


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

 Click to learn more

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

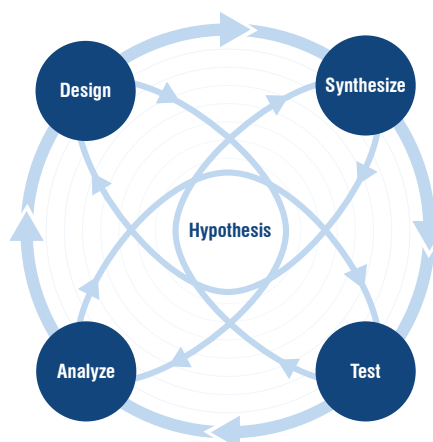
Our philosophy for medicinal chemistry is based on identifying an issue, generating a hypothesis and then interrogating in a design-synthesize-test-analyze cycle. Each compound is designed to answer a specific question to drive the optimization process and reduce overall timelines to preclinical candidate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