

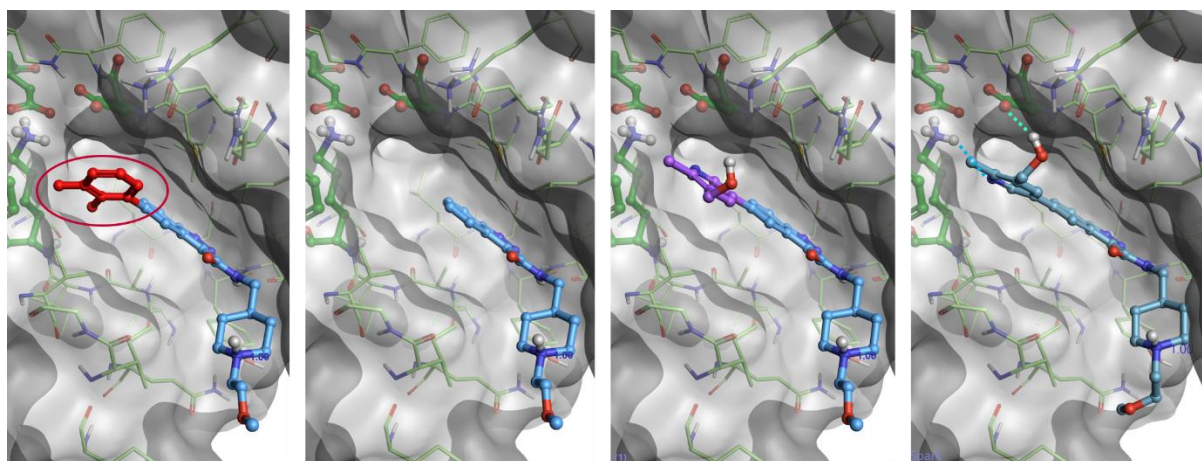
## New docking feature and improved search methods released in V10.6 of Spark scaffold hopping and bioisostere replacement software

Cambridge, UK – 18 November 2020 – [Cresset](#), innovative provider of outstanding software for molecule discovery and design, announces the [release of Spark™ V10.6](#). This release of the scaffold hopping and bioisostere replacement solution further supports the exploration of new chemical space through new and improved search methods to generate innovative ideas for drug discovery projects. A new docking feature enables medicinal and computational chemists to find novel results not mapped by an existing starter or reference molecule.

“The introduction of docking to Spark is an exciting development which will enable research chemists to explore unoccupied pockets in the target protein and map out new protein-ligand interactions.” says Dr Giovanna Tedesco, Head of Products.

“We have also made significant improvements to the more traditional Spark calculation methods, which increase the accuracy with which the tool finds new bioisosteres. These enhancements will further support researchers in their efforts to generate chemically diverse candidates to escape IP and toxicity traps.”

[Spark is available for evaluation upon request.](#)



The new docking feature enables Spark users to find fragments picking ligand-protein interactions directly from the protein active site.

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### **About Cresset**

Chemists in the world's leading research organizations use Cresset software and discovery services to discover, design and optimize the best small molecules. Our patented software and expert scientists offer unrivalled insight into protein-ligand systems, enabling chemists to accelerate their research in industry sectors including: pharmaceuticals, agrochemicals, fine chemicals and flavors and fragrances. [www.cresset-group.com/software](http://www.cresset-group.com/software)

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