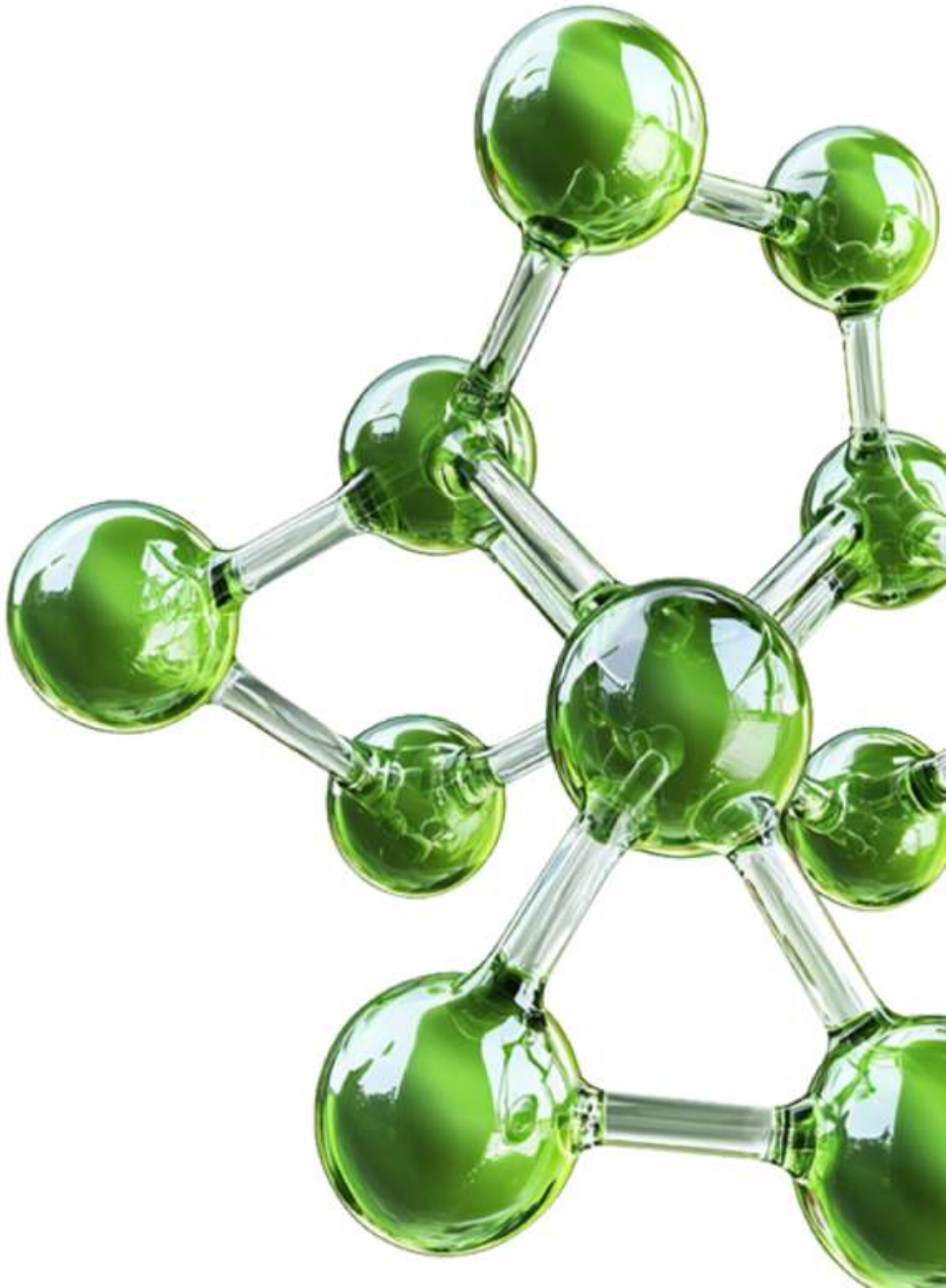
CHEMSPACE
Delivering Discovery Solutions®

3D Shape-Based Similarity Screening

September 2025



3D Shape-Based Similarity Screening - Overview

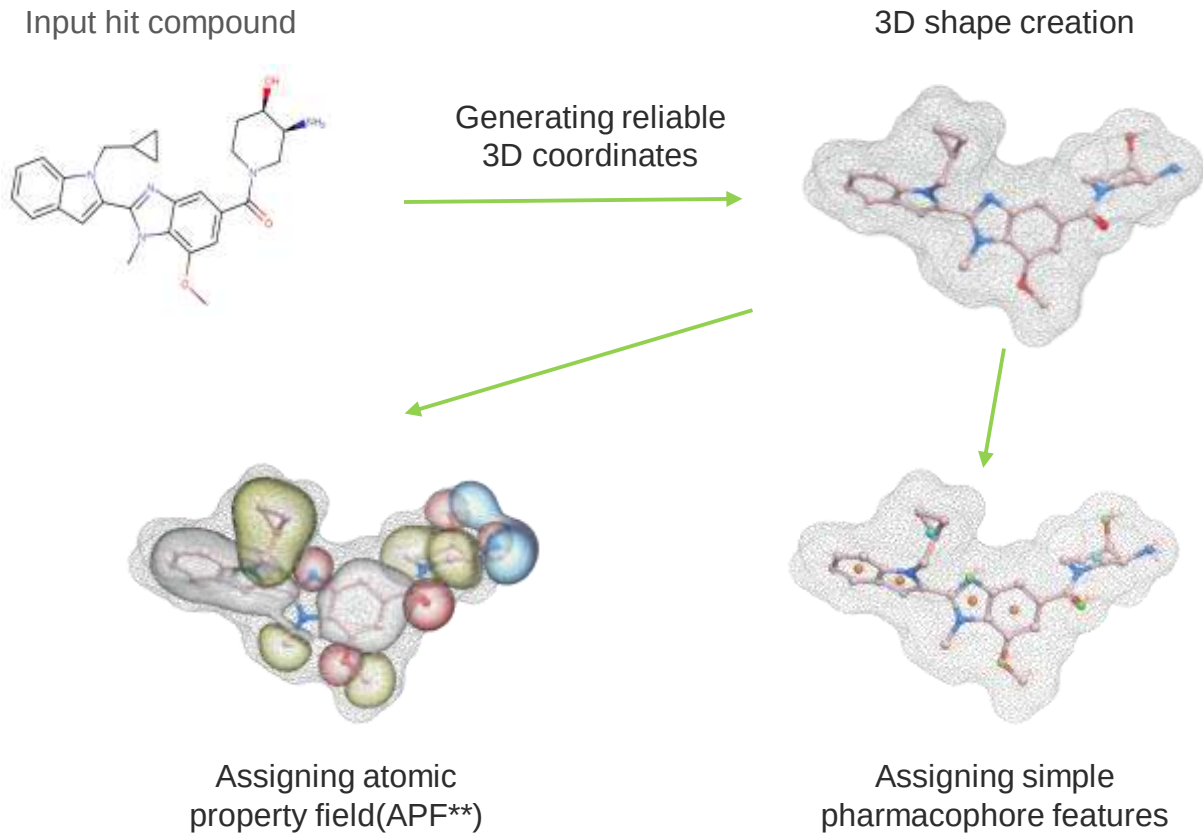
Chemspace offers a fast approach to identifying novel, diverse compounds within a biologically relevant subset of Enamine's 1.76M Screening Collection.

Powered by 3D similarity screening to uncover hidden connections and novel hits.

Limited offer

5,000 USD*

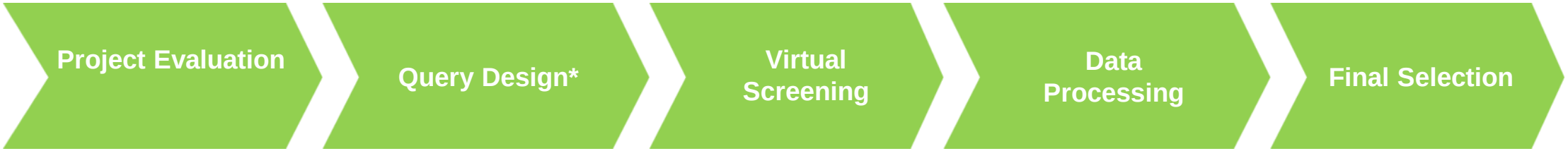
per project



*** Virtual screening of 1.7M Enamine Screening Collection** with delivery of 200 selected hits included

** The Atomic Property Field (APF) is a 3D pharmacophoric potential implemented on a continuously distributed grid which can be used for ligand docking and scoring.

3D Shape-Based Similarity Screening - Workflow



Project Evaluation	Query Design*	Virtual Screening	Data Processing	Final Selection
Initial meeting to discuss the project goals	Reference compound analysis and alignment, creating queries for shape and pharmacophore screening	Virtual screening of 3D conformer database	Data collection & analysis of shape/pharmacophore screening results**	Selection of 200 diverse compounds with report generation

***** Project cost covers creation and screening of 1 query for shape-based screening and up to 3 queries for pharmacophore screening.

****** For the final selection stage, compounds will be prioritized based on the highest similarity scores in shape-based screening, the lowest RMSD values in pharmacophore screening, as well as those identified by both methods.

3D Shape-Based Similarity Screening – Project Details

Project Requirements:

2D or 3D structure of hit compound(s)*

3D shape-based similarity screening can be performed on the carefully prepared 3D conformer dataset of Enamine's 1.76M Screening Collection

Project goal:

To discover new, diverse compounds similar to known actives to support scaffold hopping and hit expansion.

* For query design, up to 5 hit compounds will be selected based on initial assessment.

3D Shape-Based Similarity Screening – Result and Deliverables

Delivering:

- A dataset of at least 200 compounds*
- Detailed report with description of the selected compounds

Lead time:

5 business days

* The final number of selected compounds may be smaller depending on the query. In such cases, the project cost will be adjusted accordingly.

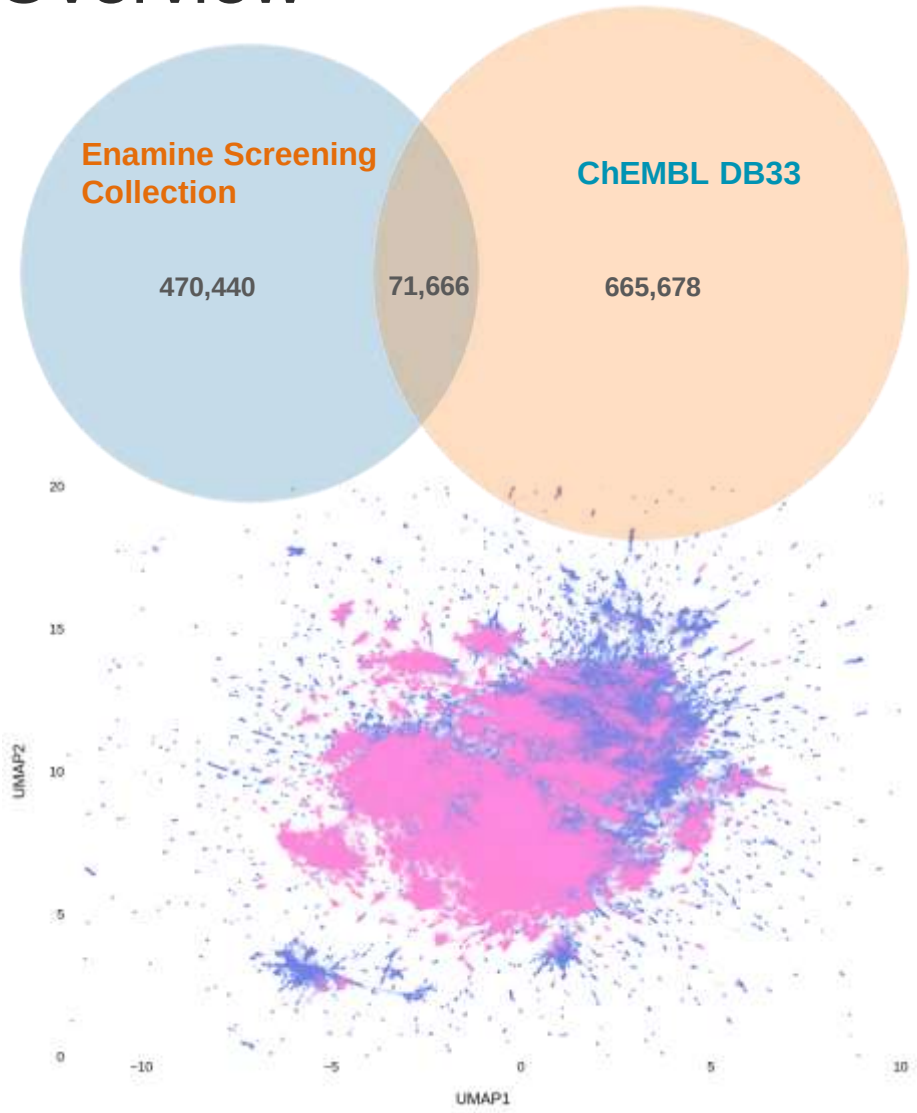
Thank you!

sales@chem-space.com

LIBRARY DESCRIPTION

Enamine Screening Compound Collection Overview

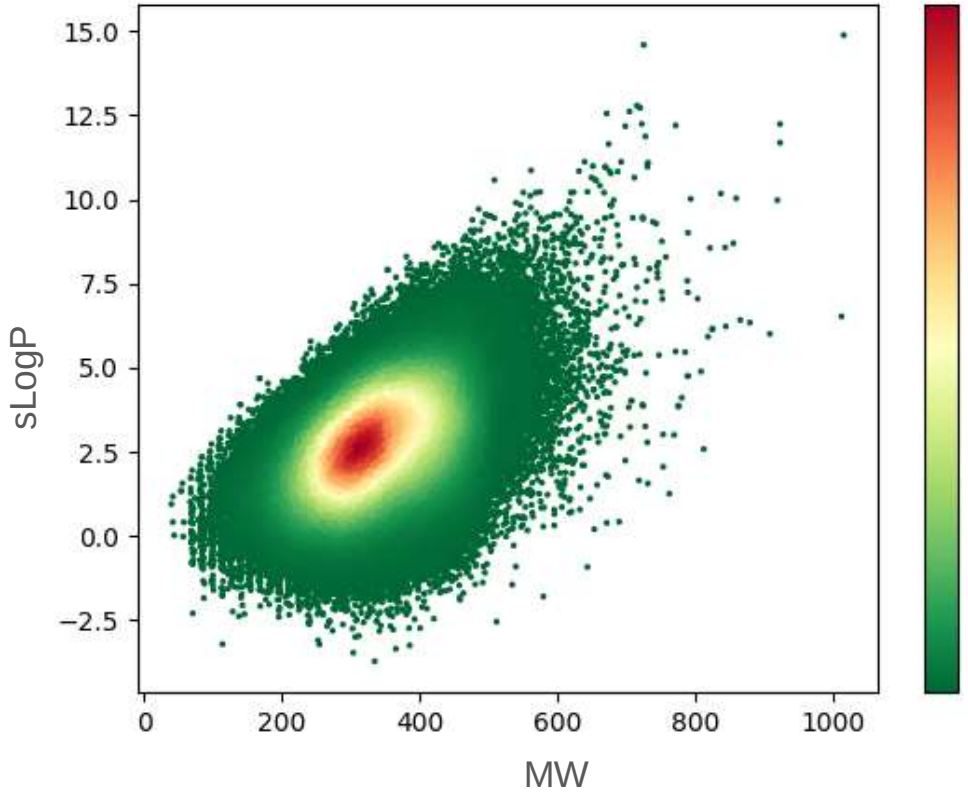
- Database size: 1.7 million molecules
- Diversity estimation:
  - ✓542,106 Bemis–Murcko scaffolds
  - ✓~3.1 compounds per scaffold (average)
  - ✓71,666 scaffolds overlapping with ChEMBL33



Scaffolds overlapping between ChEMBL (blue) and Enamine Screening Collection (pink)

Quality of Screening Compound Collection

- 51% drug-like compounds
- 44% lead-like compounds
- 11% shaped molecules
  (9% disc-like & 2% sphere-like)
- 5% compounds with high QED
  (QED>0.9)
- No PAINS
- 3% fragment-like compounds
- 1% natural-like compounds



Physicochemical Profile Of Screening Compound Collection