UNIVERSITY OF PATRAS
SCHOOL OF HEALTH SCIENCES
DEPARTMENT OF PHARMACY
UNDERGRADUATE STUDIES' COURSES

COURSE DESCRIPTION: **BIOINORGANIC CHEMISTRY – MOLECULAR SIMULATIONS**
COURSE CODE: **PHA-C11-NEW**

BIOINORGANIC CHEMISTRY – MOLECULAR SIMULATIONS
COURSE DESCRIPTION

1. GENERAL

SCHOOL	HEALTH SCIENCES		
SEPARTMENT	PHARMACY		
LEVEL OF COURSE	UNDERGRADUATE		
COURSE CODE	**PHA-C11-NEW**	**SEMESTER OF STUDIES**	**5th**
COURSE TITLE	BIOINORGANIC CHEMISTRY – MOLECULAR SIMULATIONS		

INDEPENDENT TEACHING ACTIVITIES	**TEACHING HOURS PER WEEK**	**ECTS CREDITS**
Lectures	3	6
Laboratory practice	3	

COURSE TYPE	Scientific Field course
PREREQUISITE COURSES:	-
TEACHING AND ASSESSMENT LANGUAGE:	Greek
THE COURSE IS OFFERED TO ERASMUS STUDENTS	Not offered
COURSE WEBPAGE(URL)	http://www.pharmacy.upatras.gr/images/DS/PHA-C11-EN.pdf

2. LEARNING OUTCOMES

Learning Outcomes

The course aims to enhance the knowledge of the Pharmacy Students in the field of:

(a) Biological macromolecules, which are of vital significance in a number of biochemical pathways and interesting pharmaceutical targets, with emphasis in biomolecules with inorganic centers/cofactors. For this reason, the students need to have previously acquired basic knowledge in General & Inorganic Chemistry, and Biochemistry

(b) Bioactive compounds, known or potential drugs, with metal ions (i.e. cis-platinum)

(c) Structural bioinformatics, data mining, aminoacid sequence homology, database architecture and use etc.

(d) Modelling, molecular simulation and structure prediction and analysis

(e) Application of experimental tools and methods in the structure determination of biomolecules or the simulation of biomolecular complex, including protein target – drugs complexes and the design of new potentially bioactive molecules.

Additionally, through the laboratory training the students are expected to develop their skills in the use of structural bioinformatics tools towards the study of the structure-activity relationship of biologically interesting biomolecules.
Finally, the present course, aims to enhance and extend the knowledge of the undergraduate students beyond the aspects of the Inorganic Chemistry and Biochemistry providing advanced knowledge in the field of biological inorganic chemistry and specific topics in Biochemistry (structural biochemistry).

General Abilities

Data search and mining, data evaluation using modern tools and methods
Independent thinking and work
Collaborative work and joint research efforts
Work in a competitive environment
Work in an interdisciplinary scientific environment
Producing new research ideas
Promote free, creative and inductive thinking

3. **COURSE CONTENT**

Bioinorganic Chemistry [Topic 01]

(a) Coordination compounds: Basic Principles and theory
(b) Bioinorganic Chemistry: Inorganic centers in biological macromolecules
(c) Metalloproteins & Metalloenzymes of biological and pharmaceutical interest
- Zn (zinc) Metalloenzymes (proteases, anhydrases, aminopeptidases, ligases, etc.)
- Heme and Copper proteins
- Iron-sulfur proteins
- Transcription factors and DNA repair proteins

(d) Biomimetic Chemistry (artificial enzymes)
(e) Metal complexes in pharmacy

Molecular Simulations [Topic 02]

(a) Biomolecular simulations and Structural Bioinformatics – Understanding the structural basis of biological processes
(b) Data bases organization, classifications and exploitation
(c) Basics in protein architecture, DNA & RNA, structural classification of proteins
(d) Protein Architecture, structure modeling approaches, experimental methods in protein structure determination, molecular/docking simulations
(e) Protein structure quality assessment and structural analysis

Laboratory training (Dry Lab)

Exercise 1: Data bases, data searching & mining Δεδομένων (SwissProt, PubMed etc.). Searching literature data in Pubmed and structures in PDB
Exercise 2: Sequence mining and alignment – Use of Blast & ClustalW.
Exercise 3: Protein Architecture (CATH & SCOP), Prediction of 2ndary & tertiary structure (NPS@ & 3D-PSSM servers)
Exercise 4: Molecular Display and Analysis of protein structures - use of MOLMOL software
Exercise 5: NMR conformational analysis of proteins
Exercise 6: Alignment, comparison, analysis and quality assessment of protein structures - use of PROCHECK software, Ramachandran plots, etc.

Exercise 7: Modeling of protein structures (comparative modeling & Threading)
Exercise 8: Molecular Docking, screening of virtual libraries (theory and applications)

4. TEACHING AND LEARNING METHODS - ASSESSMENT

Teaching method	Interactive teaching within a classroom
Use of information and communication technologies	• Use of modern technologies, web-based applications and software in laboratory training and in the communication with students. • Teaching process is supported by Information and Communication Technologies (ICTs).
Teaching organization	***Teaching Method*** — ***Semester Workload*** Lectures — 39 Laboratory training — 39 Un-supervised study — 72 ***Total number of hours for the Course*** **(25 hours of work-load per ECTS credit) — 150**
STUDENT ASSESSMENT	Evaluation of the students is carried out through written examination at the end of the semester and oral evaluation during the laboratory courses. Written examination and oral evaluation is carried out in Greek language. Written examination includes the description for a number of theory topics and multiple-choice exercises.

5. RECOMMENDED LITERATURE

Suggested Books: (in greek)

1) Introduction in Protein Structure, Carl Branden & John Tooze (Eds), Garland Science, NY, USA, Taylor & Francis Group, 2006

2) Bioinorganic Chemistry, D.P. Kesisoglou & G Psomas, 2010, Thessaloniki

3) Laboratory Training Topics “Molecular Simulations”, G.A.Spyroulias, 2008, Patras