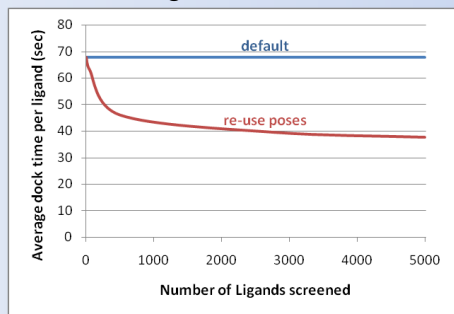


eHiTS provides an optimal balance between accuracy and speed in molecular docking. The state of the art conformational search algorithm and eHiTS' native top-performing scoring function give rise to a superb tool for pose prediction and virtual screening. Supplementary utilities offering additional capabilities from ligand-based screening to score tuning make up, together with eHiTS, one of the most advanced and versatile suites for rational drug-design.

Fragment-Based Docking

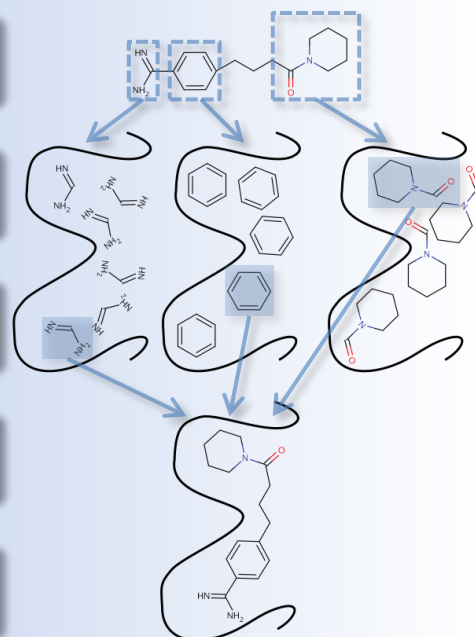
eHiTS systematically and exhaustively docks the fragments of the ligand into the binding pocket as summarized on right.



Docking time as a function of screened library size.

Known to be one of the fastest docking tools, eHiTS' fragment-based approach allows accelerating the docking process in virtual screening scenarios by re-using the poses of reoccurring fragments across the docked library.

1. The ligand is divided to rigid fragments and flexible connecting chains.
2. Each fragment is docked independently everywhere in the binding pocket.
3. Fragment poses are matched to reconstruct the ligand.
4. Flexible chains are fitted and optimized.
5. Ligand pose is fully optimized within the binding pocket.

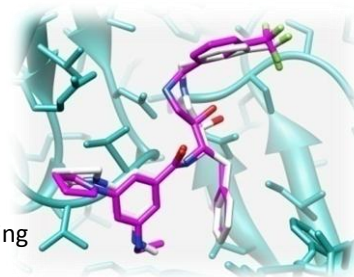
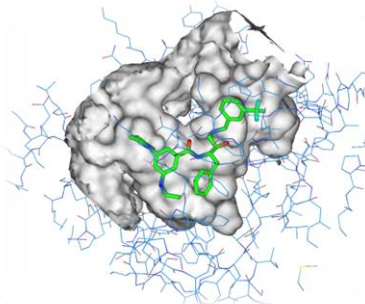


Highly Automated, Highly Flexible

With scientific accuracy and ease of use in mind, eHiTS can automate many steps in the docking process, including:

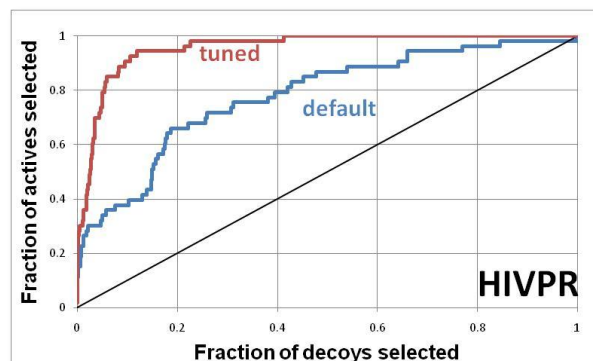
- Binding pocket detection.
- On-the-fly protonation state handling.
- Partial charges assignment.

At the same time, eHiTS allows the user to predefine all the above, and also to control many docking parameters, including pocket size and topology and accuracy level.



Tunable Scoring Function

Users are able to easily tune the eHiTS scoring function to better suit their systems of interest. A tuning utility allows three modes of tuning, designed for different docking purposes. Rank-tuning aims to improve binding mode predictions by enhancing score-RMSD correlation. Enrichment-tuning focuses on the separation of actives and inactive ligands for screening, and affinity-tuning addresses binding energy prediction. By training the scoring function with available data, the user can dramatically improve the performance of eHiTS. The tuning induced improvement in enrichment is shown on right with ROC curves for the DUD set's HIV protease target.



Evaluation copies of eHiTS and its utilities can be requested via our website or by the email below.