Statistical analysis of amino acid side chain flexibility for 1:n Protein-Protein docking

In Protein-Protein docking, the question wether and in which conformation two proteins may interact is addressed. In 1:n Protein-Protein docking, one protein is docked against many other proteins, so that the time for calculating and ranking the hypotheses for one protein pair should be kept short. Therefore no time consuming energy minimization can be done as evaluation.

In the talk two possibilities for integrating side chain flexibility in 1:n protein-protein docking will be presented. On the one hand, flexibility can be integrated by side chain demangling, in which amino acid side chains showing steric clashes are placed according to the probabilities of their conformations given in rotamer libraries. New rotamer libraries are compiled using a markov chain based approach from language processing.

On the other hand, probabilities for conformational changes are calculated for single χ angles and for the whole side chain. The knowledge about side chain flexibility can be used for weighting the penalty for steric clashes during ranking of the hypotheses. If a steric clash occurs in flexible side chains, the penalty can be lowered, whereas the penalty has to be kept high if inflexible side chains are concerned.