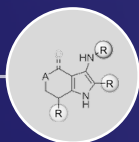
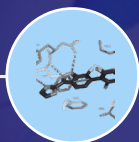


Pharmaron's CADD Consultancy Services



Chemistry



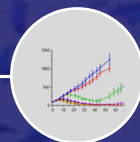
CADD



DMPK



Modelling



Biology

Pharmaron's CADD (Computer-Aided Drug Design) consulting brings together expert insights and advanced computational tools to help clients navigate complex challenges in drug discovery. Our team offers strategic guidance, project management, decision-making support, and data interpretation, combining modern computational techniques like AI with decades of hands-on drug discovery experience to deliver innovative solutions.

Our CADD experts help clients to navigate complex data and decision-making

- Target Assessment
- Protein Structure Modeling
- Virtual Screening
- Ligand-Based Design
- Cheminformatics

Target Discovery
and Hit Finding

Strategic Guidance

Hit and Lead
Optimization

- ADMET Modeling
- Multi-Parameter Optimization
- Scaffold Hopping
- *de novo* Design
- Property Prediction

For drug discovery that is accelerated, innovative and better by design

- **AI-Powered Design:** Use top-tier software and AI/ML models for virtual screening, analytics, and design.
- **High-Tech Wet Labs:** Facilitated access to expertise and capabilities from world class structural biology including cryo-EM and X-ray, biology, chemistry and DMPK.
- **Integrated Data Platforms:** Cloud-based system and dashboard to unify ADME/PK, biology, and chemical data visualization.

High Impact Work Package Examples

1 Example: Strategic Guidance for Structure-Based Virtual Screening

Target Assessment

- Evaluate target biology, structural and sequence data to
- Use AI to fill-in missing structural pieces
- Create coherent view of mechanism of target and mode(s) of interaction

Model Validation

- Combine AI and biophysics-based modeling to generate candidate atomic models
- Rank and validate models with decoys, known actives and multiple methodologies for maximum confidence in predictions

Implementation

- Choose from millions of available, to billions of synthesizable compounds for screening
- Dock on vast scale
- Iterate docking with AI model building to ensure coverage of the best docking compounds

High Impact Work Package Examples

2 Example: Accelerate Hit and Lead Finding with Confidence

Hit Finding

- Close coupling with hit finding platforms such as FBDD, HTS and DEL using virtual screening techniques ensures the right compounds are screened
- Maximize information use from high throughput platforms with AI/ML models
- Incorporate multiple predictions to get to the best series early

Data Visualization and Models

- Offer insights on SAR through structural hypotheses to guide decision-making
- Evaluate and evolve quantitative approaches to activity and property predictions
- Guide away from undesirable properties through a variety of "global" and bespoke models

Quantitatively-Enabled Drug Discovery

- Build computational pipeline to enumerate and evaluate compound ideas on project cadence.

3 Example: CADD-Driven Lead Optimization for Quality Candidates

Modern SBDD Approaches

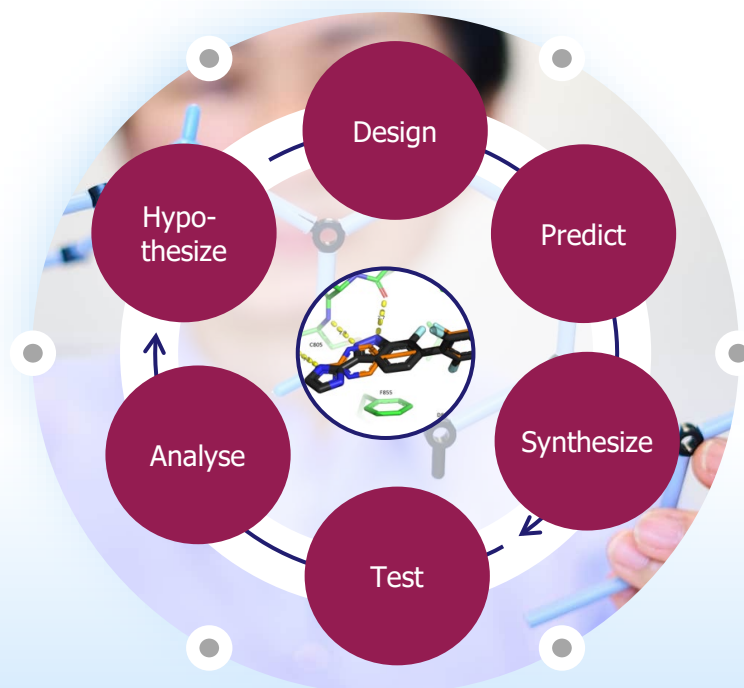
- Provide expert guidance on AI-generated protein structures, co-folded Protein:Ligand complexes, and dynamic modeling.
- Evaluate applicability of AI, MM, Free-Energy, Water Network and Quantum methods to enhance understanding and prediction of target interactions.

Maximize Data Use

- Apply AI, ML and statistical methods to quantitate SAR.
- Use feature prioritization, R-group analysis and SAR views to effectively translate models to understandable and actionable hypotheses.
- Use generative approaches to create new ligands and IP

Database-Enabled Drug Discovery

- Integrated views onto biological, chemical, DMPK and computational data



Smarter. Faster. Better.

Pharmaron's CADD Consultancy enhances the drug discovery cycle by integrating AI-driven modeling, predictive analytics, and data visualization.

We streamline hypothesis generation and improve decision-making, ensuring efficient transitions between design, synthesis, and testing for more reliable and innovative outcomes.

Why Work with Pharmaron's CADD Consultancy Team?

- **Expertise:** Our team provides deep scientific knowledge from decades of drug hunting in biotech and pharma.
- **Tailored Solutions:** We meet client needs through custom workflows and informatics.
- **Broad Modality Coverage:** Support for small molecules, peptides, ADCs, PROTACs, and molecular glues.

Book an initial conversation to explore how we can support your drug discovery journey.



Laboratory
Services



Chemistry,
Manufacturing &
Control



Clinical
Development



Biologics
& CGT

