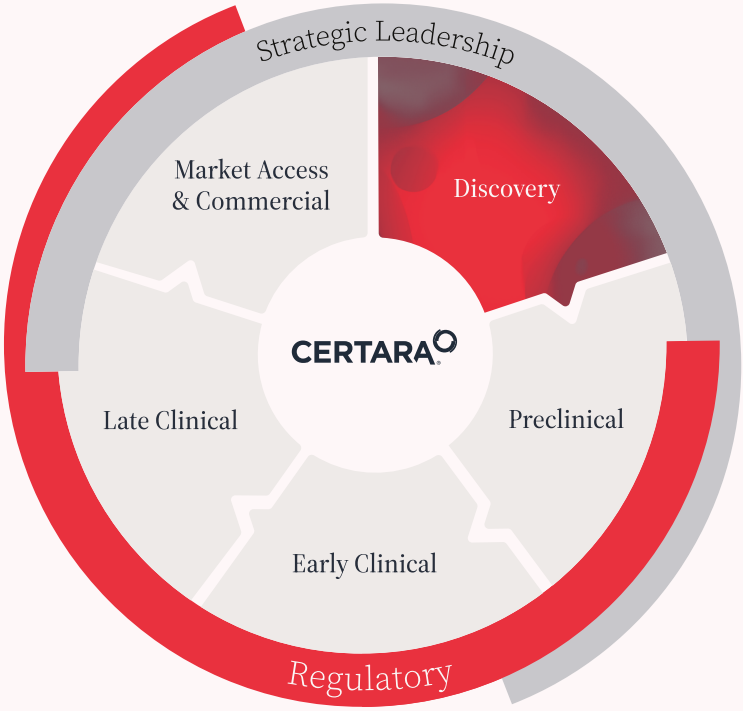
CERTARA
Discovery

Streamline Your Drug Discovery Process

Digitalizing Your Workflows in the Design-Make-Test-Analyze Cycle

Increasing efficiency in the drug discovery process is an important factor in increasing the success rate of drug development in later stages. Maximize your investment in operational excellence with analytic and predictive tools that help your scientists accelerate design cycles and make the most informed data-driven decisions.

Certara acquired Chemaxon in 2024 to unite best-in-class scientific informatics solutions, enabling chemists to improve the efficiency and quality of drug discovery. Our combined capabilities offer the industry's leading core chemistry foundation, self-service data access, data analytics leading to SAR, and tracking of scientific hypotheses and designs. Together, we're helping deliver higher quality leads more quickly and rationally to preclinical and clinical phases—and bring new medicines to patients sooner.



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Software to improve drug discovery

Our discovery focus

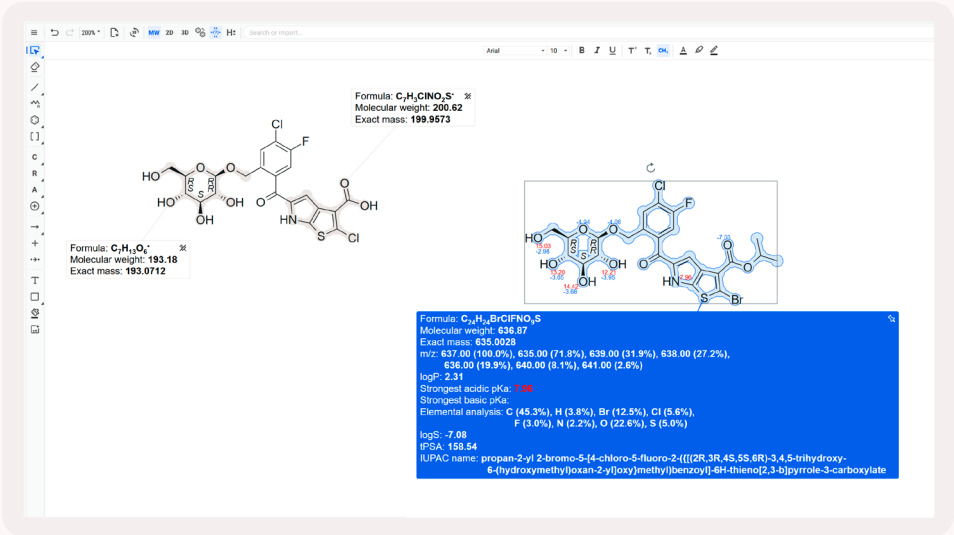
Target ID	Compound Screening	Hit to Lead	Lead Optimization	Preclinical Development	Clinical Trials
• Review of competitive landscape	• Virtual and high-throughput screening	• Property Prediction • DMTA Cycles • Structure-Activity Relationships • Synthesis & Bioactivity Measurements		• In vitro and in vivo studies • Patent & publication preparation	

Build on strong chemistry fundamentals

Improve the quality of your research data across the discovery phase. We cover core chemistry from data input via a fully featured drawing tool that can easily integrate with other software applications, to a set of high accuracy calculators, predictors and tools for structure validation and normalization.

Core Chemistry Products

- Marvin
- JChem Search Engines
- Calculators and predictors
- Standardizer and Structure Checker



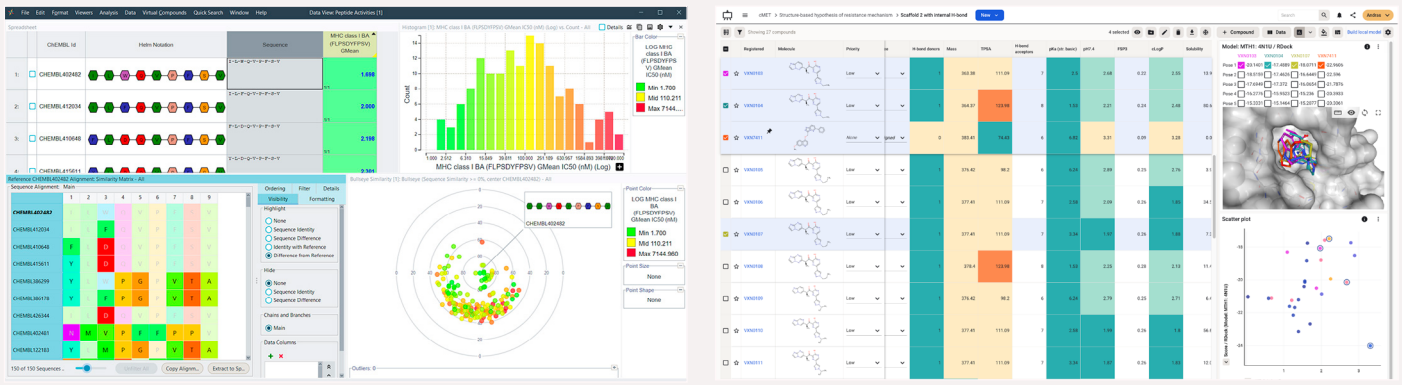
The new Marvin is a universal chemical editor that serves the needs of any chemist involved in research and drug discovery.

Close the DMTA informatics loop

Move seamlessly from data through knowledge and design all the way to realization. Our solutions give you a simple way to link virtual compounds with scientific rationale, experimental and in silico data, understand SAR, and to securely collaborate with CROs. Self-service queries, integrated analysis and visualization let discovery teams understand their data and focus on compound prioritization across therapeutic modalities, including small molecules, antibodies, peptides, oligos, and more.

Design and Analysis Products

- D360
- Design Hub



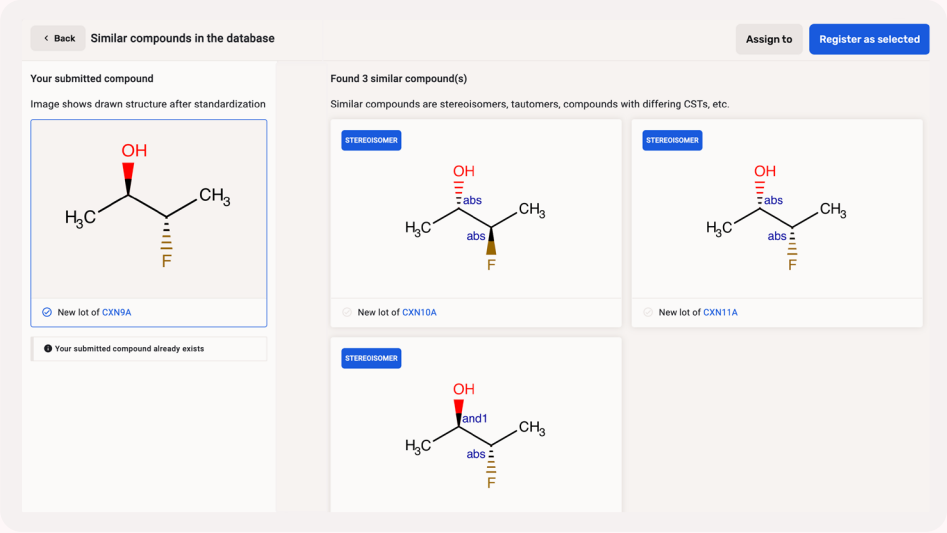
Integration between D360 (left) and Design Hub (right) lets researchers turn data into scientific hypotheses, hypotheses into designs, and designs into candidate compounds

Handle compounds with confidence

Handle your compounds with confidence across your workflows. Our solutions guarantee that all compounds in your databases are scientifically correct, follow your business rules, and keep you up-to-date on the relevant rules and regulations when shipping, storing and synthesizing substances.

Compound Management Products

- Compound Registration
- Compliance Checker
- cHemTS



Streamline compound registration with an efficient, secure, and compliant platform for managing chemical entities.

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"D360 is saving us hundreds of hours annually on data analysis. That is an important contribution to our research. The Certara team is tenacious and resourceful. They always find a solution. That's what has made our relationship so successful."

Dr. Keith Hornberger, Director of Chemistry, Arvinas

To learn more, speak with your account manager or visit certara.com/discovery

Learn more

About Certara

Certara accelerates medicines using biosimulation software, technology, and services to transform traditional drug discovery and development. Its clients include more than 2,400 biopharmaceutical companies, academic institutions, and regulatory agencies across 70 countries.

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