

## Integrated Drug Discovery Services

Pharmaron's integrated drug discovery services team leads projects from hit identification through candidate selection and beyond. We combine world-class scientific and project leadership with global resources and expertise to offer integrated end-to-end support for discovery and development of new therapeutics.

### Computational Sciences

- Cheminformatics
- Structure-based Drug Design
- Target Analysis
- ML/AI-driven Modeling

### Hit Identification

- e.g., HTS, DEL, Fragment-based or Phenotypic Screening

### Target Science

- Target Identification
- Target Validation
- Cell Line Engineering

### Chemistry

- Medicinal & Synthetic Chemistry
- Scaffold Design
- Libraries
- API Route Design
- API Scale Up

### Biosciences

- Protein Production
- Crystallization & Structural Biology
- *in vitro* Biology
- *in vivo* Pharmacology
- Biomarkers

### DMPK & Safety

- ADME
- PK/PD
- Drug Safety Assessment
- Human Projections
- Modeling and Simulations

## Integrated Drug Discovery

IND  
Application

### IND Enabling

- GLP Safety Assessment
- API Process Chemistry; GMP Synthesis
- Formulation Development and GMP Preparation
- DMPK and Pharmacology
- Regulatory Affairs

Preclinical  
Candidate  
Nomination

Co-piloting or independent delivery, FTE, risk-sharing or milestone-based, Pharmaron's integrated services team has a solution for you.

Our integrated approach provides scientific excellence combined with efficient delivery.

## Approach

The collective expertise of our seasoned drug hunting team, each member with multi-year industry experience and a proven track record, provides **strategy, decision-making** and **project coordination** to transform ideas into high-quality drug candidates.

## Expertise

Our integrated drug discovery team has operated over many years, across **therapeutic areas, target types** and **modalities**, successfully advancing projects from hit-finding through preclinical candidate selection into the clinic.

### Therapeutic Areas

- Cancer
- Metabolic diseases
- Cardiovascular diseases
- Inflammation/pain
- Immunologic diseases
- Neurologic diseases
- Rare diseases

### Target Types

- Enzymes
- GPCRs
- Transporters
- Chaperones
- Nuclear receptors
- Transcription factors
- Phenotypic
- Ion channels

### Modalities

- Orthosteric, allosteric binders
- Covalent binders
- Protein degraders
- Molecular glues
- Small and large molecules
- ADCs

## Why work with Pharmaron?

- Leverage the expertise of an experienced, multi-disciplinary scientific leadership team working in close collaboration with your team
- Benefit from nimble and flexible resource allocation, utilizing Pharmaron's comprehensive capabilities, instrumentation, and human resources across the UK, US, and China.
- Tap into scientific expertise across all relevant research fields and utilize state-of-the-art technology to facilitate efficient Design-Make-Test-Analyze cycles.
- Eliminate the coordination between different service providers and transform Pharmaron's industry leading turnaround times into accelerated drug discovery

Selected publications highlighting our scientists' expertise.

**Discovery of HC-7366: An Orally Bioavailable and Efficacious GCN2 Kinase Activator**

Journal of Medicinal Chemistry. 2024. [↗](#)

Journal of  
**Medicinal  
Chemistry**

pubs.acs.org/jmc

Drug Annotation

**Discovery of HC-7366: An Orally Bioavailable and Efficacious GCN2 Kinase Activator**

**Discovery of a novel series of selective macrocyclic PKC $\theta$  inhibitors**

Bioorganic & Medicinal Chemistry Letters. 2024. [↗](#)



Bioorganic & Medicinal Chemistry Letters

Volume 100, 1 March 2024, 129630



**Discovery of a novel series of selective macrocyclic PKC $\theta$  inhibitors**

**A novel dual ATM/DNA-PK inhibitor, XRD-0394, potently radiosensitizes and potentiates PARP and topoisomerase I inhibitors**

Molecular Cancer Therapeutics. 2024. [↗](#)

MOLECULAR CANCER THERAPEUTICS | SMALL MOLECULE THERAPEUTICS

**A novel dual ATM/DNA-PK inhibitor, XRD-0394, potently radiosensitizes and potentiates PARP and topoisomerase I inhibitors**

Tona M. Gilmer<sup>1</sup>, Chun-Hsiang Lai<sup>2</sup>, Kexiao Guo<sup>2,5</sup>, Katherine Deland<sup>3</sup>, Kathleen A. Ashcraft<sup>3,6</sup>, Amy E. Stewart<sup>2</sup>, Yaode Wang<sup>4</sup>, Jianmin Fu<sup>4</sup>, Kris C. Wood<sup>2</sup>, David G. Kirsch<sup>2,3,7</sup>, Michael B. Kastan<sup>2</sup>



**Non-specific binding of compounds in *in vitro* metabolism assays: a comparison of microsomal and hepatocyte binding in different species and an assessment of the accuracy of prediction models**

Xenobiotica. 2022. [↗](#)

XENOBIOTICA  
2022, VOL. 52, NO. 8, 943-956  
<https://doi.org/10.1080/00498254.2022.2132426>

 Taylor & Francis  
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RESEARCH ARTICLE

 OPEN ACCESS  Check for updates

**Non-specific binding of compounds in *in vitro* metabolism assays: a comparison of microsomal and hepatocyte binding in different species and an assessment of the accuracy of prediction models**

Talk to our scientists about your drug discovery program today.



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Manufacturing  
and Control



Clinical  
Development



Biologics  
& CGT