Superimposing Multiple Structures and Exploring Protein Binding Sites

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This thesis is focused on superimposing molecular structures, particularly protein binding sites. Three algorithms are presented: the first for superimposing a pair of three-dimensional structures, the second for finding a pairing of atoms in protein structures, and, finally, the third for superimposing multiple structures at once. Furthermore, models of particular binding sites can be computed using the algorithm for multiple alignment. Part of the thesis is the implementation of the algorithms in a software package called Site-Binder, that also provides a user friendly graphical interface. SiteBinder was successfully tested on real data and compared to other available software for superimposing molecular structures. The results provided by SiteBinder were better or at least as good as those provided by the other software packages.