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Optimum pH for protein-protein complexes. PETRAS KUNDROTAS, EMIL ALEXOV, Dept. of Physics & Astronomy, Clemson University, Clemson, South Carolina — The structure and function of proteins are influenced by external parameters such as pH of the environment. The pH at which proteins are most stable is the optimum pH of stability and the pH at which the binding affinity of protein-protein complexes is maximal is called optimum pH of the complexes. Therefore it is plausible to suggest that two proteins forming a complex in a particular environment should have their optimum pH's correlated as well as they should be correlated with the optimum pH of the complex. In order to test this hypothesis, we have calculated the pH dependencies of electrostatic folding free energy and total net charge for a set of 60 protein complexes previously used for protein-protein docking benchmark. The calculations have been performed for the entire complex and for each individual molecule separately. It was shown that there exists a clear correlation between optimum pH of the complex and optimum pH's of its components. In addition, the correlations between the net charges of the individual molecules and between the charges of the interfaces were also studied. The above findings could be used as additional criteria in evaluating models of protein-protein complexes.

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