BioSolveIT
expect actives!

Alexander Neumann

YoungSolvers Workshop

Introduction to SeeSAR and infiniSee

YoungSolvers Initiative

Support for the next generation of drug designers

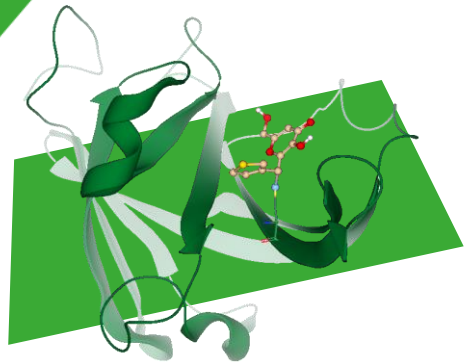
- Directed towards Master students in Europe
- 2 months free license to BioSolveIT applications
- No strings attached, no hidden fees

- Open office hours in Gathertown
- Accompanying workshops
- biosolveit.de/youngsolvers

SeeSAR

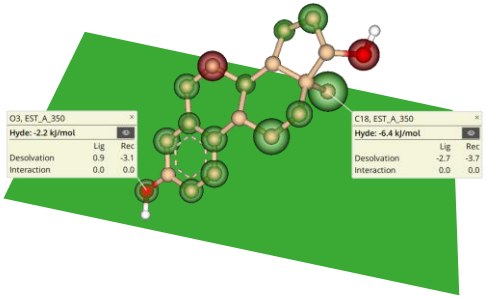
Your Everyday Drug Design Dashboard

Fast • Visual • Easy



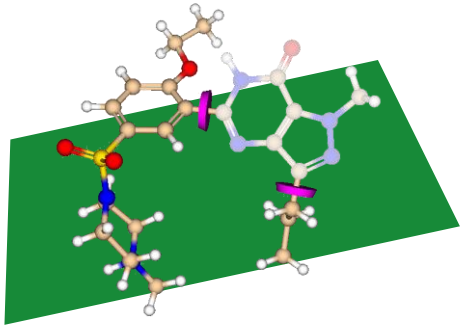
Sophisticated, Powerful Docking

Covalent Docking • FlexX Algorithm
Pocket Detection



Visual Assessment

HYDE Affinity Estimation • Torsions
Physicochemical Properties



Lead Optimization

3D Scaffold Hopping • Growing
Merging • Design On-the-Fly

SeeSAR Modes

Protein Mode

Protein Editor Mode

Binding Site Mode

Molecule Editor Mode

Analyzer Mode

Inspirator Mode

Docking Mode

infiniSee
Chemical Space Navigation Platform

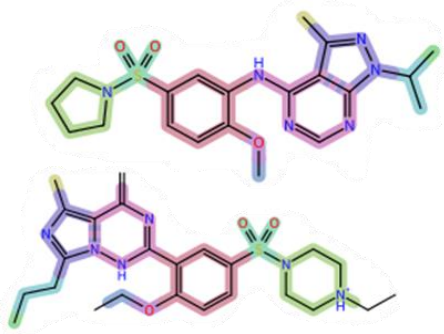
Screen large Chemical Spaces

See how molecules are related

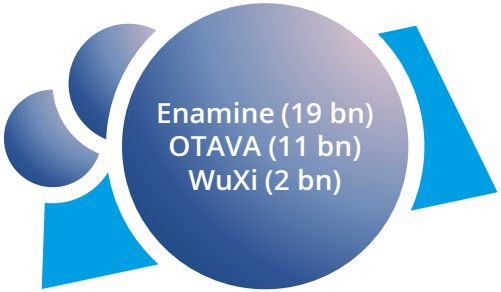
Discover novel scaffolds

Find accessible compounds

Fuzzy pharmacophore search with FTrees

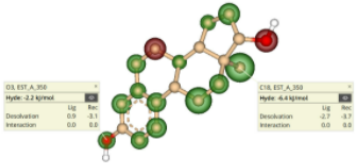


Billions of accessible, on-demand compounds



Want to know more?

HYDE - Interactive, desolvation-aware visual ΔG estimates



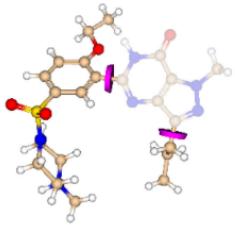
HYDE binding assessment approximates and visualizes affinities. The system has NOT been trained to specific targets, instead implicit HYdrogen bond and DEhydration are intrinsically balanced without weighting parameters as seen in all force fields. The user instantly gets interpretative feedback for lead optimization and other design tasks.
HYDE is constantly improved and originated from a collaboration with BAYER, Hamburg University, and BioSolveIT.

Find out more about HYDE here

biosolveit.de/SeeSAR#science

PDFs with elaborate information and publications on the software components (FlexX, HYDE, …)

ReCore - 3D scaffold hopping



Replace a given core and generate new intellectual property. You can specify bonds or interactions to be matched by new fragments. The arrangement of the connected residues is taken to a fragment library that has been pre-processed for speed ("indexed"). Results are retrieved using a 4-dimensional vector and the quality of the fit is computed. Indices can be custom designed with in-house compound libraries.
ReCore emerged from a collaboration with Roche Basel and Hamburg University and has been extensively augmented and extended by BioSolveIT thereafter.

Find out more about ReCore here

3D Model export