

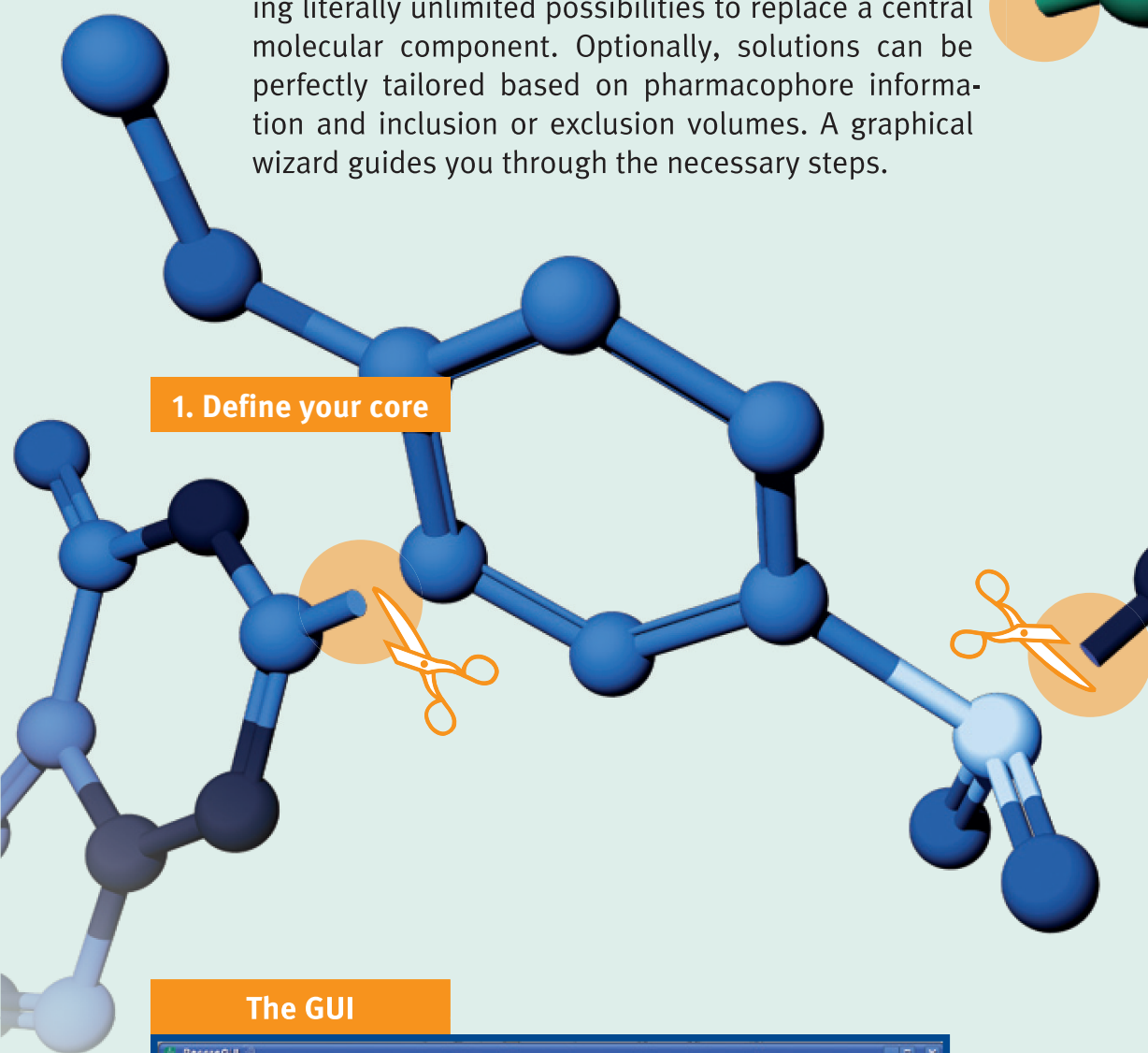


ReCore lets you replace a molecular component while leaving the anchor fragments in place. It allows you to evade patents or to link fragment binders within a few seconds.

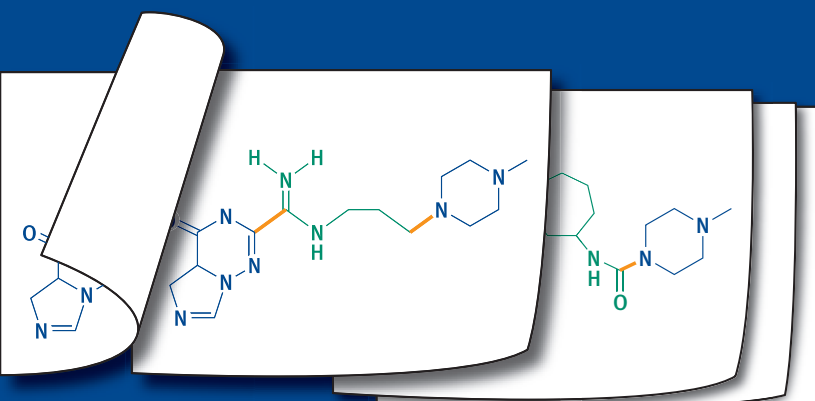
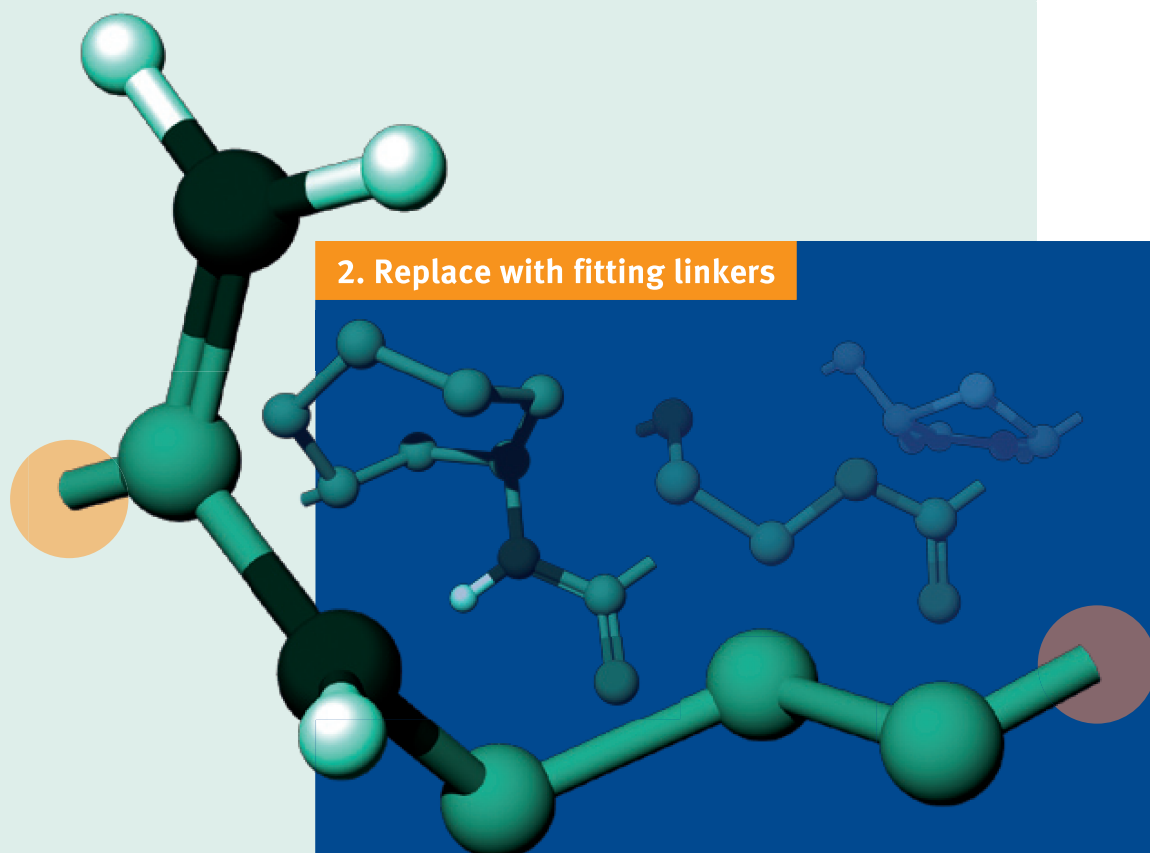
About ReCore

ReCore is a tool for 3D scaffold replacement or fragment linking: For a user-defined molecular core, a number of best geometric fits are found by searching a 3D fragment library. Jumping chemical classes, you can evade patents, or avoid ADME/T issues. ReCore is the perfect solution to link known fragment binders, offering literally unlimited possibilities to replace a central molecular component. Optionally, solutions can be perfectly tailored based on pharmacophore information and inclusion or exclusion volumes. A graphical wizard guides you through the necessary steps.

1. Define your core

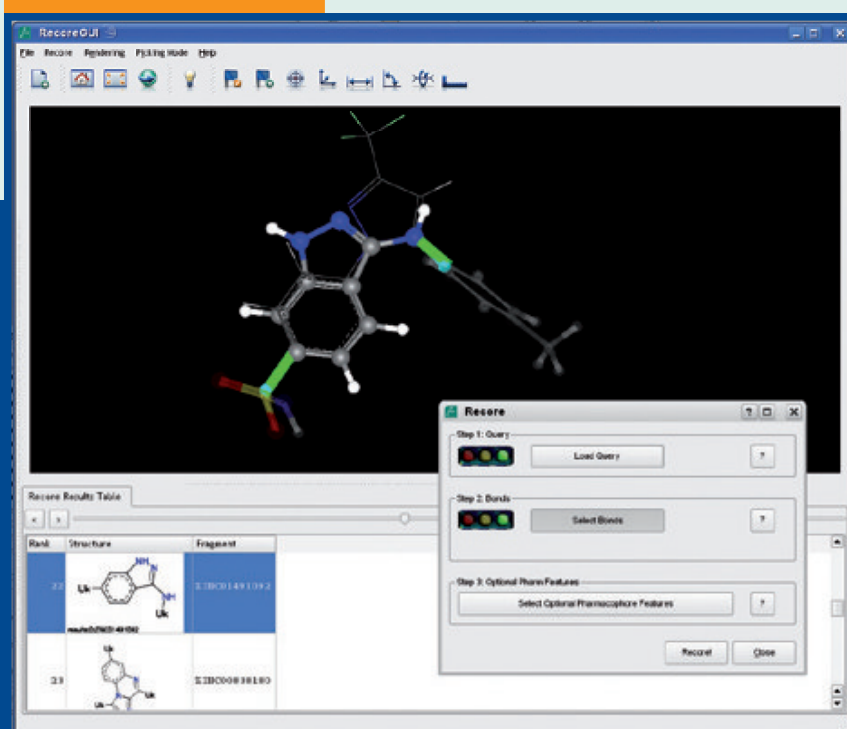


2. Replace with fitting linkers



3. Browse hits

The GUI

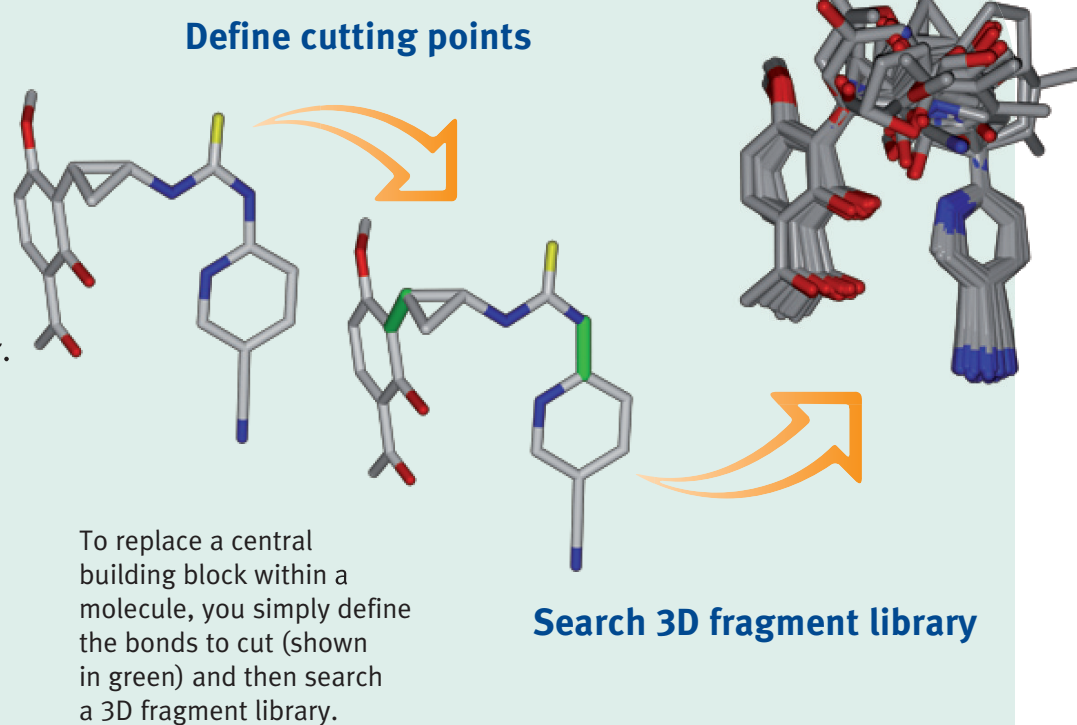


A graphical user interface lets you interactively define the core, pharmacophores and exclusion volumes. Click [ReCore!] and ReCore will find the best fitting replacements for the original core, leaving the “anchor fragments” (or “R-groups” or “binding fragments”, or ...) in place. Just seconds later, you can browse your results in 2D and stereo 3D!



Advantages

- ReCore is lightning fast: Click, click, and browse your results just seconds later.
- ReCore is interactive: Click bonds to define the core, hit the “ReCore!” button. That’s it.
- ReCore’s algorithm is parameter free. No need for adjustments.
- ReCore discovers precisely fitting core replacements that leave anchor fragments or known binding fragments in place.
- ReCore delivers virtually endless possibilities of replacement patterns; solutions are generated in the sequence of their compliance with your query.
- ReCore allows inclusion of your corporate IP by adding your proprietary compound collection to the fragment library.
- ReCore is the perfect idea generator
 - to evade a patent or IP issue
 - to overcome any issues with your lead compound
 - to join known fragment-binders
- ReCore development has been industry driven and is pre-approved: It was designed from scratch in close collaboration with Hoffmann-LaRoche AG.
- The GUI is fun and easy to use, providing both computer novices and experts access to a powerful search engine.



Complementary to ReCore

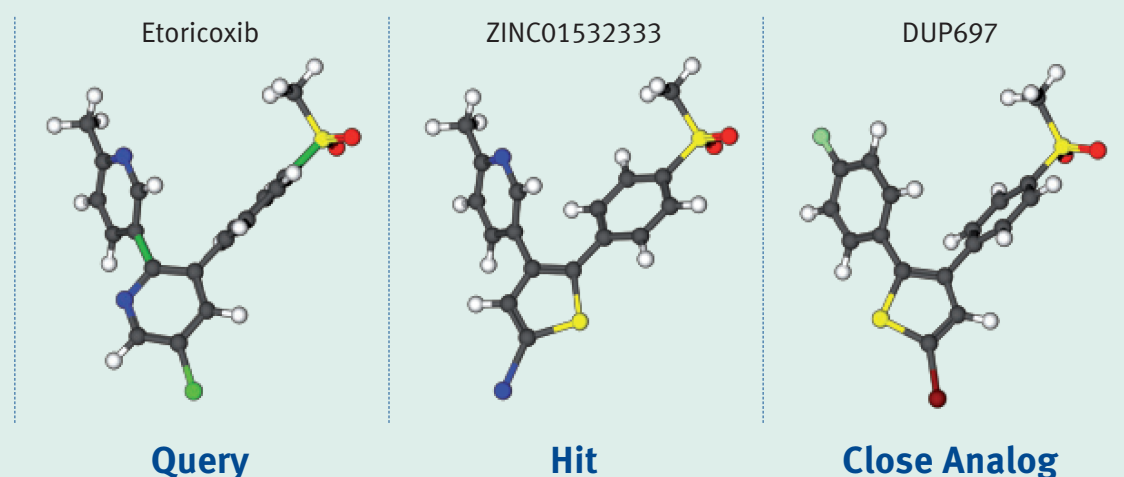
ReCore is a part of BioSolveIT’s De Novo Suite:

FlexNovo: High speed de novo ligand docking; dock ReCore solutions into your target to consolidate your ideas; or use ReCore’s shredding mechanism to generate a fragment space for FlexNovo.

FTreesFS: With a ReCore hit as a query, fuzzily search in huge, synthetically accessible fragment spaces to generate even more ideas.

Exports to any other tool: Right-click on any solutions of interest and export them to your favorite tool in mol2-format for further processing.

Application Example



This showcase illustrates how ReCore works: The goal was to find a new scaffold for a COX2 inhibitor, Etoricoxib. The bonds shown in green (left) define the core to be replaced. A promising hit on rank 7 (ZINC01532333, middle) turns out to be a close analog to DUP697 (right) – another known COX2 inhibitor.

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Reference:

[1] Maass, P. et al., *J. Chem. Inf. Model.* 47, 390-399 (2007)

Technical Requirements

ReCore is available for Linux and Windows platforms. Minimum requirement is a 1GHz CPU machine with 500MB RAM and a few GB of disk space (for the accompanying database). For more details, please visit www.biosolveit.com/ReCore

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