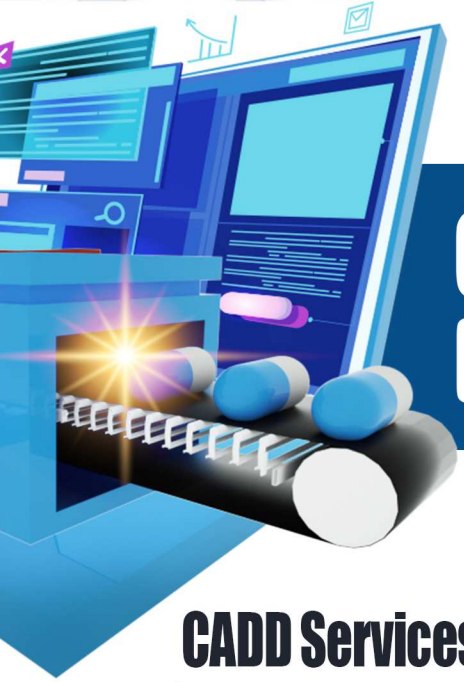


Computer-Aided Drug Discovery (CADD) Service

Computational chemistry methods are increasingly being combined with SOTA experimental techniques to enhance the success rate of drug discovery and explore the potential of new modalities.

CADD Services

1 Binding Prediction
In-house Docking & Virtual Screening Platform

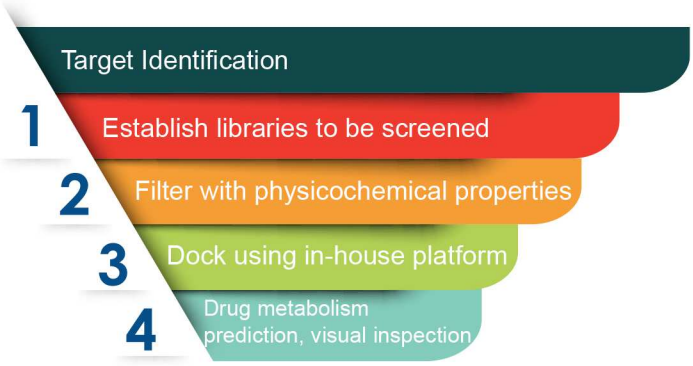
2 Scaffold & R-group Replacement
Linker Library, Molecule Generation

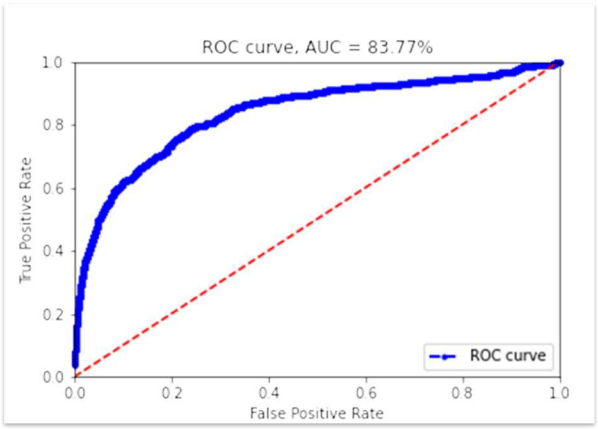
3 ADMET Prediction
Physicochemical Property Calculation, Metabolism Prediction

4 Molecular Modeling & Simulations
Proteolysis Targeting Chimera, GPCR, PPI, Modelling

Virtual Screening

- 50+ molecules delivered in Four Weeks





WEEK 1
- Kickoff

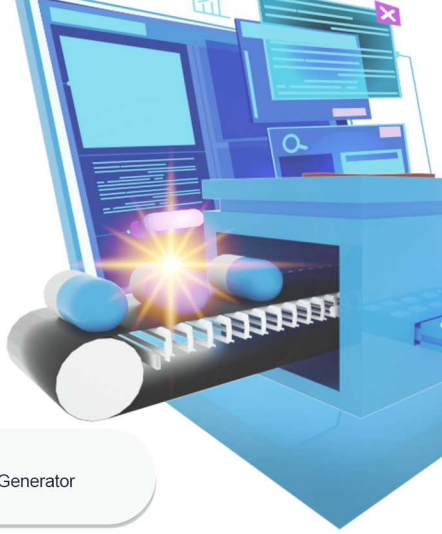
WEEK 2
- Screening commercial or virtual libraries of interest;
- Design of focused virtual library if needed

WEEK 3
- Pharmacophore filtering;
- Solubility/permeability/CYP prediction;
- Visual inspection

WEEK 4
- Final delivery

药明康德
WuXi AppTec

Scaffold and R-group Replacement



- Validity
- Uniqueness
- Novelty
- Drug-likeness and synthetic accessibility
- On-demand generation of Novel scaffolds or molecular fragments

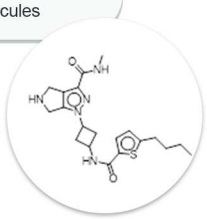
1 DEL selected hits

2 SMILES

3 ML model

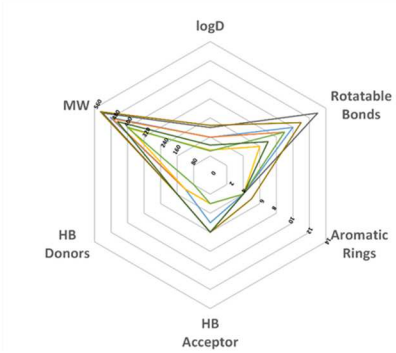
4 Generator

5 New Drug-like Molecules



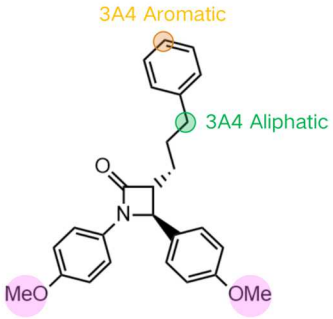
ADMET Prediction

- **Radar Chart of Calculated Physicochemical Properties**



We observed good correlations between the calculated logP (or logD) values and experimental solubility. The predicted PSA values also correlate well with measured membrane permeability. Simply calculating the physicochemical properties can provide us a hint on improving the ADME properties of small-molecule drug candidates.

- **Prediction of cytochrome P450 mediated metabolism**

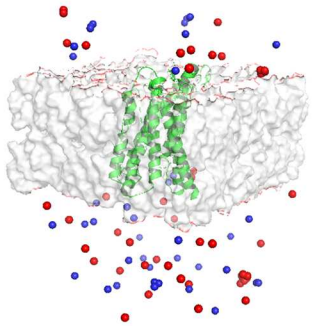


Possible metabolism sites of compounds of interest can be predicted.

Molecule source: doi.org/10.1021/jm050529c

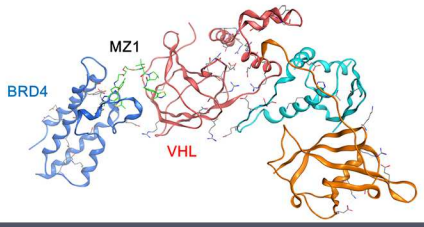
Molecular Modeling and Simulations

- **Membrane Proteins Embedded in Lipid Bilayers**



- Conformational change
- Analysis of h-bonds/salt bridges
- Mutation effect

- **Proteolysis Targeting Chimera -induced Ternary Complexes**



- Optimization of linker length and type
- Simulating PPI at all-atom level
- Predicting physicochemical properties and synthetic accessibility of Proteolysis Targeting Chimera molecules

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