ΠΑΝΕΠΙΣΤΗΜΙΟ ΚΥΠΡΟΥ
ΤΜΗΜΑ ΦΥΣΙΚΗΣ

Το Τμήμα Φυσικής του Πανεπιστημίου Κύπρου
σας προσκαλεί την

Παρασκευή, 28 Αυγούστου 2020, ώρα 10:30
στην αίθουσα LRC017, στο κτήριο της Βιβλιοθήκης του Πανεπιστημίου

στην παρουσίαση της Διδακτορικής Διατριβής της Ελένης Μιχαήλ

«* Development and application of efficient and accurate free energy models and methodologies for high-throughput computational protein design*»

Computational protein design (CPD) assists in the creation of new or modified proteins and the rationalization of experimental results and is an important biotechnology tool. We develop and test novel physics-based free-energy functions and computational methodologies for high-throughput CPD. We parameterize and test four solvation free energy models, and use one of the models for the successful full redesign of three different protein families. We develop a novel general CPD methodology that explores conformational/chemical space via molecular dynamics (MD) and Monte Carlo (MC). The methodology overcomes the typical "fixed-backbone" approximation of high-throughput CPD and improves protein structural relaxation due to mutations. Application to proton binding in several proteins yields improved results compared to traditional CPD by fixed-backbone MC. We explore the key interactions and interpret experimental binding affinities of complexes between LD-motif peptides and the Focal Adhesion (FA) targeting domains of proteins FAK and PYK2. Using CPD methods, we design novel peptides with improved affinity for FAK. Such peptides could be used as inhibitors of the Paxillin:FAK complex and contribute to the development of cancer biomarkers or cancer therapy targets.

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3. E. Michael, S. Polydorides, V. Promponas, P. Skourides and G. Archontis (2020). Recognition of LD motifs by the Focal Adhesion Targeting Domains of FAK and PYK2: Insights from Molecular Dynamics Simulations. Proteins, *In Press* https://doi.org/10.1002/prot.25992.
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