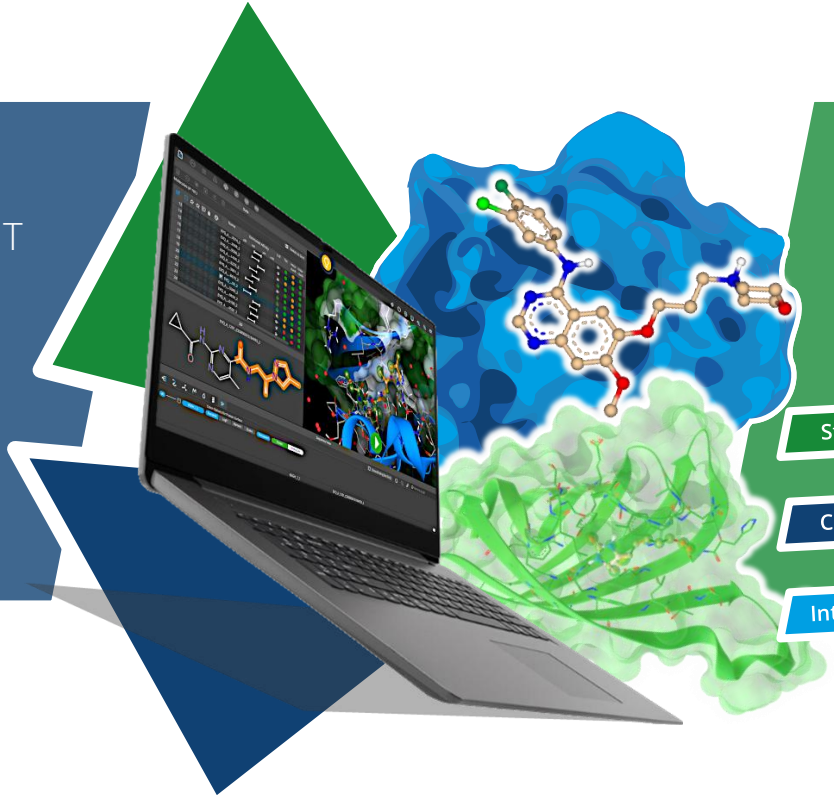
BioSolveIT

expect actives!

BioSolveIT

Revolutionizing Virtual Drug Discovery

For more than two decades, we at BioSolveIT have been dedicated to craft the most user-friendly drug discovery software infused with scientifically excellent ingredients.



Our Mission

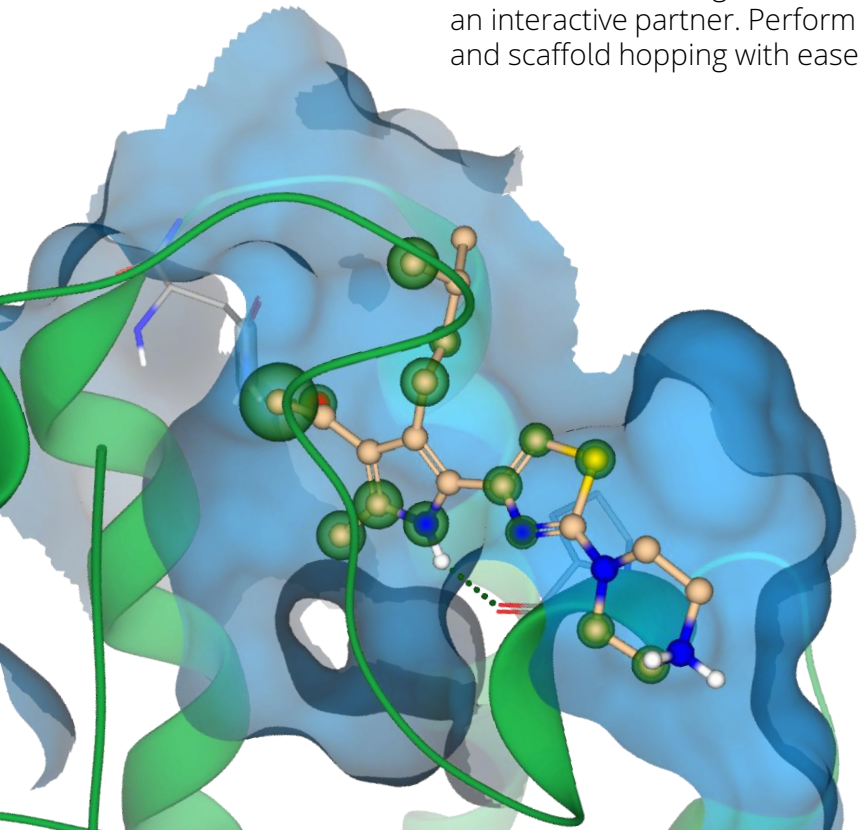
Providing domain experts with expertly developed software that empowers them to significantly enhance their performance and excel in their work.

- Structure- and ligand-based drug discovery
- Chemical Space navigation and exploration
- Interactive and fun-to-use software solutions

Fast • Visual • Easy

Our Recipe for Happy Users

Our software is designed and developed to support you in your efforts as an interactive partner. Perform tasks such as docking, lead optimization and scaffold hopping with ease in a clean graphical environment.



Fast

Effortlessly execute your tasks and gain instant understanding of the results with swift calculations.

Visual

Enhance your decision-making process with intuitive color codes to evaluate interactions **effectively**.

Easy

Beginners and veterans can experience the joy of on-the-fly drug design with our **user-friendly solutions**.

We Are Not Like Other Companies

Our Proficiency Is Surpassing the Limits of Common Methods

BioSolveIT is at the forefront of pioneering Chemical Space exploration, as well as innovative, visually engaging, and interactive structure-based drug discovery and modeling.

Exploiting all possibilities

The chemical space bears endless potential. The only limiting factor is the **number of compounds** that can be handled in a reasonable time.

Throughout the years, the size of compound collections has grown, and BioSolveIT's technology has enabled the creation of the largest molecule sets: Chemical Spaces.

Compound libraries

(what the others do)

- **Multiple/assembled long** lists.
- **Pre-combined** options.
- Takes **forever** to screen.

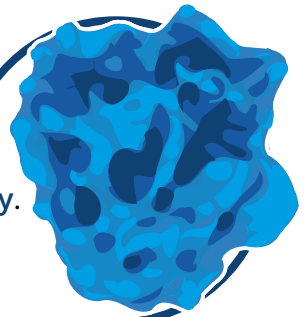
Enumerated

Next generation of molecule collections

Chemical Spaces

(what we do)

- Matching result is found **on-the-fly**.
- **Almost infinite** options.
- **Super fast** solution finding.

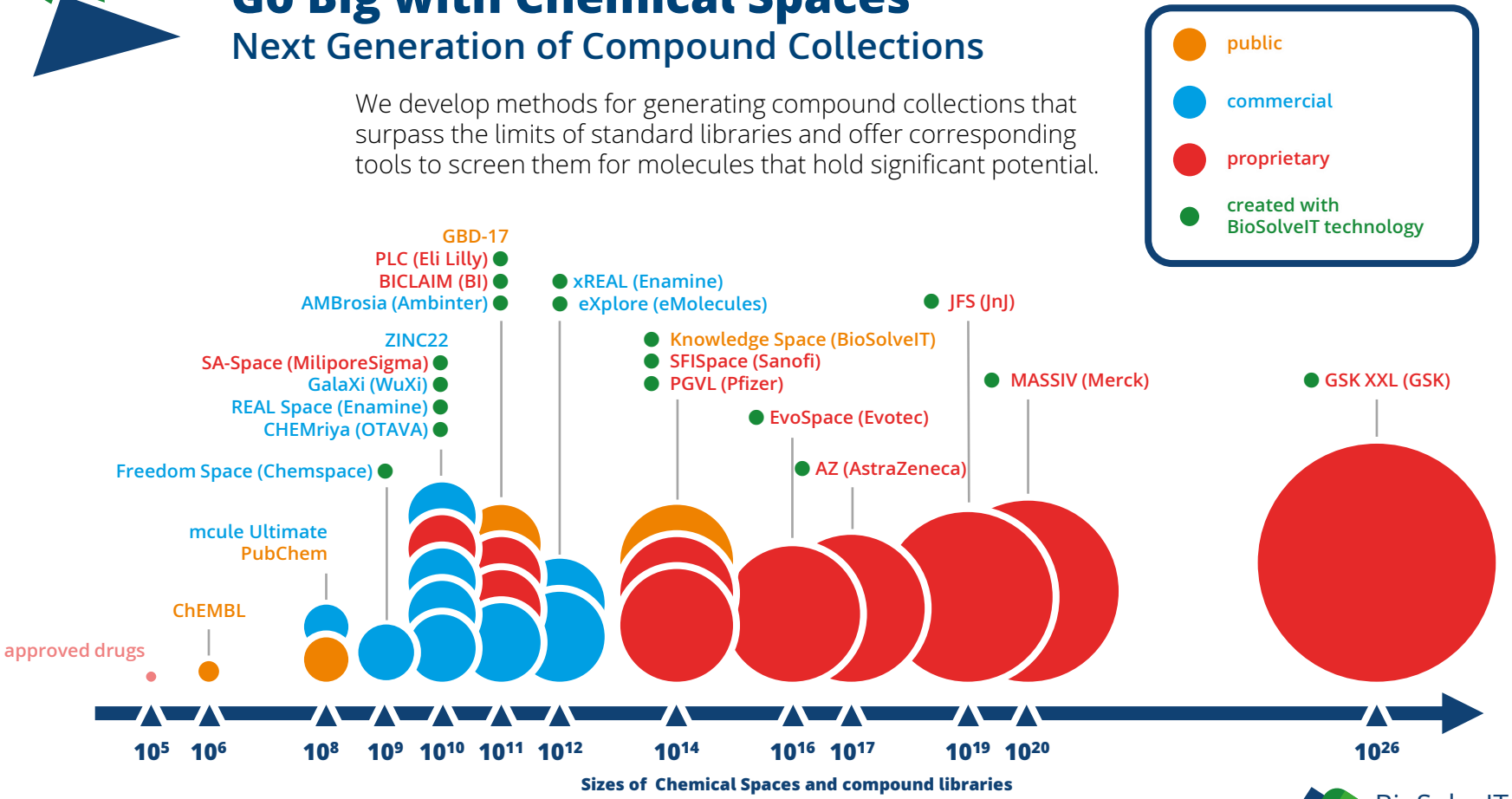


Combinatorial

Go Big with Chemical Spaces

Next Generation of Compound Collections

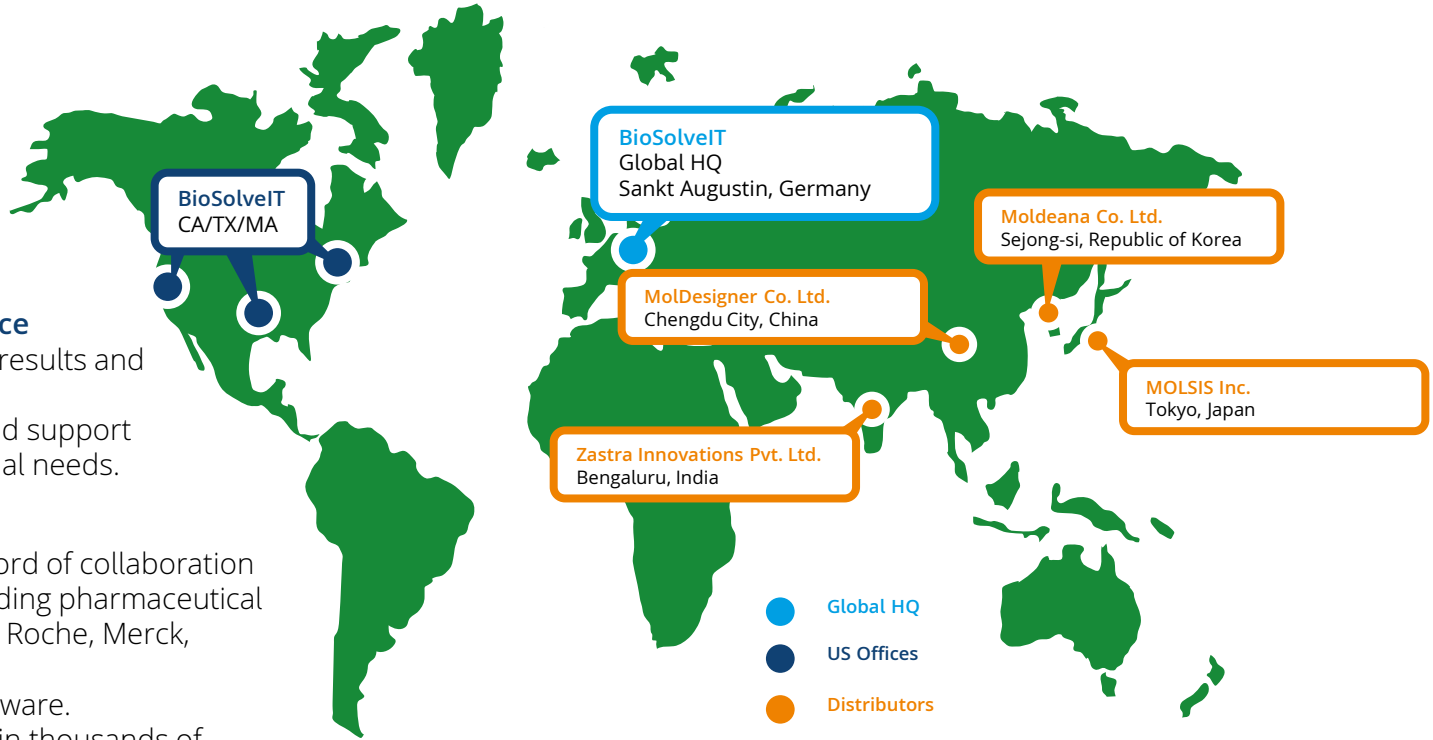
We develop methods for generating compound collections that surpass the limits of standard libraries and offer corresponding tools to screen them for molecules that hold significant potential.



Your Global Partner

Trusted and Reliable around the World

After its **establishment in 2001**, BioSolveIT now operates at a global level with offices in Europe and North America, as well as distributors in several Asian countries.



Customer-oriented service

- We aim for the optimal results and outcomes for you.
- Best possible service and support tailored to your individual needs.

Success with confidence

- Expertise and trach record of collaboration with academics and leading pharmaceutical companies (e.g., BAYER, Roche, Merck, BASF, and more).
- Secure and reliable software.
- Success acknowledged in thousands of publications.

Drug Discovery Solutions

Our Product Portfolio

SeeSAR
3D drug design dashboard

infiniSee
Chemical Space navigation platform

infiniSee xREAL
Enamine's largest compound catalog

High-performance computing

HPSee
Scalable workflow infrastructure

Structure- and ligand-based drug discovery

- **FlexX** — Molecular docking
- **FastGrow** — Pocket exploration
- **Conformator** — Molecule superposition
- **HYDE** — Affinity scoring
- **FlexS** — Molecule superposition

Chemical Space exploration

- **FTrees** — Fuzzy pharmacophore
- **SpaceLight** — Close analogs
- **SpaceMACS** — Substructure matching
- **CoLibri** — Chemical Space creation

The platform's individual components are also available as command-line tools that can seamlessly be integrated into your existing workflows.

Services we offer

Empowering Your Drug Discovery Through Tailored Solutions

Access our in-house expertise!

Contract Research
We work with your team to solve your drug discovery challenges like hit finding and optimization.

Custom Chemical Space
We can help you build a custom Chemical Space which encompasses the full spectrum of synthesizable potentials.

Chemical Space Docking™
We perform the next generation of virtual screening to mine for most promising candidates from ultra-large Chemical Spaces for you.

Scaffold Hopping and Fast Follow-Up
Need to replace an undesired core motif or IP overlap? We can generate ideas tailored for you.

Virtual Screening
Need to identify novel hits against your target? We have the expertise plus some of the most powerful tools to achieve your goals.

Covalent Docking
We can process various covalent warheads and individually expand our molecule transformation to dock uncoventional motives.

SAR Analysis and Lead Optimization
Collaborate with us to gain insights into SAR with our visual affinity tools. Explore and refine your lead compounds with confidence.

Target Analysis and Pocket Finding
We help mine the PDB to compare binding sites, discover novel ones, and assess their druggability.

Success with confidence
Let us convince you! Contact us for a free, no-obligation, and confidential evaluation or pilot project.