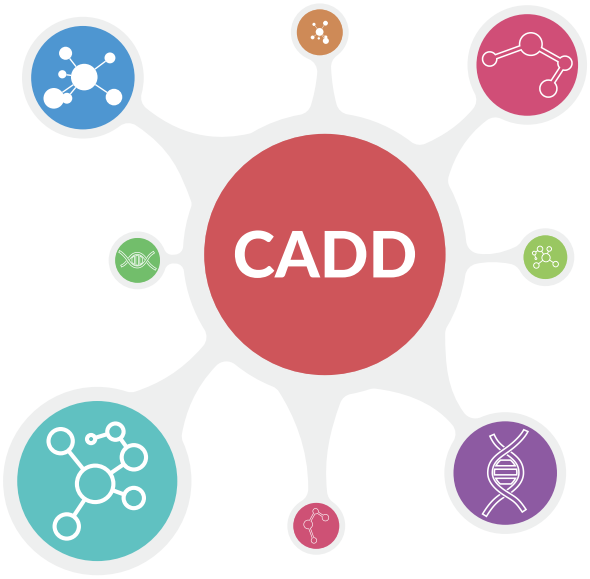
TargetMol®
A DRUG SCREENING EXPERT

Computer-Aided Drug Design

Technical Description

Computer-aided drug design is based on computational chemistry and uses computer modeling techniques to simulate, calculate and predict the relationships between drugs and biological molecules in order to design and enhance lead compounds.

The most fundamental goal of CADD is to simulate the binding between targets and candidate drugs to reduce the number of compounds to be screened in vivo, thereby improving the efficiency of lead compound discovery. (In random screening, the bioactivity rate was only 0.01%-0.1%; With CADD, the bioactivity rate can reach 5%-20%)



Target Structure Simulation & Prediction

We offer homology modeling services to predict the 3D structure of proteins from amino acid sequences; We also provide target fishing services to find possible targets for bioactive compounds.

Molecular Docking/Virtual Screening

We provide molecular docking services to explore the interaction mode between protein targets and small molecules/peptides/proteins; Meanwhile, we offer virtual screening services based on target/ligand structure, thereby reducing the number of compounds to be screened by focused screening and improving the efficiency of lead compound discovery.

ADMET Prediction

Using ADMET platform to predict the absorption, distribution, metabolism, excretion and toxicity properties of small molecules in the human body to reduce the elimination rate of candidate molecules and increase the success rate of drug development.

Molecular Design & Optimization/Scaffold Hopping

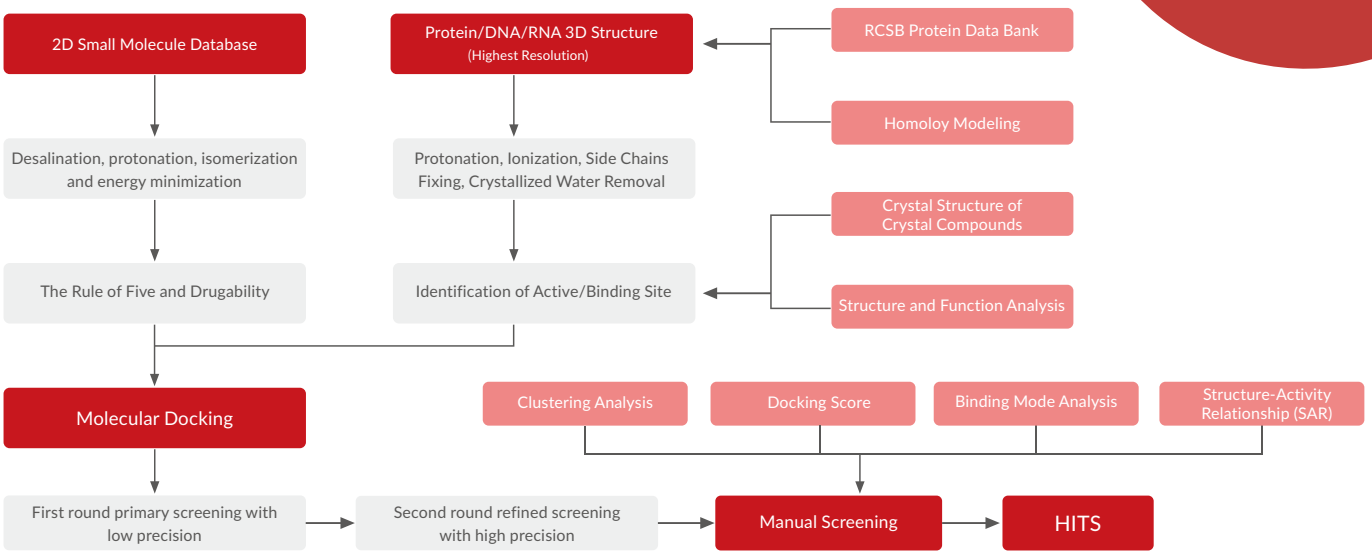
Based on the experiment requirements, design and optimize high-quality small molecule derivatives; Find drug molecules with novel structures through the method of scaffold hopping, and obtain hit compounds without intellectual property protection.

inquiry@targetmol.com
(781) 999-4286
Official Website
https://www.targetmol.com/
36 Washington Street, Wellesley Hills, MA 02481 USA
Facebook
Linkedin
Instagram

TargetMol®

A DRUG SCREENING EXPERT

Molecular Docking-based Virtual Screening



Highlighted Feature

Manual screening: Based on the docking score, we selected high-affinity target compounds by taking into account the 3D structural characteristics (hydrophilicity, hydrophobicity, hydrogen bonding) of the drug binding sites. At the same time, referring to the structure-activity relationship (SAR) of existing target drugs, we reserved the most important and conservative interaction mode of compounds, explored more new target compounds by the extension of the core scaffold, and finally by cluster analysis, obtained multiple target compounds for subsequent experimental activity verification.

Advantages of TargetMol®

Professional Team
Experienced technical team with more than 10 years experience in CADD

Compound Library
A stable supply of 20,000+ compounds to meet the needs of different clients

Screening Process
Additional manual screening significantly improves the reliability of simulated results

Screening Plan
Informative evaluation and closure reports to help clients fully understand the screening process and results

Featured Packages
Specialized natural compound and drug repurposing libraries, with well-defined targets and low prices

High Cost Effectiveness
Virtual screening at a cost much lower than the market average

Results Assurance
Free HD display of binding to meet publication requirements

Licensed Software
Multiple licensed professional CADD software, clients are safe from software intellectual property rights issues

Targetmol Chemicals Inc.

— Drug Screening Expert (Inhibitors, Natural Products, Compound Libraries)