康龙化成 PHARMARON

Computer-Aided Drug Design

With state-of-the-art tools, our CADD team routinely generates insights into data and proactively designs new compounds to guide medicinal chemistry teams in creating or expanding IP space, while addressing specific issues, such as potency, selectivity, physical properties or metabolic stability. The CADD team works directly with collaboration partners and as part of integrated drug discovery teams. The team has an excellent track record since its inception, with performance that has been recognized by partners from US, Europe, Japan and China.

Therapeutic Areas

- Anti-infectives
- Cardiovascular
- CNS and pain
- Epigenetics
- Immuno-oncology
- Inflammation
- Respiratory systems

Software/Hardware

- Schrodinger
- Boston Denovo
- ChemAxon
- CCDC
- Rosetta
- Dotmatics
- 3D Stereo Graphic Systems
- Linux Workstations
- Clusters with CPU and GPUs

Molecular Simulations

- Physical chemical properties
- Drug absorption & transport
- Drug metabolism
- Drug-drug interactions

Hit Finding and Evaluation

- Virtual screening
- Diversity analysis
- Combinatorial enumeration
- Hole-filling/library optimization
- Library comparison
- Fragment and high-throughput screening support

ChemInformatics

- ADME/toxicity prediction
- pKa Prediction
- Match pair & activity cliff analysis
- R-Group analysis, Free-Wilson
- AI and statistical

Compound Designs

Ligand-based Drug Design

- Pharmacophore modeling
- Virtual screening
- Scaffold hopping
- QSAR/QSPR
- Similarity search
- *de novo* Growth with a pseudo-receptor

Structure-based Drug Design

- Internal structural biology group
- Protein homology modeling
- Docking studies
- Virtual screening
- Scaffold hopping
- *de novo* growth and optimization
- PLDB/Crossminer/Relibase+

Targets and Modalities

- Protein-protein interactions
- PROTAC
- Covalent interactions
- Peptides
- Enzymes, proteases, kinases
- Receptors, ion channels
- GPCRs

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Laboratory Services

Chemistry, Manufacturing and Control

Clinical Development

Biologics & CGT

Pharmaron is a global life science service provider that offers a broad spectrum of research, development and manufacturing service capabilities throughout the entire drug discovery, preclinical, clinical development and commercialization process.