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Docking Studies: A Tool for Computer Aided Drug Design

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Molecular modeling has become a valuable and essential tool to medicinal chemists in the drug design process. Molecular modeling describes the generation, manipulation or representation of three-dimensional structures, all theoretical method and computational techniques used to model or mimic behaviour of molecule. It involves a range of computerized techniques based on theoretical chemistry methods and experimental data to predict molecular and biological properties. Docking studies are used to find best matching between two molecules. The major aspects of the docking studies are protein flexibility, ligand sampling, and scoring functions. The aim of this study is to explain the aspects of docking studies that has helped in the discovery process of new drugs. The emphasis will be on lead generation and optimization.