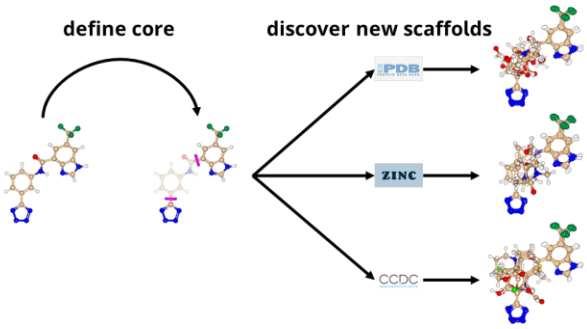
ReCore

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.
ReCore emerged from a collaboration with Roche Basle and Hamburg University and has been much augmented and extended by BioSolveIT thereafter.

You are free to use any custom compound or fragment libraries (commercial, in-house) and can apply pharmacophore constrains interactively. The diversity of solutions will maximize your possibilities and creativity.



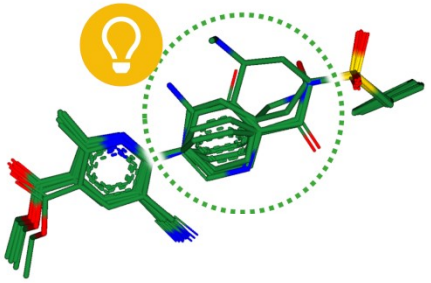
Advantages

- 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.

Fragment merging/linking is supported in SeeSAR. Even small indices capture millions of possibilities by design. Fast, local SDDs will boost the speed of delivery.

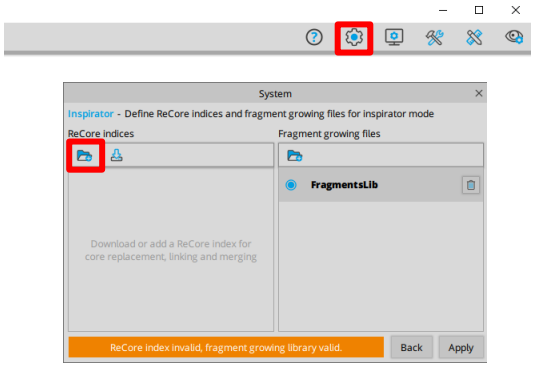


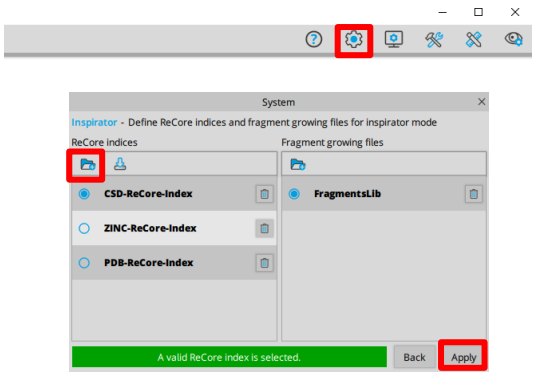
Testimonials

- *"In my opinion, software of this sort belongs on the desktop of any chemist designing bioactive molecules."* - John van Drie
- *"ReCore works well! It has a user-friendly interface, and the constraints are easy to set up."* - GSK, China
- *"The diversity of solutions from ReCore is much better than similar types of software."* - Roberto Forlani, NiKem Research Srl, Italy.
- *"ReCore proposed an elegant ring closure in a linear scaffold, not only retaining key pharmacophore features, but activity as well."* - Sander Nabuurs, LeadPharma, The Netherlands.

Getting started

After downloading the 3D molecule libraries, open the **System** dialog in SeeSAR and go to **Inspirator** settings. Click on **[Select ReCore index file]** and navigate to the unpacked *.rsx file. Select the file and press **[Open]**. The index will be available after applying.





Literature

Recore (Computer Software Review)
J. H. VanDrie
2009 131 (4), 1617-1617
http://doi.org/10.1021/ja900089h

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