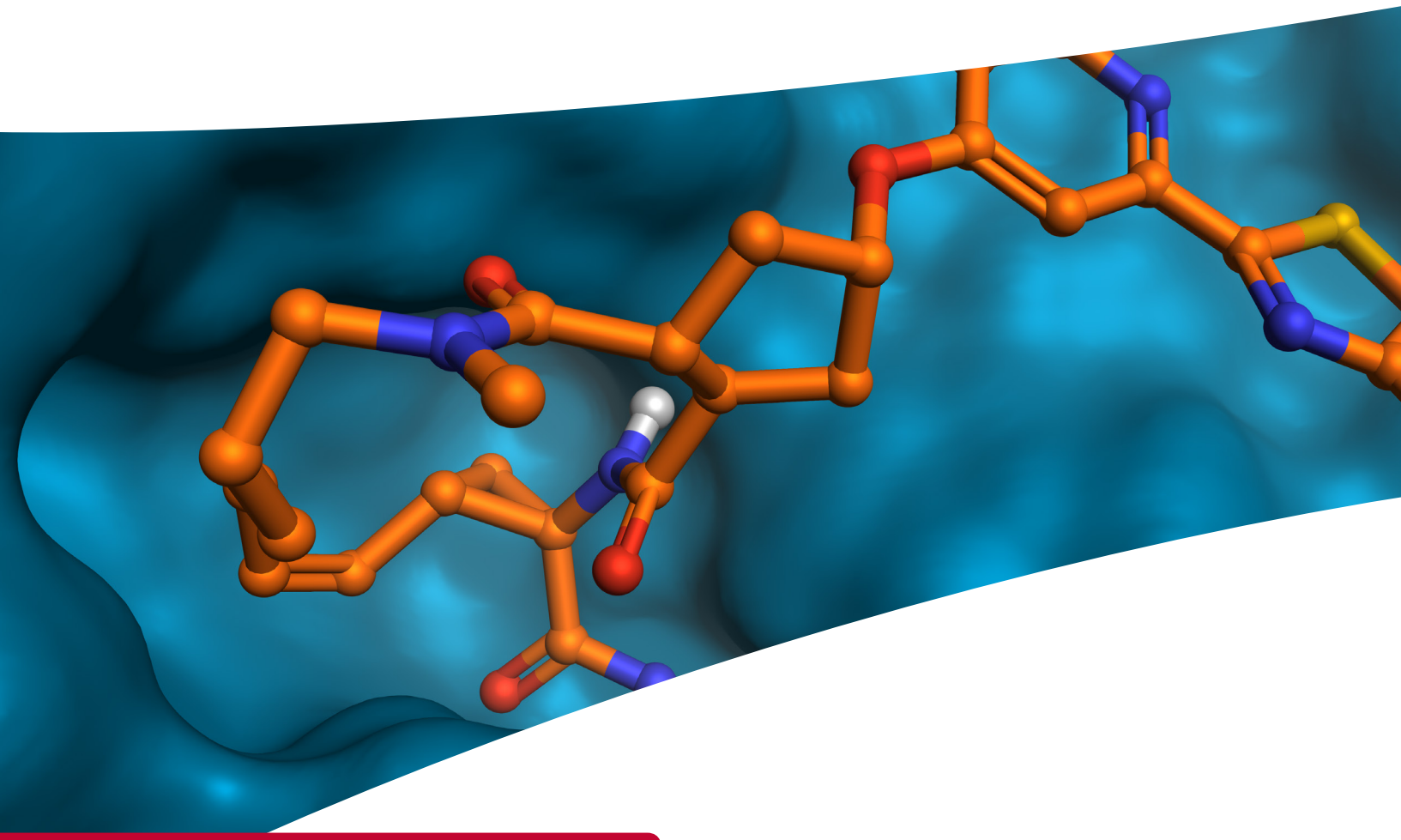
cresset
software

Outstanding software for molecular discovery

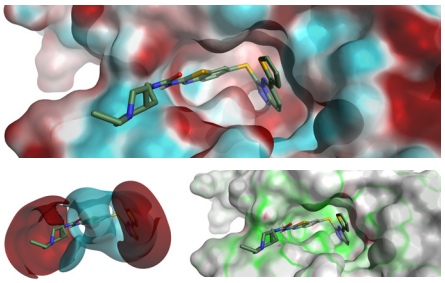


innovative science • intuitive software

Fresh insights into structure-based design

New approaches for protein-ligand analysis and molecular design

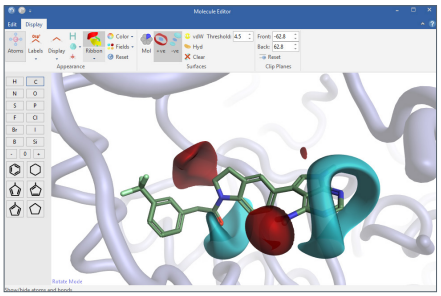
Perfect molecule design



Left: Protein electrostatic potential map within the binding pocket.

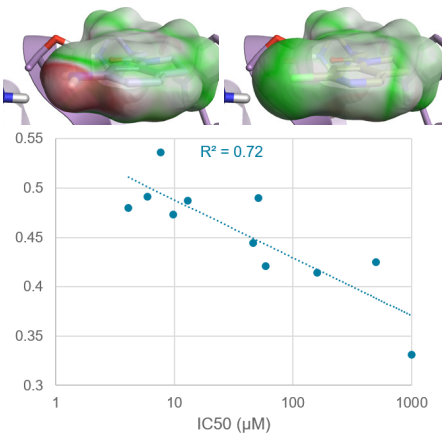
Bottom left: Ligand electrostatic map showing complementary electrostatics to the protein.

Bottom right: Electrostatic complementarity map.



Designing new ligands in Flare™ gives you immediate feedback on electrostatic changes while viewing your molecule in the protein active site.

Fast and interactive activity prediction



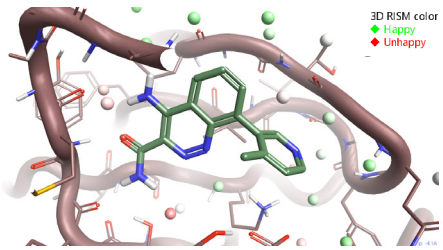
Cresset's innovative Electrostatic Complementarity™ (EC) scoring provides rapid activity prediction with visual feedback on new molecule designs.

Left: Less active XIAP analog (red) is less complementary.

Right: More active XIAP analog (green) is more complementary.

Graph: EC score versus experimental activity for 11 XIAP analogs.

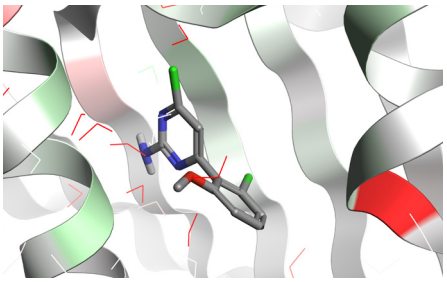
Water analysis you can trust



Knowledge of which water molecules are tightly bound and which are energetically unfavorable can give valuable insights into structure-activity relationships and help you decide where to place ligand atoms.

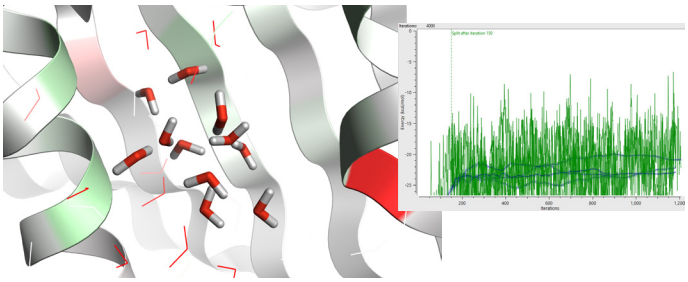
Predict detailed interaction energies

WaterSwap, a thermodynamic integration method for investigating ligand-protein energetics, gives a direct estimation of $^{\Delta G}$bind which is broken down into per-residue components.



Green residues show where the ligand is gaining the most energy from interaction with the protein.

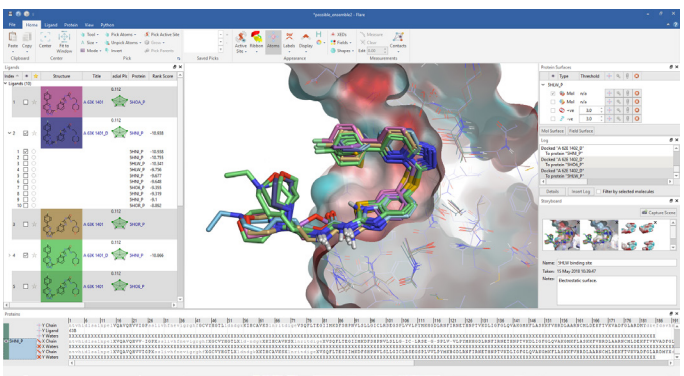
Red residues show where water binding is preferred and represent opportunities to improve ligand design.



Quick, easy and accurate docking

Rapidly and easily dock to multiple protein conformations in a single experiment.

Advanced functional forms provide excellent pose prediction, detailed feedback on new molecule designs and high enrichments in virtual screening.



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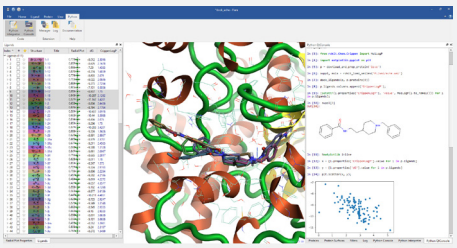
A balance of flexibility and usability

Customize and automate your tasks with the Python API

Flare has a Python API that lets you create your own workflows, automate your common tasks, expand Flare with Python modules and add custom controls.

The Python API gives full access to all of Flare's capabilities, including the RDKit cheminformatics toolkit. Flare can be upgraded with Python modules for graphing statistics, Jupyter® notebook integration and much more.



Enter Python commands into Flare and display their output inline as text or images.

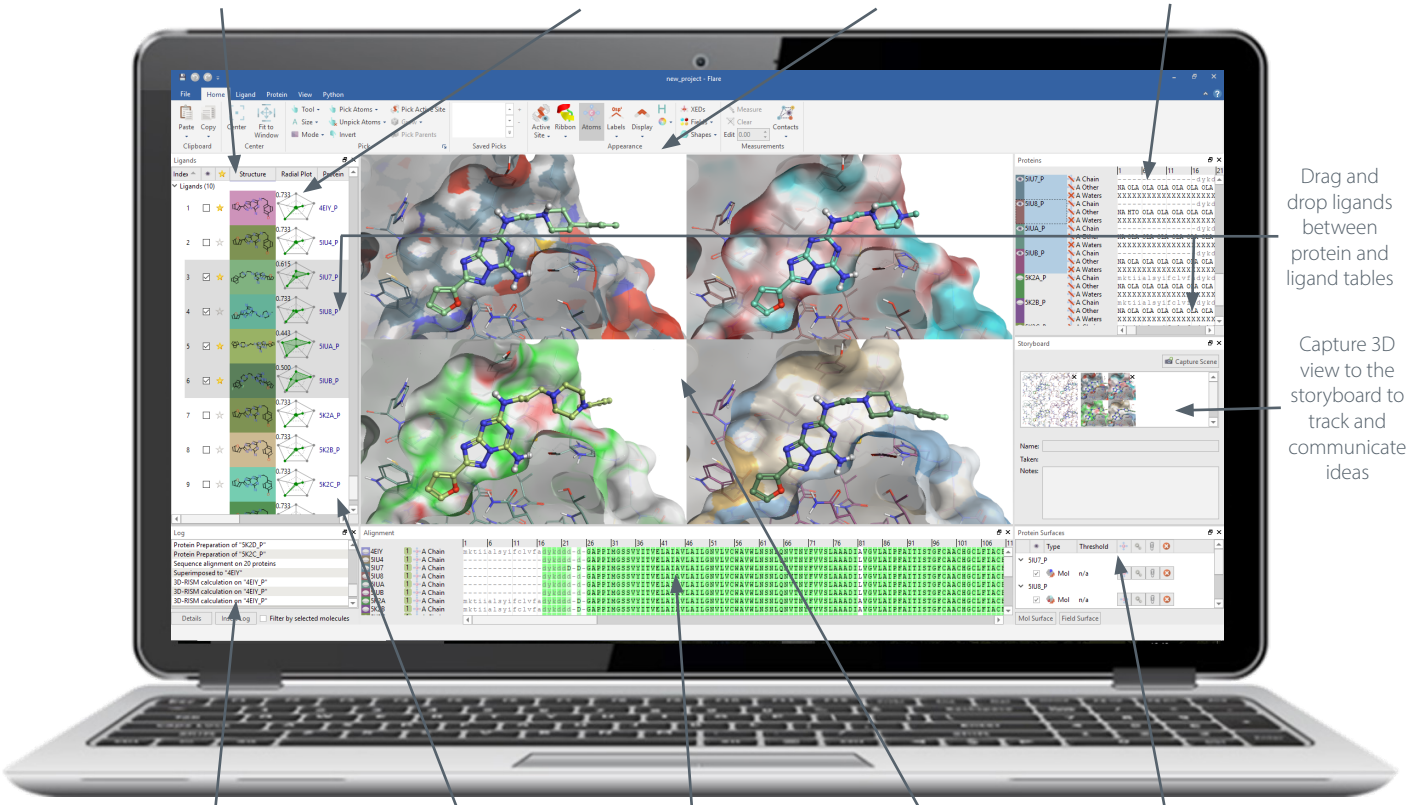
python™

Ligand-centric view gives easy access to all ligand actions: sort table on any column, control visibility and associate with proteins

Calculate physico-chemical properties and multi-parametric scores for every ligand

Convenient menu structure for quick identification of commands and controls

Protein table enables rapid inspection of specific chains or residues



Drag and drop ligands between protein and ligand tables

Capture 3D view to the storyboard to track and communicate ideas

Summary and detailed logging of calculations and events

Every ligand has a parent protein

Protein sequence alignment and superposition

Grid the 3D window by protein and ligand to compare and contrast

Control every surface with individual display options

"The protein interaction potential capability highlighted common features across the family of targets of interest that we had not been able to visualize before. We used this information to drive ligand design into a direction we have not explored before."

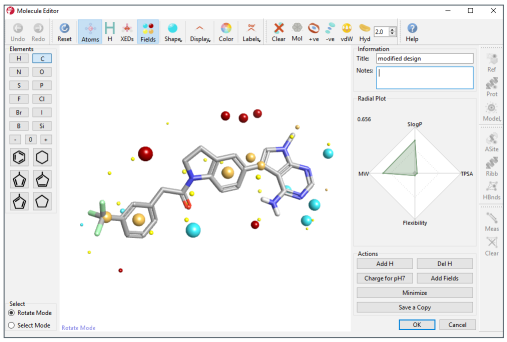
flare

Comprehensive ligand-based design

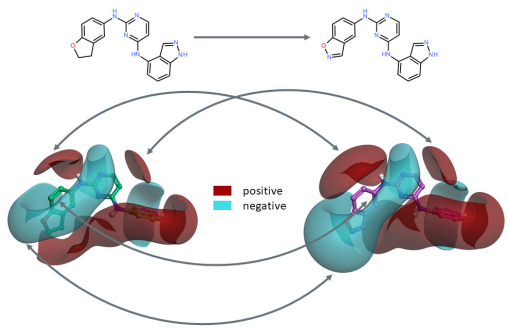
Get a deeper understanding of molecular design and SAR

Active design using electrostatics

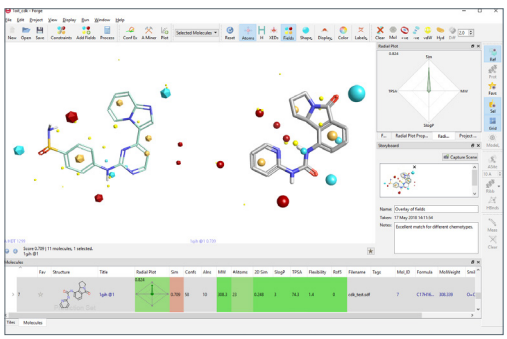
Torch™'s ligand-centric view enables 3D design whether or not you have a protein crystal structure. It makes it easy for you to focus on the designs that work and optimize their physicochemical properties.



Electrostatic and shape descriptors provide a rich informed view to help you understand the effects of chemical changes and eliminate designs that are unlikely to be active.



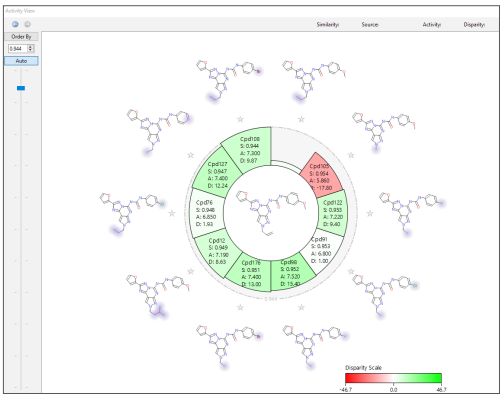
A change on one side of the molecule can often influence a distal region, especially if the moieties are electronically linked through π-systems.



Compare and score chemically different molecules based on electrostatic and shape properties.

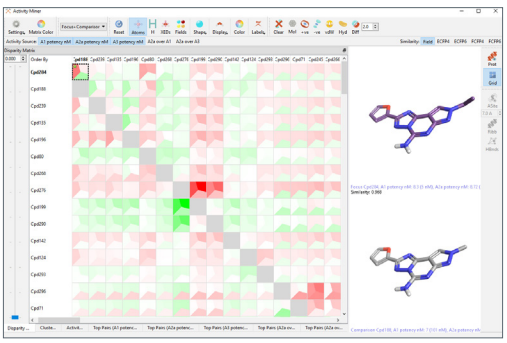
Find and understand activity and selectivity cliffs in your SAR

Activity Miner™, a component of Torch and Forge™, helps you find and understand critical regions in complex SAR. Using the concepts of activity cliffs and matched molecular pairs, you can link activity changes to electrostatic and shape changes.



Compare the similarity between a chosen focus molecule and its closest neighbors using the innovative Activity View. Easily assess the impact of small structural changes on activity and selectivity.

Pinpoint the most significant changes to your molecules using the sortable Top Pairs table. Find critical points in the SAR and understand how they relate to changes in physicochemical properties.



Display multiple activities in the Disparity Matrix to highlight key selectivity information. Rationalize changes with respect to electrostatic, shape and structural properties.

Request your free evaluation

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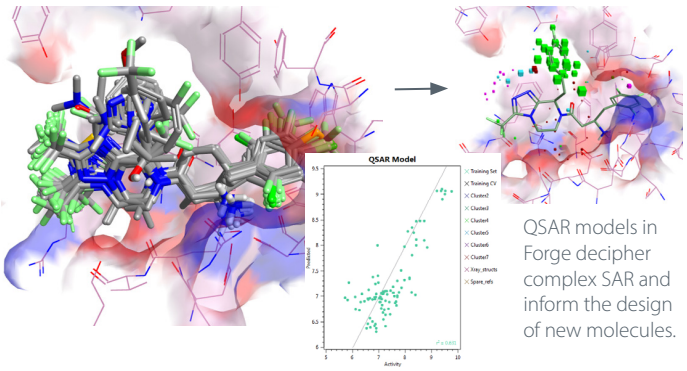
> *I have to say that your software has an extremely nice user interface and is easy to learn and use. I can tell that a lot of thought and a lot of work went into polishing these programs.*

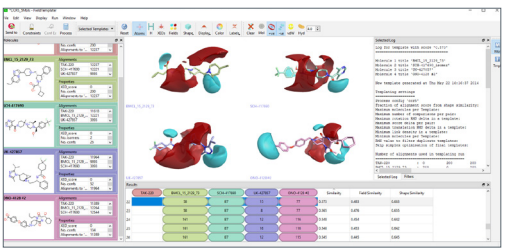
Powerful models to interpret your data

Forge uses the Cresset's patented ligand alignment algorithm to generate realistic, interpretable relationships across your molecules.

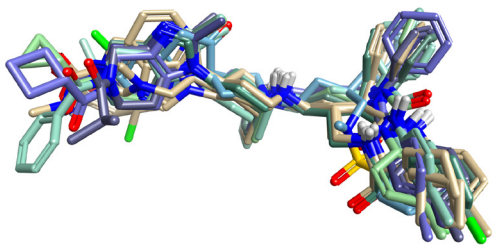
It includes an impressive range of SAR models that combine robust analysis with customizable parameters, ease of use and intuitive visualization. For SAR analysis, there is no need to look any further than Forge.



QSAR models in Forge decipher complex SAR and inform the design of new molecules.



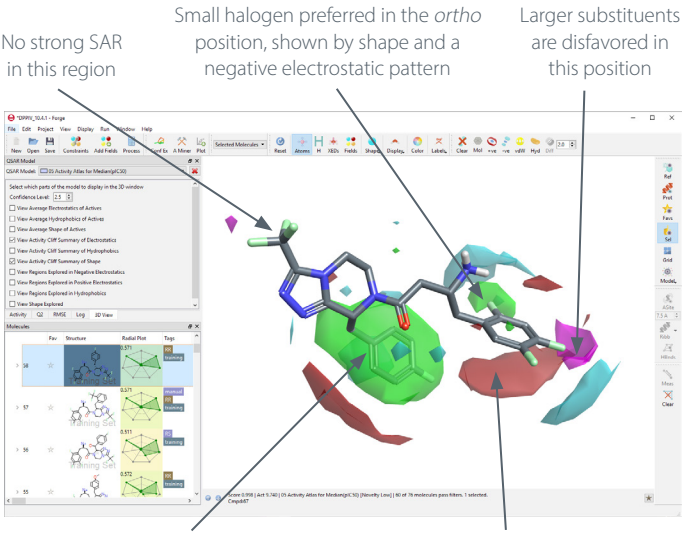
The FieldTemplater module generates bioactive conformation hypotheses using the electrostatic and shape characteristics of your molecules in the absence of protein X-ray data.

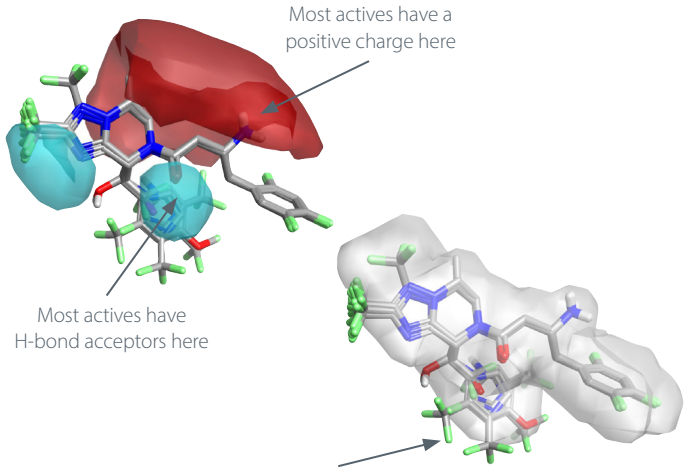


Generate realistic ligand alignments across single or multiple chemotypes with minimal manual intervention.

New SAR insights from novel methods

Activity Atlas™ is a novel, qualitative method that generates three distinct maps of the electrostatic, shape and hydrophobic properties around your molecules. It can be used with small or large data sets and is particularly useful for projects where traditional 3D-QSAR approaches fail.





Read case studies

https://cresset-group.com/case-studies

torch

forge

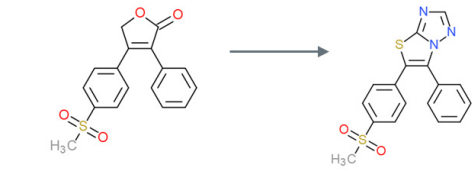
Outstanding scaffold hopping

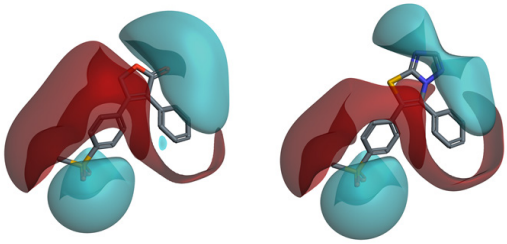
Find biologically equivalent alternatives to escape IP and toxicity traps

Novel cores to kick-start your chemistry

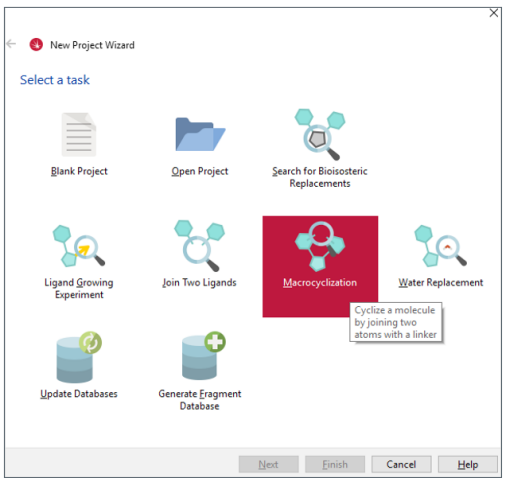
Our customers tell us that Spark™ is the best scaffold hopping and bioisostere replacement tool they have ever used.

The easy-to-use interface quickly generates a range of novel molecules from an initial structure. Profiling and scoring help you choose the most innovative and tractable leads with the properties you need.





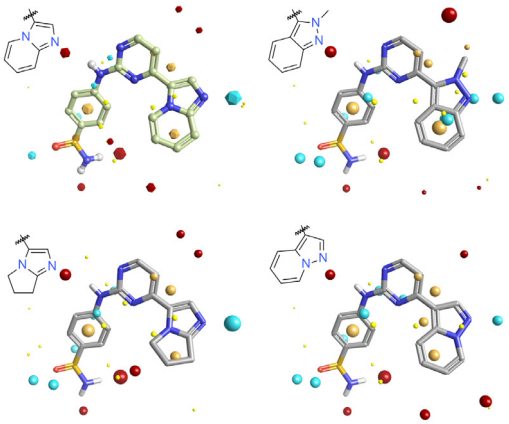
Spark generates obvious, less obvious and truly novel solutions in core hopping experiments. Searching for a replacement of the cyclic lactone of Rofecoxib unexpectedly reveals a triazolo-thiazole with similar electrostatics but completely different structure.



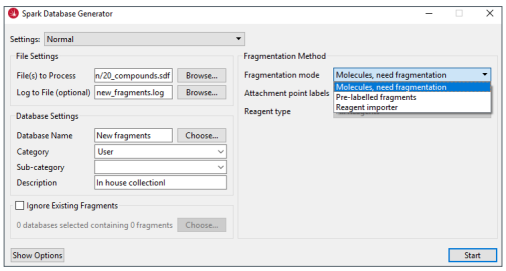
Wizard driven set-up simplifies even complex experiments, making them accessible to your whole team.

Find new R-groups from available chemistry

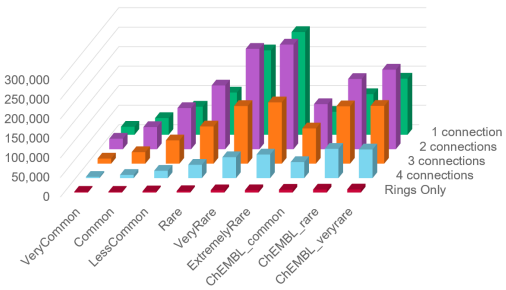
Whether your goal is R-group exploration, patent busting or IP finding, your results will include structures you have thought of yourself, plus new structures that make chemical sense and are totally unexpected. Spark's unrivalled output will ignite your chemical creativity.



Searching the Spark boronic acid database for replacements of the imidazopyridine group (top left) suggests a library that encompasses both aromatic and saturated R-groups.



Search for accessible bioisosteres in your compound collection or available reagents, using the in-built database generator.



Spark includes pre-generated databases that encompass over 3,000,000 unique fragments.

"We have had interesting and exciting results from Torch and Spark experiments which have led to us designing a novel entry inhibitor for HIV-1 with a new scaffold."

See what our customers say

https://cresset-group.com/testimonials

spark

Effective virtual screening

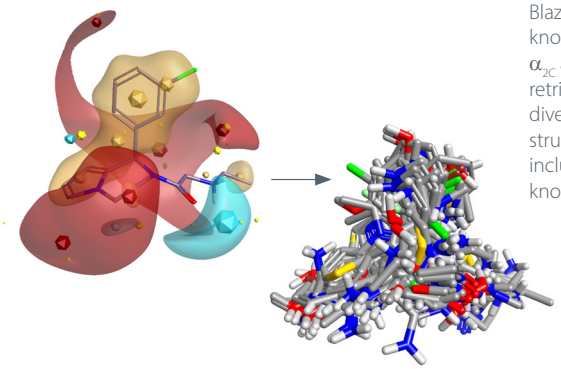
Dramatically increase your molecular diversity

Fast and effective ligand-based approach

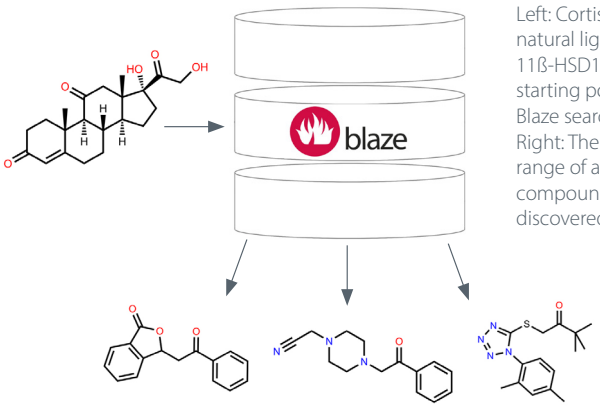
Blaze™ uses the electrostatic and shape character of known ligands to rapidly search large chemical collections for molecules with similar properties.

Hundreds of projects have been run through Blaze and we are proud of our track record. Calculations can be run overnight and our customers achieve hit rates as high as 30%.

Blaze can virtually screen 10 million structures in a few hours, making it feasible to routinely run virtual screening in parallel to wet screening.



Blaze search with a known adrenergic α_{2C} agonist retrieves a wide diversity of novel structures including many known actives.



Left: Cortisone, the natural ligand for 11ß-HSD1 and starting point for Blaze search. Right: The diverse range of active compounds discovered by Blaze.

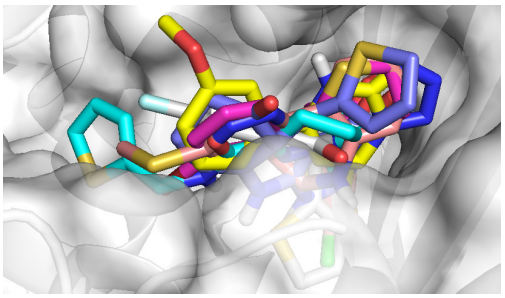
"This is a very important and exciting project for my team so thank you for your good work. The incredibly high hit rate from the Blaze compound list is intriguing."

Great leads from high-throughput docking

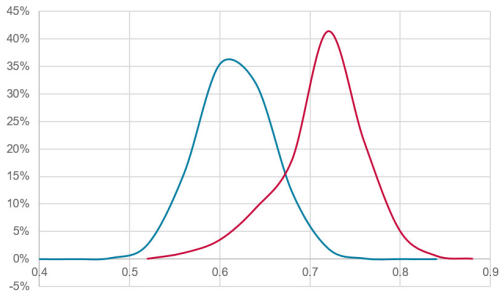
Lead Finder™ is equipped with a dedicated algorithm and scoring function for virtual screening. The algorithm is designed to rapidly dock and score ligands using a method that has been optimized to separate actives from inactives.

Lead Finder can process thousands of molecules per hour. A study on the DUD dataset showed an impressive overall ROC AUC of 0.74 and a median ROC AUC of 0.76.

Flexible licensing terms enable you to use your entire cluster, maximizing your return on investment.

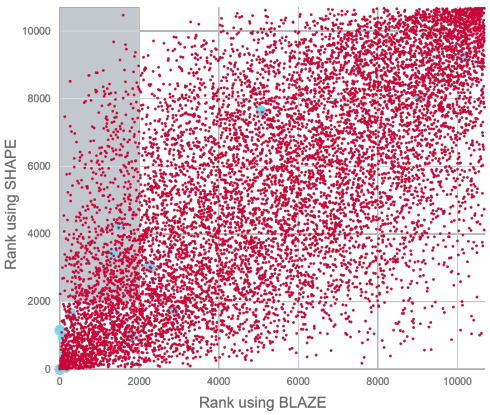


Superimposed docking results from a virtual screen of a small fragment library.



Blaze and Lead Finder perform excellently on standard test data.

Graph: Score distributions obtained by Blaze for decoys (blue) and known actives (red) for EGFR in the DUD dataset.



Blaze provides unique results. A plot of the ranking of compounds using Blaze and a shape based method demonstrates little correlation. Those in the shaded area are uniquely returned using Blaze.

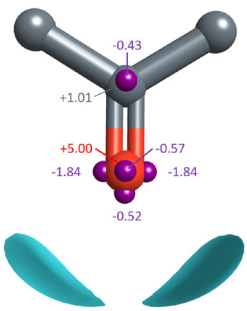
blaze lead finder

Results you can trust

Excellent science is the foundation of our software. Cresset technology centers on the application of the XED force field to the design of new small molecule bioactive compounds. These cutting edge approaches are integrated with significant open source and commercial methods from trusted partners to bring you new insights for molecule design.

XED force field, the foundation of success

The XED approach uses a complex description of atoms to model charge away from atomic centers enabling a more detailed description of electrostatics and excellent reproduction of intermolecular interactions.

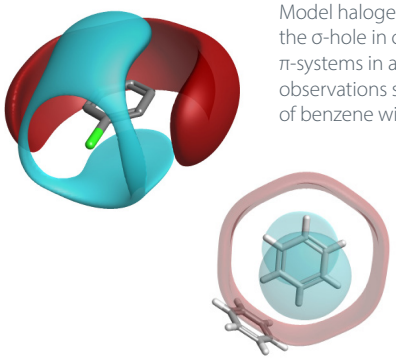


Using off-atom charges, combined with the redistribution of partial charges using a Hückel method, enables the detailed modeling of molecular electrostatics, including lone pair directionality.

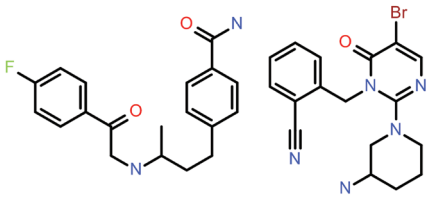
The complex charge model used in this innovative molecular mechanics force field is demonstrated by the XED partial charges for the carbonyl group of acetone. The minima in the negative interaction potential (blue) clearly show lone pairs.

The XED force field enables you to:

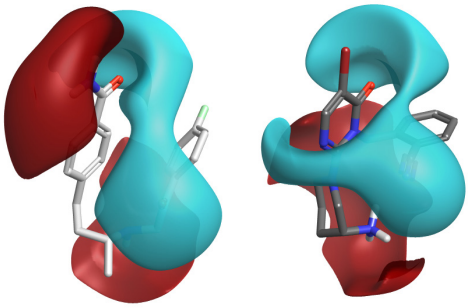
- Gain a detailed electrostatic description of your ligands and proteins
- Understand how structural changes influence your electrostatics
- See how substituents influence the electrostatics of cores and vice versa.

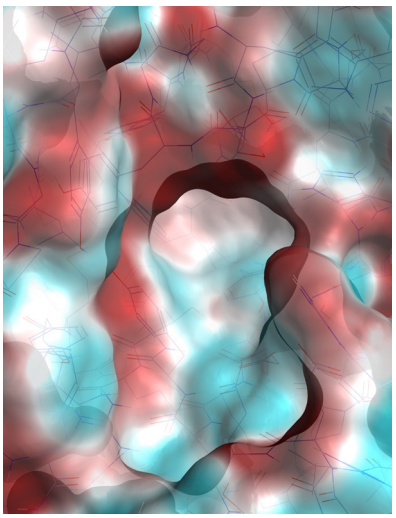


Model halogens in greater detail, such as the σ-hole in chlorobenzene, and describe π-systems in a way that mirrors experimental observations such as the T-shaped interaction of benzene with benzene.

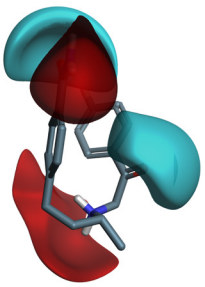


Diverse actives (top) can bind to the same protein, as shown by their 3D conformations (bottom) with electrostatic surfaces.





The electrostatics of the binding site show high complementarity to the ligand and enable the prioritization of new designs.



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cresset® software

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