A New AI-Driven Approach to Hit Identification

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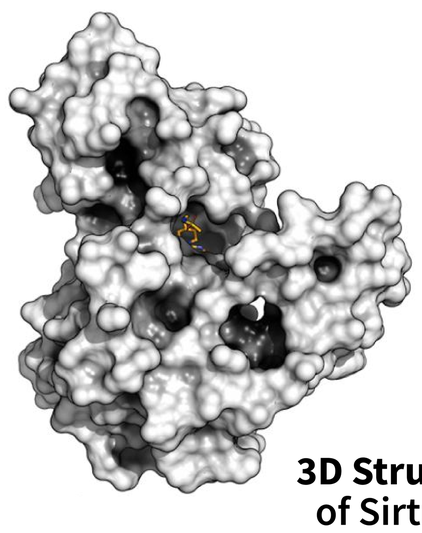
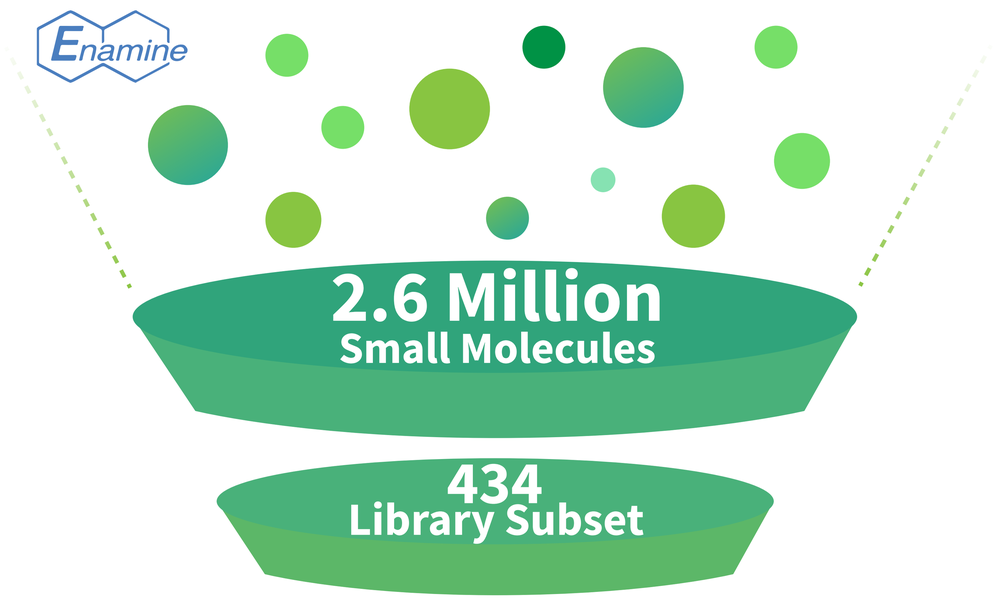
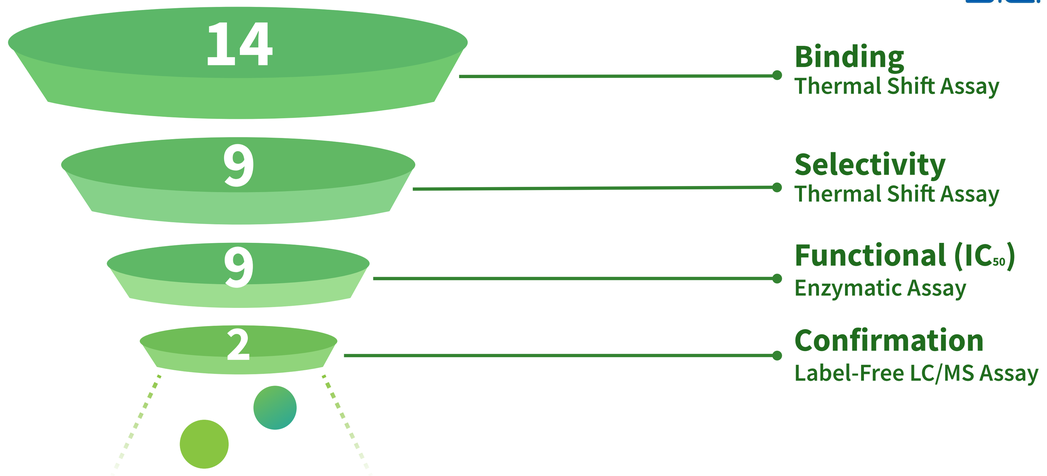


3D Structure of Sirtuin-1

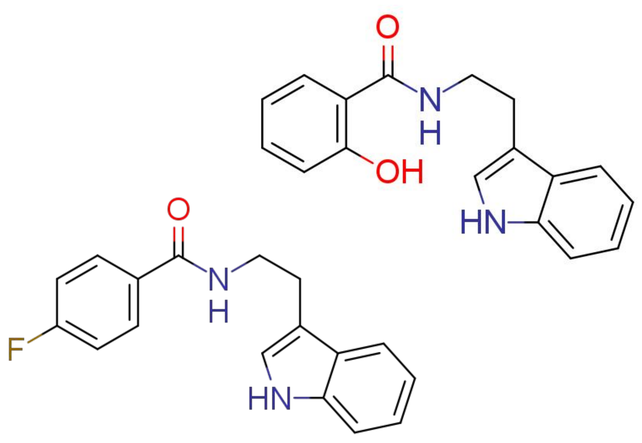
Virtual Screening by DiscoveryEngine



Hit Rate 0.46%



in vitro Validated Hits

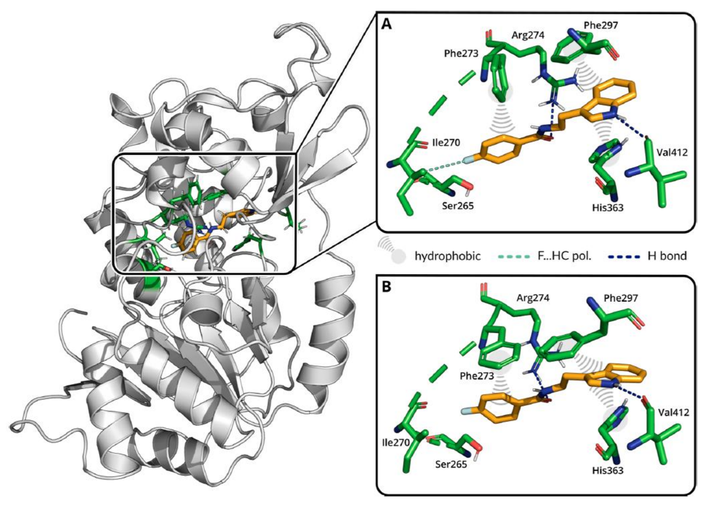


Validated Hits

The closest analog from ChEMBL with Tanimoto similarity value of 0.36

Assessment of Binding Mode

- Molecular docking
- Molecular dynamics simulation



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Chemspace Hit Discovery Solutions

V-SYNTHES

V-SYNTHES is a modular synthon-based approach for highly effective structure-based virtual screening of huge chemical spaces like the xREAL (173B compounds) using the ICM-Pro docking tool provided by MolSoft. The hit selection is done using a combination of approaches: energy minimization, AI-based scoring function, and synthon-based clustering - to name a few.

"Crystal Structure First" Approach

A great combination of crystallographic fragment hit discovery and virtual screening of vast chemical spaces. Starting from wet fragment screening using TSA we will proceed with co-crystalizing the selected fragments with the target and perform template-based virtual screening Enamine REAL (39B compounds).

DEL-ML-CS

We provide full service by conducting a DNA-encoded library (DEL), building a Machine Learning (ML) model, and providing you with low-cost, diverse compounds from synthetically accessible small molecule chemical spaces.

2D/3D QSAR

Quantitative structure-activity relationship (QSAR) methods are used to predict biological activity. We use different QSAR techniques, namely, multiple linear regression (MLR) and artificial neural networks (ANNs) to predict binding affinities. We offer high speed, good versatility, and a comprehensive compound library compliant with predefined filtering rules.

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