

Prediction details & accuracy



free structure methods

- ★Based on previous knowledge.
- ★Many different methods.
- ★Good performance.
- ★Poor information about the interaction.

Structure-based methods

Comparative Docking

- ★Outputs binding-site location.
- ★Based on structural comparisons.
- ★Applicable at wide scale.
- ★Needs the structure or a reliable 3D-model.

Virtual Docking

- ★Very precise. Ligand and receptor orientation.
- ★Needs the binding-site.
- ★Needs the structure or a reliable 3D-model.
- ★Not applicable at wide scale.

Computational time

