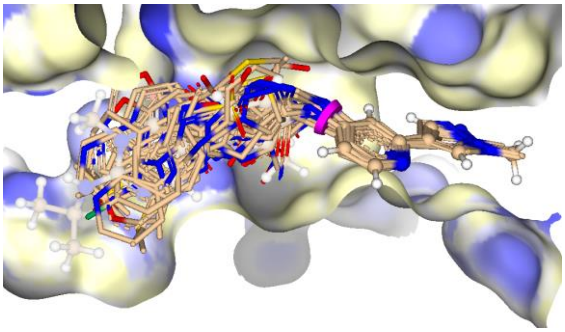
FastGrow – Pocket Exploration

BioSolveIT
expect actives!

Ultra-fast ligand growing into receptors for fragment-based compound evolution and functional group replacement.

How does FastGrow work?

FastGrow offers users an incredibly rapid search capability for ligand decorations or extensions, allowing you to explore and satisfy binding cavities within a target structure. This tool utilizes a cutting-edge and exceptionally efficient algorithm that incorporates shape-based directional descriptors. As a result, it can swiftly screen hundreds of thousands of fragments on standard hardware within a matter of seconds, generating optimized suggestions for compound design.



Developed through a collaborative effort between Hamburg University, Servier Paris, and BioSolveIT, FastGrow has undergone thorough validation in real-world scenarios involving fragment growing and replacements. This extensive validation process ensures the reliability and effectiveness of the tool. Moreover, FastGrow's early applications in the pharmaceutical industry have already yielded promising active molecules, highlighting its potential in facilitating drug discovery and design.

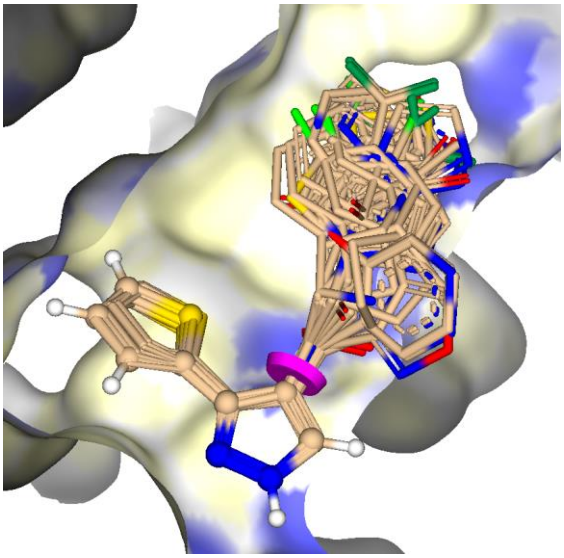
Advantages

- Interactive, explorative growing
- Possibility to apply pharmacophore constraints
- Screening of over 100,000 fragments within seconds
- Database creator to design own libraries with in-house building blocks and knowledge

Complementary decoration of ligands

Fragment growing usually requires a manual setup of a library based on the initial molecule decorated with different groups and moieties. After placement of the designed entries these are subsequently investigated for their interactions with the target (e.g., using template-based docking and scoring) using time-intensive rotational exploration around the newly formed bond.

What usually would require several hours to weeks can be performed with FastGrow within minutes in one step. This allows users to explore different com-pound evolution strategies subsequently — in a single session, on-the-fly. Fine-tuning of results can be realized through the application of optional pharmacophore constrains to include key interactions with the target. The generated results are perfectly suited as starting points for ideation and can reveal undetected possibilities for interactions. Fast-Grow is seamlessly integrated into SeeSAR's Inspirator, with affinities, logP and more at your fingertip.



Two libraries are available for users; A set of 12,000 fragments is featured by default in SeeSAR, and a more diverse set of 120,000 fragments is additionally available as download. Individual libraries can be designed with the FastGrow database generator to include individual building blocks and preferred synthesis protocols.

Application scenarios of FastGrow involve fragment-based growing approaches, group replacement to improve affinity, scaffold hopping towards particular binding motives of interest (e.g., a hinge binding motif), screening of pocket filling groups to increase selectivity, compound library generation, and many more.

Literature

Penner, P.; Martiny, V.; Gohier, A.; Gastreich, M.; Ducrot, P.; Brown, D.; Rarey, M. Shape-Based Descriptors for Efficient Structure-Based Fragment Growing. J. Chem. Inf. Model. **2020**, 60 (12), 6269–6281. https://doi.org/10.1021/acs.jcim.0c00920.

A fragment library for FastGrow containing over 120,000 entries can be downloaded for free on our website.