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Molecular docking studies: The success should overrule the doubts?

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The capability of molecular docking which is a premier approach to structure-based virtual screening in drug discovery can never be underestimated. The success of number of FDA (Food and Drug Association) approved drugs for several dreadful diseases have enhanced the speed of drug discovery. Although the uncertainties associated with scoring & computational screening may often limit the ability to confidently identify new active compounds. In this study, we explain the performance of molecular docking studies along with correlations of experimental binding affinities of ligand-enzyme complexes

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