Receptor flexibility in protein-ligand docking

Christoph Hartmann, Vigneshwaran Namasivayam, and Iris Antes

Technical University of Munich, Center for Integrated Protein Science Munich (CIPS^M) and Department of Life Science, Alte Akademie 16, D-85354 Freising

During the last decade computational methods have become an indispensable part of pharmaceutical, medical, and biotechnological research. One of the most important application areas is computer-aided drug design, in which molecular docking methods play a predominant role. Although molecular docking methods are meanwhile in a very mature state, from a methodological perspective two topics are still a challenging task: the efficient treatment of protein flexibility upon ligand binding and docking of ligands with many degrees of freedom. In this context, two approaches will be presented for the inclusion of side chain [1, 2] and backbone flexibility [3] into molecular docking algorithms. In addition, the application of the methods to protein-peptide docking and docking into flexible binding sites will be discussed.

[1] C. Hartmann C., I. Antes, and T. Lengauer, *Protein Science*, **2007**, 16(7), 1294-1307.

[2] C. Hartmann C., I. Antes, and T. Lengauer**,** *Proteins*, **2009**, 74(3), 712-726.

[3] I. Antes I., *Proteins*, **2010**, 78(5), 1084-1104.