

Παρουσίαση εργασίας την **Παρασκευή 23/11/2012**, ώρα **14:00**  
Αίθουσα Α9 του Τμήματος Πληροφορικής και Τηλ/νιών

Παρουσιάζει η μεταπτυχιακή φοιτήτρια του ΠΜΣ «Τεχνολογίες Πληροφορικής στην  
Ιατρική και τη Βιολογία» **Αγγελική Καλαμαρά**

Θέμα: "**Nearest Neighbor Searching in structural Bioinformatics**"

Abstract:

Perioxosome proliferator-activated receptors (PPARs) are a group of nuclear receptor proteins that function as transcription factors regulating expression of genes. PPARs play a major role in the regulation of cellular differentiation, development, and metabolism (carbohydrate, lipid, protein), and tumorigenesis. We have obtained sample dataset of 70 compounds as a dataset from Department of Pharmaceutical Chemistry, School of Pharmacy, University of Athens.

The dataset is described by 143 descriptors, 2 of which represent the reactivity values of compounds for the PPAR- $\alpha$  PPAR- $\gamma$  receptors and the rest 141 are physicochemical descriptors. In this project we exploit classification as well as clustering algorithms to create a model for associating the 141 descriptors with the reactivity values and test if new compounds could be classified correctly in their corresponding class of PPAR- $\alpha$  PPAR- $\gamma$  reactivity. The results indicate that there is a distinct separation between the classes with both high or low reactivity values for PPAR- $\alpha$  PPAR- $\gamma$  receptors.