



The Department of Physics at the University of Cyprus
is organizing a seminar on

Thursday, 14 April 2016, time 6:15p.m.

Room B229, Building 13, New Campus

Speaker:

Dr. Roland H. Stote
Institute de Génétique et Biologie Moléculaire et Cellulaire (IGBMC)
Director of Research
Centre National de la Recherche Scientifique (CNRS)
Strasbourg, France

**“Quantifying the Conformational Heterogeneity of a DNA
Hairpin by combining Molecular Dynamics Simulations and
Ultrafast Fluorescence Spectroscopy”**

Molecular dynamics (MD) simulations and time resolved fluorescence (TRF) spectroscopy were combined to describe the conformational landscape of the DNA primary binding sequence (PBS) of the HIV-1 genome, a short hairpin targeted by retroviral nucleocapsid proteins implicated in the viral reverse transcription. Three 2-aminopurine (2AP) labeled PBS constructs were studied. Experimentally, the complete distribution of fluorescence lifetimes was measured and the populations of conformers experimentally observed to undergo static quenching were quantified. These populations were compared to those obtained from the molecular dynamics simulations. Good agreement was found, which supports the general assumption that quenching of 2AP fluorescence results from pi-stacking interactions with neighboring nucleobases. Cluster analysis of the latter further identified predominant conformations that were consistent with the fluorescence decay times and amplitudes, providing a structure-based rationalization for the wide range of fluorescence lifetimes as well as demonstrating a general approach for the structural characterization of flexible nucleic acid motifs.

For more information please contact:
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