

Dan Zuckerman, Department of Computational Biology, Receives NSF CAREER Award

Dr. Daniel M. Zuckerman, of the Department of Computational Biology, School of Medicine, University of Pittsburgh has received a four-year NSF CAREER Award for his project entitled, “Toward Boltzmann-Weighted Protein Ensembles Using Novel Computations.”

Through this award, Dr. Zuckerman will continue development and use of novel computational approaches for equilibrium sampling for biomacromolecules, especially proteins. His goal is to generate ensembles of canonically sampled protein structures, exhibiting full fluctuations. These ensembles will be assessed systematically and will be freely available on the Ensemble Protein Database website (<http://www.epdb.pitt.edu/>), curated by Dr. Zuckerman.

The impact of generating Boltzmann-weighted protein ensembles, including large fluctuations, will be multi-faceted. Beyond providing important biochemical/functional insights, the ensembles should permit a better understanding of native-state hydrogen-exchange experiments, as well as aiding drug designers with multiple structures for docking. As Dr. Zuckerman stated in his proposal, “More than a billion dollars have been spent on structural biology—it’s time to see the full fluctuations.”

As part of the education plan for this award, Dr. Zuckerman will be writing an introductory text on statistical mechanics for students of biophysics. In this book, he will approach the topic of statistical mechanics using intuitively clear probability concepts, rather than the traditional, more abstract route of thermodynamics. He also will focus on the molecular phenomena pertinent to biophysics, rather than the typical emphasis on spin systems and phase transitions. The second part of the text will echo Dr. Zuckerman’s research, in integrating computational methods as illustrations of basic and advanced concepts.

The broad impact of this text should be substantial. Given the skyrocketing interest in molecular biophysics, there is a genuine need for a rigorous, but clear and unencumbered statistical mechanics text for the beginning graduate student and advanced undergraduate. Dr. Zuckerman’s text will fill this need.