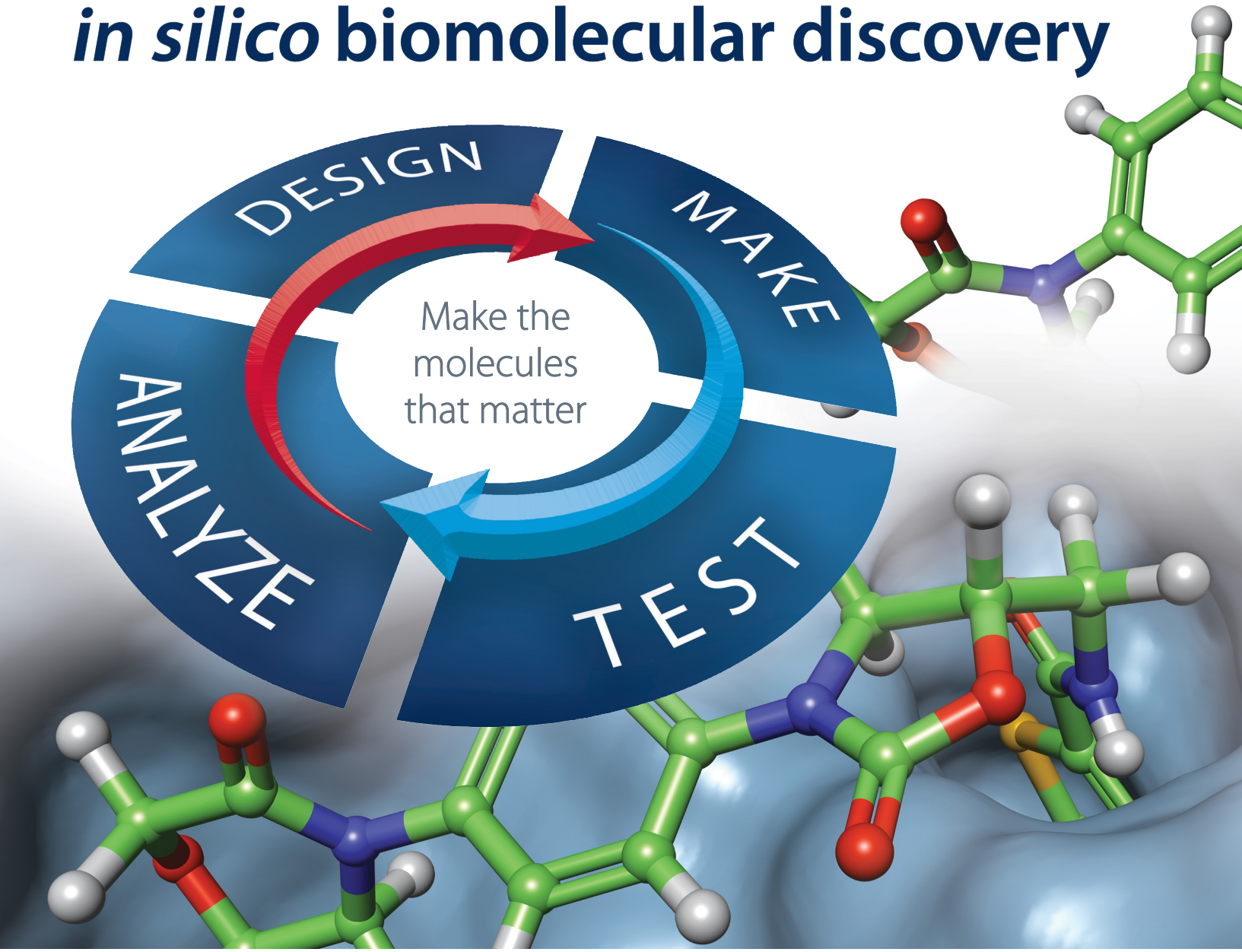
cresset®

advancing

in silico biomolecular discovery



Pharmaceutical | Biotechnology | Agrochemical | Flavor | Fragrance | Fine Chemicals | Academia

cresset®
CADD software

Intuitive software solutions

Structure-based and ligand-based desktop and server software solutions enabling computational, medicinal and synthetic chemists to accelerate their small molecule discovery projects.

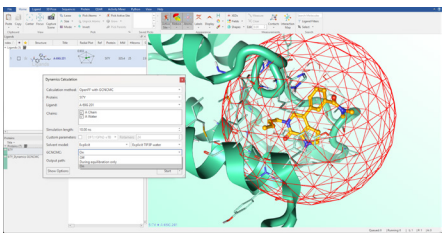
flare

Discover novel small molecules more efficiently and effectively

Through high-resolution 3D visualization and in-depth analysis of target structures and potential ligands, Flare™ enables users to optimize and prioritize new molecules efficiently and effectively.

With a variety of methods including docking and scoring, Electrostatic Complementarity™, molecular dynamics, pocket analysis, and water analysis (GIST and 3D-RISM), structure-based designers can gain new insights into protein-ligand binding to progress lead optimization with confidence.

Flare Free Energy Perturbation (FEP) calculations can be used to accurately predict the relative binding free energy of congeneric ligands.



Study the conformational changes of proteins and assess the stability of protein-ligand complexes with molecular Dynamics in Flare.

Ligand-based designers can rapidly decipher complex SAR using Activity Miner™ and Activity Atlas™. They can prioritize the best molecules to make through robust QSAR models that predict the activity and ADMET properties of new compounds.

Thanks to the Python API, Flare features are fully customizable and expandable.

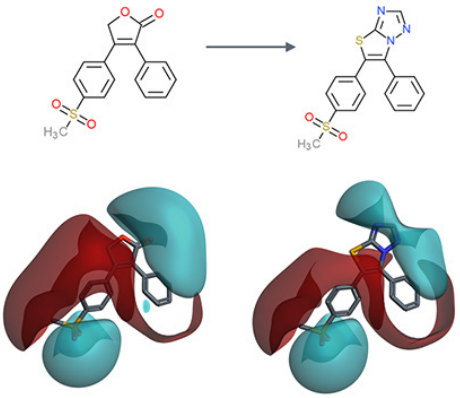
spark

Generate highly innovative ideas for your project

Our customers tell us that Spark™ is the best scaffold hopping and bioisostere replacement tool they have ever used.

Explore chemical space by quickly generating a range of novel molecules from an initial structure. Profile and score the results to choose the most innovative and tractable structures with the properties you need.

Spark's unrivalled output will ignite your chemical creativity. Whether your goal is scaffold hopping, R-group exploration, patent busting or IP finding, your results will include structures you have thought of yourself, and new molecules that make chemical sense and are unexpected.



Generate obvious, less obvious and truly novel solutions in core hopping experiments. Searching for a replacement of the cyclic lactone of Rofecoxib unexpectedly reveals a triazolo-thiazole with similar electrostatics but completely different structure.

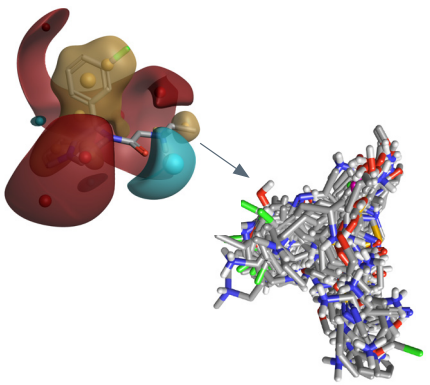
blaze

Increase your wet screening hit rate at a fraction of the cost

Blaze™ is an effective virtual screening platform. It uses the electrostatic and shape character of known ligands to rapidly search large chemical collections for molecules with similar properties.

Make efficient use of your time by routinely running a virtual screen in parallel to wet screening. A virtual screen of 10 million structures just takes a few hours.

Blaze has been delivering lead-like hits to our customers for almost 20 years achieving hit rates as high as 30%. Our customers say that what they really value is the diversity of hits returned from every Blaze screen.



Blaze search using a known A2C adrenergic agonist as query retrieves a wide diversity of novel structures including many known actives.

cresset®
Torx DMTA

Connected chemistry

A complete feature rich DMTA solution, Torx® drives productivity through effective collaboration by connecting chemists, research leaders and CROs in a secure, cloud platform.

torx

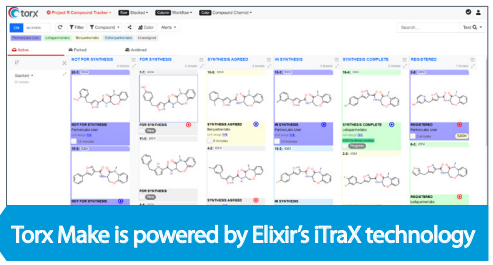
Enhance molecule design through collaboration

Torx Design helps inform design decisions by providing real-time data, connecting medicinal and computational chemists in a collaborative environment. Covalent docking enables a wide range of projects to benefit from integrated 3D pose generation, while synthetic feasibility, patentability and references can be interrogated via the seamless connection to CAS SciFinder®.

Receive live updates of key information as you sketch your new molecule design.

Track and manage compound synthesis across in-house and CRO projects

Torx Make ensures effective resource management with a top-level view of every compound in your portfolio. The real-time interface for viewing CRO workload helps to monitor and instantly share priorities and milestones securely, while the 'time in status' filter enables identification of compounds which have stalled during synthesis.

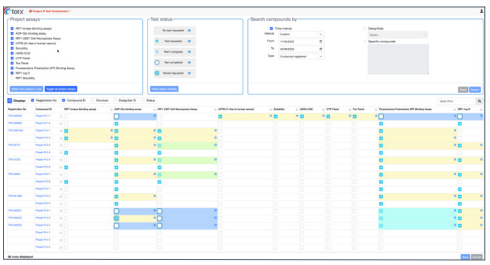


Torx Make is powered by Elixir's iTraX technology

View, track and manage the synthesis of all compounds in the intuitive, feature-rich Kanban board.

Automate assay scheduling and monitor progress in real-time

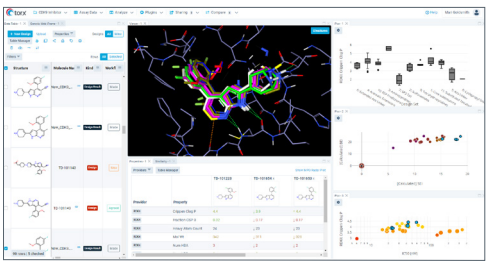
The Torx Test Orchestrator connects chemists and assay scientists with a holistic view of requests, enabling seamless test scheduling, resource allocation and results delivery. Automated requesting eliminates administrative burden and promotes open dialogue between teams.



Visualize and manage test requests at the project, hypothesis and compound level.

Inspire design through insightful analysis

Torx Analyze helps chemists gain a deeper understanding, centralizing all project data and recording key outcomes. Live merging of data from corporate repositories with the existing molecule design helps build the complete picture to enable decision-making on the next iteration of the DMTA cycle.



Analyzing the latest results, comparing 2D and 3D data with existing information enables informed decision making.

Torx is a collaboration between Cresset and Elixir Software

www.cresset-group.com/software/torx

cresset®
Discovery CRO

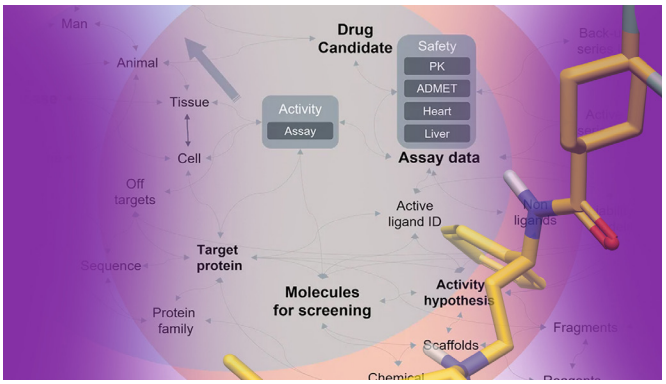
Premier computational chemistry CRO

From ideation to synthesis and biological results, our expert modelers are the best at what they do. Working alongside you from the ground up, they give expert advice and guidance on how to accelerate your assets through the pipeline.

Your scientific partner

Cresset Discovery has established an excellent success rate in contract research. Our focus is early to late phase discovery across a broad range of industries, centering on small molecule design for biological targets. We have one of the largest dedicated in-house team of expert modelers, who, in the last decade, have delivered 400+ projects with many leading pharmaceutical, biotech, agrochemical, flavor and fragrance companies.

We bring a fresh perspective, years of industry experience, outstanding science and a complete professional service. As your scientific partner, we share a real interest in your research and offer objective opinions about which avenues to pursue to advance your project. We will always choose the right technology for your project, based on your needs and your project goals.



We work alongside your scientists to solve problems, provide fresh ideas, remove roadblocks and add direction and insight. We help you reach your next milestone faster and more cost effectively through:

- Hit finding, lead generation and optimization
- Creating, broadening and protecting IP
- Supporting funding applications
- Task-driven modeling activities
- Accelerating the commercialization of assets

Outstanding science and results

Intelligent computational approaches are at the heart of our offering. We work from early to late stage research, combining expertise in medicinal and synthetic chemistry, biology, biochemistry and pharmacology. At all times our goal is to provide the best possible methods to deliver outstanding results.

- Robust science
- Experienced scientists
- Innovative methods

Collaborative working creates synergy

Every project brings a different approach, new science and a fresh way of working. We propose methods that provide answers in the most intelligent and innovative way we can. Collaboration often sparks new and better methods and ideas, and our scientists are excited by new challenges and by the synergistic nature of contract research.

- Excellent communication
- Objective advice
- Efficient project planning and execution

Flexible, cost effective resources

By accessing expertise where and when you need it, you eliminate unnecessary overheads while obtaining a world-class service. Use us as your long term CRO or to help navigate bottlenecks in your project.

- Demand-driven research
- Flexible staff resources
- Right-sized infrastructure

www.cresset-group.com/discovery