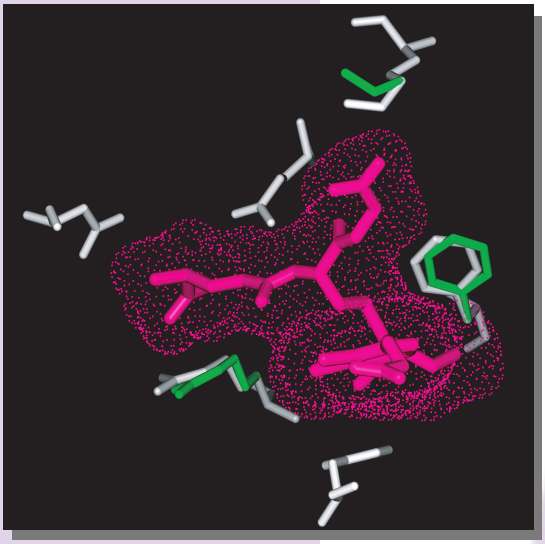
SLIDE version 3

Computational Screening and Docking Tool © MSU Board of Trustees

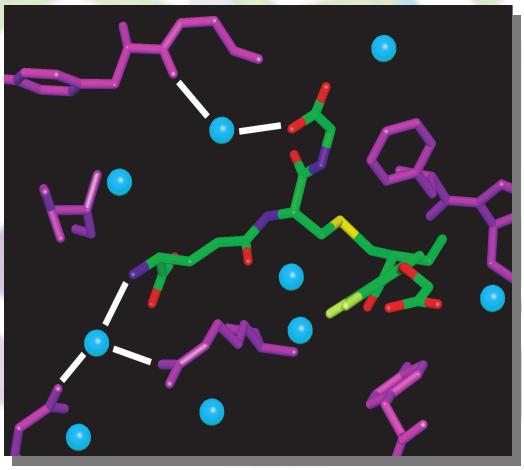


SLIDE is a computational screening and docking tool designed to find ligands with good steric and chemical complementarity to the known three-dimensional structure of a protein's binding site.

The binding site is represented by a template with hydrophobic and hydrogen bonding points. Multi-step indexing quickly tests all possible matchings of hydrophobic and hydrogen bonding interaction centers on each ligand candidate with the protein template.

Features

- Balanced protein-ligand flexibility
- Pharmacophore-based or full binding site template
- Screens, docks and scores 100,000 molecules in ~2 days on desktop hardware
- Runs on Unix workstations using C and Perl
- Includes source code



- Can screen any small-molecule database formatted as mol2 files. For ligands that are highly flexible or have 3D structures constructed from 2D, conformational sampling is recommended as input to SLIDE.

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