Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Optimization of the electrostatic interactions in protein-protein complexes EMIL ALEXOV, Clemson University, KELLY BROCK, Governor School for Math and Science, PETRAS KUNDROTAS, Clemson University — Electrostatic energy is one of the driving forces of protein-protein association. Understanding the role of the energy components on the energetics of protein-protein association will help us in engineering protein-protein interactions and could lead to development of scoring functions that can rank alternative models and decoys. Here we investigate whether the components of the electrostatic energy of protein-protein complexes is optimized in respect to random distribution of the charged residues. We report a clear tendency that coulombic electrostatic interactions are optimized, while the reaction field energy is inversely optimized. It was found that the maximum of the coulombic energy Z-score is shifted 3 units away from the origin and the maximum of the reaction field energy by 2 units. Such a large shift of the Z-score of both coulombic and reaction field energies indicates that wild-type protein-protein interactions are in most cases optimized in terms of coulombic interactions while compromising reaction field energy. Based on these finding a scoring function was developed as a linear combination of the Z-score of the coulombic interactions minus Z-score of the reaction field energy. The scoring function was tested against the decoy sets and it was shown that in majority of the cases we can identify the wild-type complex among hundreds of decoys.

Emil Alexov
Clemson University

Date submitted: 06 Nov 2006 Electronic form version 1.4