Abstract Submitted
for the SES09 Meeting of
The American Physical Society

Multivariate Analysis of Conformational Changes Induced by Macromolecular Interactions[1] INDRANIL MITRA, Dept of Mathematical Sciences, Clemson University, EMIL ALEXOV, Dept of Physics, Clemson University
— Understanding protein-protein binding and associated conformational changes is critical for both understanding thermodynamics of protein interactions and successful drug discovery. Our study focuses on computational analysis of plausible correlations between induced conformational changes and set of biophysical characteristics of interacting monomers. It was done by comparing 3D structures of unbound and bound monomers to calculate the RMSD which is used as measure of the structural changed induced by the binding. We correlate RMSD with volumetric and interfacial charge of the monomers, the amino acid composition, the energy of binding, and type of amino acids at the interface. as predictors. The data set was analyzed with SVM in R & SPSS which is trained on a combination of a new robust evolutionary conservation signal with the monomeric properties to predict the induced RMSD. The goal of this study is to undergo parametric tests and heirchiacal cluster and discriminant multivariate analysis to find key predictors which will be used to develop algorithm to predict the magnitude of conformational changes provided by the structure of interacting monomers. Results indicate that the most promising predictor is the net charge of the monomers, however, other parameters as the type of amino acids at the interface have significant contribution as well.

[1]The work was supported by grant from NIH, NLM, award R03LM009748.

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Date submitted: 05 Nov 2009 Electronic form version 1.4