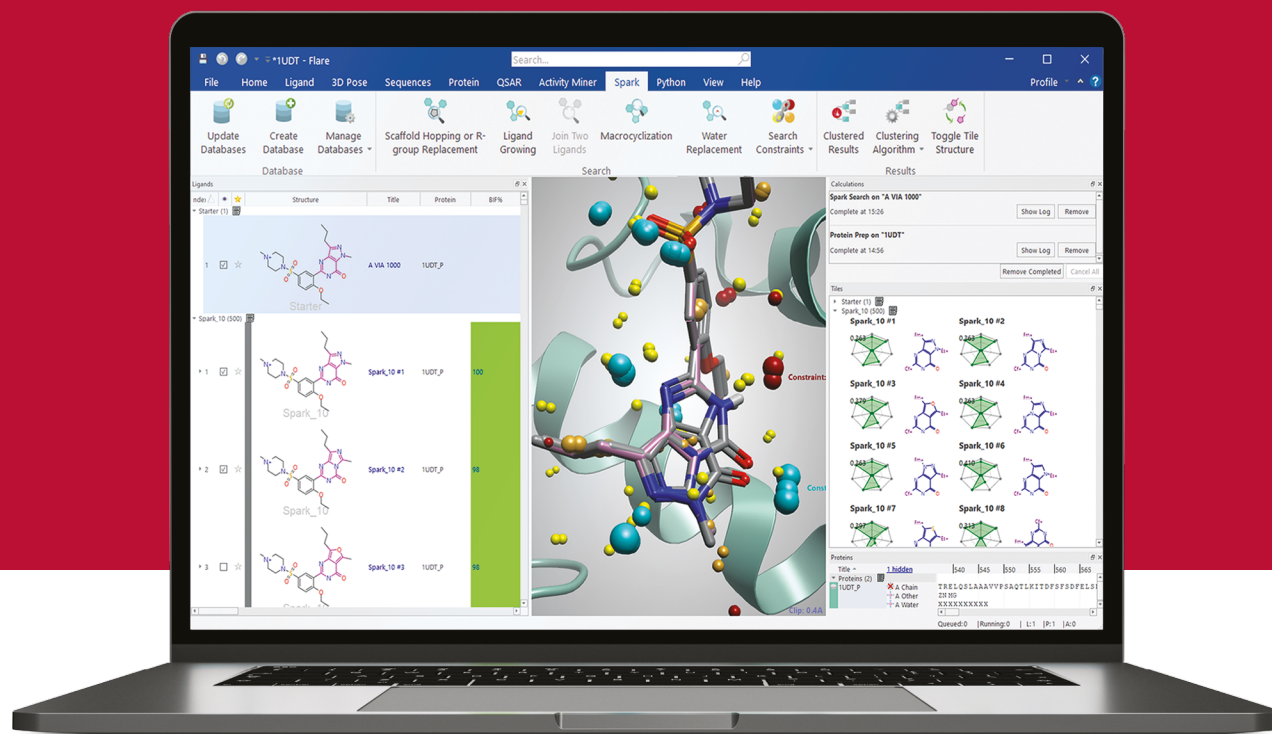# Flare™ V9

Spark™, Cresset's bioisostere replacement solution,
is now available in Flare V9.

Streamline molecule discovery from novel idea generation to extensive optimization within Flare

Bioisostere replacement in Spark works in electrostatic and shape product space to better describe the biological activity of your molecules, enabling creation of novel IP

User-friendly wizard-driven access to a wide variety of experiments

Access to an outstanding source of bioisosteres to generate new project ideas

Drive efficiency by creating custom workflows and automate tasks via the Flare Python API
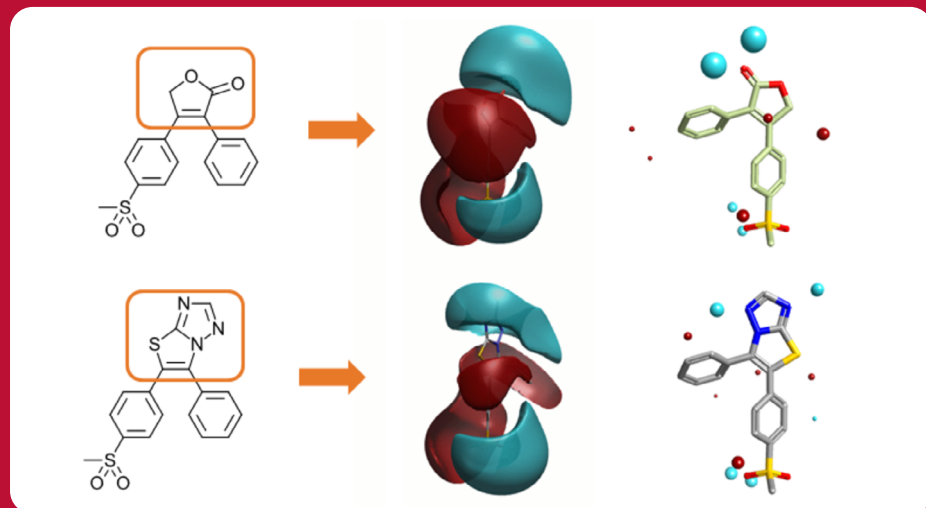
Flare for ligand and structure-based drug design

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.

Flare V9

Generate highly innovative ideas for your project using a wide variety of experiments

Find biology relevant replacements for both core and terminal groups

Grow your ligand into empty pockets

Identify linkers, from real chemistry, to join two ligands

Also new in Flare V9:

MM/GBSA Dynamics

Molecular Mechanics/Generalized Born Surface Area (MM/GBSA) is a method to calculate ligand-protein binding free energies. Estimate binding free energies for a set of ligands by averaging the MM/GBSA binding free energy over the course of an MD trajectory for more accurate results.

Homology Modeling

Homology Modeling is a method for constructing the 3D model of your target protein when its 3D structure is not yet known and only its primary sequence is available. The method relies on two requirements for building an accurate model within Flare: the 3D experimentally determined structure of a protein with similar sequence and function to that of the target, and the target sequence of amino acids.

Other new features and enhancements in Flare V9 to progress lead optimization with confidence:

- Even more highly customizable options for fine-tuning dynamics simulations
- Customize conditions for performing each step of Flare FEP calculations, along with even more visual troubleshooting tools
- Seamlessly manage Python extensions to access advanced data visualization and calculation functionalities through enhanced Extension Manager
- Write, save and run your own scripts using the JupyterLab Notebook integration

and more...