

Ruben Abagyan, Ph.D. Professor Department of Molecular Biology

October 26, 2004

Biocomplexity Faculty Search Committee c/o Professor Rob de Ruyter van Steveninck Department of Physics, Indiana University Swain Hall West 117
Bloomington, IN 47405-7105

Dear Dr. de Ruyter van Steveninck,

I am happy to write in support of Andrew Bordner's application for a Junior Faculty Position in Biocomplexity. I had the pleasure of working with Andrew for two years after he moved to my laboratory from UCSD.

Andrew's expertise in molecular modeling and biology, which is in addition to his contributions in physics, covers several fields including properties of chemical compounds, molecular mechanics and force fields, biomolecular electrostatics, and peptide docking. Andrew started in the laboratory from working on predictions of transfer energies for small drug-like molecules. In a paper we published recently he demonstrates convincingly that using simple physical principles and just a few adjustable parameters one can predict water-octanol or water-vacuum transition energies with an error comparable with non-physical, fragment-based methods, in-set predictors using hundreds of adjustable parameters. Andrew also joined our force field project and made a substantial contribution to it by building a procedure to automatically derive and refine hundreds of van der Waals parameters from the quantum mechanical data. As far as biological applications of modeling, Andrew participated in an immunology project in which we tried to predict the binding energies of MHC-bound peptides using flexible peptide docking. Later he got involved in the modeling and docking of some proteins of DNA damage recognition and repair system.

Most recently, Andrew has made a serious contribution to the field of bioinformatics and functional characterization of protein structures. After he left my lab, he moved to Molsoft and became the Principle Investigator on the Genomic Annotation Platform grant. As a part of that he completed a project on prediction of the effect of mutations, critical in our understanding of SNPs, and a new algorithm for predicting protein interaction interfaces using SVM training.

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Andrew has a searching, analytical and critical mind. He never takes anything for granted and intends to test every statement or assumption. He presents results well and is very active at group seminars. For example, during the Trilateral Symposium on Structural Biology in Japan, Andrew presented our research on predicting molecular interactions and was an excellent representative for our laboratory.

Andrew is very kind person; he is friendly and fair. It was always a pleasure for me to communicate with him on the research projects. His formulations of the problems were always lucid and well-presented. In summary, I respect Andrew Bordner as a scientist and as a person and recommend him with high enthusiasm and with no reservations. I can predict that he will continue to make important contributions in the fields of computational structural biology.

Sincerely,

Ruben Abagyan, Ph.D.