



THE CHINESE UNIVERSITY OF HONG KONG
Department of Physics
SEMINAR

Folding Landscape of Green Fluorescent Protein

by

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Place: G06 Y.C. Liang Hall, CUHK

ALL INTERESTED ARE WELCOME

Abstract

Green Fluorescent Protein (GFP) is extensively used to study gene expression, protein localization and as a biosensor of heavy metals. The effect of temperature and denaturants on the folding mechanism of GFP is studied using molecular dynamics simulations and molecular transfer model. In the temperature quench folding simulations, kinetic partitioning is observed and the protein folds in four distinct pathways. In the dominant pathway, GFP folds as a two state folder i.e from an unfolded state to a folded state. In the other three pathways kinetic intermediates are observed. On disabling the chromophore formation, thermodynamic data shows GFP is primarily a two state system with a very small probability of observing an intermediate. The intermediate observed has missing C-terminal Beta-strands and it is in agreement with the structure proposed from Hydrogen-Deuterium exchange NMR experiments. We further studied the effect of Guanidinium Chloride on the thermodynamic properties of GFP such as the fraction of the protein in the folded state as a function of Guanidinium Chloride concentration using the molecular transfer model, and the agreement between simulations and experiments is excellent.