Virtual Drug Screening

Virtual screening is widely used in the pharmaceutical industry to identify promising compounds for synthesis. However, current methods predict binding affinities with a very low degree of precision. The aim of this project is develop a new accurate approach to calculating the affinity of a small molecule for a protein binding site. We have developed a method that accurately predicts interaction energies for complexes formed between two small molecules, based on an analysis of molecular surfaces calculated using ab initio methods. This project will develop new computational tools that allow us to extend this analysis to more complex systems like protein binding pockets and hence predict drug-receptor interaction energies.