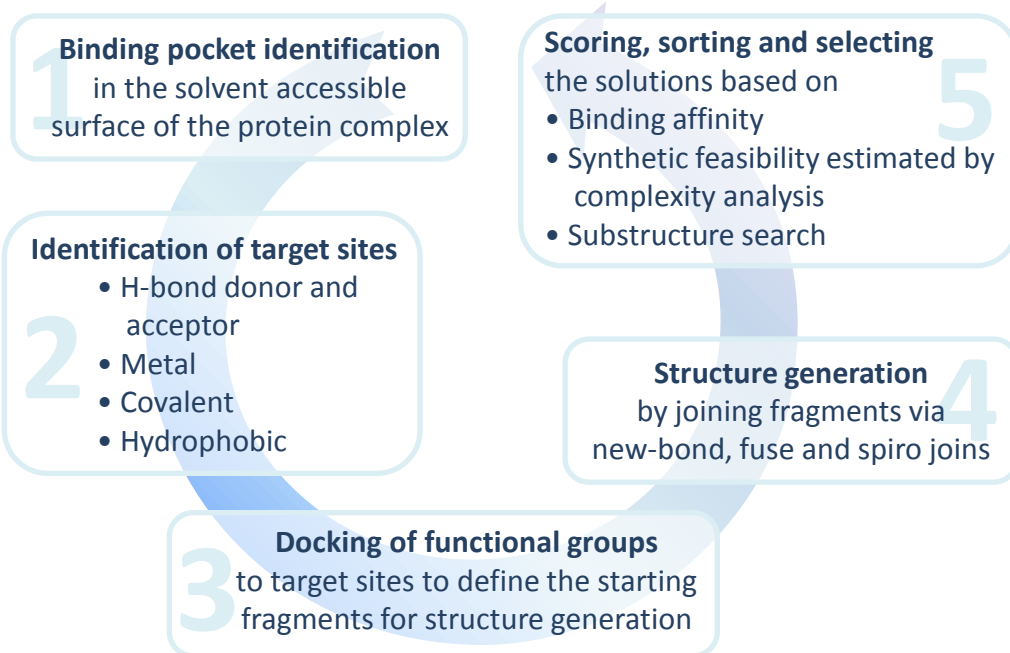


De novo Ligand Design

SPROUT Classic

Sophisticated *de novo* design tool

SPROUT Classic is a sophisticated tool for the design of drug-like, biologically active molecules. New hit molecules can be designed within the active site of your target either from scratch or starting from imported fragments. Providing several facilities for different design scenarios (including ReCore for replacing and redesigning the central unit of your molecule), SPROUT Classic is an excellent synergy with fragment-based hit discovery.

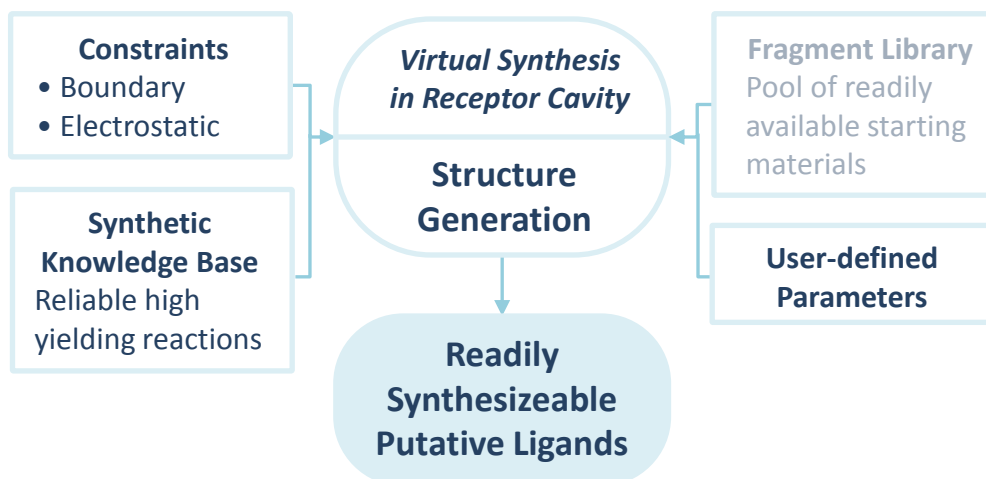


Workflow in SPROUT Classic

SynSPROUT

Design synthetically accessible ligands

SynSPROUT is aimed at generating synthetically accessible ligands by de novo design. This is achieved by applying synthetic constraints during structure generation. Skeletons are generated from fragments by using joins which correspond to chemical reactions specified in a user-defined knowledge base. SynSPROUT uses a library of readily available starting materials (monomers) for initial docking and structure generation.



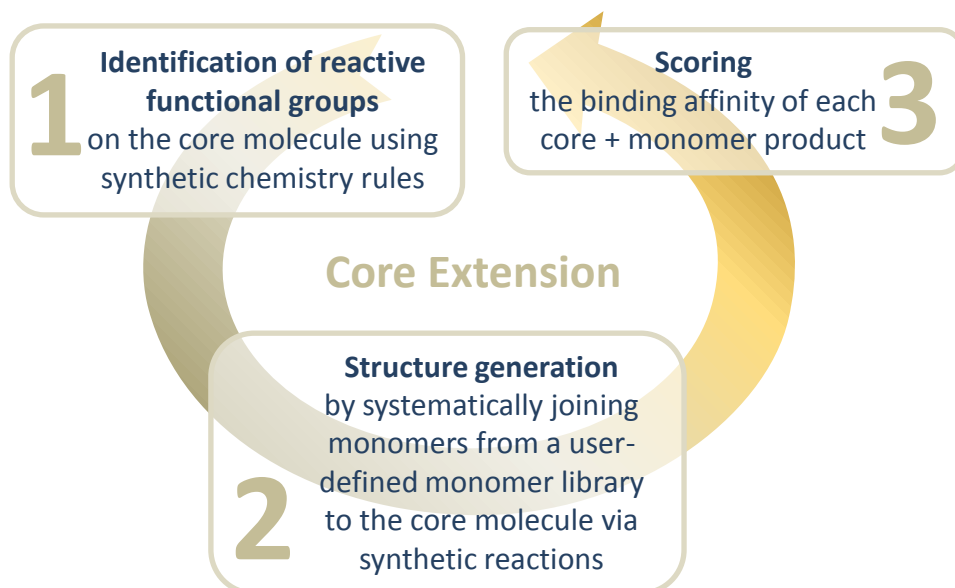
SynSPROUT's approach to generate ligands

Hit Optimization

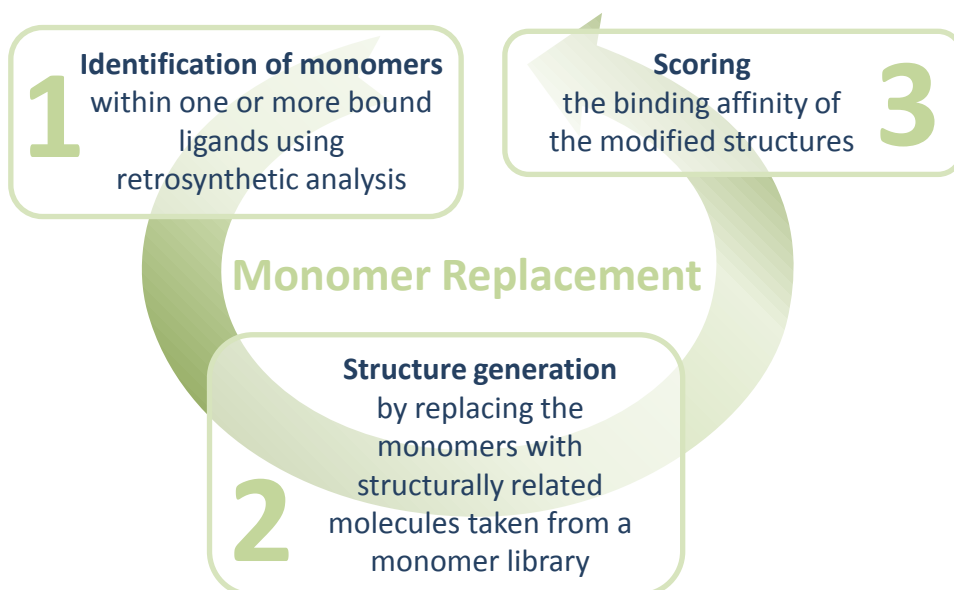
SPROUT-HitOpt

Optimize hit compounds within the target's active site

SPROUT-HitOpt is specifically designed to aid in the hit optimization process of drug discovery. There are two ways to perform hit optimization in SPROUT-HitOpt: *Core Extension* and *Monomer Replacement*.



Workflow of Core Extension in SPROUT-HitOpt



Workflow of Monomer Replacement in SPROUT-HitOpt

Supported platforms (all SPROUT variants):



About Keymodule

Keymodule Ltd. is a cheminformatics software company which specializes in the development of toolkits and applications for chemical and pharmaceutical research.

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