About PharmaResources

PharmaResources is a fast-growing CRO/CDMO company based in China and provides one-stop service for small molecule drug discovery and manufacturing. Currently we have around 1,000 scientists, focusing on medicinal chemistry, process development, DMPK, pharmaceutical researching and GMP manufacturing.

Computer-Aided Drug Design

Computer-aided drug design (CADD) is dedicated to the application of various computer simulation techniques to accelerate drug discovery and design processes, and combines with chemical and biological experiments to drive drug development programs more efficiently. Based on physics, structural chemistry, pharmaceutical chemistry, biochemistry, molecular biology and other disciplines, and based on the theory of quantum chemistry and molecular mechanics, it has developed structure-based drug design with the help of computer numerical calculation and logical judgment, database, graphics, artificial intelligence, and other

processing technologies.

Our Computer-aided Drug Design (CADD) team has standardized procedures and highly-skilled scientists for solving complex problems related to discovery. The CADD team routinely supports discovery projects starting from target identification to lead optimization. We can provide virtual screening, scaffold hopping and de-novo molecule design. We have a wide range of tools available for compound optimization. Also, we have proven expertise in collaborative small molecule, PROTAC and peptide drug discovery projects.

Structure-Based Drug Design

- Docking and Virtual Screening (AIDD, Internal Algorithms)
- Core Hopping
- Homology Modeling
- *De Novo* Ligand Growth and Optimization (AIDD, internal algorithms)
- Free Energy Perturbation Calculations
- QM Calculations
- PROTAC, Molecular Glue Modeling (Internal Algorithms and Workflows)

Ligand-Based Drug Design

- Pharmacophore Modeling and Virtual Screening
- Conformational Analysis
- QSAR
- Similarity Search/Clustering,
- R-group Decomposition
- Matched Pair Analysis, and Potency Cliff Analysis (Internal Algorithms and Workflows)

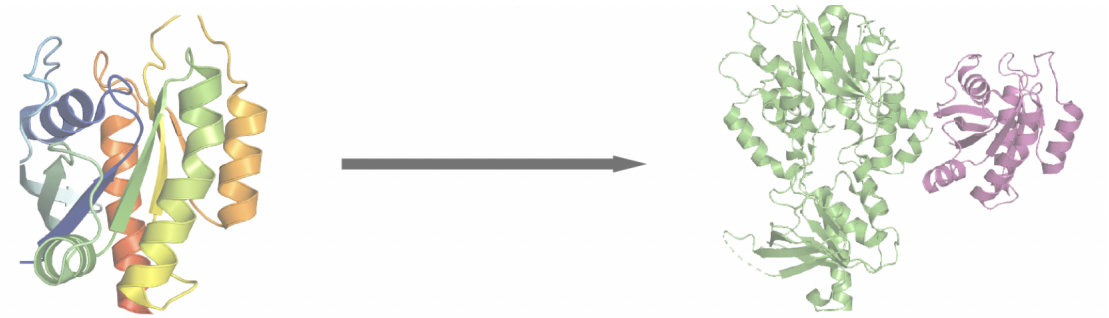
In Silico ADMET and Druglike Property Calculations

- Prediction of Physical-Chemical Properties (AIDD, Internal Algorithms and Workflows)
- Ligand-Based or Structure-Based Modeling for hERG, UGT and P450 Enzymes

Expert Consultancy in Computational Chemistry

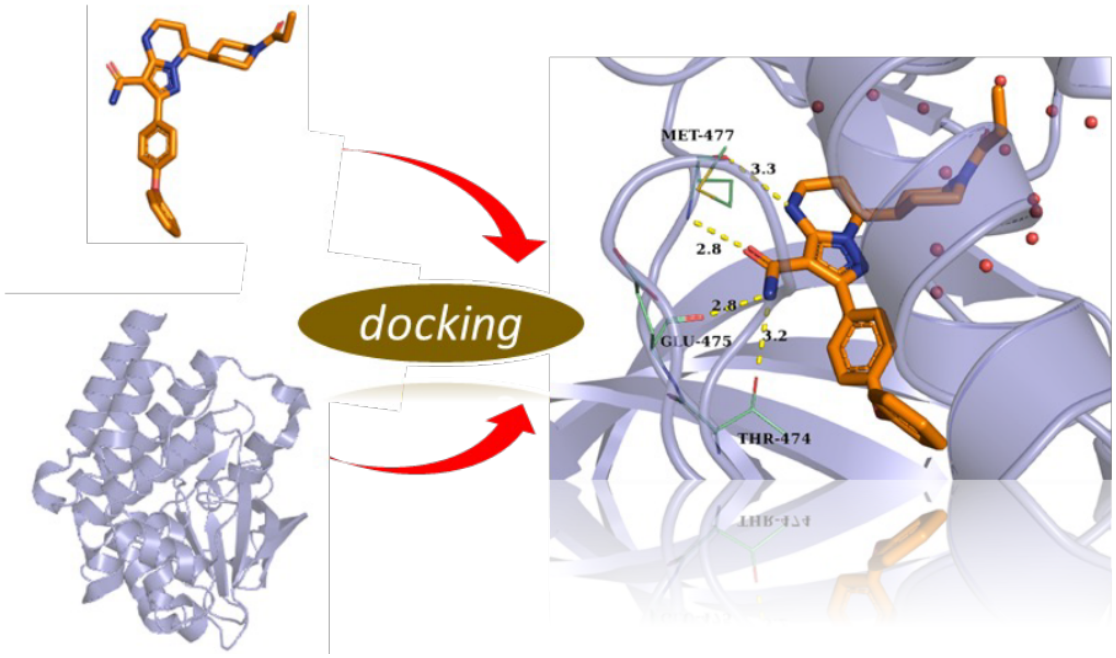
- Industry-Standard Software and Hardware
- Proprietary Design Concepts and Tools
- Highly Experienced Scientists
- Strong Track Record of Success

- Tight Integration with Allied Disciplines
- Extensive Experience in Small Molecule Modeling
- Work Closely with Internal Chemistry and Biology Teams
- Quick Respond to Our Customers' Needs



Homology Modeling

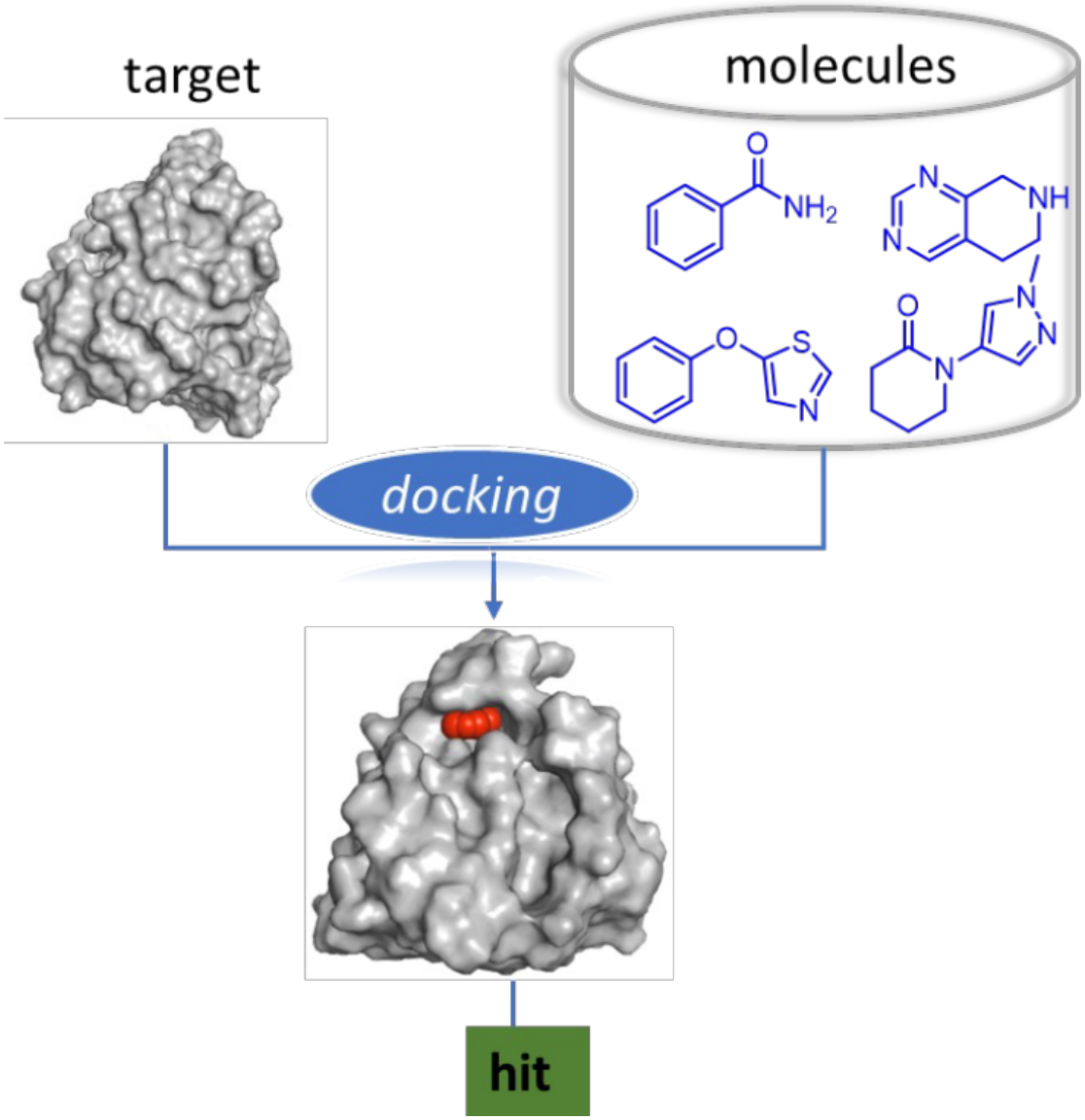
- Accurate Prediction of 3D Structure of Given Proteins
- Predict the 3D structure of complexes in protein-protein, including local docking, global docking, and flexible docking, to help the subsequent design of PROTAC and molecular glue.



Molecular Docking

Structure-based design approach exploits disease-related targets by experimentally determining 3-dimensional structure (e.g. X-ray, NMR, or Cryo-EM) or homology model (in case of unavailability of experimental structure). This method is performed to predict the binding pose of the molecule in the binding site and estimate probable binding affinity or a score representing the strength of binding.

We use docking and molecular dynamics simulation to shortlist compounds that may become a good hit or lead for a project.



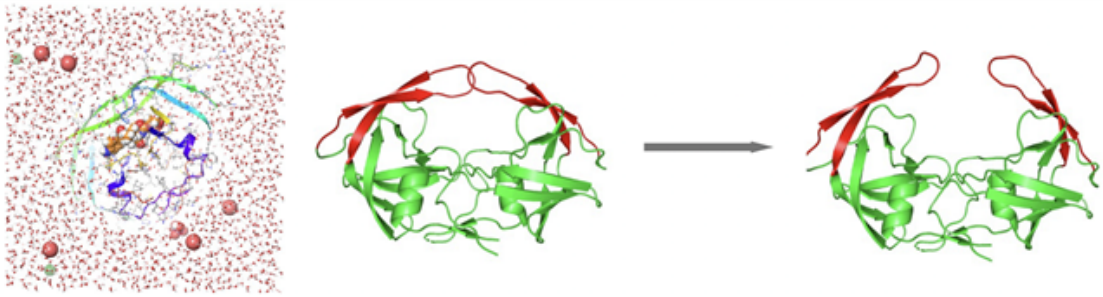
Virtual Screening

Virtual screening is a powerful modeling tool to identify novel hit compounds in any discovery program. It is routinely deployed in drug discovery projects for compound ideation and conceptualization. Virtual screening has multiple applications including hit scouting and hit-to-lead optimization.

The techniques deal with computational or in silico analog of biological screening to score, rank, and/or filter a set of structures using one or more computational procedures. This helps to decide which compounds to screen, which libraries to synthesize, and which compounds to purchase from an external source. Virtual screening uses both structures, ligand or compound-guided computational

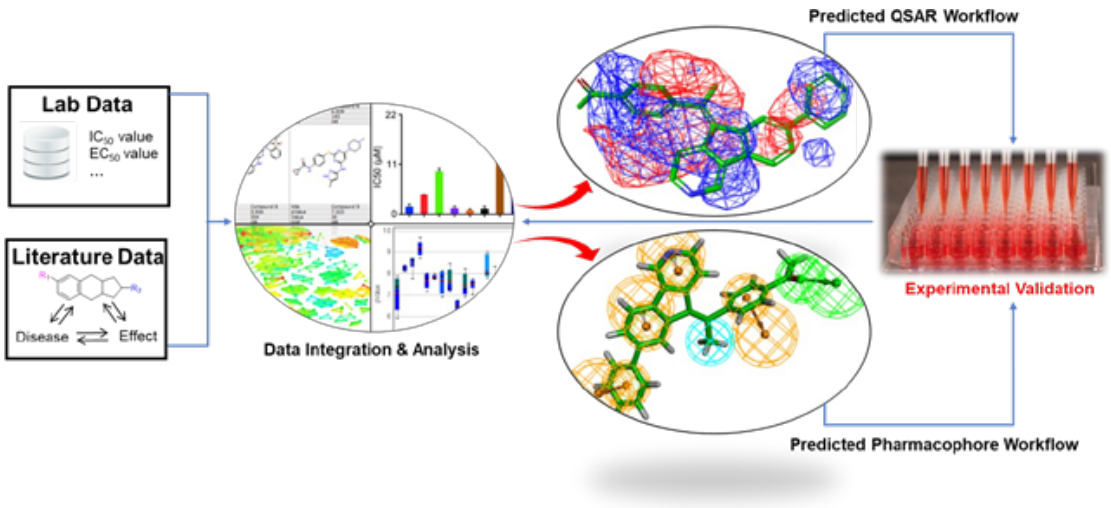
methods, or a combination of both.

We have access to more than two billion commercially available compounds' databases. This database is routinely used to carry out virtual screening studies to facilitate the compound design and ideation.



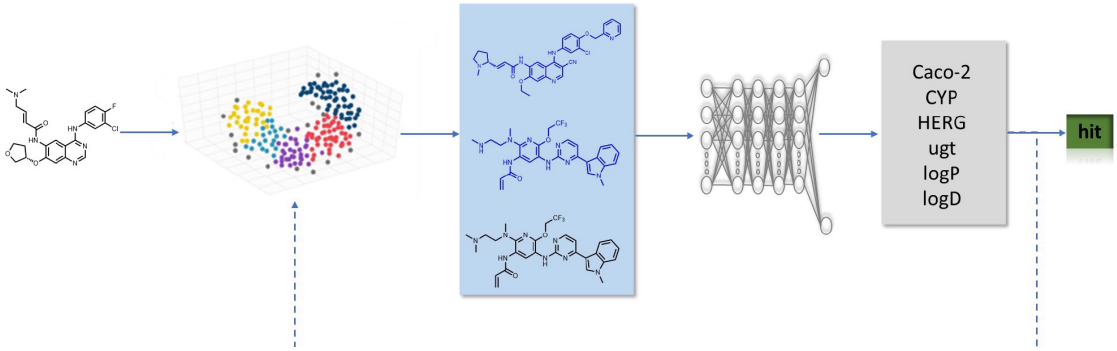
Molecular Dynamics

Molecular dynamics (MD) simulations have rapidly become an integral part of computer-aided drug design applications, allowing us to examine the flexibility of protein structures since X-ray crystallography typically provides a single "snapshot" of a highly mobile system. This can lead to the identification of an ensemble of binding site models, sometimes used in structure-based virtual screening. MD simulations can also be applied to assess the stability of binding modes proposed by protein-ligand docking studies and for conformational analysis of ligands, including an accurate treatment of their solution environment.



QSAR and Pharmacophores

Ligand or compound-based design is another powerful modeling technique used in CADD. Some of the most used techniques routinely deployed at PharmaResouces include pharmacophore modeling, quantitative structure-activity relationship (QSAR), or knowledge-based expert methods, for compound design and ideation. We use a ligand-based design approach in de novo, scaffold hopping, ligand hybridization, fragment-linking and related techniques. The ligand-based approach is not limited to compound designs but is also deployed in a predictive model. Predictive models built using AI/ML techniques are used at our facility to determine compound potency, selectivity and Physico-chemical properties. This in turn facilitates project progress.



Molecular Generation and ADMET Prediction

AI-based molecule generation can expand the new chemical molecule space beyond the existing molecular library, and learn various structural information and target relationships of small molecules combined with ADMET prediction for targeted molecular generation and lead compound optimization.

Quantum Chemistry

Quantum chemistry is the study of chemical problems by applying the basic principles and methods of quantum mechanics, including the following:

Structural Optimization
Discover the chemical structure and calculate the lowest energy conformation.

Single Point Energy Calculation
Discover the chemical structure and calculate the overall energy.

Gibbs Free Energy
Determined the direction of the reaction process by calculation.

pKa

Calculate the ability of a compound to dissociate hydrogen ions.

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