Change the Way You Think About and Work with Small Molecules

Benefit from Unparalleled Experience in Drug Discovery Research

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cresset™
smarter chemistry | smarter decisions

Transform Molecular Design and Discovery

Chemists use Cresset's software to:

- Visualize electrostatics to make better chemistry decisions
- Analyse SAR data to pinpoint and understand activity and selectivity cliffs
- Build more comprehensive chemical libraries
- Run virtual screens from the desktop
- Scaffold hop to new series and non-obvious new IP.

Cresset's software and services transform molecular design and discovery with a 'protein's eye view' of chemistry.

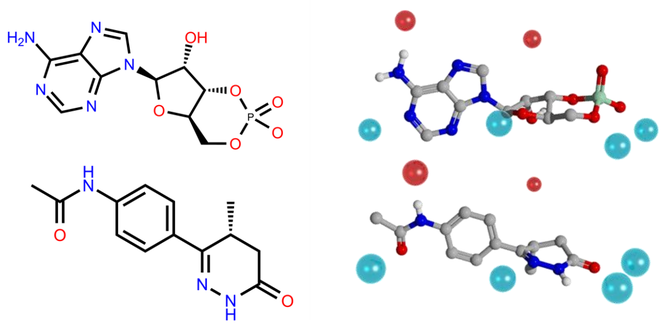


Figure 1: Top left: 2D structures of structurally diverse bioisosteres both active at PDE3, cAMP (the natural substrate) and SKF93741, a PDE3 inhibitor. Top right: The field patterns of the compounds reveal that they are biologically similar and share the same activity.

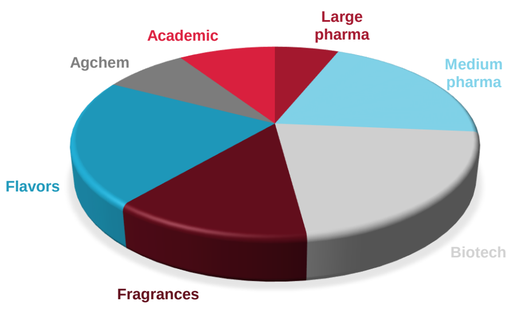
Consulting Services

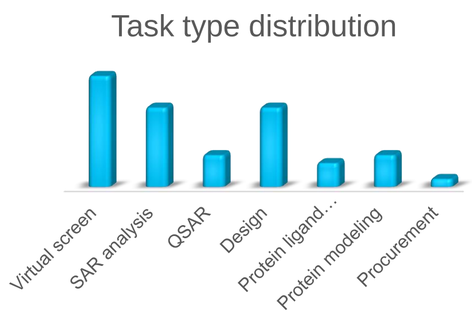
Cresset has established an excellent success rate, working on over a hundred consulting projects tailored to client's research needs.

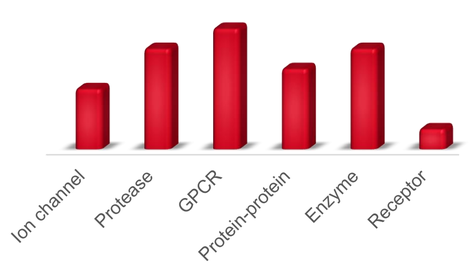
Areas of expertise, where customers use Cresset's services time and again include:

- Virtual screening
- Scaffold hopping
- Library design
- SAR analysis.

Examples of consulting projects in the last 12 months:



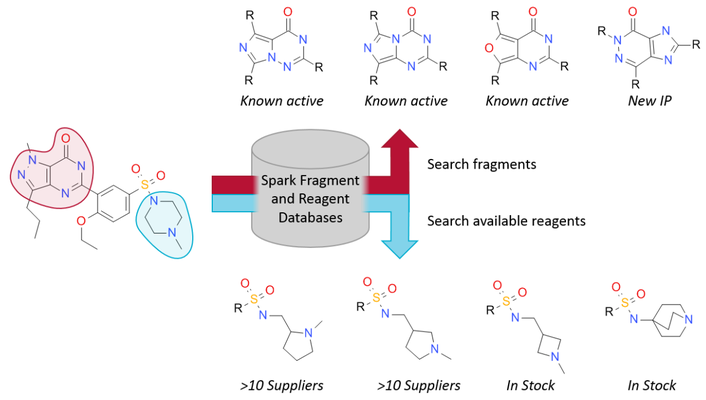




Software

sparkV10

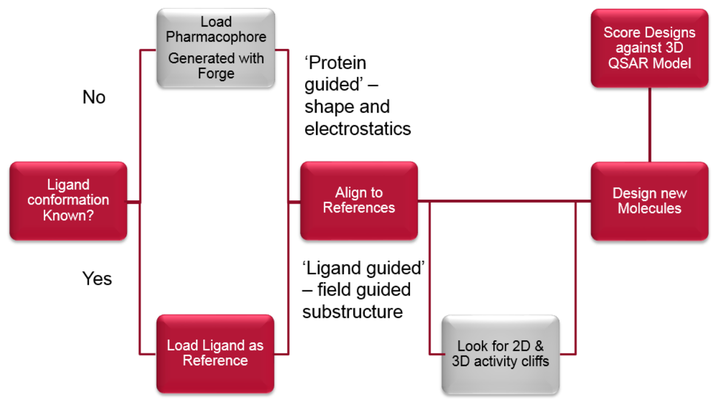
Whether your goal is R-group exploration, patent busting or IP finding, Spark will provide structures you have thought of yourself, plus new structures that make chemical sense and are totally unexpected.

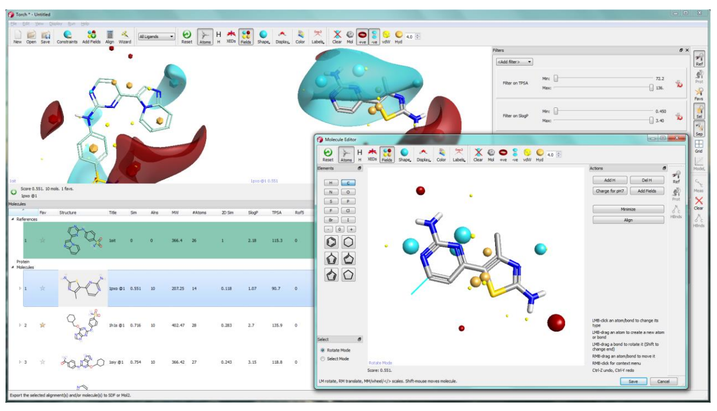


Quickly generate a range of lead molecules from an initial 2D structure.

torchV10

Torch is a powerful design and 3D structure activity relationship (SAR) workbench. Synthetic/medicinal chemists use Torch to design the next compound for synthesis or to understand their SAR.





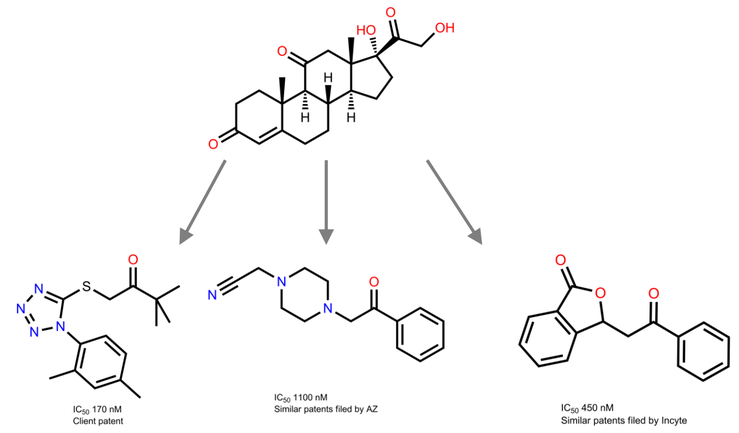
Compare the molecules' fields to generate the best 3D alignment for your compounds.

torchV10lite

TorchLite is a free molecular viewer that gives a rich, informative view of how your molecules behave in biological systems.

blazeV10

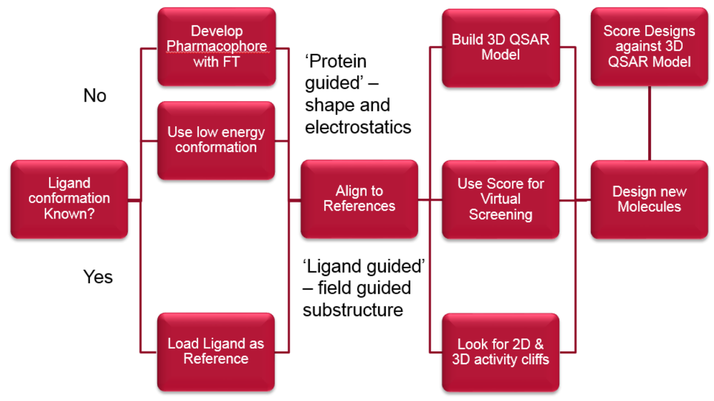
Dramatically increase your wet screening hit rate at a fraction of the cost with a biologically intelligent virtual screen of large chemical databases. Using Blaze you will increase the diversity of your project's lead compounds and jump into new areas of chemical space giving substantial improvements in the properties of your hits.



Three diverse chemotypes with high activity, identified in a virtual screen using Blaze.

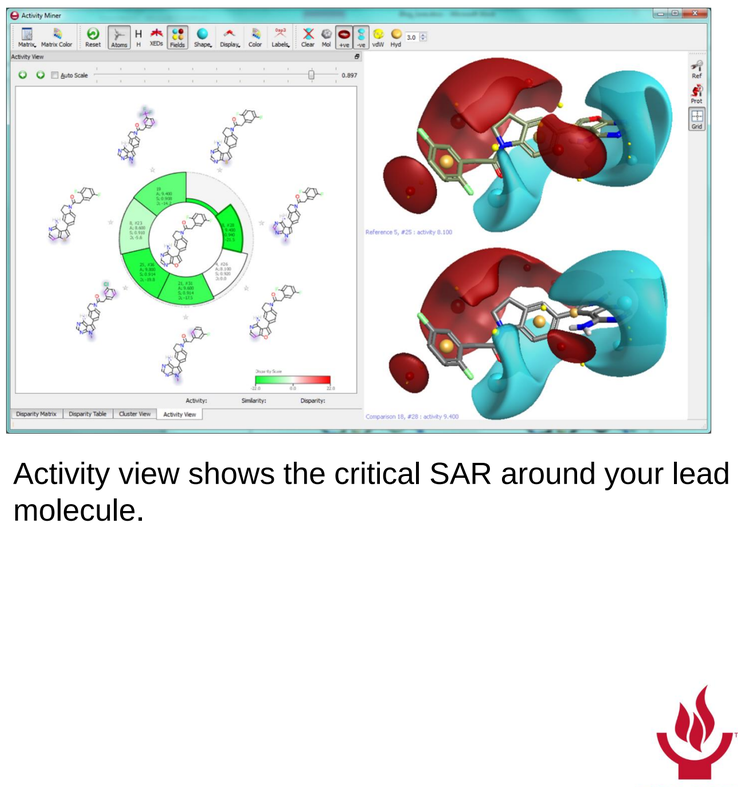
forgeV10

Forge is a powerful computational chemistry suite for understanding SAR and design. Using the shape and electrostatic character of your molecules, Forge creates qualitative and quantitative 3D models of activity. These models are visually stimulating and easy to communicate to your team.



Activity Miner

Activity Miner is a module for Torch and Forge that enables rapid navigation of complex SAR, highlighting key activity changes.



Activity view shows the critical SAR around your lead molecule.

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