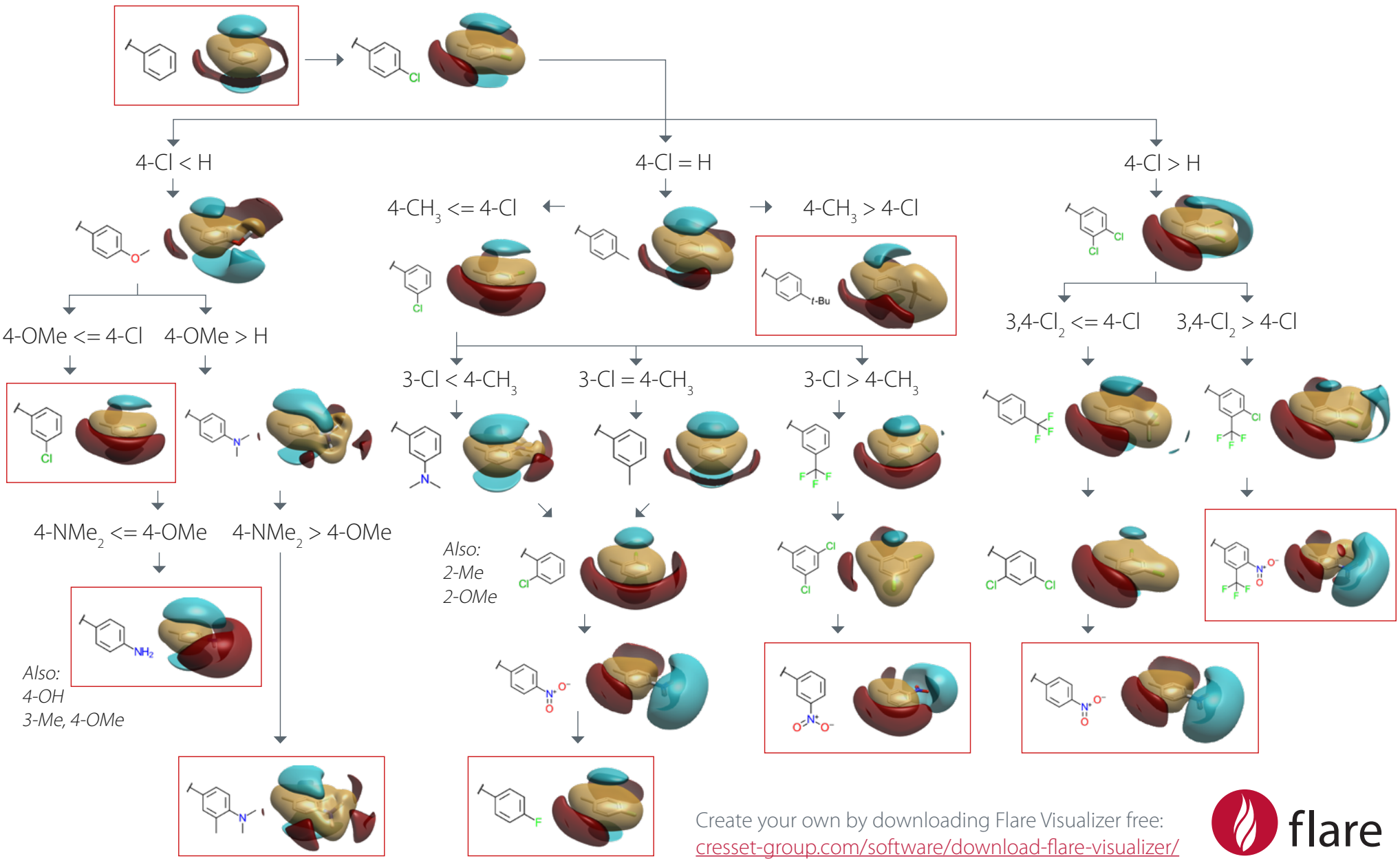
Electrostatics of the Topliss tree

Key: Positive Negative Hydrophobic

cresset CADD software



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Results you can trust

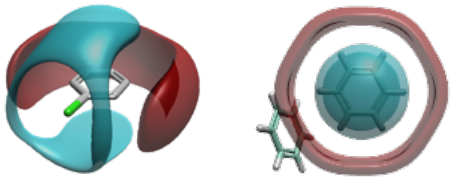
Excellent science is the foundation of our software. Cresset technology centers on the application of the XED force field to the design of new small molecule bioactive compounds. We integrate cutting edge approaches that we develop in-house with significant open source and commercial methods from trusted partners to bring you new insights for molecule design.

XED force field, the foundation of success

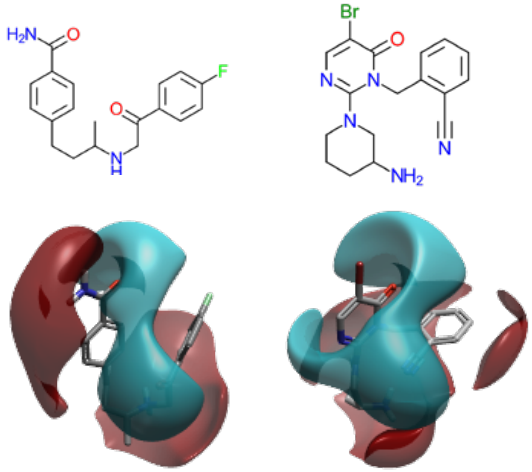
Cresset's proprietary XED force field is one of the most innovative molecular mechanics force fields in existence. Unlike traditional molecular mechanics, the XED approach uses a complex description of atoms to model charge away from atomic centers enabling a more detailed description of electrostatics and excellent reproduction of intermolecular interactions.

The XED force field enables you to:

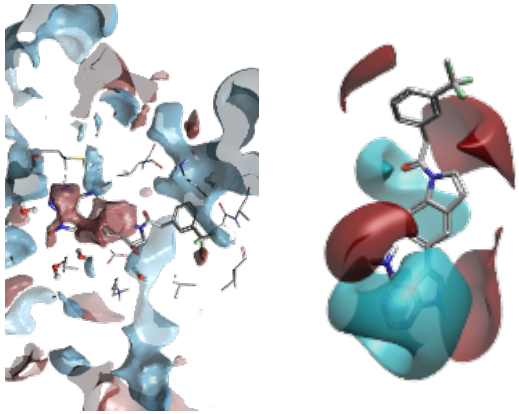
- Gain a detailed electrostatic description of your ligands and proteins
- Understand how structural changes influence your electrostatics
- See how substituents influence the electrostatics of cores and vice versa.



The XED force field enables you to 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 (center) with electrostatic surfaces.



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

Read more about the science that's unique to Cresset applications:
cresset-group.com/science

"The protein interaction potential capability [in Flare] 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.

When dealing with systems where SAR is flat and thin, Flare could pick out and identify most of the very weak hits we have, including a novel hit that is still under examination.

Flare is predicting my known ligand's co-crystallized pose more accurately than any other program I have used. I can perform focused docking, blind docking, visualization, and saving images all in one place."

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CADD software