

## COURSE OUTLINE “ADVANCED THEMES OF COMPUTATIONAL BIOLOGY”

### 1. GENERAL

<b>SCHOOL</b>	HEALTH SCIENCES		
<b>DEPARTMENT</b>	MOLECULAR BIOLOGY AND GENETICS		
<b>STUDY LEVEL</b>	ISCED LEVEL 6		
<b>COURSE CODE</b>	<b>MBG506</b>	<b>SEMESTER</b>	4 <sup>th</sup> and 8 <sup>th</sup>
<b>COURSE TITLE</b>	ADVANCED THEMES OF COMPUTATIONAL BIOLOGY		
<b>TEACHING ACTIVITIES</b> <i>In case credits are awarded to individual components of the course eg. Lectures, laboratory practicals, etc. If credit units are awarded for the whole course, indicate the weekly teaching hours and total credits</i>	<b>HOURS/WEEK</b>	<b>ECTS CREDITS</b>	
	2	3	
<b>COURSE TYPE</b> <i>General, Background, Scientific field course, Expertise Course, Skills Development etc</i>	SCIENTIFIC FIELD		
<b>PREREQUISITE COURSES:</b>	NO		
<b>LANGUAGE OF TEACHING AND EXAMINATIONS:</b>	GREEK		
<b>THE COURSE IS OFFERED TO ERASMUS STUDENTS</b>	NO		
<b>COURSE WEBSITE (URL)</b>	<a href="https://eclass.duth.gr/courses/ALEX01191/">https://eclass.duth.gr/courses/ALEX01191/</a>		

### 2. LEARNING OUTCOMES

<p><b>Learning outcomes</b></p> <p><i>Describe the learning outcomes of the course, the specific knowledge, skills and competencies that students will acquire after successfully completing the course. Refer to Appendix A.</i></p> <ul style="list-style-type: none"> <li>• Description of learning outcomes for the course according to the level of study - refer to the European Higher Education Area Qualifications Framework</li> <li>• Descriptive Indicators of Levels 6, 7 &amp; 8 of the European Qualifications Framework for Lifelong Learning and Annex B Curriculum Vitae Summary Guide</li> </ul>		
<ul style="list-style-type: none"> <li>• Gain a basic understanding of Structural Computational Biology</li> <li>• Understand the principles of the various methods for determining the atomic resolution structures of biomolecules.</li> <li>• Understand the intricacies and complexities of the protein folding problem.</li> </ul> <p>After completing the course, students will be able to:</p> <ul style="list-style-type: none"> <li>• Understand the basic principles of Structural Computational Biology</li> <li>• Understand the fundamental ideas behind X-ray crystallography and the electron microscopical three-dimensional reconstruction.</li> <li>• Understand the basic ideas and problems associated with the protein folding problem</li> </ul>		
<p><b>General Skills</b></p> <p><i>Which of the general competencies that the student will have acquired on the completion of the studies (see also the Diploma Supplement and below) are relevant to this course?</i></p> <table style="width: 100%; border: none;"> <tr> <td style="vertical-align: top; width: 50%;"> <ul style="list-style-type: none"> <li>Research, analysis and synthesize of data and information, using the necessary technologies</li> <li>Adaptation to new situations</li> <li>Decision making</li> <li>Autonomous work</li> <li>Team work</li> <li>Work in an international environment</li> </ul> </td> <td style="vertical-align: top; width: 50%;"> <ul style="list-style-type: none"> <li>Work in an interdisciplinary environment</li> <li>Production of new research ideas</li> <li>Project design and management</li> <li>Respect for diversity and multiculturalism</li> <li>Respect for the natural environment</li> <li>Development of social, professional and moral responsibility and gender sensitivity</li> <li>Promotion of free, creative and inductive thinking</li> </ul> </td> </tr> </table>	<ul style="list-style-type: none"> <li>Research, analysis and synthesize of data and information, using the necessary technologies</li> <li>Adaptation to new situations</li> <li>Decision making</li> <li>Autonomous work</li> <li>Team work</li> <li>Work in an international environment</li> </ul>	<ul style="list-style-type: none"> <li>Work in an interdisciplinary environment</li> <li>Production of new research ideas</li> <li>Project design and management</li> <li>Respect for diversity and multiculturalism</li> <li>Respect for the natural environment</li> <li>Development of social, professional and moral responsibility and gender sensitivity</li> <li>Promotion of free, creative and inductive thinking</li> </ul>
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<ul style="list-style-type: none"> <li>• Promotion of free, creative and inductive thinking</li> <li>• Research, analysis and synthesize of data and information, using the necessary technologies</li> <li>• Decision making</li> <li>• Autonomous work</li> <li>• Production of new research ideas</li> <li>• Project design and management</li> </ul>		

### 3. COURSE CONTENT

Computational Structural Biology: from crystallography and Fourier transforms, to energy minimization and molecular dynamics simulations.

A non-mathematical introduction to crystallography: waves, crystals, scattering, diffraction, the phase problem, the crystallographic experiment, production of X-rays, interaction between matter and X-rays, X-ray detectors, phase determination: an example, electron density maps, resolution.

Introduction to computational crystallography: scattering of electromagnetic radiation from an arbitrary (non-periodic) object, introduction to Fourier transformations, scattering of electromagnetic radiation from periodic objects: the structure factor, the convolution theorem and applications, the Patterson function, methods for solving the phase problem (MIR, MAD, molecular replacement, direct methods), optimization. The problem of protein folding.

#### 4. TEACHING and LEARNING METHODS - EVALUATION

<b>TYPE OF TRAINING</b> <i>Face-to-face, Distance learning, etc..</i>	Face to face	
<b>USE OF INFORMATION AND COMMUNICATIONS TECHNOLOGY</b> <i>Use of ICT in teaching, laboratory education, and in communication with the students</i>	Use of ICT in Teaching Use of ICT in Laboratory Education Use of ICT in Communication with students	
<b>MODES OF DELIVERY</b> <i>Describe the teaching methods in detail. Lectures, seminars, laboratory practice, fieldwork, study and analysis of bibliography, tutorials, practicum, placements, clinical practice, art workshop, interactive teaching, educational visits, project, essay writing, artistic creativity, etc. 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</i>	<b>Activity</b>	<b>Workload/semester</b>
	Lectures	30
	Bibliographic research & analysis	30
	Laboratory practice	30
	<b>Course Total</b>	<b>90</b>
<b>STUDENT PERFORMANCE EVALUATION</b> <i>Describe of the methods of evaluation language, methods of evaluation, types of exams, 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</i>  <i>Are evaluation criteria known to the students?</i>	<b>Student evaluation languages</b> Greek  <b>Method (Formative or Concluding)</b> Formative  <b>Student evaluation methods</b> Written exam with multiple choice test (100%)	

#### 5. SUGGESTED READING

A non-mathematical introduction to X-ray Crystallography, N. M. Glykos  
 Principles of Protein X-Ray Crystallography, Drenth Jan.

Επιλογές Συγγραμμάτων:

Βιβλίο [68406297]: ΥΠΟΛΟΓΙΣΤΙΚΗ ΧΗΜΕΙΑ: ΘΕΩΡΙΕΣ ΚΑΙ ΕΦΑΡΜΟΓΕΣ, ΑΝΤΩΝΗΣ ΚΟΛΟΚΟΥΡΗΣ

Πρόσθετο Διδακτικό Υλικό:

Βιβλίο [176048]: Introduction to Computational Biology [electronic resource], Bernhard Haubold / Thomas Wiehe

Βιβλίο [176385]: Principles of Protein X-Ray Crystallography [electronic resource], Jan Drenth

Βιβλίο [320293]: Μία μη μαθηματική εισαγωγή στην κρυσταλλογραφία πρωτεϊνών, ΝΙΚΟΛΑΟΣ ΓΛΥΚΟΣ