Summary:
Proteins play a central role in various cellular processes with various interactions with other proteins, DNA, lipids or small ligands. Because the determination of these interactions is fundamental for understanding key biological processes, several experimental methods have been developed to characterize them. Experimental studies can take a long time and are expensive. Computational methods can therefore be of great help to guide future biochemical experiments. Development of docking software is a long process involving cycles of algorithm conception, programming and tests. During my thesis, I developed an object-oriented library to help and speed-up development and tests of docking methods. This library was programmed in C++ with Python bindings, and has been used to test new methods applied to protein-DNA docking and multicomponent docking. Programs made with the help of this library are presently used to study the binding of DNA to the RecA complex, responsible for homologous recombination.