

### Summary

Medicinal chemistry is an integral part of bringing a drug through development. Our medicinal chemistry approach enables clients to benefit from efficient navigation of the early drug discovery process through to delivery of preclinical candidates.



DISCOVERY

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### Medicinal Chemistry Services:

- Target identification
  - Capture Compound® mass spectrometry (CCMS)
- Hit-finding strategies
  - Optimizing high-throughput screening (HTS) hits
- Hit-to-lead
- Lead optimization
- Patent strategy
- Preparation for IND filing

Questions for our chemists?  
Visit <https://www.criver.com/consult-pi-ds-questions-for-our-chemists>

## Medicinal Chemistry for Drug Discovery

### A Proven Track Record in Drug Discovery

Our medicinal chemistry team has experience in progressing small molecule drug discovery programs across a broad range of therapeutic areas and gene families. Our scientists are skilled in the design and synthesis of novel pharmacologically active compounds and understand the challenges facing modern [drug discovery](#). Together, they are cited as inventors on over 350 patents and have identified 80 preclinical candidates for client organizations across a variety of therapeutic areas. As project leaders, our chemists are fundamental in driving the program strategy and have consistently empowered our clients' success. A high proportion of candidates regularly progress to the clinic, and our first co-invented drug, Belinostat, received marketing approval in 2015. As an organization, Charles River has worked on 85% of the therapies approved in 2018.

We have a deep understanding of the factors that drive [medicinal chemistry](#) design: structure-activity relationship (SAR), biology, physical chemistry, drug metabolism and pharmacokinetics (DMPK), pharmacokinetic/pharmacodynamic (PK/PD) modelling, and *in vivo* efficacy. Charles River scientists are skilled in structure-based and ligand-based design approaches utilizing our in-house [computer-aided drug design \(CADD\)](#) expertise. We also bring expertise in oral, intravenous (IV), inhaled, and topical routes of administration.

### The Driving Force Behind Successful Preclinical Candidates

Medicinal chemistry is at the core of the early discovery process and critical to the success of efficient, cost-effective and scientifically significant drug discovery programs.

We support drug discovery programs at all stages of the process: target identification through methods such as our proprietary technology CCMS, hit-finding strategies including optimizing [high-throughput screening](#) (HTS) hits, [hit-to-lead](#) and [lead optimization](#). We also guide clients with developing patent strategies and preparation for [IND](#) filing. We understand our client's requirements and consistently deliver high quality preclinical candidates that meet target product profiles within agreed timelines and budgets.

EVERY STEP OF THE WAY

## Hypothesis-Driven Optimization - Minimizes Time to Decision Point

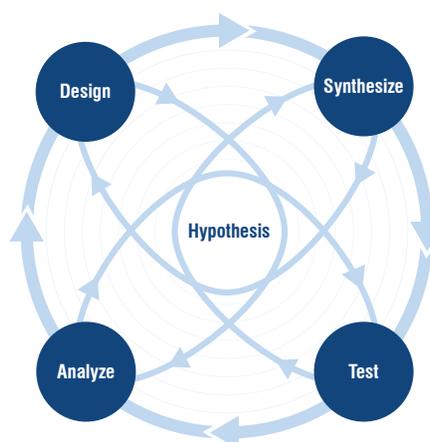
Our philosophy for medicinal chemistry is based on identifying an issue, generating a hypothesis and then interrogating in a design-synthesize-test-analyze cycle. Each compound is designed to answer a specific question to drive the optimization process and reduce overall timelines to preclinical candidate delivery.

### Design

- Multi-disciplinary design teams
- Calculated properties capability (ACD/Labs Percepta)
- Expert CADD support and Maestro desktop visualization tools
- Review ideas and prioritizations

### Analyze

- Dotmatics data repository
- Vortex visualization tool
- QSAR analysis
- Predictive Model Building



### Synthesize

- Highly skilled chemists
- Modern synthesis capabilities
- Parallel synthesis
- Hit explosion toolkit
- Purification services (SFC)

### Test

- Charles River or client
- Multiple read-outs
- Measured properties

## A Holistic View

In order to deliver success for our clients, we need to find a balance of attributes within a candidate compound. We take a holistic approach to balance different parameters when designing compounds such as potency, stability, selectivity, bioavailability, efficacy, [PK/PD](#), safety and patentability. Our chemists have the expertise, experience and processes to optimize and deliver preclinical compounds to our clients.

## Flexible Business Models

Our medicinal chemists work in various ways with clients to progress programs quickly and efficiently. In addition to FTE-based and fee-for-service pricing models, we also offer in-sourced chemistry collaborations. In all cases Charles River chemists are recognized as integral parts of our client's project teams.