UNIVERSITÀ DEGLI STUDI DI BARI ALDO MORO

DIPARTIMENTO DI FARMACIA-SCIENZE DEL FARMACO

General information		
Academic subject	**Physical Methods in Organic Chemstry**	
Degree course	CTF	
Year of study	III	
European Credit Transfer and Accumulation System (ECTS)		8 CFU
Language	Italian	
Academic Year	2021/2022	
Academic calendar (starting and ending date)	March 2022 – June 2022	
Attendance	YES	

Professor/ Lecturer	
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Department and address	**Dept. of Pharmacy – Drug Sciences**
Virtual headquarters	**Teams platform**
Tutoring (time and day)	**Monday – Friday, 15:00 – 17:00**

Syllabus	
Learning Objectives	By a combination of lectures, exercises and individual semester assignment, the principles of UV/VIS-;IR-;1H- and 13C-NMR (1D and 2D spectra); and mass spectrometry are discussed. The course is especially focused on analysing and interpreting spectral data of organic compounds. Spectroscopic determination of the structure of organic molecules.
Course prerequisites	Basic knowledge of organic chemistry and physics
Contents	Course layout Overview of electromagnetic spectrum and its application to the study of chemical molecules UV-Vis. • Principle of UV-Vis spectroscopy. • Interpretation of UV-Vis spectroscopy. • Electronic transitions in organic molecules, selection rules, application of Beer Lambert law, qualitative and quantitative analysis by UV-Vis spectroscopy. • Instrumentation and Application of UV-Vis spectroscopy. IR. • Principle Infra-Red Spectroscopy. • Basic concepts, experimental methods, functional group analysis and identification using IR spectroscopy, structural effects on vibrational frequency. • Interpretation of Infra-Red Spectroscopy. • Instrumentation and Application of Infra-Red Spectroscopy NMR • Principles of Nuclear Magnetic Resonance Spectroscopy. • Spin ½ nuclei, 1H and 13C-NMR spectroscopy, FT-NMR method. Chemical shifts, spin-spin coupling, spin-spin splitting pattern recognition for structure elucidation, coupling constants. • Interpretation of Nuclear Magnetic Resonance Spectroscopy. • Second order effects in NMR spectrum, AB and AA'BB', ABC spin systems. • Solving simple structure elucidation problems with 1H and 13C NMR spectroscopy.

	• Stereochemistry determination using NMR techniques. Study of dynamic processes by NMR spectroscopy. • Various ionization methods – EI, CI, ESI and MALDI methods, fragmentation patterns of simple organic molecules, Use of HRMS. • Fragmentation patterns of simple organic molecules (continued), solving structure elucidation problems using mass spectrometry. • Mass spectrometry and the combined use of spectroscopic techniques for structure elucidation. • Instrumentation and Application of Nuclear Magnetic Resonance Spectroscopy MS spectrometry • Solving structure elucidation problems using multiple spectroscopic data (NMR, MS, IR and UV-Vis).
Books and bibliography	R. M. SILVERSTEIN, F. X. WEBSTER- Identificazione Spettroscopica di Composti Organici- Casa Editrice Ambrosiana. M. HESSE, H. MEIER, B. ZEEH - Metodi Spettroscopici nella Chimica Organica- EdiSES WHITTAKER D. - Interpretation of Organic Spectra - RSC. E. PRETSCH, P. BUHLMANN, C. AFFOLTER - Structure Determination of Organic Compounds Table of spectral data - Springer. D. L. PAVIA, G. M. LAMPMAN E G. S. KRIZ - Introduction to Spectroscopy: a Guide for Students of Organic Chemistry - Saunders Golden Sunburst Series - Saunders College Publishing - Philadelphia. London - Toronto.
Additional materials	Additional files will be provided to all students.

Work schedule			
Total	Lectures	Hands on (Laboratory, working groups, seminars, field trips)	Out-of-class study hours/ Self-study hours
Hours			
200	70	10	120
ECTS			
8	70	10	

Teaching strategy	
	Classroom lectures, case studies, group problem solving. Lectures (4 hours per week), practical exercises (1 hours per week). E-learning not allowed.
Expected learning outcomes	
Knowledge and understanding on:	After having completed the course, the student should be able to: ○ Explain principles of UV, IR, MS and NMR spectroscopy. ○ Explain construction/design of spectrometers. ○ Operate UV and IR spectrometers, execute runs, acquire, and process spectra. ○ Analyse and interpret spectral data. ○ Use spectral data to elucidate an unknown structure or solve a structure related problem. ○ *Design the most suitable set of spectroscopic methods for a given structure-related problem.*
Applying knowledge and understanding on:	○ Spectroscopy and instrumentation ○ Method to approach structure elucidation ○ Capacity to analyse organic samples

	○ Capacity to assign structure to organic molecules
Soft skills	• *Making informed judgments and choices* ○ Appropriate technical language. ○ Capacity to elaborate scientific data • *Communicating knowledge and understanding* ○ Capacity to transfer technical information • *Capacities to continue learning* ○ Capacity to expand knowledge in the field of chemistry and spectroscopy.

Assessment and feedback	
Methods of assessment	*Compulsory exam assignment (written report): structure elucidation of an unknown compound by spectroscopic methods. An approved individual report counts for 50% of the exam. An oral assessment follows the written assignment.* - *Written exam duration (150 min)* - *Supplementary material allowed for the written exam.* - *Results published on the esse3 platform* - *Exercises available for all students*
Evaluation criteria	• *Knowledge and understanding* ○ Appropriateness of the knowledge. ○ Capacity to use spectroscopic techniques. • *Applying knowledge and understanding* ○ Critical reasoning and correct technical terminology • *Autonomy of judgment* ○ Capacity to self-assess the correct sequence in a structural analysis. • *Communication skills* ○ Clarity of the exposition • *Capacities to continue learning* ○ Acquisition of advanced knowledge of spectroscopy, which are propaedeutic for the study of Medicinal Chemistry and for the synthesis of pharmaceutically relevant compounds
Criteria for assessment and attribution of the final mark	*Mark is minimum 18 out of 30 and maximum 30 out of 30.* *50% of the maximum mark score is given to the written exam, and 50% tor the oral exam. Problem solving capability, clarity of exposition and correctness of the information will be the main criteria of the evaluation.*
Additional information	