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Cresset releases Flare: Powerful structure-based design application with outstanding new methods for protein-ligand systems

Cambridge, UK – 29 June 2017 - Cresset, innovative provider of software and contract research services for small molecule discovery and design, announces the release of Flare, an intuitive desktop application that provides outstanding new methods for understanding protein-ligand systems. Flare enhances Cresset's existing excellent product range focused on ligand-based design, and becomes their first product explicitly designed to support structure-based design.

"Cresset has been pushing the boundaries of ligand-based design for many years," says Dr Robert Scoffin, CEO of Cresset. "Flare introduces structure-based design into our portfolio, giving companies access to outstanding new methods for investigating protein-ligand systems."

Computational, medicinal and synthetic chemists working on small molecule design and optimization will use Flare to:

- Gain vital knowledge of protein and ligand electrostatics to improve new molecule design
- Compare electrostatic patterns across a protein family to design more selective ligands
- Design new molecules and dock them to a protein target
- Minimize protein-ligand complexes to achieve the optimal interaction for each compound
- Calculate the location and stability of water molecules in a protein to guide compound design.

“Flare represents the next generation of structure based design applications,” says Dr Tim Cheeseright, Director of Products. “It has a modern, intuitive interface and is easily configured to enable cloud-based calculations, making excellent science immediately available to all users whatever their experience level.”

Users will benefit from:

- Simple drag and drop to import/export molecules to the desktop or other compatible applications
- Ready access to powerful tools through a modern ‘ribbon bar’ interface
- Simple yet powerful selection capabilities and cutting-edge display options producing highly insightful molecular graphics.

“Flare integrates cutting edge approaches from Cresset with significant open source and commercial methods,” explains Dr Mark Mackey, CSO. “Throughout the product development we have worked alongside users from major pharmaceutical and biotech companies to ensure that we deliver the best science in the most intuitive format.”

Flare can be evaluated free of charge.

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Contact

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About Cresset

Cresset's software and discovery research services are used by chemists from the world's leading research organizations. Our patented methods deliver novel, realistic results for discovering, designing and optimizing the best small molecules in industry sectors including: agrochemicals, fine chemicals, flavor, fragrance and pharmaceuticals. For more information visit www.cresset-group.com