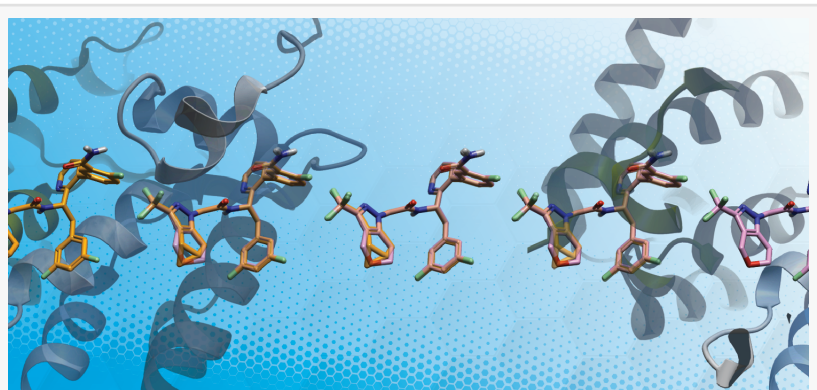


Cresset releases Flare V12 to cut synthesis and testing cycles with faster, more flexible FEP

Cresset has released a new version of its computer-aided drug design solution, focussed on improving access to Free Energy Perturbation (FEP) in drug discovery.

CAMBRIDGE, UNITED KINGDOM, June 18, 2026 /EINPresswire.com/ -- Cresset has released Flare V12, a new version of its computer-aided drug design (CADD) solution for the discovery, design and optimization of small molecules. Flare V12 is focussed on improving access to Free Energy Perturbation (FEP) in drug discovery.



Scaffold Hopping Transformation. Copyright Cresset Biomolecular Discovery.

FEP is used to predict how strongly drug candidates bind to their targets, helping guide compound selection. However, despite its recognised accuracy, adoption has often been limited by computational cost, usability barriers and challenges in modeling complex chemical transformations.

Flare V12 is designed to address these challenges.

Reducing computational cost improves throughput

One of the main barriers to wider use of FEP has been computational expense and runtime. Flare V12 introduces a new simulation engine and workflow designed to aggressively cut calculation times by more than 50% compared with the previous version, while maintaining excellent predictive performance.

For discovery teams, the impact is less about individual calculations and more about how quickly decisions can be made. Molecule discovery programs often involve large numbers of plausible design options but limited capacity to synthesize and test them, making compound prioritization a central challenge. Faster and accurate calculations help increase throughput, enabling teams to

evaluate more compounds and focus effort on the most promising molecules.

Expanding FEP to more complex chemistry

FEP in Flare V12 provides expanded support to complex chemical transformations commonly investigated in medicinal chemistry.

Ring-breaking transformations enables researchers to model scaffold hopping, cyclizations and ring size modifications in a single step, providing streamlined support to these common types of medicinal chemistry changes.

Flare FEP in this release also introduces methods to improve predictive accuracy, such as Replica Exchange for broader conformational sampling and Grand Canonical Monte Carlo during the production phase for enhanced water sampling , especially of buried binding sites.

Beyond FEP, Flare V12 extends molecular dynamics capabilities to support covalent ligands, non-standard amino acids and post-translationally modified proteins. These systems are becoming more relevant in areas such as targeted covalent therapeutics and peptide drug design. With Flare V12, enhanced parameters are automatically calculated and seamlessly used in the simulation.

Supporting better compound progression decisions

Taken together, the updates reflect a shift toward making Flare more usable beyond specialist simulation teams and more practical as part of routine drug discovery workflows. Flare is a complete molecule design solution, where FEP can be combined with a large offering of complementary methods to rigorously evaluate and validate sets of high-value design ideas before synthesis.

“The core challenge in discovery is deciding which compounds to make when synthesis is expensive and timelines are tight,” said Tim Cheeseright, CEO of Cresset. “FEP has the potential to bring clarity to those decisions, but historically it has been difficult to apply consistently. With Flare V12, we have focused on making these methods faster, easier to use and applicable to a much broader range of chemistry so teams can prioritize compounds with greater confidence and reduce unnecessary synthesis.”

[Learn more about Flare FEP: Flare™ FEP - Cresset](#)

About Cresset

Cresset® is leading the digital revolution in molecule design and cross-team communication, combining cutting-edge science with AI/ML to enable customers to discover new compounds faster and more efficiently. Built from 20 years of computational chemistry innovation from

solving customer challenges, they provide an unrivalled platform for discovery organizations to achieve scientific success. By harnessing digital transformation, Cresset's trusted, cutting-edge in silico solutions empower organizations to make informed decisions and design the molecules that matter.

www.cresset-group.com

Sally Jennings

Cresset Biomolecular Discovery

[email us here](#)

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