Surfs Chemical Spaces. Hops Distant Relations. Yields Accessibles.

infiniSee
infinite 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 hits from partners, e.g. Enamine.

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 front-runner 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 REAL Space® [5] has proven success rates around 85%, and our partner delivers within approximately 3 weeks.

Merck’s MASSIV space 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.

You can navigate the REAL Space® and KnowledgeSpace with infiniSee.

If you are a pharma company, another research organization, or a compound provider and would like us to create your own 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**

- **Enamine REAL Space®**: Billions of tangible molecules to mine. Delivery rates of 80% guaranteed within approximately 3 weeks time. https://biosolveit.com/CoLibri/spaces.html

- **KnowledgeSpace**: A space of $10^{19}$ virtual molecules built from publicly 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:

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Corporate / proprietary

Merck MASSIV [3] leads the field with $10^{20}$ possibilities.
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**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 in post-processing tasks.

**Acknowledgments and Remarks**

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**


