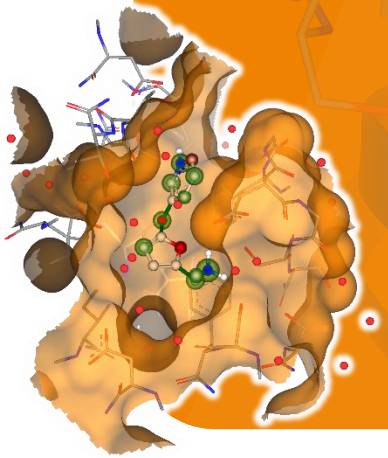
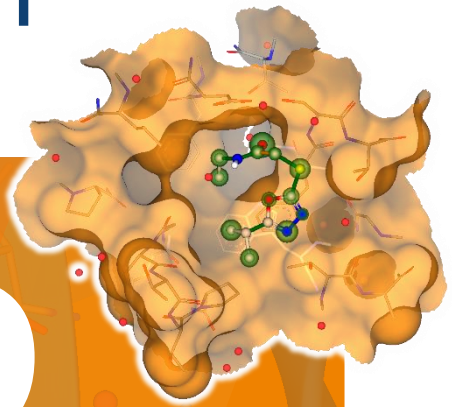
BioSolveIT
expect actives!



FBDD

Fragment-Based Drug Design



And How To Be Successful In It

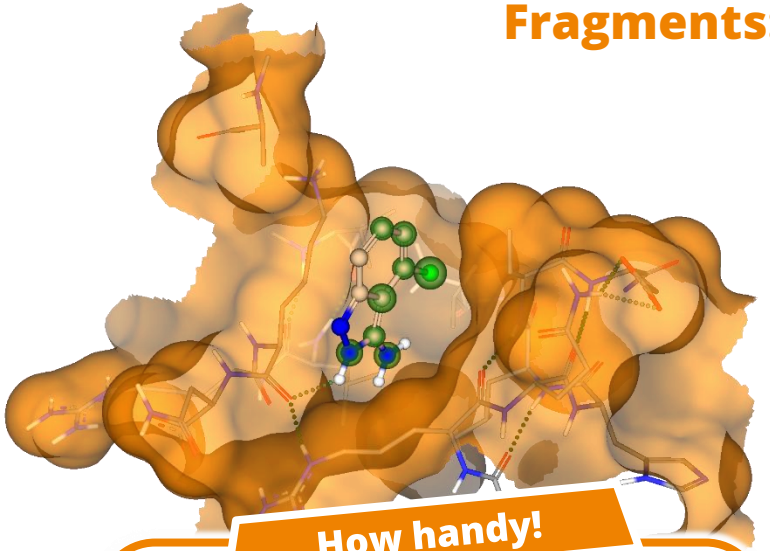
What is Fragment-Based Drug Design (FBDD)?

Fragment-Based Drug Design (FBDD) focuses on screening small, low-molecular-weight compounds (fragments) that bind to biological targets. These fragments serve as starting points for drug discovery, and through optimization and development, they grow into more potent, high-affinity molecules.

Rule of Three (RO3) defining fragment-like compounds:
logP ≤ 3 • MW < 300 • H-bond donors ≤ 3
H-bond acceptors ≤ 3 • rotatable bonds ≤ 3

Fragments are small molecules that are grown into larger compounds by adding functional decorations.

Fragments: Small, Efficient Beauties



How handy!

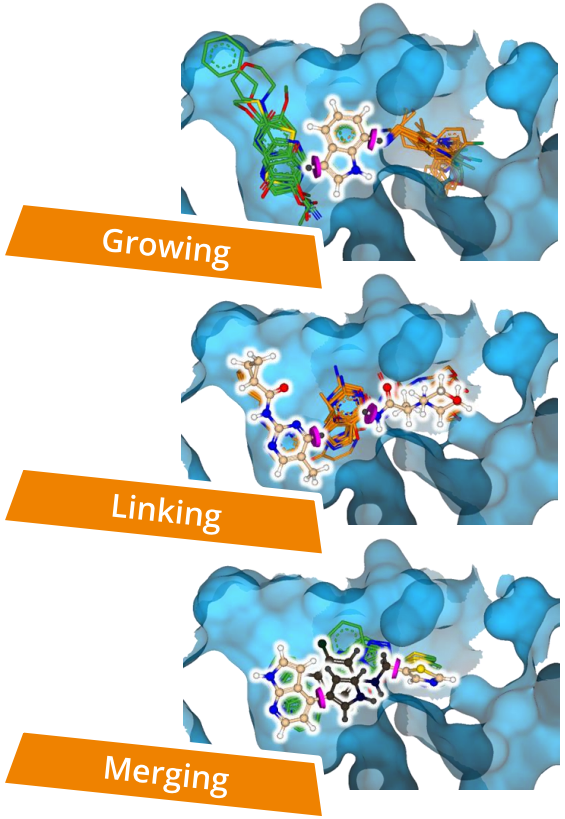
A driving force for the binding of fragments is their ability to form high-quality interactions with the target structure.
Visual support of SeeSAR helps you to see the individual contributions of each atom to the overall binding affinity. Use this to assess predicted binding modes of your ligands!

Fragments cover a broad chemical space, offering more opportunities to identify novel drug candidates. This makes the approach cost-effective as fewer resources to screen and optimize are required.

As FBDD can identify molecules that form high-quality interactions to bind to a target structure, hits represent perfect starting points for rational design of more potent candidates.

The BioSolveIT platforms **SeeSAR** and **infiniSee** facilitate fragment-based campaigns from the 3D and 2D world.

The Journey into Drug-Like in 3D



SeeSAR can perform the three most prominent methods applied in FBDD: **Growing** of a fragment into unoccupied binding pockets, **linking** of two fragments binding in separates sites, and **merging** of two fragments to find a scaffold replacement with features of both molecules.

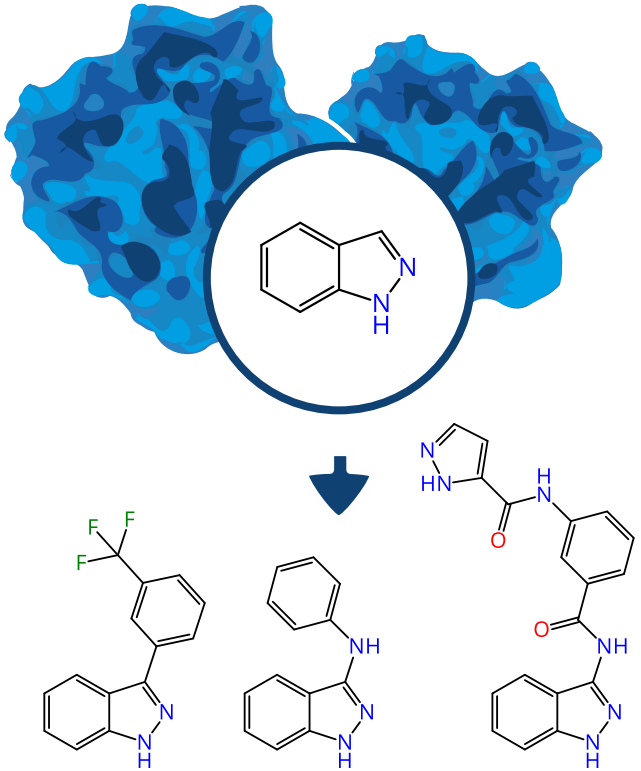
Several databases are available to address different challenges in modern drug discovery.

Tools:

SeeSAR

Inspirator

Chemical Spaces: The Land of Milk and Honey for FBDD



Chemical Spaces are ultra-vast compound collections, containing trillions of drug-like, commercially available entries.
Thus, they represent the largest catalogs featuring a plethora of molecular motifs and scaffolds.

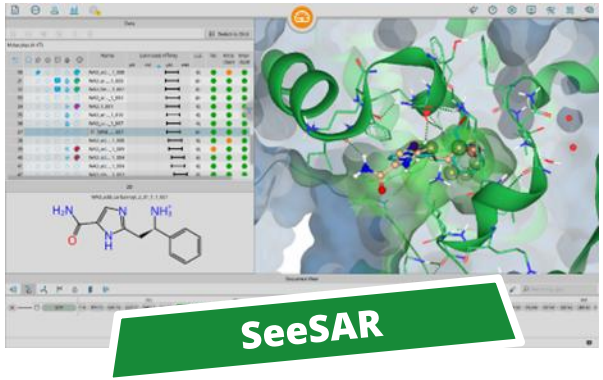
By searching several commercial Chemical Spaces, you get access to millions of compounds containing your substructure of interest that are not listed anywhere else.

Tools:

infiniSee

Motif Matcher

Supercharge the Smallest Opportunities into Big Success



Ready to take your Fragment-Based Drug Design to the next level?

Experience the power of BioSolveIT's tools and accelerate your drug discovery process.

Learn more using the QR code below: