
**ANNOUNCEMENT**

The laboratory of Molecular Analysis (LMA) performs research activity which is grounded on the ***utilization of Mathematical Physics methods and Programming methodology*** in order to promote the ***Rational Design of Pharmaceutical products.***

Doc Nikolas P. Benetis is a research associate of LMA who contributes to the above aim with the ***investigation of the structural and the dynamic properties of lipid bilayers*** and their ***interaction with bioactive and pharmaceutical molecules*** by producing and applying new simulation software on solid state spectra of P-31 NMR

A great deal of our software can be found in our www page
http://www.eie.gr/nhrf/institutes/iopc/researchgroups/lma-group/lma-group-simulationsw-en.html .
Additional developments of the software are necessary toward two following described directions:

**A.** Incorporation of the computational nucleus (FORTRAN) as well as certain intermediate stages of the simulation procedure, e.g. the ***introduction of the starting parameters*** for the fitting and the ***graphical presentation of the results***, inside a larger functional shell in the form of WINDOWS which will be written in a higher lever programming language such as C++. That shell will establish a friendly environment in the applications of our simulation software and will attract a greater number of interested scientists, such as biochemists, biologists, as well as scientists who specialize in pharmaceutical branches of chemistry for the exploitation of the physicochemical results of the simulations.

B. ***Further devolvement of the mathematical-computational model of the broadline NMR simulations*** aiming to improve the evaluation of the structural details and the complicated

dynamics of the lipid bilayers. This project can be most appropriately carried out by students of ***physical chemistry, applied mathematics or physics*** who will be given the opportunity to exploit their basic education in the branches of Quantum Mechanics, Statistical Thermodynamics and Spectroscopy, under the continuous supervision of Dr. N.P. Benetis.

**For additional information, the people interested to contribute in the above research project are kindly asked to communicate with the responsible for the project Dr. Nikolas P. Benetis niben@eie.gr or the director of the Laboratory of Molecular Analysis Dr. Thomas Mavromoustakos tmavro@eie.gr**

Our web page is:
http://www.eie.gr/nhrf/institutes/iopc/researchgroups/lma-group/lma-group-en.html

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