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# Scoring Functions for Molecular Docking Studies

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Computational approaches that dock ligands into the protein target and score their potential complimentarily to binding sites are widely used in identification and opti-mization of the structures.

The scoring functions are one of the most important parts in structure-based drug design. These fast approximate mathematical methods are used to predict the binding affinity between two molecules and to rank the docking poses.

In this paper we discuss key concepts and specific features of the scoring functions used in the molecular docking studies.

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