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

COURSE TITLE: BIOMOLECULAR NMR & PROTEIN ARCHITECTURE

CODE: DPHA_A03

BIOMOLECULAR NMR & PROTEIN ARCHITECTURE
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_A03**	**SEMESTER**	**B'**
COURSE TITLE	**BIOMOLECULAR NMR & PROTEIN ARCHITECTURE**		

INDEPENDENT TEACHING ACTIVITIES	**WEEKLY TEACHING HOURS**	**CREDITS**
Lectures and Dry-Lab Exercises	3	5

COURSE TYPE	• Specialized General Knowledge
PREREQUISITE COURSES	Biochemistry
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_A03_EN.pdf

2. LEARNING OUTCOMES

Learning Outcomes
What it is expected as learning outcomes is that the students will acquire new knowledge about the other than analysis, uses of NMR spectroscopy and on the use and analysis of the appropriate methods in the study of biomolecules according to the Level 7 of the European Qualifications Framework for Lifelong Learning. Thus, at the end of the course the students will acquire knowledge on the use of the: (a) NMR spectroscopy in the study of biomolecules and the strategy for the study of strongly and weakly interaction molecules, thus the basic principles for the NMR-driven in drug design (b) methods and protocols in the preparation of the suitable (in labeled, 15N, 13C and/or 2H forms), protein samples for NMR studies (c) multidimensional homo- or hetero- nuclear NMR experiments analysis (resonance assignment) in the study of the conformational, dynamics and interaction of biomolecules and the way to extract information relative with the structure and the function of these biomolecules

(d) Biomolecular NMR in the discovery and optimization of lead compounds and new applications in structural biology, i.e. in-cell NMR, and
(e) NMR as a powerful analysis tool in clinical research and diagnosis

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 new research ideas
- Production of free, creative, and inductive thinking

3. SYLLABUS

- Theory and Principles in NMR Spectroscopy – Strategies in 1H 1D resonance assignment – Examples & Practical Exercise.
- Basics of Structural Bioinformatics, Computational & Structural Biology – Methods, Tools, Data bases & Data mining.
- Preparation of biomolecular samples (proteins, RNA, DNA, etc) suitable for NMR studies – Methods in protein/RNA uniform labeling, selective/specific and reverse selective labeling of aminoacids in proteins.
- 2D homo- & hetero- nuclear NMR Spectroscopy – Methodology and Experimental set-up – Applications in peptides/polypeptides.
- 3D homo- hetero- nuclear NMR Spectroscopy – Methodology and Experimental set-up – Applications in proteins.
- Approaches in NMR studies of biomolecules and biomolecular high molecular weight complexes.
- 15N-relaxation measurements, H/D exchange and protein dynamics.
- Determination of 3D structural models using NMR data.
- Study of protein – protein/nucleic acids/RNA/DNA/small molecules interaction through NMR, calculation of Kd, design of bioactive molecules through biomolecular NMR.
- NMR in drug design.
- NMR spectroscopy in lead discovery and optimization process.
- Modern approaches in Structural Biology & Magnetic Resonance Diagnostics -– in cell NMR, NMR-metabolomics, etc.
- NMR in metabolomics and clinical research

4. TEACHING and LEARNING METHODS - EVALUATION

DELIVERY	Face to face
USE of INFORMATION and COMMUNICATIONS TECHNOLOGY	• Teaching and learning processes are supported by the Upatras e-class platform. • Teaching process is supported by Information and Communication Technologies (ICTs).
TEACHING METHODS	***Activity*** — ***Semester Workload*** Lectures — 39 Unsupervised study — 12 Laboratory practice — 74 ***Course Total*** **(25 hours of work-load per ECTS credit) — 125**
STUDENT PERFORMANCE EVALUATION	Language of Evaluation: Greek / English Written exams: • Multiple choice questions, short answer questions, matching questions, problem solving, writeen work

5. RECOMMENDED BIBLIOGRAPHY

Suggested Bibliography:

- NMR Primer for Life Scientists. Rattle Henry, ISBN 10: 0951643630 ISBN 13: 9780951643631 Publisher: Partnership Press, 1995
- BioNMR in Drug Research, Zerbe, Oliver (Editor), Methods and Principles in Medicinal Chemistry (Series Nr. 16), Edition November 2002, XVIII, 484 Pages, Hardcover, ISBN: 978-3-527-30465-3, Wiley-VCH, Weinheim
- S. Jurt, O. Zerbe "*Applied NMR Spectroscopy for Chemists and Life Scientists*" 1st Edition, Wiley-VCH, Weinheim, 2013.
- L. Garrido, N. Beckmann (Eds), "*New Applications of NMR in Drug Discovery and Development*" (Volume 2), RSC Publishing, 2013.
- E. R. Zartler, M. Shapiro (Eds), "*Fragment-Based Drug Discovery: A Practical Approach",* 1st Edition, Wiley, 2008.

Related Academic Journals:

Primer, Protein NMR spectroscopy,
https://edisciplinas.usp.br/pluginfile.php/5322096/mod_resource/content/0/protein%20NMR%20spectroscopy%20currnt%20biology.pdf