REAL Space Navigator™ — From Virtual to Vials in Your Lab.

Expect Actives

REAL Space Navigator

- Navigate & select favorite compounds from a **3.8 billion** virtual compound space
- Within **less than 3 weeks**, **more than 80%** of your favorites will be delivered to you
- Fuzzy pharmacophores ensure sensible results — far **beyond substructure** searches

REAL Navigation — Super Big Data

REAL Space Navigator is a new software for chemists to search the **vast spaces** of compounds from our partner **Enamine**.

Molecules are pulled from the REAL Space — the world's first commercial chemical search space, conceived with care by Enamine. **80% synthetic access** is guaranteed. Often even better.

Today, it contains more than **3.8 billion orderable compounds** to order from and thus exceeds anything offered before in size.

Compounds are delivered in 3 weeks or less.

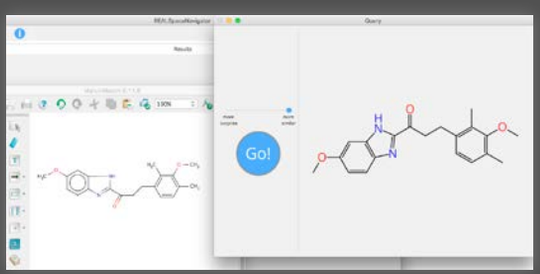
3.8 billion compounds — REAL-ly

It is not about increasing the size of the haystack — it is about expanding the realms of possibility for you by orders of magnitude: BioSolveIT's FTrees navigation technology finds the most appropriate compounds in this vast space within **2 minutes**.

A standard PC with 4GB will do. Safely.

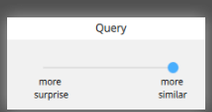
The REAL Space Navigator runs behind your firewall and keeps **your compounds secret**. Drag and drop your query, press "Go!". Cherry-pick your favorite solutions. Then contact Enamine to obtain a quote. 3 weeks later, the compounds are yours.

Drag and drop, press Go!



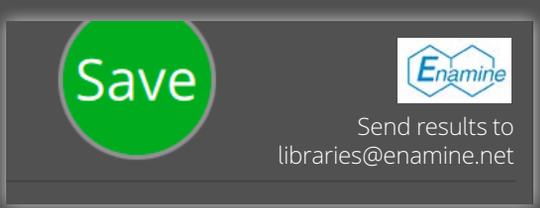
Copy and paste from your 2D sketcher, go!

REAL Space Navigator reads your sketches from the clipboard. Supported: SDF, PDB, smiles, mol2, or simply a drag and drop.



Targeted similarity sliders let you choose to go for library enrichment, scaffold hops, or new inpirations.

Guaranteed: 80% will arrive. In < 3 weeks.



Our partner Enamine will deliver at least 80% of the hits. In less than 3 weeks time. To your desk.

All data stay with you. The compound IP is yours.

Technical Requirements
REAL Space Navigator 2 runs on Windows, Macs, Linux. The software needs the latest graphics card drivers installed.

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

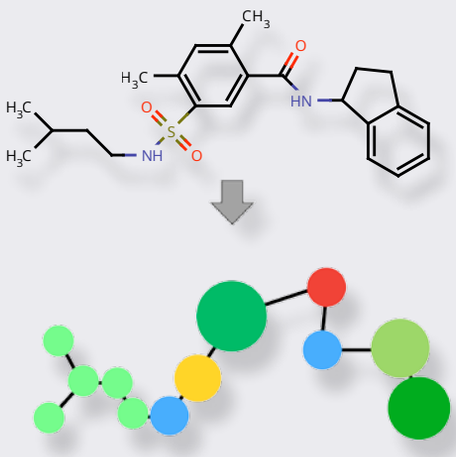
www.biosolveit.com
contact@biosolveit.com
biosolveit.com/linkedin
facebook.com/BioSolveIT

REAL Space Navigator

Fuzzy similarities, powered by FTrees™

REAL Space Navigator exploits FTrees technology — ultrafast **pharmacophore-based** alignment algorithms that go far beyond 2D substructure searches.

Molecules are transformed into "informed trees" that we use to find other hits. For example:



FTrees contain information about connectivity and physico-chemical parameters, they deliver scaffold hops by design, in no time.

Boost your choice with your own space !

Can you create your own chemical space? Sure!

We can help you create your own, corporate chemical spaces. BioSolveIT has a proven track record with several big pharmas (see the list to the right).

Using CoLibri™, our space administration and creation software, we can be quick at transforming your knowledge into a vast space of chemical possibilities that you will enjoy navigating within minutes with our software.

Connecting with your IT infrastructure

- **Pipelining** — connect with your favorite package:
  - **KNIME**
    Nodes for the popular, free pipelining toolkit KNIME from knime.org are available straight from our website at https://www.biosolveit.com/KNIME
  - **PipelinePilot**
    We support the PipelinePilot enviroment. All components are available to licensees and can readily be downloaded from https://www.biosolveit.com/PipelinePilot.
- **Web embedding** — Please ask us for support for your infrastructure. We are happy to target the software to your chemical space !
- **Commandline** — If you prefer to shell script your workflows, the commandline interface is the best choice.

Published space navigation successes

Several organizations have already created in-house search spaces of vast sizes. Our globally unique technology for navigating through this incomprehensibly large amount of possibilities shows very high likelihoods of synthetic tractability — a resource for fast, novel IP generation. A selection:

- **Pfizer's PGVL: 10^{16} compounds**
  Boehm M et al., JMC 2008 51:2468-2480
- **Merck's MASSIV: 10^{20} compounds**
  Krier M et al., Curious Conference 2018 — 10^{20} Molecules. A gigantic pool of possibilities at your fingertips.
- **Boehringer-Ingelheim's BI-CLAIM: 10^{11} compounds**
  Wellenzohn B et al., JMC 2012 55(24) 11031-11041

Just think of the possibilities...

If the REAL Space Navigation were the size of a truck... When you search the largest available molecular library of a few hundred million compounds, then this would be like searching only a pool of possibilities, the size of a bee, compared to the **billions** that the REAL Space Navigator offers today. Immeasurably more possibilities to choose from!

Acknowledgments:

Real Space Navigator is a collaboration between Enamine and BioSolveIT. The core technological idea behind the tool is from Prof. Dr. Rarey at ZBH, Hamburg University, Germany.[1] The FTrees code has been rewritten and parallelized and exploits state-of-the-art molecular initialization powered by NAOMI and ProToss.[2]

References:

[1] a. Rarey M & Dixon JS, JCAMD 1998 12:471-490;
b. Rarey M & Stahl M, JCAMD 2001 15:497-520
[2] Bietz et al., JCheminform, 2014, 6(12):1-12

Tool Website:

http://www.biosolveit.com/realspacenavigator

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