UNIVERSITY OF PATRAS
SCHOOL OF HEALTH SCIENCES
DEPARTMENT OF PHARMACY
POSTGRADUATE PROGRAM: **DRUG DESIGN AND DEVELOPMENT**

COURSE TITLE: DESIGN AND DISCOVERY OF BIOACTIVE COMPOUNDS

CODE: DPHA_1

DESIGN AND DISCOVERY OF BIOACTIVE COMPOUNDS
COURSE OUTLINE

1. GENERAL

SCHOOL	HEALTH SCIENCES		
ACADEMIC UNIT	DEPARTMENT OF PHARMACY		
PARTICIPATING INSTITUTIONS	-		
TITLE of POSTGRADUATE PROGRAM	DRUG DESIGN AND DEVELOPMENT		
LEVEL	POSTGRADUATE		
COURSE CODE	**DPHA-1**	**SEMESTER**	**A'**
COURSE TITLE	**DESIGN AND DISCOVERY OF BIOACTIVE COMPOUNDS**		

INDEPENDENT TEACHING ACTIVITIES	**WEEKLY TEACHING HOURS**	**CREDITS**
Courses	5	8

COURSE TYPE	General Background, Specialised general knowledge (Medicinal Chemistry, Pharmacognosy, Computational Chemistry), Skills Development.
PREREQUISITE COURSES	None
LANGUAGE of INSTRUCTION and EXAMINATIONS	Greek
COURSE OFFERED to ERASMUS STUDENTS	Yes, with guided self-study in English
COUSRSE (URL)	http://www.pharmacy.upatras.gr/images/DS/DPHA_1_EN.pdf

2. LEARNING OUTCOMES

Learning Outcomes
Upon successful course completion, students will acquire knowledge, skills and abilities related to level 7 of the European Qualifications Framework for Lifelong Learning. In particular, students will: 1. understand the strategy and logic of relating the activity of a drug to its chemical structure, as well as the role of "molecular targets". 2. have been introduced to the techniques and methodology underlying the discovery of bioactive natural products from natural sources. 3. have understood the basic approaches to the discovery of Lead compounds, as well as the methodologies for designing a specific bioactive compound. 4. have familiarized themselves with the techniques of optimizing physicochemical properties of a molecule with the aim of making it a better "medicine".

5. They will be able to understand the principles of QSAR and modern computational methods and how they can work synergistically and/or independently in the context of new drug design and discovery.

General Competences

- Search for, analysis and synthesis of data and information, with the use of the necessary technology
- Working independently
- Team Work
- Decision-making
- Working in an international environment
- Working in an interdisciplinary environment
- Production of free, creative and inductive thinking
- Adapting to new situations

3. SYLLABUS

LECTURES

1. Molecular targets in drug discovery.
2. Principles in Structural Bioinformatics, Computational and Structural Biology - Methods & Tools, Database mining, Data analysis and classification.
3. Prediction, experimental study/determination and analysis of 3D structures of pharmaceutical targets and bioactive compounds - Conformational analysis of biomolecular structures.
4. Strategies in the search for new lead compounds (serendipity, analogue design, compound screening, rational drug design).
5. Discovery of bioactive natural products: raw materials and strategies of study and isolation (random control, ethnopharmacological approaches, chemical ecology, bioactivity-driven fractionation, biotechnological approaches).
6. Structure-based and ligand-based design of bioactive molecules.
7. Optimization of drug-target interactions (structural modifications, structure-activity relationships).
8. Optimization of drug access to the target (optimization of hydrophilic/hydrophobic properties, drug metabolism, prodrugs).
9. Enzyme inhibitors in drug discovery:
   a. Enzymes as attractive drug targets
   b. Mechanisms of enzymatic reactions
   c. Reversible inhibitors (Slowly and tightly bound inhibitors)
   d. Irreversible inhibitors
   e. Transition-state analogues as enzyme inhibitors
   f. Kinetics of enzymatic reactions

PUBLIC PRESENTATIONS

Selected case studies in modern drug discovery.

Individual Assignment & Presentation

4. TEACHING and LEARNING METHODS - EVALUATION

DELIVERY	Face to face
USE of INFORMATION and COMMUNICATIONS TECHNOLOGY	• Use of ICT - e-class platform • Communication with students
TEACHING METHODS	***Activity*** — ***Semester Workload*** Lectures — 65 Presentations of Case Studies — 13 Case Studies' Preparation & non-directed Study — 122 ***Course Total*** **(25 hours of work-load per ECTS credit)** — **200**
STUDENT PERFORMANCE EVALUATION	Language of Evaluation: Greek / English Written exams • Multiple choice questionnaires, Short answer questions, Open ended questions (60% of final grade) Public Presentation • Presentation of a Case study (Greek or English) (40% of final grade)

5. RECOMMENDED BIBLIOGRAPHY

Suggested Bibliography:

1. Graham L. Patrick, "An Introduction to Medicinal Chemistry", 5th Edition, Oxford University Press, 2013.
2. Thomas L. Lemke, David A. Williams, "Foye's Principles of Medicinal Chemistry", 7th Edition, Lippincott Williams and Wilkins, 2012.
3. Richard B. Silverman, "The Organic Chemistry of Drug Design and Drug Action", 3rd Edition Academic Press, 2014.
4. Gareth Thomas, "Medicinal Chemistry: An Introduction", 2nd Edition, Wiley, 2008.

Related Academic Journals:

Journal of Medicinal Chemistry
ACS Medicinal Chemistry Letters
European Journal of Medicinal Chemistry
ChemBioChem, ChemMedChem
Bioorganic and Medicinal Chemistry
Bioorganic and Medicinal Chemistry Letters
Angewandte Chemie International Edition
Medicinal Research Reviews