Πανεπιστήμιο Κύπρου

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

Friday, 7th of December 2018, time 4:00 p.m.

Room B228, Building 13, New Campus

Assistant Professor Phanourios Tamamis
Department of Chemical Engineering
Texas A&M University

"Development of molecular thermodynamics-based tools to investigate the molecular recognition properties of proteins by compounds and modified RNAs"

Computational molecular-thermodynamics-based methods are becoming increasingly powerful tools in the delineating the structure of interactions formed in biomolecular complexes. Our lab focuses on two different types of such interactions, involving (A) protein : RNA binding, and (B) protein : small compound binding.

(A) There are over 150 currently known, highly diverse chemically RNA modifications, which modulate RNA–protein interactions. The field of modified RNA-protein interactions has been in dormant state until very recently, when experimental studies started revealing the importance of RNA modifications in biological functions.Yet, little is known about the wealth of such interactions due to experimental limitations. To address this, we developed and published the first molecular-thermodynamics computational protocol for the study of interactions between proteins and RNA containing post-transcriptional modifications. We are further advancing the protocol to broaden our understanding of protein interactions with all known RNA modifications in several systems of key biological importance. The talk will focus on the development of the protocol to explore the wealth of modified RNA interactions with proteins.

(B) Computational docking methods aim to predict how compounds bind to receptors are highly important for understanding key biological axes as well as for the discovery of novel drugs. Such methods rely on the combination of a search algorithm to generate possible binding conformations and a scoring function to evaluate the conformations. Interestingly, according to a comprehensive evaluation, the docking program with the greatest sampling power is not more than 60% accurate in predicting the structure with at least 2 Angstrom accuracy. Undeniably, the improvement of existing or the development of novel programs is of utmost importance. We have been developing a novel molecular-thermodynamics -based computational docking protocol which nearly exhaustively searches a compound's binding site through mean field potential energy functions constraining the compound at different positions in the binding site and which uses all-atom MD simulations and free energy calculations to elucidate the most favorable binding mode of a ligand bound to the receptor. The protocol will be demonstrated using example cases of structures delineated by our lab in high-accuracy, in accordance with experiments.

For more information, please contact:
Department of Physics, telephone: 22892826