HELLENIC REPUBLIC
National and Kapodistrian
University of Athens

DEPARTMENT OF INFORMATICS AND TELECOMMUNICATIONS

TEI ATHENS (DEPT. OF BIOMEDICAL TECHNOLOGY ENGINEERING)

ACADEMY OF ATHENS (BIOMEDICAL RESEARCH FOUNDATION)

NCSR DEMOKRITOS (INSTITUTE OF INFORMATICS AND TELECOMMUNICATIONS)

Postgraduate Program
INFORMATION TECHNOLOGIES
IN MEDICINE AND BIOLOGY

Computer Modeling of Biomolecules

PhD Zoe Cournia

Researcher, Biomedical Research Foundation of the Academy of Athens, Center for Basic Research I, Pharmacology-Pharmacotechnology Division.

Phone: 210-6597195, email: zcournia@bioacademy.gr

Short Description: This interactive course will introduce students to the principles and applications of biomolecular modeling, and pinpoint how biomolecular problems, such as computer-aided drug design and protein folding, are being currently addressed by computational techniques. The students will be taught fundamental concepts of both basic and applied biomedical science using a highly interdisciplinary approach.

Course Objectives: The seminar focuses on several areas in which computer modeling is having a direct impact: 1) Protein structure and folding, 2) Membrane structure and membrane proteins, 3) Protein Dynamics, 4) Computer-aided drug design, 5) Enzymes as molecular machines.

Students who take this course will:

1. Reinforce and deepen their understanding of fundamental biological concepts.
2. Gain hands-on experience with modeling tools and techniques.
3. Gain a window into modern methods of scientific research and drug design principles.
4. Understand the power of molecular modeling for science.
5. Build a foundation for future study in medicine, pharmaceutical industry, etc.

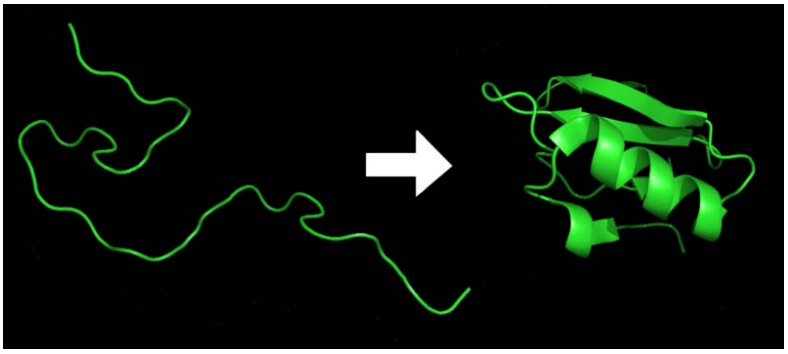
Requirements: This course is intended for medical or science Master's students who are interested in the impact of molecular modeling in natural sciences and medicine. Students should have a good understanding of biological concepts (Biology, General Chemistry).

Weekly Schedule

- **1st Week:** Introduction in the basic principles of molecular modeling and the software to be used throughout the course

- **2nd Week:** Protein structure and visualization of biomolecules

- **3rd Week:** Exploring Protein Folding



- **4th Week:** Membranes and Membrane Proteins

- **5th Week:** Structure-resolving techniques in biology (X-ray crystallography, NMR spectroscopy, neutron scattering)

- **6th -7 th Week:** Molecular Dynamics of Proteins

- **8 th Week:** Normal Mode Analysis

- **9th Week:** DNA, Structure and Function studied by Molecular Modeling Tools

- **10th – 11th Week:** Computer-aided drug design

- **12th Week:** Enzymes as Molecular Machines. Large scale assemblies and limitations of Biomolecular Modeling

Short Bio

Zoe Cournia graduated from the Chemistry Department in the University of Athens and subsequently pursued doctoral studies in the University of Heidelberg, Germany, with Dr. Jeremy Smith. She obtained the Ph.D. degree in 2006 in the field of computational biophysical chemistry. Cournia then joined Dr. Bill Jorgensen's lab in the Department of Chemistry, Yale University to perform post-doctoral studies in computer-aided drug design. At Yale, she focused on the design and discovery of novel anti-cancer agents using computational techniques. Her research, sponsored by the American Association for Cancer Research Fellowship in Angiogenesis, focused on the protein Macrophage Migration Inhibitory Factor (MIF), which has been recently identified as a pro-oncogenic and pro-inflammatory factor. Aided by state of the art computational methods, her work led to the discovery of several small-molecule inhibitors of MIF-receptor binding, which are now employed in pre-clinical studies at the Yale School of Medicine. Dr. Cournia became a Lecturer in Yale College in 2009 where she taught the course "Computer Modeling of Biomolecules". During 2007-2008 she served as a co-President of the Yale Pharmaceutical and Biotechnology Society and in 2009 she was also honored with the "Women of Innovation Award" from the Connecticut Technology Council.

Since October 2009 she is a member of BRFAA, where as a researcher (Lecturer Level) she works on targeting the mutated cancerous PI3Kα protein with small molecule inhibitors, inhibition of the c-Myc-Max interaction with small molecule inhibitors, and the design of small molecule inhibitors of the Arp2/3 complex in order to discover new anti-cancer agents. For these studies the Cournia lab employs a combination of MD simulations, virtual screening, de novo drug design, free energy perturbation calculations, pharmacological property prediction and Monte Carlo simulations.