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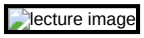

Special Guest Lectures

"Application of the UNRES force field to simulations of folding pathways of multi-chain proteins"

Ana Rojas
Physics and Astronomy Department, LSU
Johnston 331
December 12, 2005 - 10:00 am

Abstract:
Predicting the native structure and folding pathway of proteins remains one the most difficult problems in contemporary computational biology. The two fundamental ingredients to solve this problem are the protein's force field and the method used to find the global minimum of energy on the context of that force field. I will present the implementation of the molecular dynamics technique to predict the folding pathway of oligomeric proteins in the context of a reduced model, the United Residues Model (UNRES). In UNRES, each amino acid residue is represented by only two interaction sites, which makes the model simple enough to carry out large-scale simulations. I will discuss the efficiency of the method based on test simulations and the implications of "real life" simulations.

Speaker's Bio:
N/A

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