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Daniel Zuckerman

Assistant Professor
Department of Computational Biology
School of Medicine
University of Pittsburgh

http://www.ccbb.pitt.edu/Professor_Websites/Zuckerman/index.htm

***Title: Computing Protein Fluctuations --
Coarse-Grained Models and Beyond***

Host: Ron Elber, ron@cs.cornell.edu, 255-7416

Abstract:

Structural biology faces a major challenge: although proteins are little machines which make cells work, we mostly have static snapshots of proteins available to us. In principle, computations can fill the gap by depicting the functional motions of proteins, but in reality, there is a huge under-sampling problem. Simulation approaches which combine coarse-grained models and Monte Carlo exchange simulation therefore may be useful in the future.