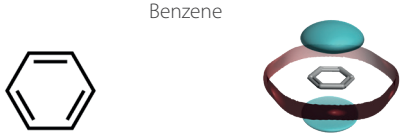
# Electrostatics of heterocyclic rings

cresset software

innovative science • intuitive software

Key: Positive Negative

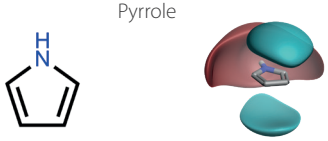
Benzene



Furan


Pyridine

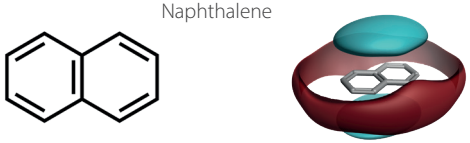

Pyrrole



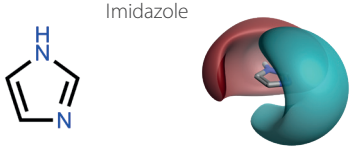

Pyrimidine


Oxazole


Naphthalene



Imidazole




Quinoline

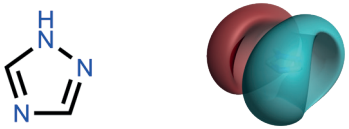

1H-Pyrazole


Isoquinoline


1,2,4-Oxadiazole


Quinazoline


1H-1,2,4-Triazole




Benzofuran


Indolizine


Indole

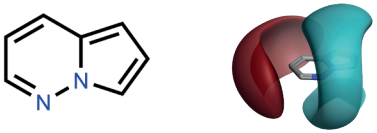

2H-Isoindole


1,3-Benzoxazole


Imidazo[1,5-a]pyridine

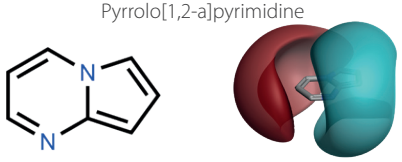

Benzimidazole


Pyrrolo[1,2-b]pyridazine




1H-Indazole


Pyrrolo[1,2-a]pyrimidine




1H-Pyrrolo[2,3-b]pyridine


1H-Benzotriazole


Create your own by downloading Flare Viewer free
www.cresset-group.com/software/flare

flare

# Results you can trust

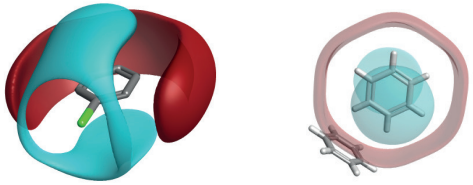
Excellent science is the foundation of our software. Cresset technology centers on the application of the XED force field to the design of new small molecule bioactive compounds. We integrate cutting edge approaches that we develop in-house with significant open source and commercial methods from trusted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

## XED force field, the foundation of success

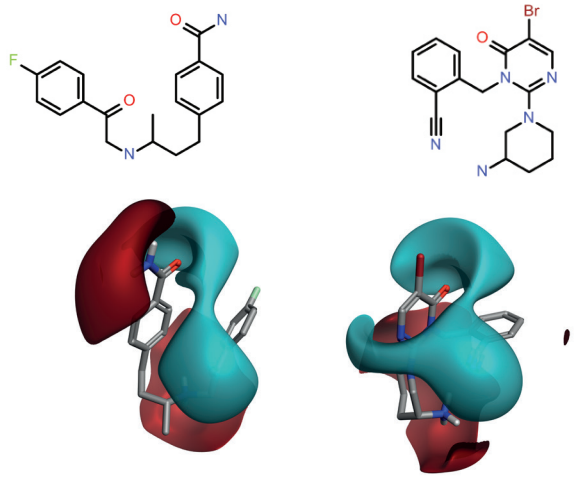
Cresset's proprietary XED force field is one of the most innovative molecular mechanics force fields in existence. Unlike traditional molecular mechanics, the XED approach uses a complex description of atoms to model charge away from atomic centers enabling a more detailed description of electrostatics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

The XED force field enables you to:

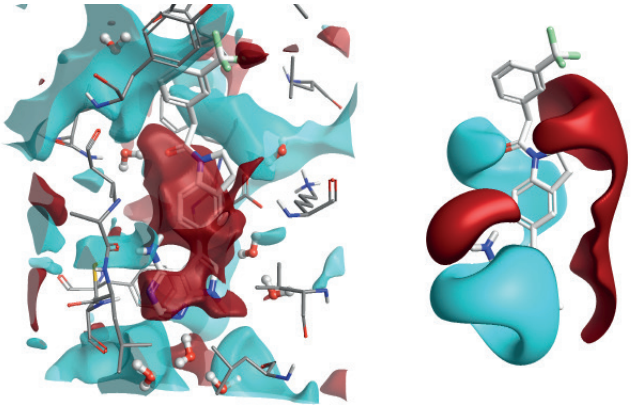
- Gain a detailed electrostatic description of your ligands and proteins
- Understand how structural changes influence your electrostatics
- See how substituents influence the electrostatics of cores and vice versa.



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**

*"Flare gives us an excellent assessment of the potential binding of hits. We use it to triage hits from Blaze and Forge experiments in the absence of 3D-QSAR, narrowing them down to an affordable subset of the most promising hits. Flare gives us the luxury of choosing the best hits from a far larger pool than we could purchase directly.*

*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 has made some nice fragment predictions which we had previously identified, further increasing our confidence in Flare."*

cresset® software