The Best Solution For Your Drug Design

About PharmaResources

PharmaResources is a fast growing CRO/CDMO company based in China, which is an one-stop service provider of small molecules for new drug discovery and manufacturing. Currently we have around 1000 scientists, focusing on medicinal chemistry, process development, DMPK, pharmaceutical researching and GMP manufacturing.

Computer-Aided Drug Design

Our computer-aided drug design (CADD) team supports drug discovery projects all the way from hit identification through lead optimization. Offering virtual screening, scaffold hopping and de-novo design to predict and optimize the binding mode of small molecules in protein structures by means of crystal structures and predict the affinity between ligands and target proteins.
CADD is an efficient tool in the field of drug discovery and development, through which you can find the most promising drug candidates in a very cost-effective manner. It always gives hope for improvement in the drug discovery field.

PharmaResources CADD Skills and Expertise

- Structure-Based Drug Design
- Ligand-based drug design
- ADMET and Druggability Prediction

Why Work With us for CADD Services?

- Extensive Experience in Product and Patent Strategy
- Diversified Computing Simulation services
- CADD & AIDD Dual Platform
- Work Closely with the Chemical and Biology Department
- Sufficient Computing Resources
- Respond Quickly to Customer Needs

Homology Modeling Docked with Protein

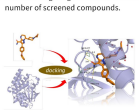
- Fast predict the 3D structure of proteins, by unknown structure sequences and proteins of 3D structures with certain homology.
- Predict the 3D structure of complexes in protein-protein, including local docking, global docking, and flexible docking, to help the subsequent design of PROTAC and molecular glue.

Molecular Docking

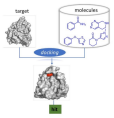
- Docking small molecules into large molecule binding pockets helps to precisely investigate ligand-receptor interaction patterns.

Virtual Selection

- Simulate target-ligand interactions computationally to reduce the actual number of screened compounds.



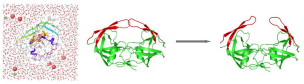
Molecular Docking



Virtual Selection

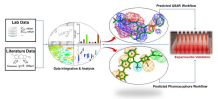
Molecular Dynamics

- Molecular dynamics is an important research method to study the molecules or the structure and properties of molecules through computer simulation, and is commonly used in the field of new drug research to investigate the stability of systems and key roles, and is also often used to predict binding sites.



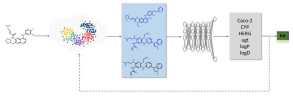
QSAR and Pharmacophores

- Based on the available data, we predict the activity of unknown compounds by establishing quantitative structure-activity relationship models and pharmaco phore models, and assist in the design and optimization of compounds.



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:

1. Structure, Properties and Relationship between Stable and Unstable Molecules and Their Structure and Performance
2. Molecule-to-Molecule Interactions
3. Molecules Collide and React with Each Other

- **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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Got Questions? Contact Us