BioSolveIT
expect actives!

And How To Be Successful In It

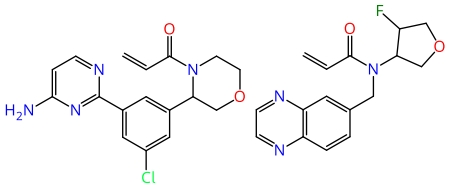
What is Ligand-Based Drug Design (LBDD)?

Ligand-Based Drug Design (LBDD) is a computational approach that leverages knowledge of existing ligands, or small molecules that bind to biological targets, to design and optimize new drug candidates. By comparing known ligands, researchers can predict how similar molecules will interact with the same target, offering faster insights and improving lead discovery.

Similar ligands
=
Chance to target the same structure

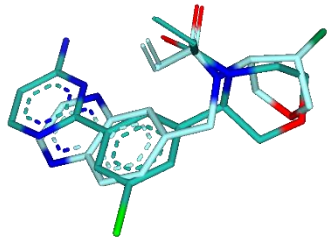
No Target Structure?
No Problem!

The BioSolveIT product portfolio features several powerful applications facilitating LBDD in the 2D and 3D world.



2D – Mining Chemical Spaces for similar compounds

We have developed several methods to retrieve similar compounds to a query structure from trillion-sized molecule collections based on the needs of the project.

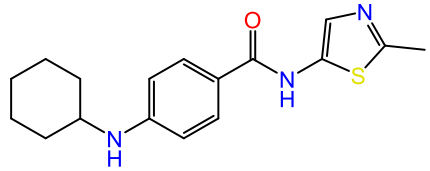


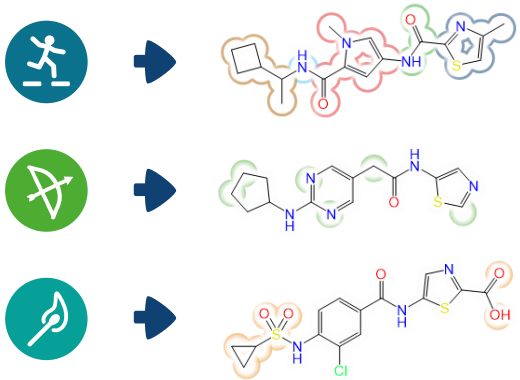
3D – Molecule superpositioning

Align a set of molecules to a conformation of your template ligand to match its shape and features.

Dive into the Largest Hunting Grounds for Drug-Like Compounds: Chemical Spaces

Query Molecule





Chemical Spaces are combinatorial compound clusters featuring trillions of entries.

We at BioSolveIT develop methods to screen these vast molecule collections for relevant chemistry. Our Chemical Space navigation platform **infiniSee** retrieves similar and accessible compounds tailored to the aims of the projects.

Tools:

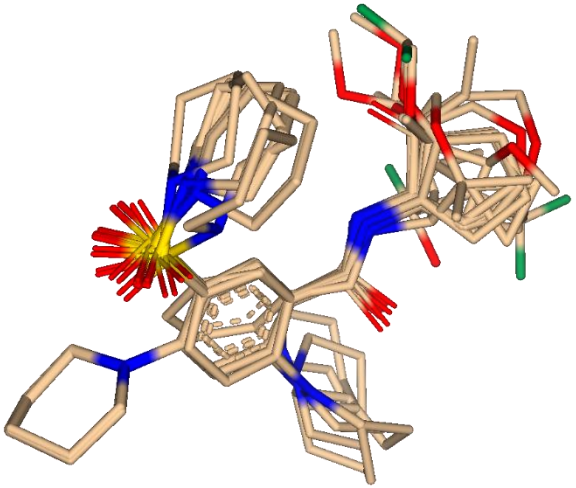
infiniSee

Scaffold Hopper

Analog Hunter

Motif Matcher

Explore Shape Similarities and Functional Overlaps with SeeSAR



Another way to assess the similarity between two molecules is by using 3D methods to align them and score how well they overlap.

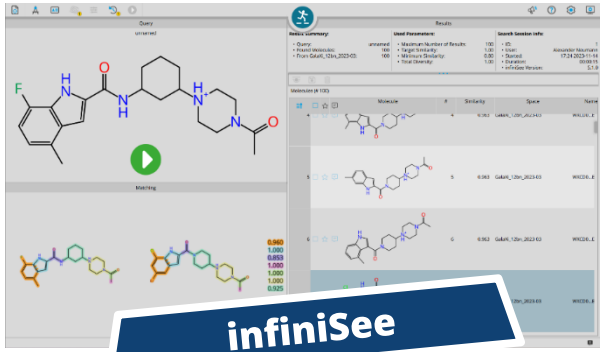
In our drug discovery dashboard **SeeSAR** and its **Similarity Scanner** Mode, users can perform ligand-based virtual screening to screen for most similar compounds based on features like shape, aromaticity and arrangement of H-bond donors and acceptors.

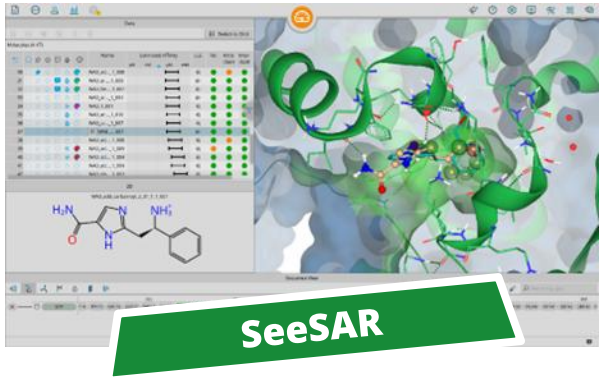
Tools:

SeeSAR

Similarity Scanner

Fill Your Drug Discovery Pipeline with BioSolveIT!





Ready to take your ligand-based projects to the next level?

Experience the power of BioSolveIT's applications and accelerate your drug discovery process.

Learn more using the QR code below: