ReCore – Rescaffolding

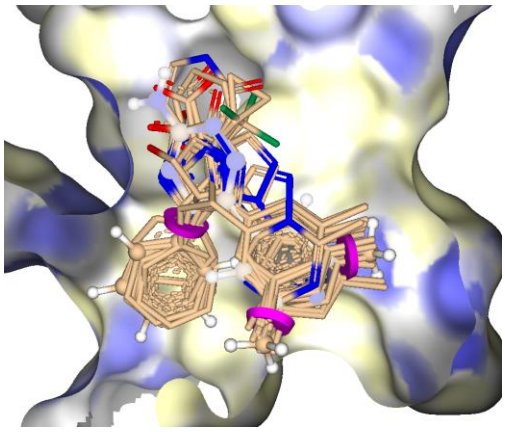
BioSolveIT
expect actives!

Generate new scaffolds, evolve and merge fragments, or explore subpockets in the blink of an eye with ReCore.

How does ReCore work?

The ReCore rescaffolding functionality in SeeSAR requires a 3D fragment library to search in — we call this an "index". Our ReCore indices are created using 3D-compound databases like PDB, ZINC or CSD. Fragments are generated based on shredding rules that define cutting points and filter rules to get rid of fragments with unfavorable properties.

You have the flexibility to utilize a wide range of compound or fragment libraries, whether they are commercially available or developed in-house. Additionally, you can interactively apply pharmacophore constraints during the design process. This allows you to tailor your search and exploration of compounds based on specific molecular requirements.



By having access to diverse solutions, your possibilities and creative potential will be maximized. This means you can explore a multitude of options and combinations, enabling you to generate innovative and unique compounds that align with your desired criteria.

Advantages

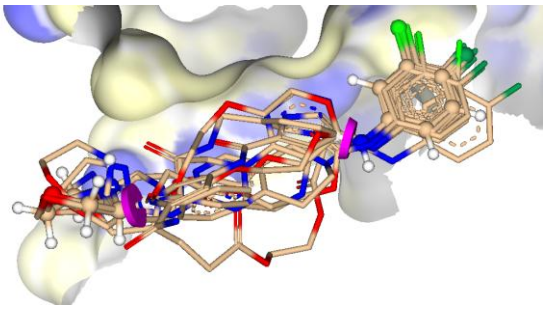
- Replace central elements in known bioactive molecules
- Generate new scaffolds in 3D in the blink of an eye
- Impose pharmacophore constraints interactively
- Custom design your own fragment database for scaffold replacement

3D Scaffold hopping. Guaranteed

Generate new IP or get rid of a problem with a molecule, specify bonds or interactions to be matched by new fragments. The arrangement of these vectors is taken to a fragment library that has been pre-processed for speed ("indexed"). From this, results are retrieved within fractions of a second, and using a 4-dimensional vector, the quality of the fit is computed. The fragment library ("index") can be generated from crystals or computer-generated files, or the user can certainly also index corporate structures.

Combine fragments

Fragment linking is a powerful feature supported by SeeSAR. It enables you to identify the optimal motif or molecular structure that can connect two or more fragments while preserving their respective binding sites. By doing so, fragment linking allows scientists to design new compounds that combine the desirable features of multiple fragments, enhancing their binding affinity and potential therapeutic effects.



In addition to fragment linking, SeeSAR offers the capability of fragment merging. By merging fragments that exhibit specific molecular interactions or functional groups, you can create new chemical entities that possess desired pharmacological properties.

To ensure efficiency and quick results, ReCore employs fast and local similarity detection algorithms (SDDs). These algorithms optimize the speed of compound delivery by rapidly comparing the chemical structures and properties of fragments and scaffolds. The integration of fast, local SDDs significantly accelerates the generation and evaluation of potential compounds, enabling you to streamline their workflow and make informed decisions in a timely manner.

Even with relatively small indices, the software can explore millions of possible molecular combinations. This expansive search capability provides researchers with a diverse pool of potential compounds to consider during the drug discovery process, greatly increasing the chances of finding promising leads.

Literature

Maass, P.; Schulz-Gasch, T.; Stahl, M.; Rarey, M. Recore: A Fast and Versatile Method for Scaffold Hopping Based on Small Molecule Crystal Structure Conformations. *J. Chem. Inf. Model.* **2007**, *47* (2), 390–399. https://doi.org/10.1021/ci060094h.

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