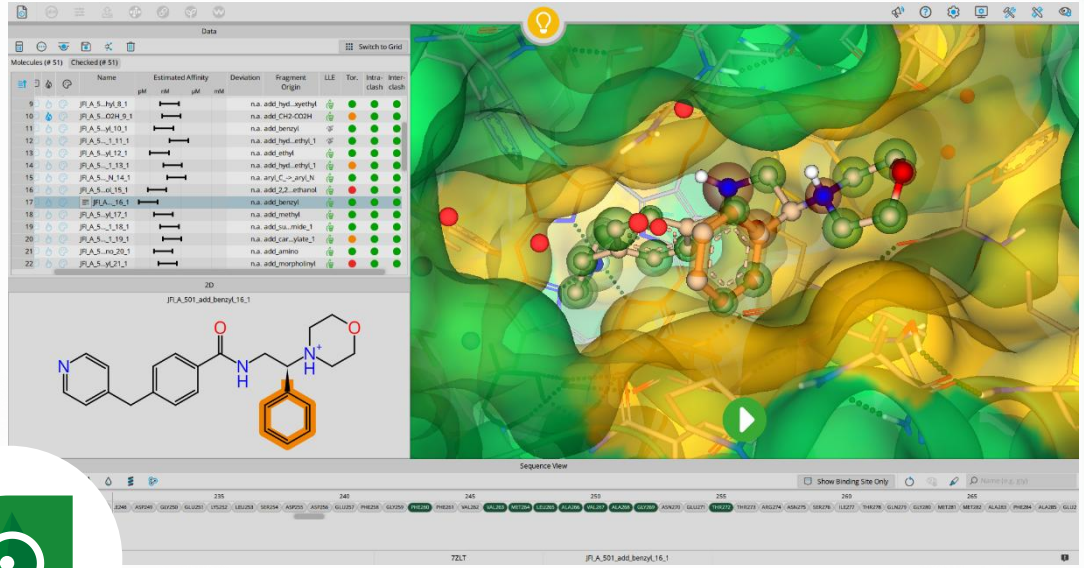
BioSolveIT
expect actives!



SeeSAR

Drug Discovery Dashboard

Fast

Visual

Easy

SeeSAR

fast • visual • easy

SeeSAR is your intuitive, visual drug design platform. Covering every step of your drug discovery process – from virtual screening to fragment-based design – SeeSAR fosters ideation in the most fun and comprehensive way.

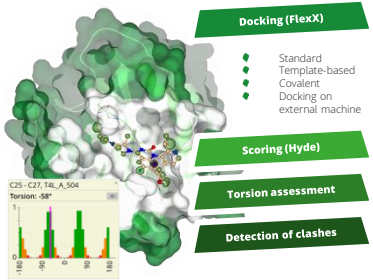
What SeeSAR Does

- Visual and interactive assessment of your target-ligand complex.
- Bread-and-butter of modeling: Docking, scoring, prioritization.
- Source for ideation, scaffold hopping, and compound evolution.

Enhancing Drug Design for Everybody

The synergy between fast, visual and easy creates a sophisticated drug discovery experience that encourages on-the-fly design and rewards with groundbreaking results.

Meanwhile, SeeSAR is extremely easy to use. Drug discovery veterans and beginners can perform tasks in a clean software environment to reach their goals fast and efficiently.



Hyde Scoring Desolvation-Aware ΔG Estimates

Assess the contributions of individual atoms to the overall binding affinity of the ligand and understand how and where to improve your compound with a single glimpse.

What's Inside?

The app includes all tools vital for handling your compounds and target structures which have been fine-tuned to the needs of any medicinal or computational chemist as well as drug hunters in general.

Protein Mode
Drag and drop your protein, or search comfortably in an online database. Within seconds, your target is prepared, and you can get started.

Protein Editor Mode
Modify your protein according to your needs. Explore rotamers, introduce mutations, and customize side chains.

Binding Site Mode
SeeSAR automatically detects the binding site of a ligand for you. In addition, you can precisely expand it by adding individual residues — or with a single click to find empty pockets in your protein.

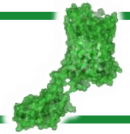
Molecule Editor Mode
Modify molecules to your taste in 2D or 3D on-the-fly. Once you are done, the molecules are directly prepared for your tasks.

Analyzer Mode
Estimate affinities and interpret the results using the visualized HYDE score. Filter your compounds for relevant parameters, calculate ADME properties, and gain full control over ligand-target interactions.

Inspirator Mode
Ideate without limits! Discover new scaffolds, explore, and grow into free cavities, or link molecules using fragment libraries for elegant solutions.

Docking Mode
Dock your compounds with one single click (standard, template-based or covalent)! Screen libraries for actives, and instinctively evaluate your results.

Similarity Scanner
Align your compounds without the need of a target structure based on their molecular similarity with the FlexS algorithm.



Nice to know for Comp Chems

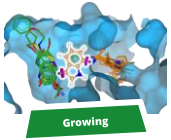
Following components can be run in command lne on your computer, server, or cloud:
FlexX • Hyde • FlexS • FastGrow

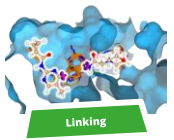
Powerful Tools for Creative Solutions

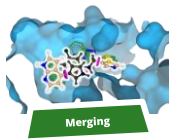
SeeSAR was developed to support you in your compound ideation and design process. A wide range of functionalities helps you to find unexpected results for modern drug discovery challenges.

Launchpad for Fragment-Based Drug Discovery

SeeSAR contains various features tailored to augment the design of compounds using the smallest molecules.

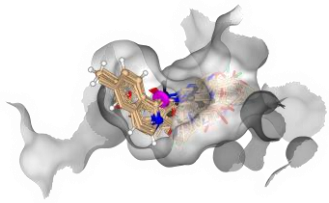






Satisfy Binding Pockets with FastGrow

Browse through millions of fragment conformations to discover ideas how to complement your binding site within seconds. Select the extension direction on your ligand and start the ideation process.



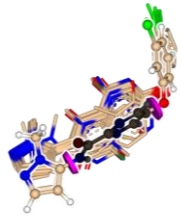
Several chemically diverse FastGrow libraries are available to expand the hunting grounds for the most promising solution.
This features a set for medchem-like compounds, sp3-enriched fragments and hinge binder motifs.

Profit from Your Expertise

You have complete control over what happens on the screen. Leverage your expertise with SeeSAR's help to evaluate the results and determine which compounds to prioritize.

Replace Unwanted Motifs
Browse through tens of millions of high-quality 3D fragments with ReCore to find novel scaffolds according to your needs in a flash.

Ligand-Based Drug Discovery
Perform ligand-based alignment for small libraries or as a virtual screening campaign with the Similarity Scanner and the FlexS algorithm.



Download SeeSAR and start your drug discovery process

following this link