ΙΔΡΥΜΑ ΤΕΧΝΟΛΟΓΙΑΣ ΚΑΙ ΕΡΕΥΝΑΣ

ΕΡΕΥΝΗΤΙΚΟ ΙΝΣΤΙΤΟΥΤΟ ΧΗΜΙΚΗΣ ΜΗΧΑΝΙΚΗΣ
ΚΑΙ ΧΗΜΙΚΩΝ ΔΙΕΡΓΑΣΙΩΝ ΥΨΗΛΗΣ ΘΕΡΜΟΚΡΑΣΙΑΣ
Οδός Σταδίου, Ρίο, Τ.Θ. 1414, 265 04 Πάτρα
Τηλ.: 2610 965 300 & 3, Fax: 2610 990 987
www.iceht.forth.gr

ΣΕΜΙΝΑΡΙΟ

ΟΜΙΛΗΤΗΣ: Dr. Θέμης Λαζαρίδης
City College of New York/CUNY, USA

ΘΕΜΑ: Modeling peptide and protein interactions with membranes

ΤΟΠΟΣ: Αίθουσα Σεμιναρίων ΙΤΕ/ΕΙΧΗΜΥΘ

ΗΜΕΡΟΜΗΝΙΑ: Τετάρτη, 2 Ιουνίου 2004

ΩΡΑ: 17:00

ΠΕΡΙΛΗΨΗ

Membrane proteins comprise about one fourth of all proteins in the cell and perform essential biological functions. Understanding of the mechanism of their action requires knowledge of their three-dimensional structure and the changes it undergoes during function. Experimental determination of the structure of membrane proteins, in addition to being exceedingly difficult, provides only static snapshots. A more comprehensive picture of membrane protein function could be obtained by computer modeling. Most computer studies so far either neglect the membrane environment entirely, or treat the membrane in full atomic detail. The former approach may miss significant effects arising from protein-lipid interactions and the heterogeneity of the membrane environment. The latter approach is computationally very expensive and does not easily provide thermodynamic information (e.g. the free energy of membrane insertion). We recently developed a third approach where the lipid membrane is treated implicitly, through a term in the energy function that describes the solvation free energy of the protein in a heterogeneous lipid-water system. This energy function (IMM1) gives reasonable energies of insertion into or adsorption onto a membrane, and allows stable 1 ns MD simulations of the glycophorin A dimer. We find that the lowest energy orientation of some peptides in bilayers varies depending on the thickness of the hydrocarbon layer.