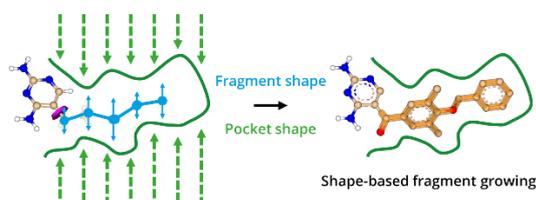




Ultra-fast ligand growing into receptors for fragment-based compound evolution and functional group replacement.

How does FastGrow work?

FastGrow enables users to breathtakingly fast search for ligand decorations or extensions that explore or fill binding cavities of a target structure. The tool uses a novel and highly efficient algorithm with shape-based directional descriptors to screen hundred-thousands of fragments within seconds on standard hardware to create optimized suggestions.



Having been developed at Hamburg University in a joint collaboration with Servier Paris and BioSolveIT, FastGrow was thoroughly validated on real fragment growings/replacements in various scenarios. Beyond this, early applications in pharma already led to active molecules.

Advantages

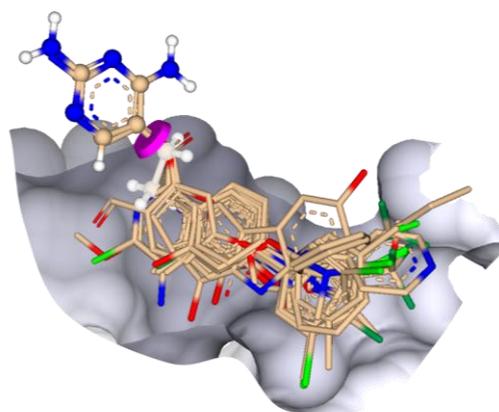
- Interactive explorative growing
- Possibility to apply pharmacophore constraints
- Screening of over 100,000 fragments within seconds
- Database creator to design own libraries with in-house building blocks and knowledge

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 compound evolution strategies subsequently — in a single session, on-the-fly. Fine-tuning of results can be realized through the application of optional pharmacophore constraints 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. FastGrow 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.

Talk to us to learn more and test it for yourself.

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](#).