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Accounting for conformational flexibility when targeting proteins

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Molecular simulation techniques are well-established tools for understanding protein motion and complementing experimental observations. Molecular conformations from such simulations provide insight into receptor flexibility, particularly with respect to the binding of activity-modulating molecules, such as drugs. With the ultimate goal of predicting and designing these favorable interactions, incorporating information about flexibility can enhance structure-based drug design. While modeling all receptor degrees of freedom can be challenging due to conformational space sampling restrictions, advances in computing technology, hybrid and hierarchical protocol, as well as enhanced sampling algorithms are making an impact now, and will continue to do so in the future. An overview of these topics and applications to specific therapeutic targets will be presented.