BioSolveIT
expect actives!

And How To Be Successful In It

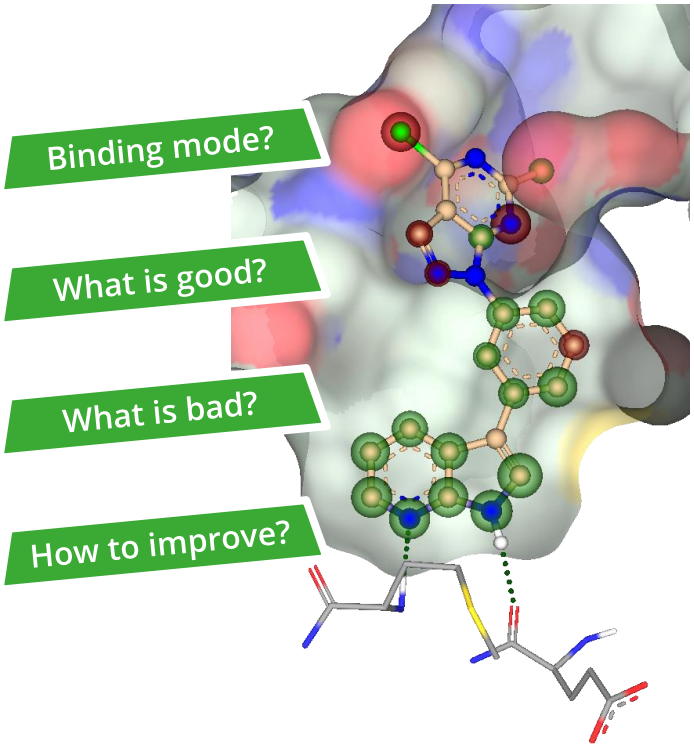
What is Structure-Based Drug Design (SBDD)?

Structure-Based Drug Design (SBDD) is a method of designing drug candidates by using the 3D structure of a biological target, usually a protein. By understanding how a ligand (drug candidate) interacts with a specific binding site, researchers can design molecules that fit perfectly, improving efficacy and reducing side effects.

SBDD is applied in:
Lead discovery • Compound optimization • Target assessment

Information about a ligand's binding mode is used to predict compounds with improved potency

Understanding Your Complex Is Imperative to Write Success Stories

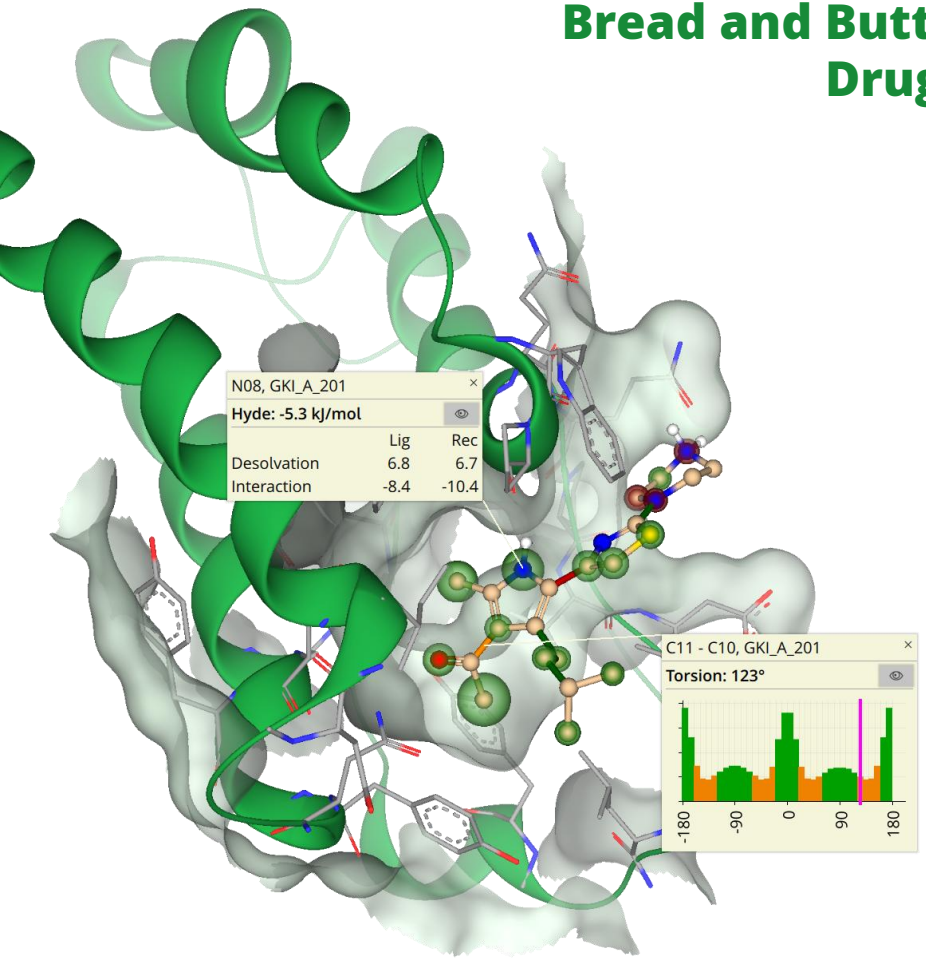


In order to make informed decisions on the next steps during a drug discovery project, it is crucial to understand how your ligand interacts with the target structure.

For this, a thorough understanding of the binding mode of the ligand, as well as the areas with favorable interaction patterns and those that should be improved, is required.

Our drug discovery dashboard **SeeSAR** is your sparing partner for interactive compound ideation. Visual support helps you to easily assess your ligand-target complex.

Bread and Butter of Computer-Aided Drug Discovery



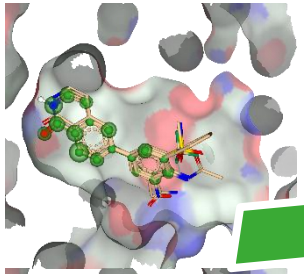
With SeeSAR, common tasks like the prediction of druggable binding sites, pose generation of ligands and their assessment become intuitive, efficient and visually guided.

Our scoring algorithm HYDE highlights the individual contributions of each atom to the overall binding affinity to help you spot areas to improve.

Tools:

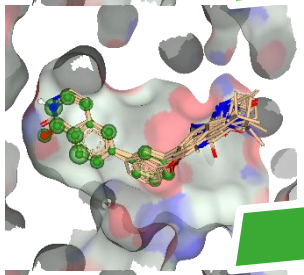
- SeeSAR
- Binding Site Mode
- Docking Mode

SeeSAR's Inspirator Mode: Sometimes Medicinal Chemists Need Help As Well



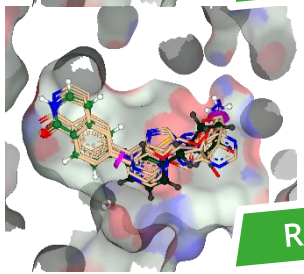
290 commonly used medicinal chemistry transformations to improve the compound.

Analoging



Browse through hundred-thousands of extensions in seconds.

Growing



3D screening for the topologically best matching motifs.

Re-scaffolding

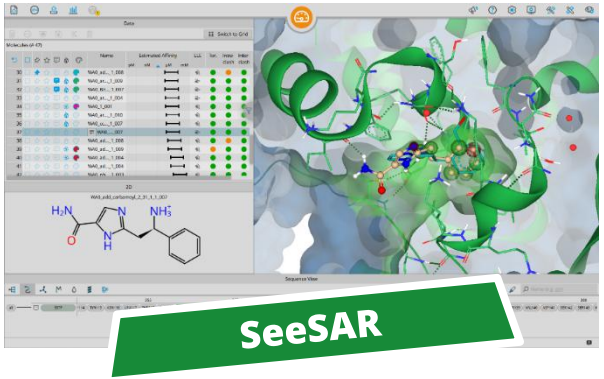
Every drug discovery project comes with its own challenges and goals. This can lead to quickly exhausting one's knowledge repertoire and heading straight towards a dead end. The Inspirator Mode helps you to generate sound solutions for several scenarios: Replacing an undesired scaffold, generating promising analogs or grow your compound into unoccupied binding pockets.

Tools:

SeeSAR

Inspirator

Advance Your Compound to Their Highest Potential



- Sophisticated and easy-to-use drug discovery dashboard.
- Binding site prediction and docking of molecule libraries.
- Compound ideation and lead optimization to guide you to success!

The only thing standing between you and the most promising drug candidates is the download button.

Unlock the full potential of your project with BioSolveIT's tools!

Learn more using the QR code below:

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