✓ Synthon-based space creation
- ✓ Applicable to commercial collections of choice



## Proprietary building blocks collection

Analysis of diversity and overlap with commercial catalogs

## Create building blocks pool for reaction types

Building blocks undergo SMARTS filtering for specific reactions. Supports 40 protocols across 29 reaction types.

## Filtering building blocks with ML models

Each building block set is filtered using ML models trained on Enamine REAL success data.

## Space Enumeration

The space will be provided in both enumerated (up to 100B) and synthon-based formats

## Property Filtering

The enumerated version of the space can be filtered according to the properties of choice.

## Space Support and Update

The space can be updated based on the updates on the building blocks collections.

# CUSTOM SPACE COMPOUND SYNTHESIS



Receiving PO and list of compounds



Sourcing of building blocks

Up to 1 week



Delivery of final molecules

Up to 1 week

Synthesis & Purification

3-4 weeks



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