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Predicting 3D structures of transient protein-protein complexes

PETRAS KUNDROTAS, EMIL ALEXOV, Dept. of Physics & Astronomy, Clemson University, Clemson, South Carolina — Predicting transient protein-protein complexes is a major task of the post genomic era since the ultimate goal is to understand how proteins interact in the living cell. Apparently experimental methods as X-ray and NMR cannot be used at such large scale and therefore numerical methods for predicting protein-protein complexes should be applied. In this presentation we propose homology based approach to predict 3D structure of protein complexes. The underlying presumption is that if two proteins are homologous to other two proteins that form a complex then they will form a complex, 3D structure of which should be similar to the 3D structure of the existing complex. In order to test our method we have created a database of template complexes. The methodology of database creation will be presented and discussed. Due to very limited number of protein-protein complexes in the Protein Data Bank we expanded our database by including proteins containing loosely connected domains. A jack-knife test was performed and the quality of the models was evaluated against existing protein-protein complexes. It is shown that including interfacial information and residue pairing restrains in the sequence alignment improves the results.

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