The Department of Biophysics, Institute of Physics, Faculty of Science,

Pavol Jozef Šafárik University

would like to invite you to the two-day

LECTURE

of

Francesca Mocci

(University of Cagliari, Italy)

- her scientific activity is mainly directed to the study of conformational preferences of organic and bio-organic molecules, their interactions with other molecules and ions. These researches are carried out by means of modeling techniques often combined with NMR techniques. The employed computational techniques are based either on quantum or classical mechanics, and recently she became involved in the development of coarse grained models. Part of these studies involve collaborations either with national or international groups.

Introduction to NMR spectroscopy

Tuesday and Wednesday (20-21.09.2016) at 10:00

- the introduction to the basic principles behind NMR spectroscopy, factors influencing the NMR chemical shift, how to identify the molecular structure based on NMR spectra. Effects of the molecular dynamics on the NMR spectra will also be considered. Examples of application on organic and bioorganic molecules will also be given, possibly including the combination of NMR with molecular modeling.

Place: Jesenná 5, Košice, Laboratory of molecular simulations and advanced visualizations

*funding by the **Erasmus+** project*