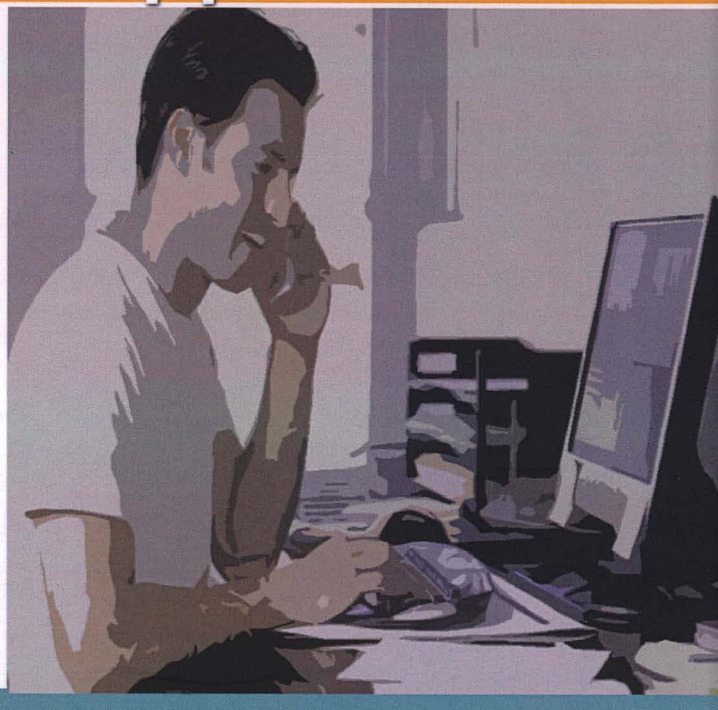
Computer Applications

Theories and Applications

Imad Fakhri Taha Al Shaikhli
Akram M. Zeki
Asadullah Shah



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Edited By:

Imad Fakhri Taha Al Shaikhli
Akram M. Zeki
Asadullah Shah

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ABSTRACT

With the rapid development in the amount of molecular biological structures, molecular docking approaches become one of the vital tools in the rational drug design. Many efforts are devoted to large-scale analysis of 3D structures protein. The primary aim of using molecular docking is to achieve scientific and commercial breakthrough in drug design and discovery. Today, there are some applications that used to predict the interaction between receptors and ligands. For example, AutoDock is one of the popular tool that used in this filed. It used to fit the ligand into the correct active site accurately. The molecular docking simulation helps the researcher to conduct experiments widely. This chapter discussed the enormous uses of docking algorithm techniques in the rational drug design field.