DIPARTIMENTO DI SCIENZE

COURSE: **Spectroscopic Methods for the study of Bioactive Molecules**			
ACADEMIC YEAR: **2019-2020**			
TYPE OF EDUCATIONAL ACTIVITY:			
TEACHER: **Prof. Antonietta Pepe**			
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phone: **0971/205486**		mobile (optional):	
Language: Italian (english on request)			
ECTS: 6 (4 of lessons and 2 of tutorials/practice)	n. of hours: 56 (32hr of lessons and 24hr of tutorials/practice)	Campus: **Potenza** Dept./School: **Dipartimento di Scienze**	Semester: **I (from 01/10/2019 to 20/01/2020)**

EDUCATIONAL GOALS AND EXPECTED LEARNING OUTCOMES

The main aim of the course is to give the student a working knowledge of the applications of modern spectroscopic techniques in Biology and Chemistry. This knowledge will allow the identification of the molecular structure of small natural organic molecules using spectroscopic data. The course will present the physical bases of the main spectroscopic methods currently used in biological research. Mathematical formalism will be kept to a minimum and specific biological applications will be considered.

After having completed the course, the student should:
1) Understand principles of all of the above mentioned spectroscopic methods.
2) Be able to extract specific information about structure of a compound from various spectra.
3) Be skilled enough to elucidate an unknown structure, or solve a structure-related problem, by combining information obtained from various spectroscopic methods.
4) be able to analyze and discuss spectroscopic results in the context of the scientific literature in the fields of biology, biochemistry, and biophysics.
5) know the potentialities of the studied spectroscopic approaches in biological and biochemical studies.

PRE-REQUIREMENTS

In order to understand the basis of the spectroscopic techniques and the main applications in Biology, the student should have good knowledge of the basic principles of General and Organic Chemistry and of Physics

SYLLABUS

General introduction to the structural determination of organic molecules (1h)

Spectroscopic methods: Basic Principles. (2h)

Electronic spectroscopy (8h) Electronic transitions. Lambert-Beer law. Cromophores. Fluorescence. Main fluorophores used in Biological studies. Circular dichroism: basic principles. CD spectra of Proteins.

Infrared spectroscopy (IR) (4h) . Harmonic oscillator model. Infrared spectra. Types of vibrations that give rise to signals in the IR region (stretching ,bending, wagging, rocking vibrations). IR of major functional organic compounds. Fingerprint region. IR spectra of proteins.

Mass spectrometry (MS) (6h): molecular weight determination. Main ionization techniques: EI, Chemical ionization, FAB, electrospray. MALDI-TOF. Principal fragmentations of organic compounds.

Nuclear magnetic resonance spectroscopy (NMR) (10h). The nuclear spin. Basic principles of NMR . ^{1}H- NMR. Chemical shift. Integration. Scalar coupling. First order spectra. Analysis of simple spin systems. Nuclear Overhauser effect (nOe). ^{13}C-NMR. ^{13}C chemical shift. Broad-band decoupling. Imaging MR in medical diagnosis.

Classroom tutorials on the identification of organic molecules from the spectroscopic data. (12h)

Laboratory tutorials (12h):

1. ***Electronic spectroscopy tutorial:*** *Sample preparation and UV, CD and fluorescence spectra acquisition of an unknown protein.*
2. ***Infrared spectroscopy tutorial:*** *Sample preparation and IR spectrum acquisition of an unknown compound.*
3. ***NMR spectroscopy tutorial:*** *Sample preparation and ^{1}H and ^{13}C NMR spectra acquisition of an unknown compound.*

TEACHING METHODS

- Theoretical lessons (32h) with Classroom tutorials (12h) on combined analysis and interpretation of spectra of organic compounds in order to determine the molecular structure. Examples of exercises are proposed in the classroom with the active participation of student.
- Laboratory tutorial (12h). The students have to prepare a report for each laboratory tutorial.

EVALUATION METHODS

The aim of the final examination is to evaluate the level of achievement of the educational goals .
At least 3 days before the examination day the student has to send the 3 reports of the laboratory activities. (score 6 max.)
The final examination consists of two parts. A written examination (1h) where the student has to identify the molecular structure of an unknown organic compound by the combined analysis of IR, NMR and MS spectra. (score 6 max) Once the written examination is approved, an Oral examination on the theoretical aspects of the spectroscopic and spectrometric techniques has to be taken. (Score 18 max)

TEXTBOOKS AND ON-LINE EDUCATIONAL MATERIAL

- *Pedulli, G.F. Metodi fisici in chimica organica ; casa Editrice PICCIN.*
- *Silverstein R.M., Webster F.X., Kiemle D.J. Identificazione Spettrometrica di Composti Organici, II Edizione Casa Editrice Ambrosiana 2006.*
- *Hesse M, Meier H, Zeeh B: Metodi spettroscopici in Chimica organica. Seconda Edizione. Casa editrice EDISES.*

Course slides will be available from the University E-learning platform , whose access is free for students attending the classroom. Furthermore, links to websites, where exercises are available, will be provided.

INTERACTION WITH STUDENTS

At the beginning of the course the teacher will describe the educational goals, the syllabus and the examination methods to the students and ask for the institutional emails of the attending students. All course information will be send to the provided email addresses.

Office hour: by email appointment

EXAMINATION SESSIONS (FORECAST)[1]

10/02/2020; 24/02/2020; 10/03/2020; 22/6/2020; 2/07/2020; 03/09/2020; 6/10/2020; 15/12/2020

SEMINARS BY EXTERNAL EXPERTS YES □ NO x

FURTHER INFORMATION

[1]Subject to possible changes: check the web site of the Teacher or the Department/School for updates.