Virtual Screening by Docking Method

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The effective integration of the detailed structural information with computational chemistry, medicinal chemistry and informatics makes the dream of virtual screening into reality. One of the most important technologies essential for virtual screening is an effective docking method to find molecules that efficaciously interact with their target molecules.

Since the efficient docking method can be a powerful tool for virtual screening, many different approaches to solving the docking problems have been proposed. The docking problems are not solved yet and none of the currently available programs are perfect in predicting all possible cases. To increase the success rate and quality of realistic problems, a new method that overcomes the existing pitfalls should be developed.

The molecular weight of about 85% of currently applied drugs ranges between 200 and 600. Therefore docking problems in which the size of drug candidates falls into this range are most important from the practical point of view. We have developed a docking procedure specifically adapted to the problems and applied it to a test set of high-quality X-ray structures of the complexes between target and small molecules. The overall success rate of more than 90% was attained in the redocking problems.

The present study has clearly shown that if a reliable crystal structure of the protein-ligand complex is available the modern docking method can predict the docking modes of other possible drug candidates with reasonable accuracy and speed.