99. Ranking Protein Docking Results by knowledge-based Potentials

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Abstract

Two knowledge-based potentials have been developed to discriminate native protein-protein complex structures from non-native ones. One potential is based on the *inverse* Boltzmann equation [1] while the other one represents an empirical approach. Both potentials include seperate weighting factors for functional groups and h-bonds to stress the importance of these type of interactions. Furthermore a solvent-dependent part is introduced, as well as a trapeze function for smoothing the distribution functions. The generated distribution functions for both potentials are critically examined. To compare the performance of both potentials several unbound protein-protein docking studies are carried out. Besides criteria such as geometric, hydrophobic and electrostatic complementarity an appropiate "energy"-function can be used to rank complex structures [2]. The dockings are performed with CKORDO, a modified and improved reimplementation of KORDO [3] based on the Fourier Correlation Technique [4]. The results indicate that the empirical potential in combination with the introduced weighting of functional groups shows the highest discriminatory power.

References

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