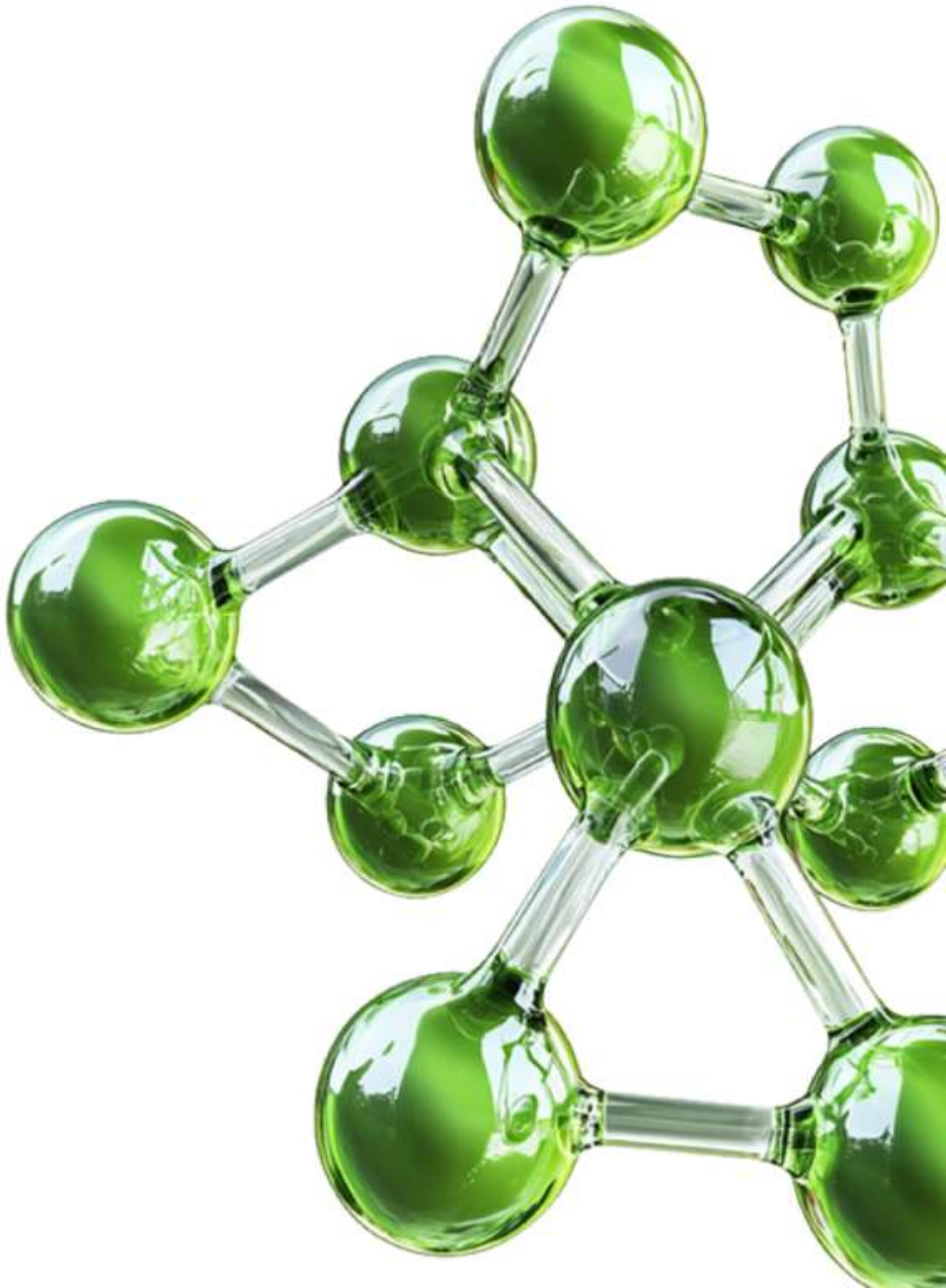
CHEMSPACE
Delivering Discovery Solutions®

AL-ACCELERATED DOCKING

September 2025



AL-Accelerated Docking - Overview

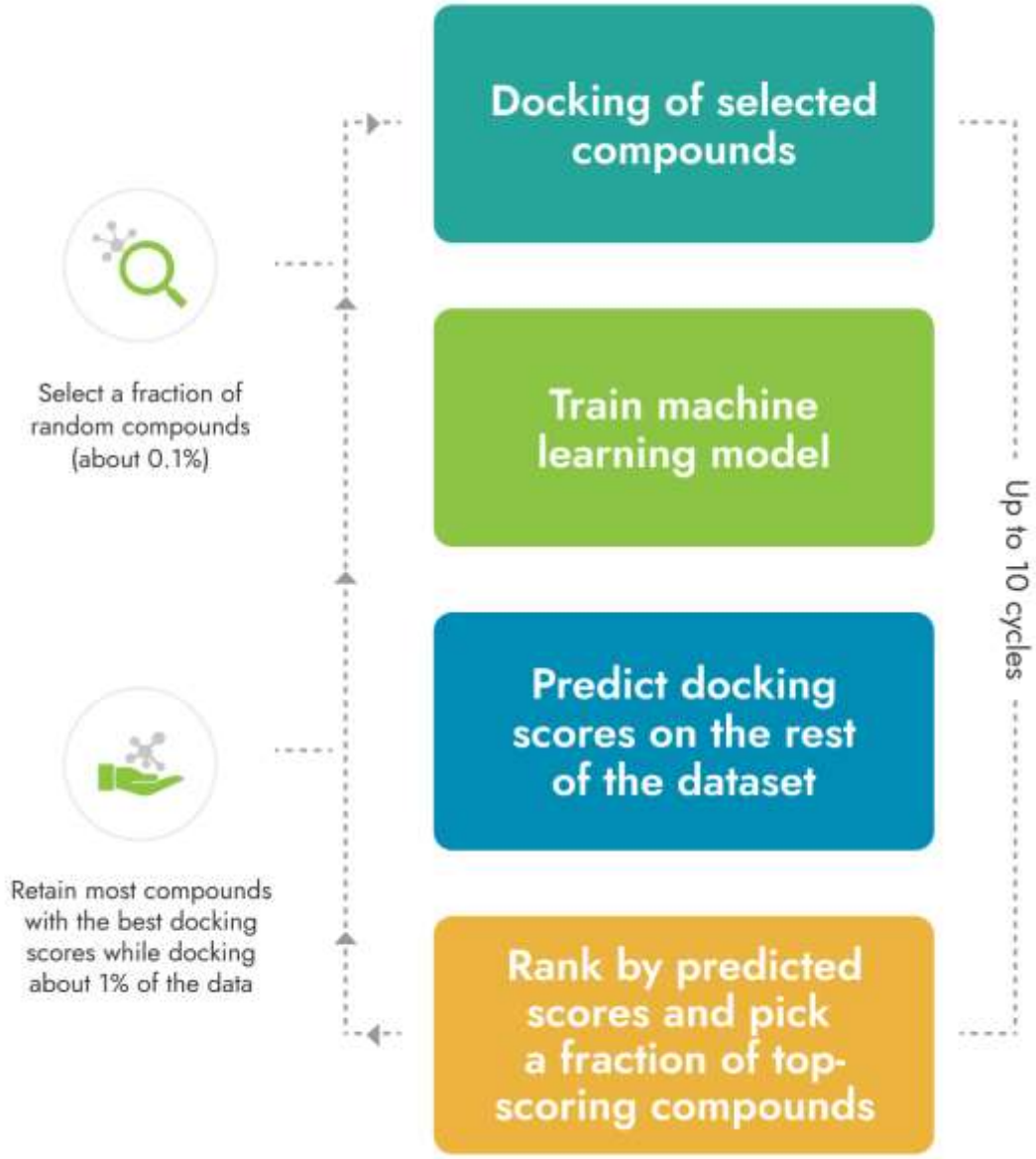
Active learning is a powerful technique that allows exploring large molecular datasets by performing only a fraction of calculations.

This allows to perform exploration of spaces up to 100M molecules.

Limited offer

35,000 USD*

per project



* Docking up to 100M, SQM for 10k and synthesis of **200 compounds** included!

Workflow

Project evaluation

Initial meeting to discuss the project goals

Docking model creation & validation

The docking model is prepared using either data provided by the client or open-source data.

The preparation process and docking simulations are performed in ICM-Pro software (Molsoft).

The model is then validated to ensure reliability before proceeding to large-scale screening.

AL-accelerated docking

Performing the cycles of AL-accelerated docking. 5 to 10 cycles needed depending on the target

SQM calculations

SQM* calculations performed on the top 10k compounds selected based on docking score, pocket occupancy, and interactions with key residues.

Final selection

Selection of 200 diverse compounds for synthesis

Optional – Creation of custom set for screening

You can request creation of a custom subset from Enamine REAL up to 100M based on your requirements or use one of the subsets provided by us

* Pecina, A., Fanfrlík, J., Lepšík, M., & Řezáč, J. (2024). SQM2.20: Semiempirical quantum-mechanical scoring function yields DFT-quality protein–ligand binding affinity predictions in minutes. Nature Communications, 15(1). https://doi.org/10.1038/s41467-024-45431-8

Project Details

Project Requirements:

A reliable 3D structure of the target protein (X-ray crystallography, Cryo-EM, or a high-quality homology model).
Information about the binding pocket, obtained from co-crystallized ligands, cofactors, pocket-detection software, or experimental data*

Project goal:

Highly efficient exploration of vast (and even custom-built) chemical space for effective hit identification

Available datasets (from the Enamine REAL Space of 77B compounds):

- ✓ 100M Ro5 Diversity Subset
- ✓ 100M Beyond Ro5 Diversity Subset
- ✓ 100M Lead-Like Subset
- ✓ 100M CNS-Penetrant Subset
- ✓ Custom Subset (up to 100M compounds)

* Additional target preparation, like MD simulation for binding pocket optimization, are not covered by this offer

Result and Deliverables

AL-accelerated docking

Lead time

15 business days

What you will receive after Stage 1:

- Detailed report featuring the docking model validation
- 10,000 top-scoring compounds
- Selection of 200 compounds for synthesis*

Compound synthesis

Lead time

3-4 weeks

Synthesis of up to 200 compounds – included in the price

The REAL compounds are synthesized using an assembly line with 80%+ synthesis success rate

* The selection can be refined by the customer based on the provided 10k top-scoring compounds

Thank you!

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