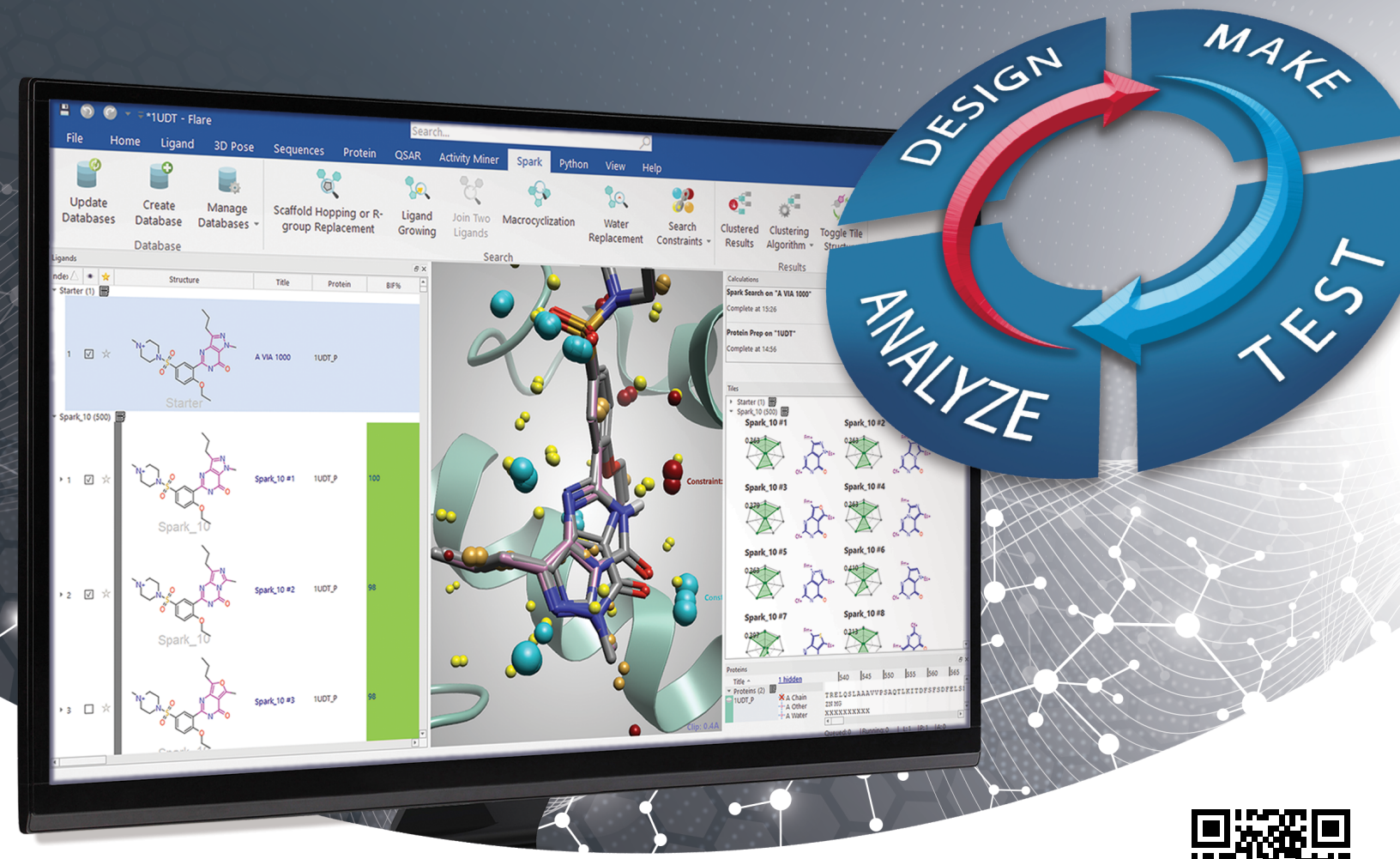
cresset®

AICPA SOC aicpa.org/soc4so SOC for Service Organizations | Service Organizations

CYBER ESSENTIALS CERTIFIED

Accelerate drug discovery with integrated *in silico* **DMTA** solutions

MAKE THE MOLECULES THAT MATTER



cresset® CADD software

cresset® Discovery CRO

cresset® Torx DMTA

cresset®
CADD software

Intuitive software solutions

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

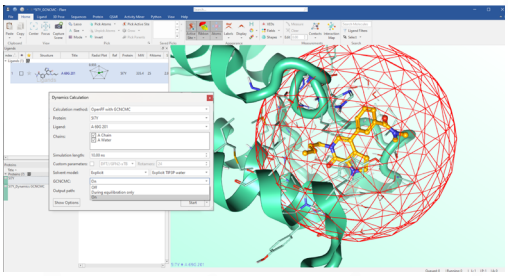
flare

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 efficiently optimize and prioritize new molecules, while full integration of Spark, Cresset's best-in-class bioisostere application allows creation of novel IP.

Methods include:

- Docking and scoring
- Electrostatic Complementarity™
- Molecular Dynamics
- Water analysis (GIST and 3D-RISM)
- Free Energy Perturbation (FEP)
- MM/GBSA



Study conformational changes of proteins and assess the stability of protein-ligand complexes

Ligand-based designers can rapidly decipher complex SAR using Activity Miner™ and Activity Atlas™, prioritizing molecules 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.

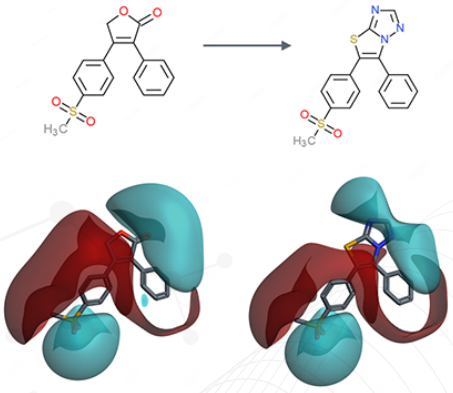
spark

Inspire chemical creativity and generate innovative ideas

Explore chemical space with Spark™ to quickly generate a range of novel molecules from an initial structure.

- Scaffold hopping
- R-group exploration
- IP finding & patent busting
- Integration of Enamine Linker Libraries
- Patent busting

Profile and score the results to choose the most innovative and tractable structures with the properties you need. Flare includes full integration of Spark.

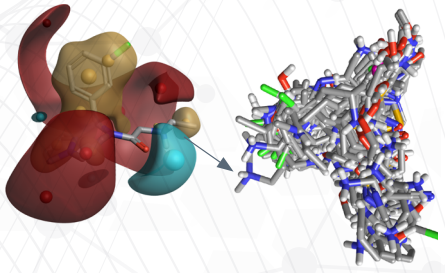


Generate obvious, less obvious and truly novel solutions to ignite your discovery projects.

blaze

Intuitive virtual screening of compound collections

Blaze™ uses the electrostatic and shape character of known ligands to rapidly search large collections for molecules with similar properties. Run virtual screening in parallel to your wet screening. A virtual screen of 10 million structures takes only a few hours and achieves hit rates as high as 30%.



Retrieve a wide diversity of novel structures with every screen

cresset®
Torx DMTA

Connected chemistry

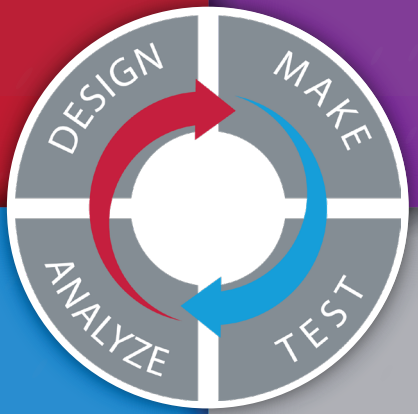
Dedicated standalone molecules work in synergy for a complete DMTA solution. Seamless integration with third party applications such as CDD Vault* enables automatic registration of new compounds.

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. Protein-ligand docking, including covalent, 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®.

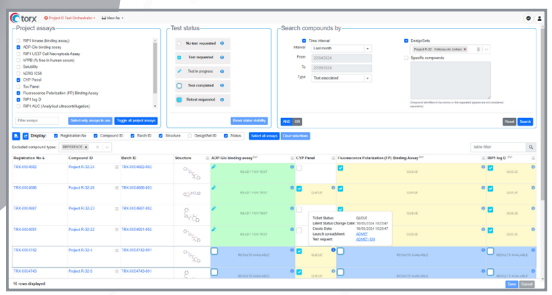
Track and manage compound synthesis across in-house and CRO projects

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.



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.



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.

Torx is a collaboration between Cresset and Elixir Software™

cresset®
Discovery CRO

Premier computational chemistry CRO

Cresset Discovery has established an excellent success rate in contract research. Our expert computational chemistry team can support every step of the discovery process, accelerating your asset no matter the modality. through your pipelne

Your scientific partner

Our dedicated in-house team has an excellent success rate in contract research, having delivered over 450 projects with leading pharmaceutical, biotech, agrochemical, flavor and fragrance companies.

We do not seek to own any intellectual property from your project; all scientific materials relating to the work belong to you.

Optimize the value of your research investment and reach your next milestone faster!

Collaborative working creates synergy

Intelligent computational approaches are at the heart of our offering, combining expertise in medicinal and synthetic chemistry, biology, biochemistry and pharmacology.

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

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 Contract Research Organization or to help you to navigate demanding bottlenecks in your drug discovery projects to reach your goals faster.

Gain access to the latest in silico and AI modeling technologies