infiniSee

BioSolveIT
expect actives!

Surfs Chemical Spaces.
Hops Distant Relations. Yields Accessibles.

- Ultrafast chemical space navigation: 10^{20} in minutes
- Easy scaffold hopping: FTrees reveal hidden similarities
- Visualized similarities: Informed decisions through clear graphics

infiniSee: Infinite accessibles

Navigate in vast chemical spaces of size 10^{20} or even larger with infiniSee®. Find novel compounds for example during hit exploration, or for SAR expansion and patent escape.

- Navigate through chemical spaces
- Neat graphics help you rationalize results
- Purchase from partners, e.g. Enamine or WuXi.

infiniSee searches these spaces in minutes on a laptop. infiniSee is the world's **fastest** and most **visual** tool for navigating the chemical cosmos **easily**.

Why mine chemical spaces?

Novel intellectual property (IP) is urgently needed in the hunt for drugs. It can be shown that success in finding new molecules is connected to the size of space searched: Increasing the size by 10% will lead to 10 times more active hits.

The size of the chemical cosmos is estimated to be 10^{63}. Classical searches only cover spaces up to 10^{9} today. Use infiniSee to navigate breathtakingly large spaces of 10^{20} and more.

Pfizer, Boehringer-Ingelheim, and several frontrunner companies have documented their success — see the back of this flyer. Merck cut costs down by 90%, and sped up projects by 100% [3].

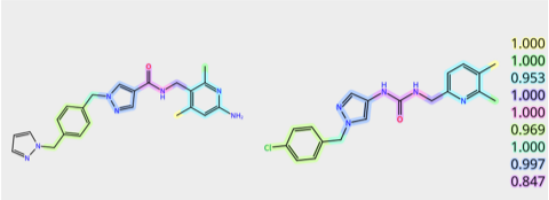
Use infiniSee together with downloadable chemical spaces to find compounds that can be purchased or are tangible within a few weeks:
From virtual to vial within days is now reality.

Distant in 2D, neighbors in action.

infiniSee uses award-winning FTrees [1,2] technology to spot molecules that are distant at first sight, yet very close in chemistry and pharmacophore-based action. Ultrafast and multidirectional navigation in multidimensional hypercubes deliver convincing molecules within minutes.

Visualization:
The key to staying in the driver's seat.

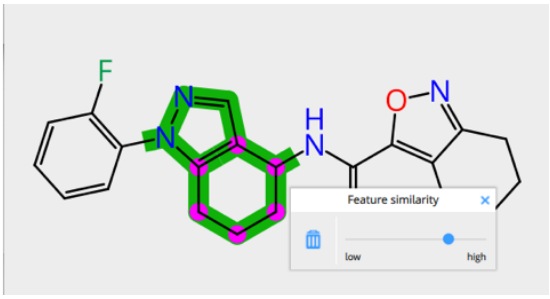
infiniSee will show you *why* it considers something similar. You will not be left alone with mere numbers; instead an intuitive, visual explanation will reveal hidden similarities between a query and hit molecules.



Here is an example: The color coding shows how the molecules align. Local similarities are displayed to enhance understanding.

Your pharmacophores: Keeping what's important.

Using a visual graphical definition you can impose pharmacophore boundary constraints. A minimum similarity for parts of your query molecule has then to be obtained in the results. This guides your navigation within the chemical space (or library of compounds).



In the background, very robust and fast FTrees technology [1,2] is used, while ProToss [4] takes care of protonation within milliseconds, including consistent tautomers.

Technical Requirements

infiniSee runs on Windows 64bit, Macs, Linux 64bit. It will automatically use all your CPUs in parallel. infiniSee needs the latest graphics card drivers installed. We recommend 16GB RAM.

How to get it

Just download and use for free for 3 days:
http://www.biosolveit.de/infiniSee
If you are happy, the software will help you with licensing.

www.biosolveit.com
contact@biosolveit.com
biosolveit.com/linkedin
facebook.com/BioSolveIT

infiniSee

Synthetic tractability built in.

Only what is highly likely to be formed in the lab will be formed during infiniSee's chemical space navigation. Therefore, the results will be extremely likely to be accessible in reality.

Enamine's 14 billion REAL Space® [5] has proven success rates around 85%, and deliver within approximately 3 weeks.

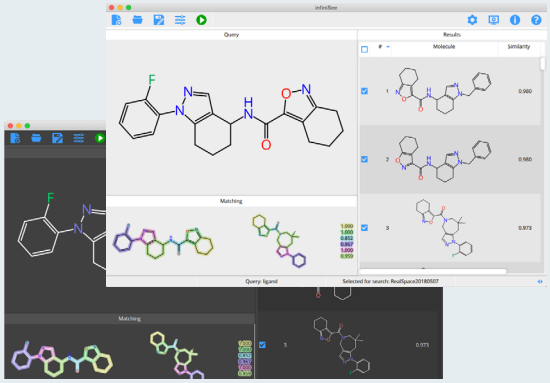
Merck's MASSIV space of likely accessible molecules led to a ten-fold cost saving and a doubled speed-up in projects [4].

The KnowledgeSpace by BioSolveIT delivers results created from publicly available building blocks and reactions.

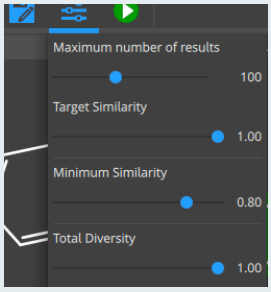
Beyond REAL Space®, WuXi's new 2 billion GalaXi® space of on-demand molecules can be searched with infiniSee alike.

If you would like us to create your own vast fragment space, then please get in touch.

A versatile interface, very easy to use.



Computer screen or presentation: Dark or light themes enhance your interactive experience with infiniSee.



Close neighbors or distant scaffold hops, infiniSee has the relevant sliders for you to control navigation.Fine-tune your result diversity and create and save up to 100,000 solutions.

Contents and chemical space partnerships

- **On-demand Molecules: Enamine REAL Space®** and **WuXi GalaXi®** More than 16 billion of tangible molecules to mine and order straight away. Enamine guaratees delivery rates of 80% within approximately 3 weeks time.
  Details at biosolveit.com/CoLibri/spaces.html
- **KnowledgeSpace:** A space of 10^{15} virtual molecules built from publically available reactions and building blocks: https://biosolveit.com/KnowledgeSpace
- **Your own, in-house chemical space — contact us:** You can potentially increase your minable IP pool by creating your own chemical space. Here are a few examples:

Merck's MASSIV [3] leads the field with 10^{20} possibilities.

Complementary software

CoLibri: BioSolveIT's chemical space creation tool, available at: https://biosolveit.com/CoLibri

SeeSAR: Really interactive 3D design before your eyes, more at: https://biosolveit.com/SeeSAR

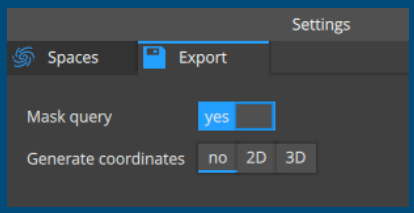
KNIME, PipelinePilot, commandline support. Start here: https://biosolveit.com/KNIME and biosolveit.com/PipelinePilot

FTrees, FTreesFS: The fast search machinery as a standalone executable: https://biosolveit.com/FTrees

Your ideas are safe and secure.

All computations run on your own computer, behind your firewall. Except for new software version checks, no information is pushed or pulled over the internet.

Your results will ensure the query remains undisclosed upon export, and we can include 2D or 3D coordinates for you for post-processing tasks.



Acknowledgments:

infiniSee is powered by BioSolveIT's FTrees and FTreesFS technology, ideas originally conceived by Prof. Rarey at Hamburg University, Germany.[1-2]

A chemical space review with more details recently appeared in Drug Discovery Today [6].

References:

[1] Rarey, M.; Dixon, J. S., JCAMD 1998, 12, 471–490.
[2] Rarey, M.; Stahl, M., JCAMD 2001, 15, 497–520.
[3] Krier, M.; Klingler, F., curious Conference 2018
[4] Bietz, S. et al., JCheminform. 2014, 6, 1–12.
[5] REAL Space, Enamine 2019, enamine.net/library-synthesis/real-compounds/real-space-navigator
[6] Hoffmann, T; Gastreich M., DDT 2019, Review: https://doi.org/10.1016/j.drudis.2019.02.013

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SeeSAR

BioSolveIT
expect actives!

SeeSAR™ — Every Chemist's SAR and ADME Dashboard

- Visual 3D Guidance for Lead Optimization for bench chemists and experts alike
- Entropy-aware ΔG estimates, torsional analyses, and explorability — visualized on-the-fly
- Now includes the rigorous Optibrium™ ADME models

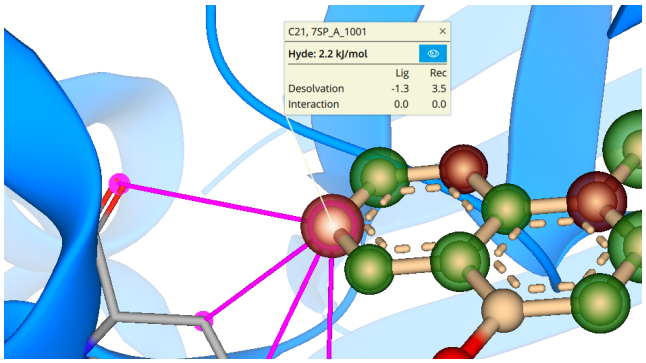
SeeSAR: Visual SAR and ADME

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

Atoms increasing affinity are colored green, unfavorable ones red. Explore and fill free cavities, see torsional implications, check crystal structures for artifacts, and much more — and keep an eye on the scientifically rigorous ADME properties by Optibrium™. SeeSAR is award-winning, next generation software from BioSolveIT, tailored to your everyday ligand optimization work.

SeeSAR Rationalizes Your SAR

Affinity is not only about forming new bonds.
It is 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.

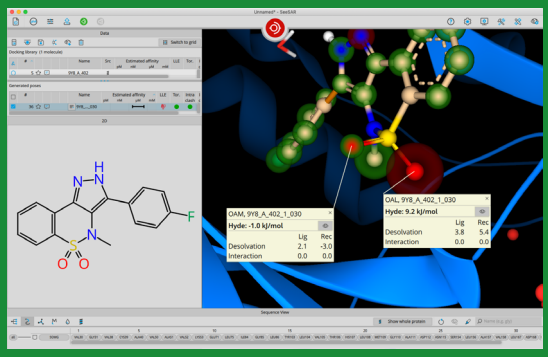


More than a mere number: SeeSAR lets you drill into details so you can see what happens exactly. For example this ligand covering a backbone's C=O, entailing a strong desolvation penalty (PDB: 3T7P).

More than a few ligands? Triage & Filter!

SeeSAR sports a luxuriously designed filter dialog. Not only can you sort and filter by the properties we compute, but also your own SD-file properties are taken into account. And duplicates? Forget about them!
Just download & go! No admin rights are needed!

Strictly Visual Dashboarding

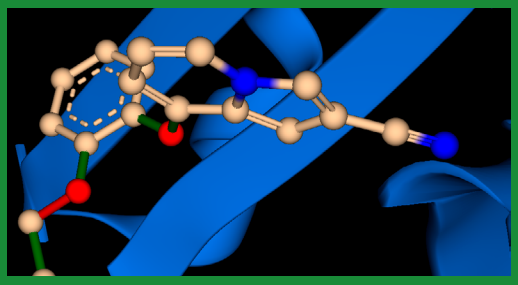


Visual SAR and ADME alerts before your eye:

Green atoms are good, red ones unfavorable; solubilities, blood-brain-barrier penetration, hERG properties and much more, all in a crisp interface.

Rapidly rationalize your SAR — know what to do next and why.

Graphics & Reporting: We Thought of You!



Exploiting your modern hardware, graphics are smooth, and report generation will be a pleasure.

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:
http://www.biosolveit.de/SeeSAR
If you are happy, the software will help you with licensing.

www.biosolveit.com
contact@biosolveit.com
biosolveit.com/linkedin
facebook.com/BioSolveIT

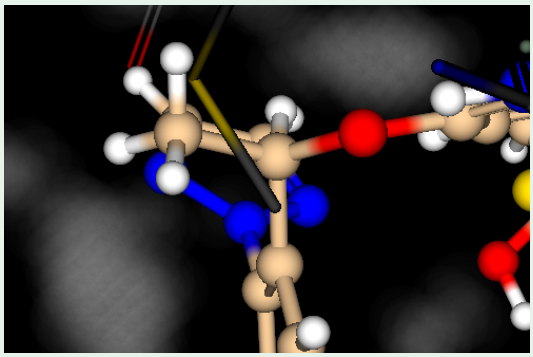
SeeSAR

MedChem 3D Editing, Auto H⁺/Tautomers

SeeSAR features a new 3D editor which relaxes your edits on the fly — and shows effects on the **explorability volume** or **torsional significance** and estimated ΔG.

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, for every pose! Clash visualization, protein editing, and tons more, all nice and easy.

See Explorability and Tighten Your Fit!



Unoccupied space where you can improve the tightness of fit is intuitively visualized:

White 'fog' tells you where at least one fluorine atom would fit between ligand and protein. Also perfect for fragment growing: It is interactively pushed out or modified while you edit or grow automatically.

Recent Success Stories

Improving GPCR Dockings: Mason et al., 2016, J.Comput.Inf.Model. ASAP, DOI: 10.1021/acs.jcim.5b00660

SAR for Dynamic Combinatorial Chemistry: Mondal et al. , 2014, Angew.Chemie.Int.Ed.Engl., 53, 3259

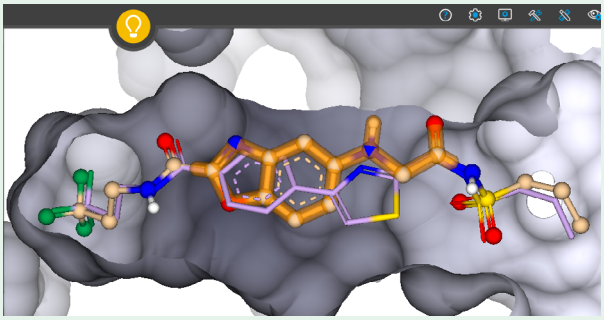
SAR in MAO-B Elucidated: Tzvetkov et al., 2014, J.Med.Chem., 57, 6679

ADME by optibrium

Optibrium StarDrop™-based ADME properties are available! For example: 2C9 pK_i, PPB90 plasma binding, 2D6 affinity, P-glycoprotein-binding, BBB-penetration, hERG pIC_{50}, logD, solubility — and more!

The New Inspirator — FBLD On-the-Fly

Link/merge, grow, rescaffold at world record speed. Millions of possibilities, in seconds.



Complementary to SeeSAR

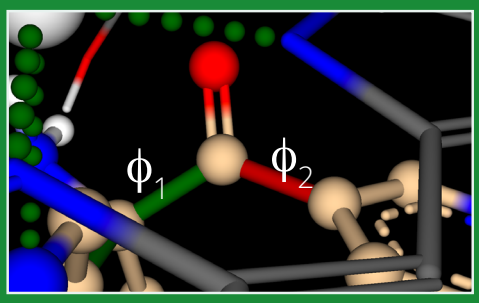
- LeadIT — our full-featured SBDD and FBLD suite:
  - ReCore
    Google-like fragment and structure based design (FBLD, SBDD): Replace or grow from a binder, generate merging and linking proposals in seconds; everything visualized in 3D.
  - FlexX
    Fast & accurate docking: With more than 8,000 citations, FlexX is great tool, pushing the boundaries over the years.
- infiniSee — The fastest navigation across the biggest chemical spaces Navigation Sleek 2D sketches of protein-ligand complexes [4].

Torsion Checks at Your Fingertips

Torsion angles around rotatable bonds are colored by how often they have been observed in small molecule crystals. An approach first used by Hoffmann-LaRoche [2].

Coloring is by occurrence:

Red: Seldom
Yellow: Occasional
Green: Frequent



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 (ZBH), Dr. Tanja Schulz-Gasch, and Dr. Martin Stahl at Hoffmann-LaRoche in Basel, Switzerland.[2]
The ADME models are © Optibrium™, Ltd.: www.optibrium.com.

References:

[1] Schneider et al., JCAMD 2013, 27(1):15-29
[2] Schärfer et al., JMedChem 2013, 56 (6):2016-28
[3] Bietz et al., JCheminform, 2014, 6(12):1-12

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