Inspires Design. Delivers Fast. Wins Awards.

BioSolveIT
Expect Actives

SeeSAR™

- 2D and 3D visual design guidance for **bench chemists** & experts alike
- Entropy-aware **ΔG estimates, torsion/clash/explorability** analyses — visualized on-the-fly
- Now includes the **FBLD** Inspirator® and Optibrium™-powered **ADME** models

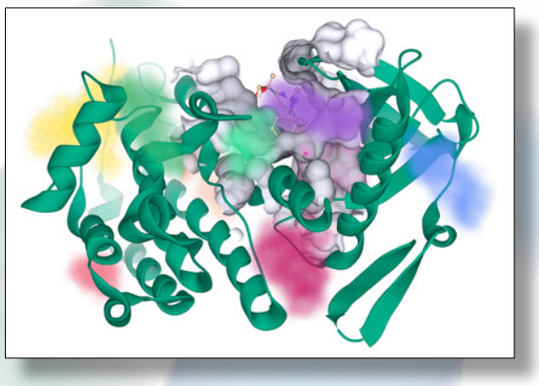
See your **SAR** — In realtime!

SeeSAR is **fast**, **visual**, and radically **easy** to use. It estimates and visualizes **SAR** and **ADME** with technolgies that we have developed with Bayer, Roche, Hamburg University [1-3], Optibrium, and others.

Atoms that improve **affinity** are surrounded by a green "Corona", unfavorable atoms carry red ones. Explore and **fill free cavities**, see **torsional** implications, check crystal structures for artifacts, analyze potential **clash** risks, and keep an eye on the scientifically rigorous Optibrium™ **ADME** properties. SeeSAR is award-winning, next generation software from BioSolveIT, tailored to your everyday ligand optimization and all your **fragment-based design needs**.

Playful Inspiration, Starting with Pocket Detection

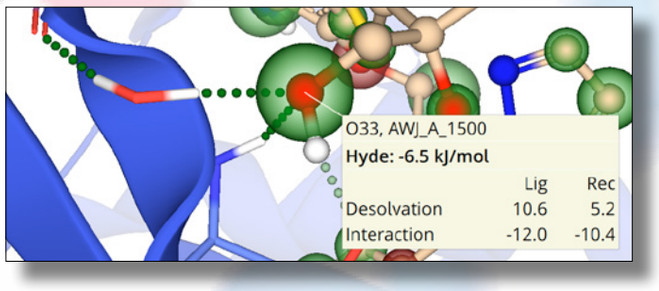
Fast and visual binding site proposals within SeeSAR: Find the correct pocket with >90% accuracy within the top 3 ranks. Select an allosteric pocket with one simple click using Hamburg University's integrated DoGSite **pocket finder** as also seen from Merck [4].



SeeSAR's new mode also sports parallelized, quick **docking**! With more than 8,000 citations, the docking algorithm is a great helper to obtain binding proposals. The clean interface gives you control over the output.

SeeSAR Rationalizes Your SAR

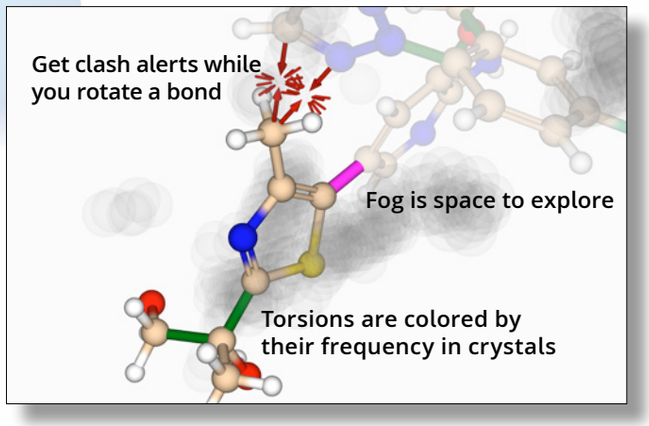
Affinity is not only about forming new bonds, it's also about **entropic** energy terms, e.g., freeing water from an unbound ligand first before it can be accomodated in a pocket. SeeSAR will show you what happens — with great, simple graphics.



Visual HYDE [1] computations will let you understand desolvation effects, and bridging waters will automagically be oriented and displayed in the H-bonding network. All this happens on-the-fly.

Explorability? Tightness of Fit? Clash? — Everything *in situ*!

The 3D editor relaxes your newly created lead ideas on the fly — and shows the effect on **explorability volume, torsional implications** and estimated **ΔG**. Moreover: **H_2O**, **protonation**, and **tautomer** selection are taken care of within milliseconds using the world's best and fastest technology: ProToss [3]. This applies to both protein, incl. His/Asn/Glu flips, and ligand, individually for every pose!



Technical Requirements
SeeSAR runs on Windows, Macs, Linux. It will automatically use all your CPUs in parallel. SeeSAR needs the latest graphics card drivers installed.

How to Get It
Just download and use for free for 7 days: https://biosolveit.de/SeeSAR
If you are happy, the software will help you with licensing.

https://biosolveit.com
contact@biosolveit.com
biosolveit.com/linkedin
facebook.com/BioSolveIT

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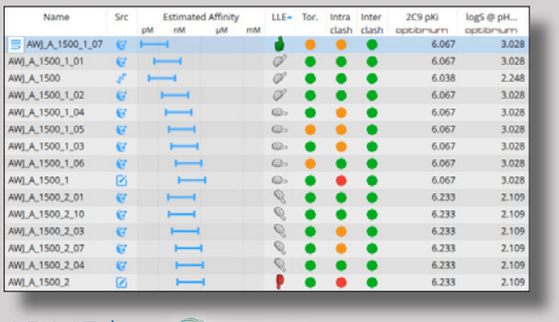
SeeSAR™

You may ask: "Why SeeSAR?"

- SeeSAR is the only **interactive & visual design ideation** tool available. Computed estimates are visualized, and so the actual *design decisions stay before your eyes and in your hands*.
- No other tool available gives you such **instant** & **visual** feedback: ΔG, torsions, clash... Use the HYDE Coronas to see where atoms are likely to improve ΔG, rotate a bond to see resulting clash...
- There is **no learning curve** — Promise: Within 30 minutes, you will use it productively. @CADD experts: Complementing your favorite cheminformatics package, SeeSAR will give you visual and orthogonal information.

Strictly Visual Dashboarding

Predict (or load your own) properties, browse them conveniently, or use the new **filter dialog**. Select, export, post-process to your liking.

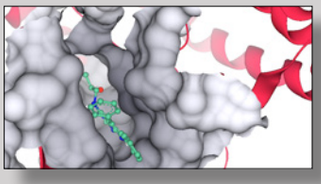


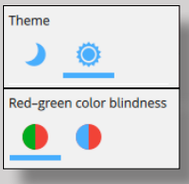
ADME by optibrium

Optibrium StarDrop™-based ADME properties are integrated! See immediately: 2C9 pK_i, plasma binding, 2D6 affinity, P-glycoprotein-binding, BBB-penetration, hERG pIC_{50}, logD, solubility — and more!

Graphics & Reporting: We Thought of You!

High resolution scene shots for publications, support for the red-green blind, dark modes — SeeSAR is at the forefront of all visual drug design.

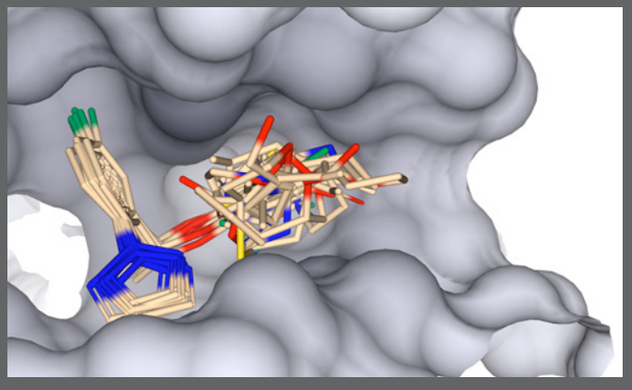




The Inspirator® — Fragment-Based Design

The new Inspirator® provides **instantaneous ideation for FBLD**: Exploit swift indexing techniques like Google does, and grow and link fragments in parallel on your laptop. Save that hardware money.

- **Merge fragments** ("Mix & Match", link different parts)
  Connect parts from different ligands with something new.
- **Rescaffold in 3D in no time with ReCore®**
  Recplace an unwanted core by alternatives that fit well. [5]
- **Grow / explore a pocket from a fragment binder**
  Take a fragment, define a growing vector, grow!



Grow & explore a cavity:
Define a vector, press 'Grow!'
Seconds later, the pocket is populated with proposals from a library of typical medicinal chemistry fragments, the parallel computation is completed in seconds.

Recent Success Stories

SeeSAR is widely used in universities, biotechs, crop protection companies, and big pharma across the world. Below is a selection of diverse applications that have recently been published:

- **A New Fragment-Based Inhibitor**:
  Brethon A et al., 2017, Bioorg. Med.Chem. Lett., **27**, 5375
- **Improving GPCR Dockings**:
  Mason J et al., 2016, JCIM 2016, **56**, 642
- **SAR for Dynamic Combinatorial Chemistry**:
  Mondal M et al. , 2014, Angew. Chemie. Int.Ed. Engl., **53**, 3259

Acknowledgments:

SeeSAR exploits patented HYDE Visual Affinities technology from Bayer AG and Prof. Rarey's group at ZBH, Hamburg University, Germany.[1] Our statistical significance visualization for torsions are rooted in ideas from Dr. Christin Schärfer, Dr. Tanja Schulz-Gasch, and Dr. Martin Stahl at Hoffmann-LaRoche in Basel, Switzerland.[2]
The ADME models are © Optibrium, Ltd.: https://optibrium.com.

References:

[1] Schneider et al., JCAMD 2013, **27**, 15
[2] Schärfer et al., JMedChem 2013, **56**, 2016
[3] Bietz et al., JCheminform, 2014, **6**, 1
[4] a) Volkamer et al., JCIM, 2012, **52**, 360
b) Volkamer et al., JCIM 2010, **50**, 2041
[5] Maass et al., JCIM 2007, **47**, 390

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