Interface between Docking Study and Bioinformatics

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Docking study and Bioinformatics are being used at different stages of drug discovery and discussed independently. However, since these two *in sillico* approaches are more effective when they are cooperatively utilized.

Although human genome project is over, still around a half of human sequences are lack of functional annotation. Sequence analysis of sophisticated bioinformatics tools to detect distant homologue is useful to predict molecular function of "un-annotated" sequences, and it is difficult to say exact natural ligand or catalyzed reaction. Additional prediction of natural ligand of the protein by docking study would let experimental researcher to confirm the function with less difficulty.

Recently many pieces of structural information of target protein is available. Superposition of protein's tertiary structures of the common family or superfamily and analysis of them by protein bioinformatics tools enable one to extract important information for docking study.