

## COURSE OUTLINE

### (1) GENERAL

<b>SCHOOL</b>	Sciences		
<b>ACADEMIC UNIT</b>	International Graduate Program in Biological Inorganic Chemistry		
<b>LEVEL OF STUDIES</b>	Graduate		
<b>COURSE CODE</b>	<b>3</b>	<b>SEMESTER</b>	<b>1</b>
<b>COURSE TITLE</b>	Biophysics of pharmaceutical action		
<b>INDEPENDENT TEACHING ACTIVITIES</b> <i>if credits are awarded for separate components of the course, e.g. lectures, laboratory exercises, etc. If the credits are awarded for the whole of the course, give the weekly teaching hours and the total credits</i>	<b>WEEKLY TEACHING HOURS</b>	<b>CREDITS</b>	
		5	
<i>Add rows if necessary. The organisation of teaching and the teaching methods used are described in detail at (d).</i>			
<b>COURSE TYPE</b> <i>general background, special background, specialised general knowledge, skills development</i>	Scientific field Special background Specialised general knowledge		
<b>PREREQUISITE COURSES:</b>	No		
<b>LANGUAGE OF INSTRUCTION and EXAMINATIONS:</b>	Greek / English		
<b>IS THE COURSE OFFERED TO ERASMUS STUDENTS</b>	Yes		
<b>COURSE WEBSITE (URL)</b>	<a href="http://bic.chem.uoi.gr/BIC-En/biophysics-en.html">http://bic.chem.uoi.gr/BIC-En/biophysics-en.html</a>		

### (2) LEARNING OUTCOMES

<p><b>Learning outcomes</b></p> <p><i>The course learning outcomes, specific knowledge, skills and competences of an appropriate level, which the students will acquire with the successful completion of the course are described.</i></p> <p><i>Consult Appendix A</i></p> <ul style="list-style-type: none"> <li>• <i>Description of the level of learning outcomes for each qualifications cycle, according to the Qualifications Framework of the European Higher Education Area</i></li> <li>• <i>Descriptors for Levels 6, 7 &amp; 8 of the European Qualifications Framework for Lifelong Learning and Appendix B</i></li> <li>• <i>Guidelines for writing Learning Outcomes</i></li> </ul>
<p>After successfully completing the course, descriptive marker 6 of the European Qualifications Framework, students should be able to:</p> <ul style="list-style-type: none"> <li>• know basic principles of biophysics of biomolecules and drugs</li> <li>• know the effect of functional groups and stereochemistry on the biological activity of compounds</li> <li>• know basic websites in order to find structural biology information</li> <li>• know types of software and the principles of molecular simulation</li> <li>• know basic meanings of multiparametric statistical analysis</li> <li>• be aware of the basic principles governing the Quantitative Relationships Action - Structure (QSAR)</li> </ul> <p><b>Knowledge</b></p> <p>Protein-ligand interactions (molecular binding and molecular dynamics) Thermodynamics of interactions (electron, steric, topological and hydrophobic parameters) QSAR methodology</p>

**Skills**

Molecular modeling  
Biophysicochemical properties analysis through multi-parameter methods

**Abilities**

Team work and working independently  
Learning opportunities for relevant computational packages

**General Competences**

*Taking into consideration the general competences that the degree-holder must acquire (as these appear in the Diploma Supplement and appear below), at which of the following does the course aim?*

*Search for, analysis and synthesis of data and information, with the use of the necessary technology*

*Adapting to new situations*

*Decision-making*

*Working independently*

*Team work*

*Working in an international environment*

*Working in an interdisciplinary environment*

*Production of new research ideas*

*Project planning and management*

*Respect for difference and multiculturalism*

*Respect for the natural environment*

*Showing social, professional and ethical responsibility and sensitivity to gender issues*

*Criticism and self-criticism*

*Production of free, creative and inductive thinking*

*.....*

*Others...*

*.....*

The general competences that students should have acquired are:

Search for, analysis and synthesis of data and information, with the use of the necessary technology

Working independently

Team work

Learning opportunities for relevant computational packages

Acquiring bibliographic research publicity skills

Acquire the appropriate theoretical base to allow further education at a doctoral level (theoretical and laboratory).

**(3) SYLLABUS**

1. Drug design. Introduction: Correlation of parameters (geometry, stereochemistry, bioavailability, toxicity, side effects, interactions).

2. The biophysics of the 3D structure. Structure of proteins and macromolecules. Flexibility, Wrap - Energy Paths.

3. Structural Biology. Experimental techniques (X-ray, NMR)

4. Databases. Protein Data Bank (PDB)

5. Introduction to molecular modeling. Modeling techniques and algorithms.

6. Joint compounds. Theoretical study of joint anticancer compounds and their anti-tumor mechanisms.

7. Equilibrium ratio model. Drug planning

8. Molecular dynamics of biomolecules. Protein-ligand interactions (molecular binding and molecular dynamics). Thermodynamics of interactions (electron, steric, topological and hydrophobic parameters). Force fields.

9. Meanings of multiparametric statistical analysis

10. QSAR - Drug Design. Introduction: Correlation of parameters (geometry, stereochemistry, bioavailability, toxicity, side effects, interactions).

11. Available software (demonstration and / or hands-on training)

12. Project - Presentation

**(4) TEACHING and LEARNING METHODS - EVALUATION**

<b>DELIVERY</b>	Face to face
<i>Face-to-face, Distance learning, etc.</i>	

<p><b>USE OF INFORMATION AND COMMUNICATIONS TECHNOLOGY</b> Use of ICT in teaching, laboratory education, communication with students</p>	E-mail, PowerPoint	
<p><b>TEACHING METHODS</b> The manner and methods of teaching are described in detail. Lectures, seminars, laboratory practice, fieldwork, study and analysis of bibliography, tutorials, placements, clinical practice, art workshop, interactive teaching, educational visits, project, essay writing, artistic creativity, etc.</p> <p>The student's study hours for each learning activity are given as well as the hours of non-directed study according to the principles of the ECTS</p>	<b>Activity</b>	<b>Semester workload</b>
	Lectures	65
	Essay writing	60
	Individual study, preparation	70
<b>Course total</b>	<b>195</b>	
<p><b>STUDENT PERFORMANCE EVALUATION</b> Description of the evaluation procedure</p> <p>Language of evaluation, methods of evaluation, summative or conclusive, multiple choice questionnaires, short-answer questions, open-ended questions, problem solving, written work, essay/report, oral examination, public presentation, laboratory work, clinical examination of patient, art interpretation, other</p> <p>Specifically-defined evaluation criteria are given, and if and where they are accessible to students.</p>	<p>Student evaluation is done either by presenting to a committee of teachers and a public audience or by the final written examination. The final examination includes: Multiple Choice, short-answer, open-ended, and Problem Solving Questions</p>	

## (5) ATTACHED BIBLIOGRAPHY

<ul style="list-style-type: none"> <li>• Molecular Biophysics for the Life Sciences Norma M. Allewell; Linda O. Narhi; Ivan Rayment Springer, 9781461485476</li> <li>• Computational Biochemistry and Biophysics Oren M. Becker; Alexander D. Mackerell Jr; Benoit Roux; Masakatsu Watanabe Marcel Dekker Ltd, 082470455X</li> <li>• A Primer on QSAR/QSPR Modeling: Fundamental Concepts (Springer briefs in Molecular Science) Kunal Roy; Supratik Kar; Rudra Narayan Das Springer, 9783319172804</li> <li>• Statistical Modelling of Molecular Descriptors in QSAR/QSPR Matthias Dehmer; Kurt Varmuza; Danail Bonchev; Frank Emmert-Streib Wiley-Blackwell, 9783527324347</li> </ul> <p>- Related academic journals:</p> <ul style="list-style-type: none"> <li>• Journal of Chemical Information and Modeling</li> <li>• Journal of Medicinal Chemistry</li> <li>• RSC Advances</li> <li>• Journal of Biological Physics</li> <li>• Biophysical Journal</li> <li>• Biophysical Chemistry</li> </ul>
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