The Department of Chemistry and Biochemistry

Seminar Series

Presents a Seminar Titled:

"The Use of Thermal Unfolding Molecular Dynamics Simulations to Study Protein Folding"

Presented By

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In order to gain a better understanding of protein folding, researchers have been attempting to design two proteins that have maximal sequence identity but different folds and functions. The most successful to date is the mutation of *Streptococcus* protein G, subunits G_A, a 3α helix fold, and G_B, a 4β/α fold such that only 3 residues out of 56 are non-identical, G_A95 and G_B95, respectively. Understanding how such a small difference can cause a change in fold could provide new insights into the relationship between primary sequence and tertiary structure. The role of long range interactions in these two proteins were studied using thermal unfolding molecular dynamics simulations. Persistent contacts were identified and correlated with the non-identical residues. Our results suggest that differences in the primary sequence affect the contacts present in the unfolded state and at the beginning of folding and it is these interactions which dictate the folding pathway.

Thursday, October 18, 2012 at 12:20 in DRAGAS 1117