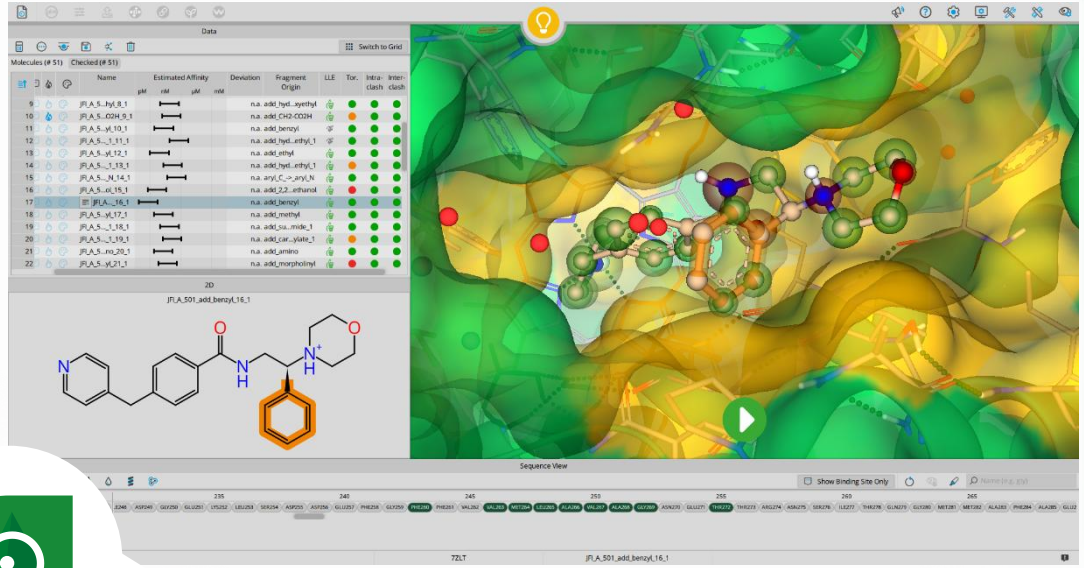
BioSolveIT
expect actives!



SeeSAR

Drug Discovery Dashboard

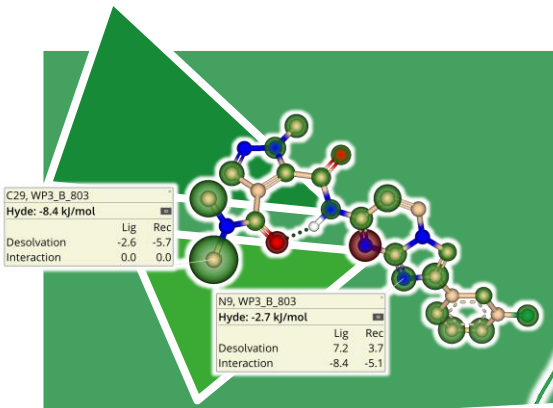
Fast

Visual

Easy

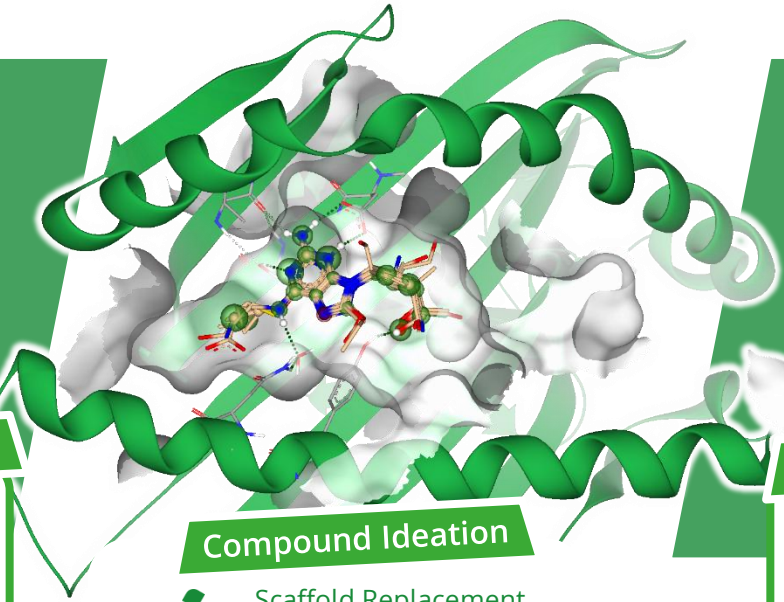
SeeSAR

Your Everyday Drug Design Dashboard



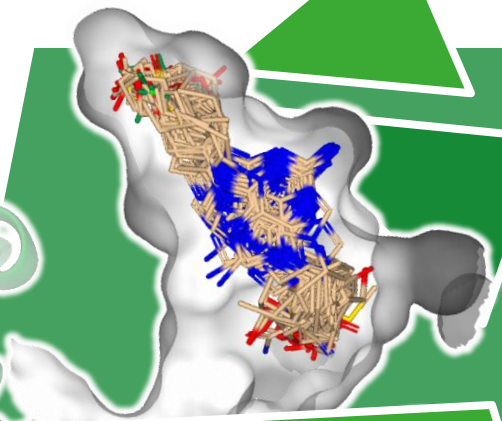
Interactive, Visual Assessment

- Comprehensive Feedback
- Affinity Estimation (Hyde)
- Physicochemical Property Prediction
- Molecular Torsion and Clash Assessment



Compound Ideation

- Scaffold Replacement
- Compound Growing
- Substituent Sampling
- Analoging
- On-the-Fly Design



Augmented Drug Discovery

- SBDD, FBDD, LBDD
- Docking (standard, template-based, covalent)
- Virtual Screening
- Chemical Space Docking™
- HPC Support

What's Inside?

Covering all needs

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

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.
SIENA

Inspirator Mode

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

Docking Mode

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

Chemical Space Docking™

Efficiently perform the structure-based docking assessment of billions or even trillions of molecules for the most promising compound candidates.
FlexX, Hyde

Binding Site Mode

Detect binding sites for a ligand. In addition, precisely expand it by adding individual residues — or find empty pockets in your protein with a single click.
DogSiteScorer

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

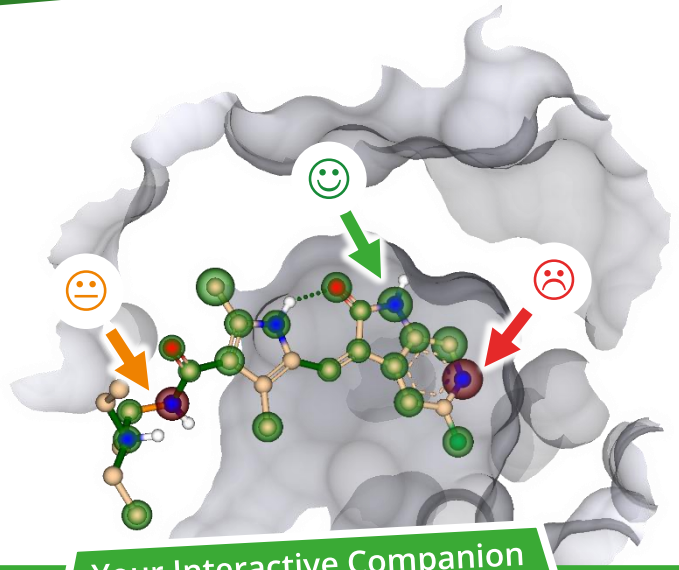
Estimate affinities and interpret the results using the visualized HYDE score. Filter your compounds for relevant parameters, calculate ADME properties, and gain full control over ligand-target interactions.
Hyde

Similarity Scanner

3D align your compounds without the need of a target structure, based on their molecular similarity and shape.
FlexS

Enhancing Drug Design

Gratifying Interplay for Trailblazing Results



Your Interactive Companion

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

Fast

Instantly understand your complex to design, analyze, and evolve your compound with **swift and informative calculations**.

Visual

Intuitive color codes enable sighting of key interaction spots and where to improve and expand your ligand.

Easy

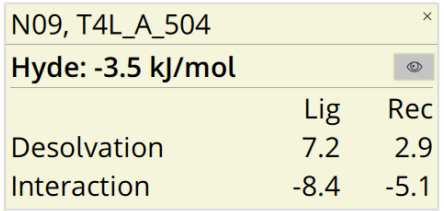
Straightforward operation in clean user interface which is fun to use **for beginners and veterans alike**.

Visually-Informed Assessment

Interactive Dialog with Your Complex

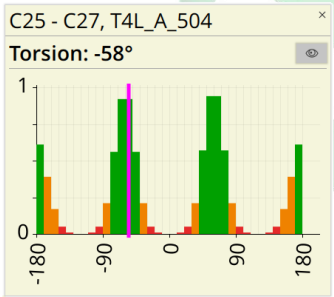
Hyde scoring – Desolvation-aware ΔG estimates

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.



Molecular torsions

Perform your tasks with confidence due to the traffic light implementation for the molecule torsion angles based on rigorous statistical analysis of small molecules in crystal structure databases.



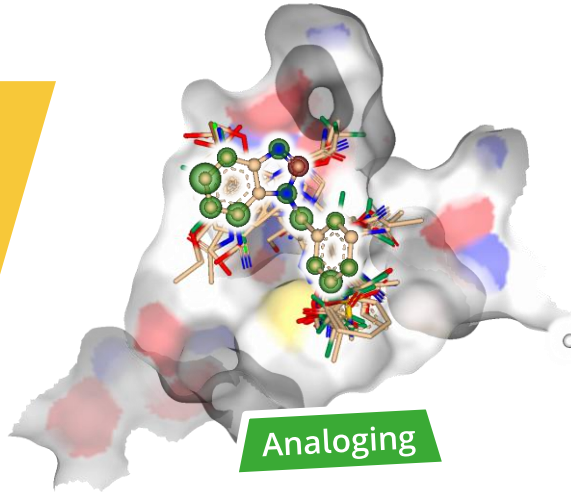
Inspirator Mode

Miracle Bag for Compound Ideas

The Inspirator Mode was developed as your sparring partner in molecule design sessions. It provides you with suggestions for scaffold replacements and compound decorations.

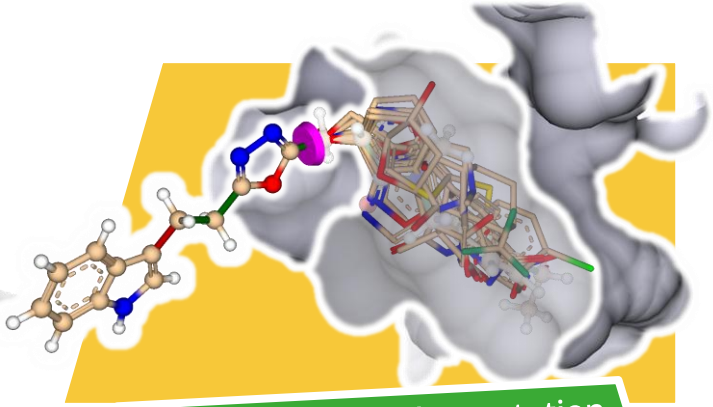
Replacing Scaffolds

Get rid of unwanted motifs and browse through tens of millions of high-quality 3D to find novel scaffolds according to your needs in a flash.



Analoging

Given a ligand and a binding site, SeeSAR can sample 290 commonly used medchem transformations to suggest promising modifications.



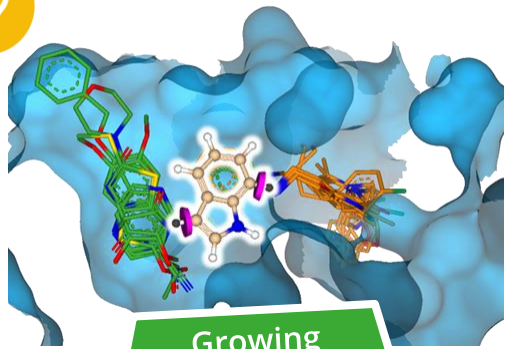
Binding Site Complementation

Screen hundreds of thousands of molecule decorations for a ligand to extend into a binding cavity – within seconds!

Evolve Your Hits

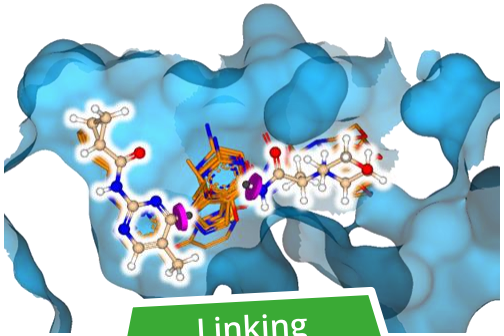
Launchpad for Fragment-Based Drug Discovery

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



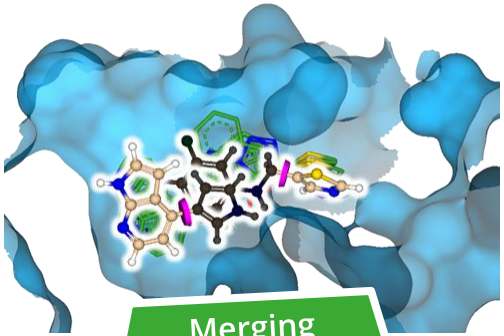
Growing

Extend your fragment binder to complement the binding site with FastGrow.



Linking

Connect distinct fragments using ReCore, carefully accounting for their 3D poses, to identify the optimal scaffold that aligns geometrically with the attaching vectors.



Merging

Amalgamate overlapping moieties of binders for synergistic improvement of the potency in the unified compound.

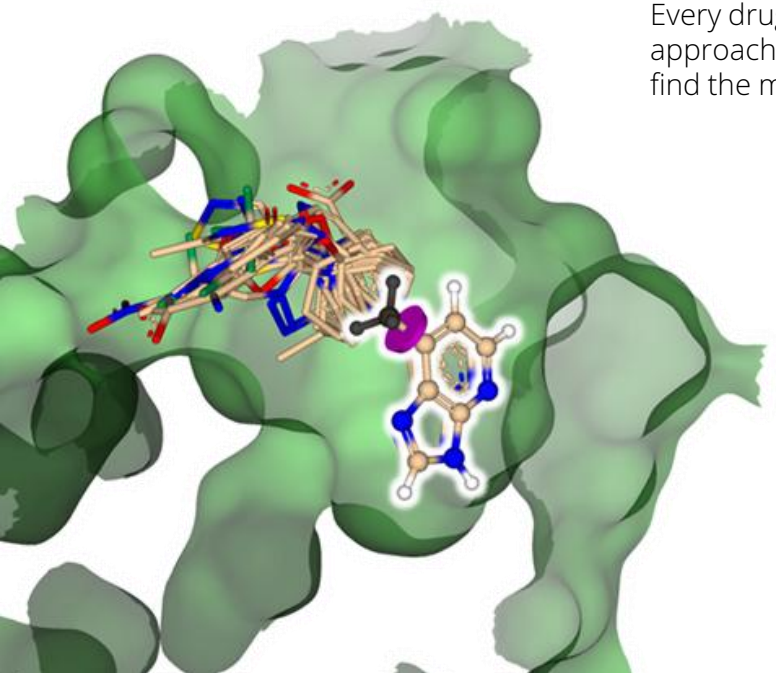
Handy Advice

Apply pharmacophore constraints to guide your results and focus on key features known to you.

FastGrow: Lightning-Fast Pocket Filling

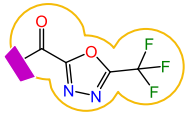
Quickly Satisfy Your Binding Site

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.

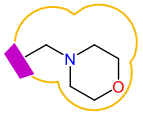


Various sets for diverse challenges

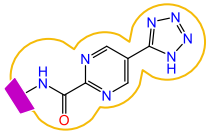
Every drug discovery project comes with its own hurdles and can require different approaches to be successful. To address this, we provide several FastGrow libraries to find the most fitting solutions to your problem.



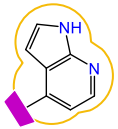
Default set
SeeSAR incorporates a set of 12k medchem-like growing fragments right from the start.



sp³ carbon
In this set, an sp³ carbon is the first atom after the extension vector. It can be used to decorate nitrogen-containing groups.



Medchem
The larger medchem growing set contains 120k fragments derived from common drug motifs, building blocks and structures observed in PDBs.



Hinge binder
Features computationally validated hinge binders derived from bioactive molecules encompassing 51k entries.

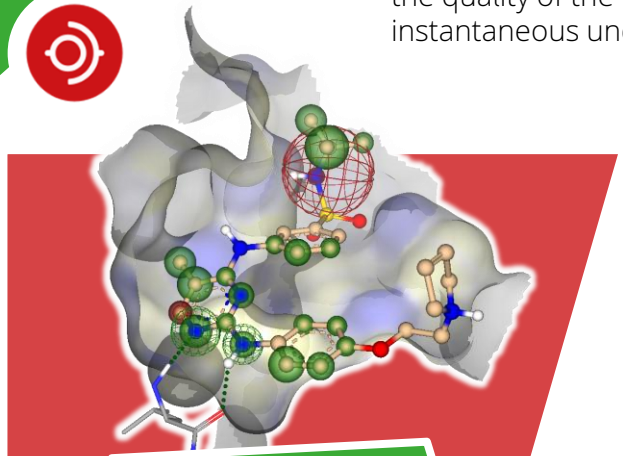
Utilize your resources

You can create your own FastGrow sets incorporating your in-house molecules as extensions to profit from your IP.

Docking Mode

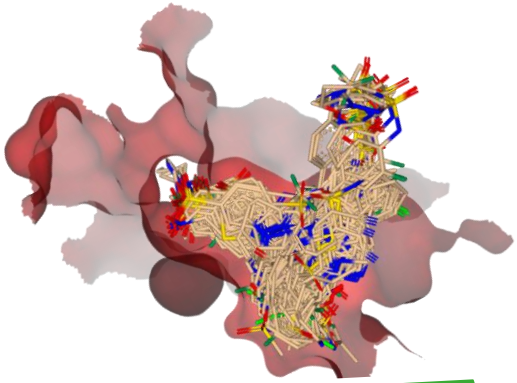
Pose Generation and Assessment

Predict the binding mode of ligands at your target binding site and assess the quality of the poses. The comprehensive traffic light guarantees instantaneous understanding of your complex.



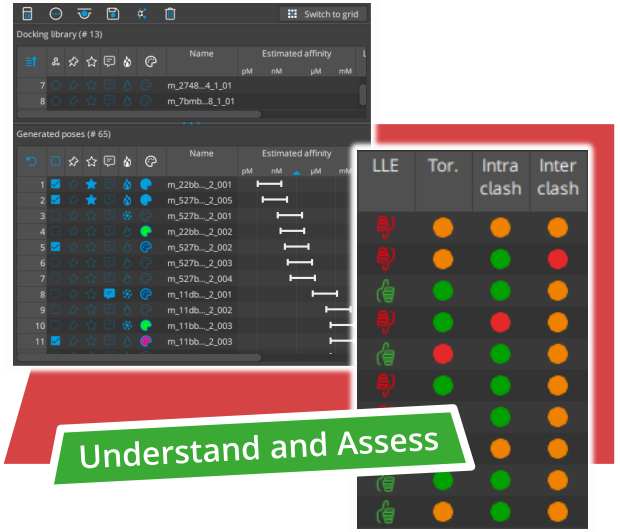
Guide Your Search

Apply a broad selection of **pharmacophore constraints** and allowed conformers to fine-tune your results.



Prepared for All Scenarios

In addition to the standard docking, **template-based** and **covalent docking** are available to address the needs of individual projects.



Understand and Assess

Streamlined compound handling helps you to check for best pose parameters in order to select the best candidates for follow up.

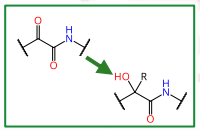
Covalent Docking
Warhead Handling

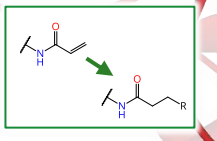
SeeSAR automatically detects and transforms 36 of the most commonly used covalent warheads in medicinal chemistry during a docking run.

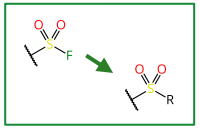
After a covalently targetable residue was selected, your molecule library will be sampled for the best poses, taking all potential resulting stereoisomers into account.

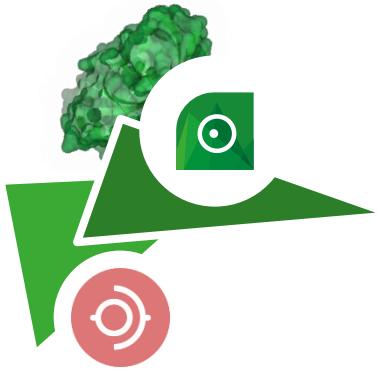
Supported Warheads

- acrylamide
- acrylester
- aziridine
- aldehyde
- alkynylyl
- alkynylylamine
- acrylimidazole
- acrylpyzarole
- (o-, m-, p-) arylators
- azide
- bicyclobutane
- boron
- boronate
- carbamate
- cyanamide
- diazerine
- disulfides
- epoxide
- haloacetamide
- iscocyanate
- ketoalkynyl
- α-ketoamide
- ketoamine
- lactam
- maleimide
- nitrile
- nitroalkanes
- nitroalkenes
- oxetane
- sulfonyl fluoride
- thioles
- urea
- vinylnitrile
- vinylsulfones









Made to Scale

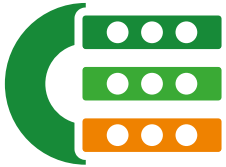
High-Performance Computing Support

Efficiently perform large-scale virtual screening campaigns on remote hardware with SeeSAR's **External Docking Mode**.

Powered by HPSee

HPSee is BioSolveIT's scalable virtual screening workflow environment. It enables the effortless handling of large compound collections in computational drug discovery scenarios

- Management of Libraries
- Team Orchestration
- Streamlining of Workflows



Simply select one **remotely stored** compound library for a virtual screening campaign and start the whole process with a single click.

Once the docking has finished, download **only the top scoring poses** for visual assessment on your local machine.

No more data juggling or terabytes of trash data. Work **conveniently** with only the most relevant results!

Chemical Space Docking™

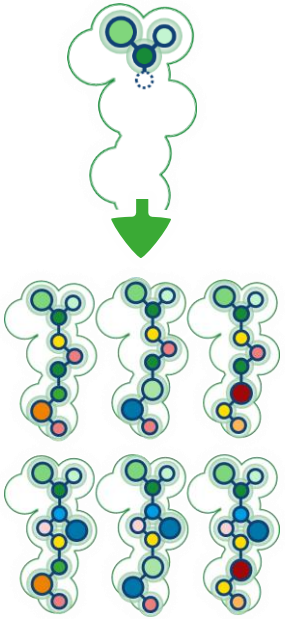
Unlocking the Molecular Universe

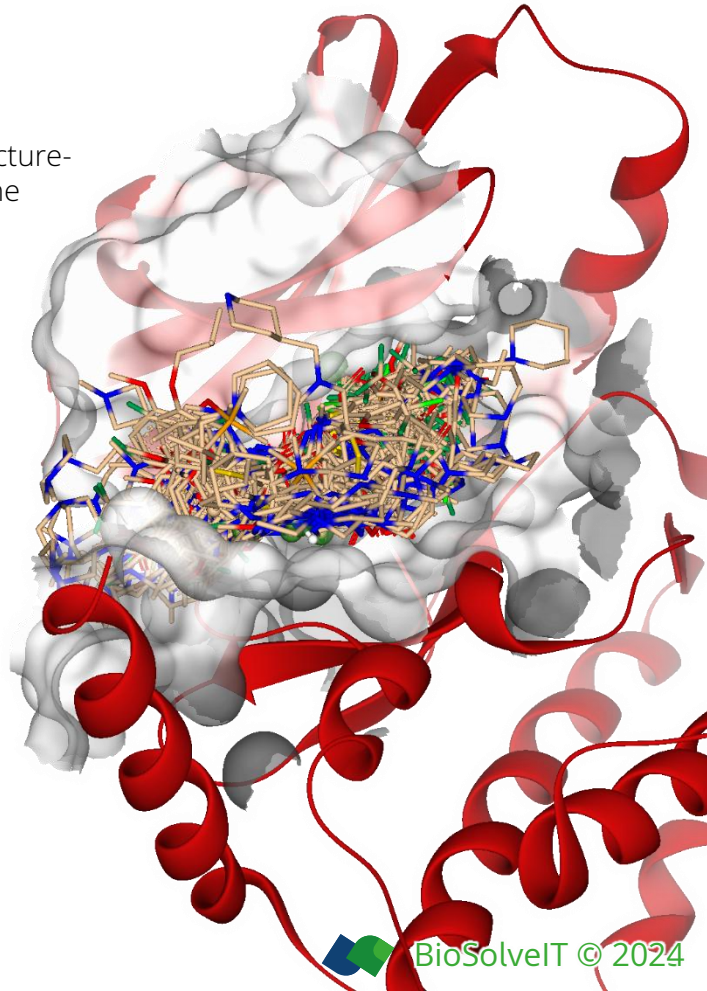
Chemical Space Docking™ is BioSolveIT's response to structure-based exploration of more than billions of compounds. The novel approach mines the best drug candidates with exceptional efficiency.

Chemical Space Docking™ provides you with the best **accessible** and synthesizable results out of trillions of molecule, requiring **only a fraction** of the typical computational resources

We collaborate with globally known compound suppliers in the creation of Chemical Spaces featuring commercially available, **make-on-demand** entries.

- Ambinter (**AMBrosia**)
- eMolecules (**eXplore**)
- Enamine (**REAL Space**)
- Freedom Space (**Chemspace**)
- OTAVA (**CHEMriya**)
- WuXi Labnetwork (**GalaXi**)

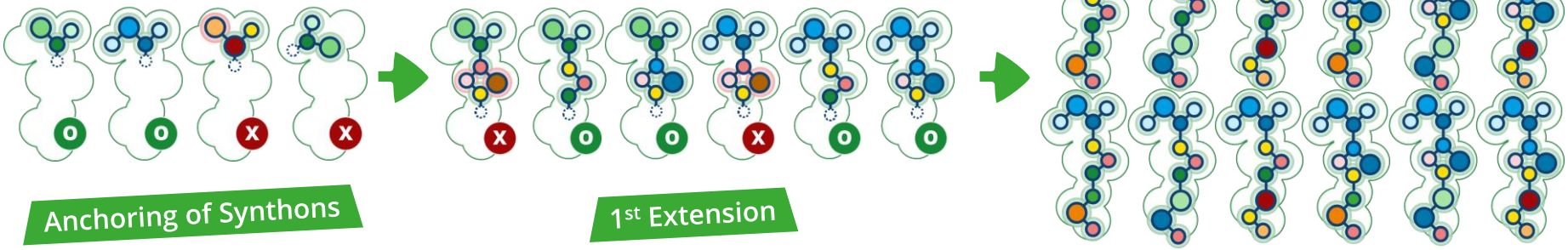




Interactive Workflow

Extracting the Most Relevant Chemistry

Assessing trillions of molecules using just a small portion of the typical computational resources, thanks to a novel approach.



Docking and scoring of the building blocks containing an **extension vector** (“synthons”) to spot the best candidates forming high-quality interactions with the target.

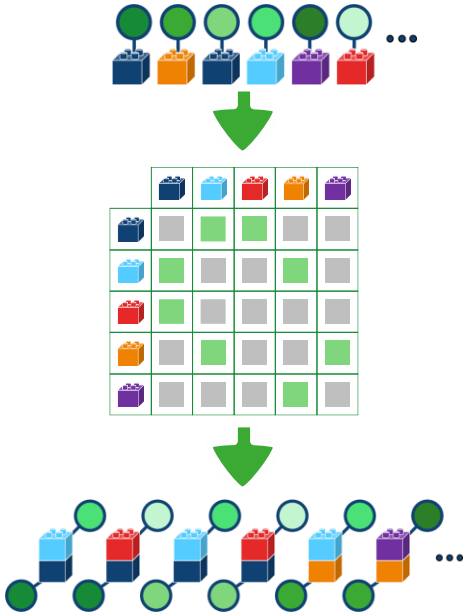
All possible, chemically accessible compounds originating from the selected synthons are created and docked. Since synthons with bad scores were discarded, only a fraction of resources is required to efficiently screen the whole Chemical Space.

Some compounds are already complete after the first extension. In some cases, a second extension is possible leading to the final molecule. Given the nature of the approach, all results are **synthetically accessible**.

Combinatorial Chemical Spaces

Handling Trillions of Tangible Compounds

The defined combination of commercially available building blocks results in trillion-sized compound catalogs featuring chemically diverse molecules.

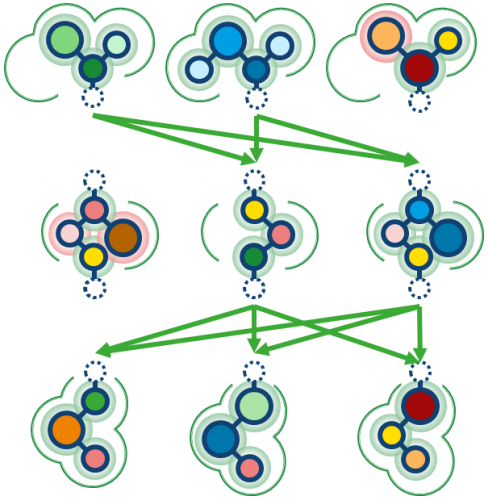


Combinatorial built-up

The combinatorial Chemical Spaces feature reactions that determine which compounds can be created, ensuring that every entry is synthetically accessible. Results from one of our partners' Chemical Spaces can be ordered and delivered to you within a few weeks.

Mining for gems

Only synthons displaying high-quality interactions are considered during the extension steps. Scoring, visual support and other parameters help you to identify the best candidates for follow-up.
It was proven that Chemical Space Docking™ outperforms brute-force docking in **enriching high-scoring candidates**.



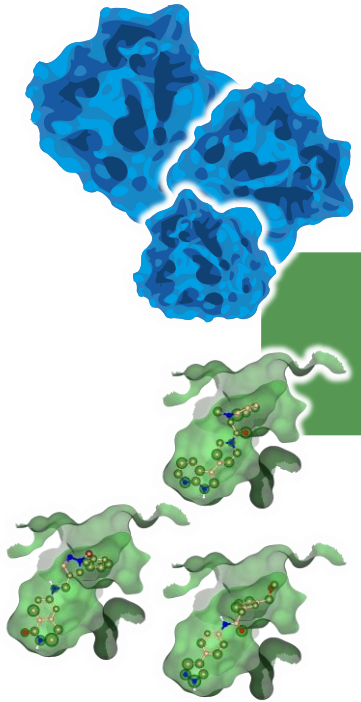
More Than Virtual Screening

Special Traits of Chemical Space Docking™

Our Approach represents the next generation of augmented hit finding.
Several advantages set this method apart from standard procedures.

Chemical Space Docking™ runs **on your own hardware**. No need to share your data with third parties and to rely on a service provider.

Furthermore, slim hardware is enough. Although more is always better, you can achieve high computational efficiency without the need for expensive, high-performance machines, allowing for **cost-effective and secure in-house operations**.



Several commercial Chemical Spaces are available, each coming with their own building blocks and reactions.

SeeSAR was developed to cater towards beginners and experts alike. Every stage of the workflow is **easy to understand and to operate**.

The method retrieves **diverse chemistry** complementing different subpockets of the target, fueling your pipeline with a variety of scaffolds.

YASARA: Energy Minimization

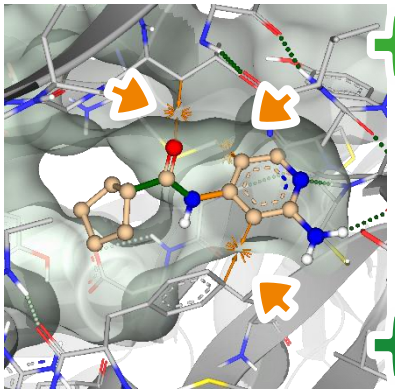
Refine Your Target Complex

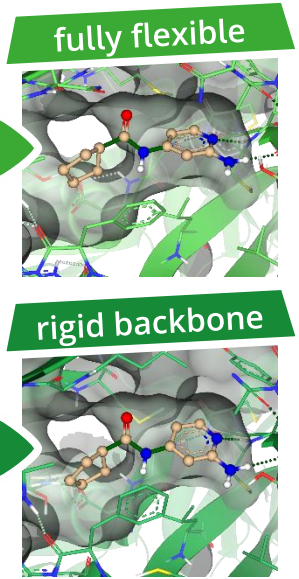
The YASARA module is an optional third-party integration in SeeSAR that allows users to optimize their target structures and models.

Take your structures to the next level

Enhance the starting points for molecular modeling approaches or virtual screenings, or refine your docking predictions for additional insights. Energy minimization is a versatile tool for achieving better predictions.

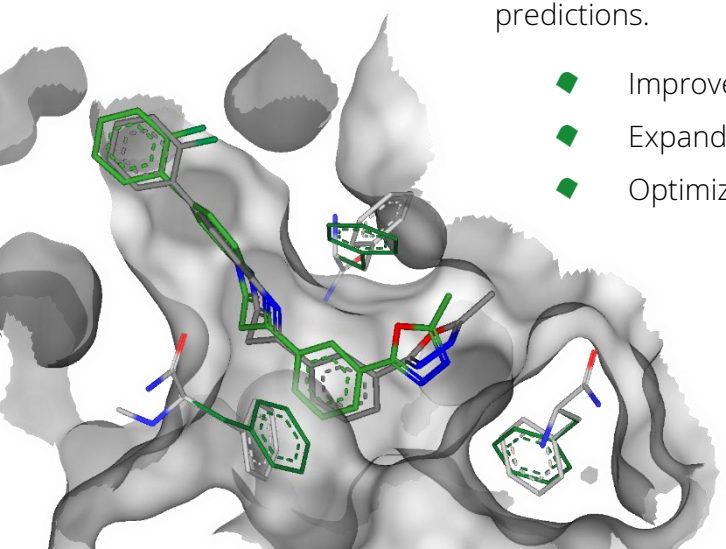
- Improve the quality of models
- Expand and sample binding sites
- Optimize poses and complexes





Adapt your complex

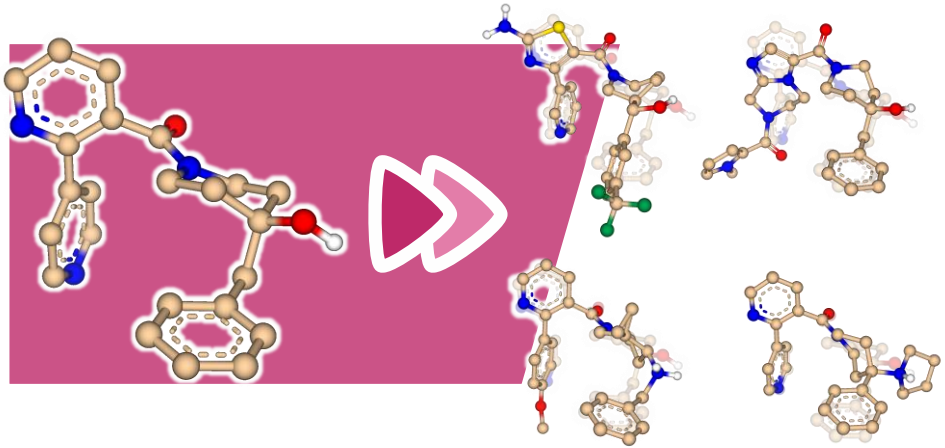
Energy minimization can be used to refine molecular torsions and clashes within a complex. The user has the option to choose whether to keep the target flexible or maintain the protein backbone as rigid.

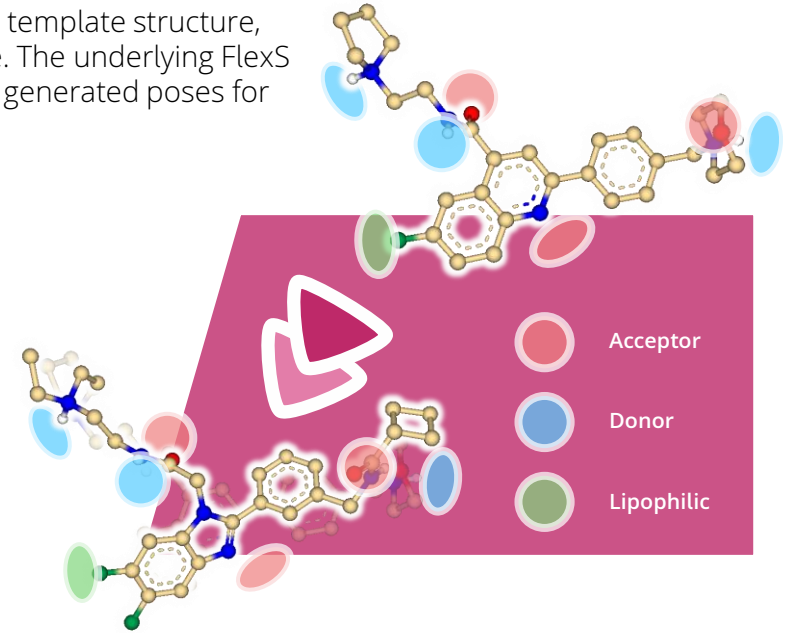


No Target Structure? No Problem!

Ligand-Based Virtual Screening

The Similarity Scanner 3D aligns molecules with a template structure, based on interaction features, volume, and shape. The underlying FlexS algorithm provides users with a score to rank the generated poses for selection of the best candidates.





Novel structures
FlexS retrieves structures similar to your query compound – a great source for scaffold hopping and functional group replacement. You may guide your search by applying pharmacophore constraints to fine-tune your results.

For 3D alignment, **pharmacophore features** such as hydrogen bond donors/acceptors as well as the molecular shape and volume are considered.

Let Science Speak for Itself

Stylize Your Complex

Augment your communication and presentations with powerful figures to highlight the impactful findings.

Customizable perspectives

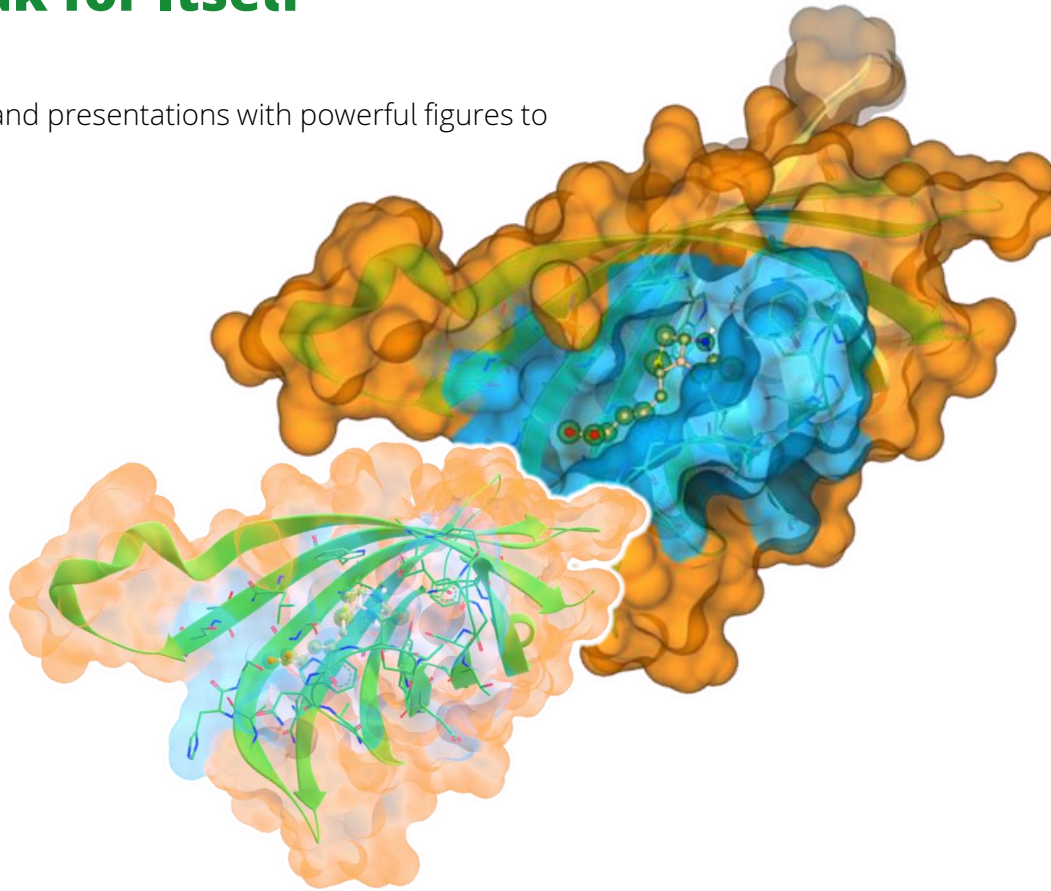
Highlight what's important with individual coloring and display of target structure, surface and binding site. Screenshots can conveniently be made with any preferred dpi resolution. Perfect for publications and reports!

Or take your visualization to the next level and export 3D models (.glb format) of your structures to embed them in your presentations, videos or websites.

Discuss your results

You can highlight molecules of interest, mark them as favorites or add annotations. Thus, people can easily follow your thoughts when you share the project with them.

Furthermore, SeeSAR also comes with a **colorblind mode** to accommodate all needs.



Master Your Challenges

The German Army Knife of Drug Discovery

Invaluable source for ideation
- Improve your compound on the fly
- Discover novel scaffolds and bioisosteres
- Find molecule decorations
- Satisfy unoccupied binding sites

Target handling
- Align and compare binding sites
- Detect druggable pockets
- Modify your binding site
- Work on proteins, DNA and RNA
- Screen for similar binding sites
- Work with in-house structures
- Directly download PDB-IDs

Stimulating fragment-based drug discovery
- Grow your ligand with FastGrow
- Fuse, link and merge fragments
- Mix-and-match
- Rescaffolding in no time

Bread-and-butter of computational chemists
- FlexX Docking (standard, template-based, covalent)
- Scoring of poses with Hyde
- Assessment of binding poses by molecular torsions and clashes
- Ultrafast prediction of tautomers and protonation states
- Manage and filter molecule sets
- Apply pharmacophore constraints
- Scalable KNIME workflows
- Convenient molecule edition
- Create compound libraries to test hypotheses

Innovative ligand-based drug discovery
- 3D virtual screening
- Compound alignment
- Hypothesis generation

Valuable insights
- Measure and label distances, torsions, residues, angles
- Predict ADME and physicochemical properties of your compounds
- Visualize parameters with diagrams

Present and discuss your results
- 3D model export (glb/pptx file)
- SDF and excel output
- Highlight favorites and (in)actives
- Intuitive color coding
- Annotations
- Capture scenes
- Adjustable binding site representation

Flexible, adaptable interface
- Light and dark theme
- Adjustable layout
- Support for color blindness