

**Course title ECTS** code 13.3.0727 Spektroskopia chemiczna / Chemical spectroscopy Name of unit administrating study Faculty of Chemistry **Studies** Field of study **Type Form** Chemical Business Bachelor / Engineer Full-time studies Teaching staff prof. Sylwia Rodziewicz-Motowidło, dr hab. Emilia Sikorska, prof. Zbigniew Kaczyński Forms of classes, the realization and number of hours **ECTS** credits A. Forms of classes, in accordance with the UG Rector's classes - 45 h regulations tutorial classes - 10 h lectures, auditorium classes student's own work - 45 h B. The realization of activities multimedia presentation, in-class learning Total: 100 h - 4 ECTS C. Number of hours 45 h (15 h lecture, 30 h auditorium classes) The academic cycle Third year, winter semester Type of course Language of instruction obligatory Polish **Teaching methods** Form and method of assessment and basic criteria for evaluation or examination requirements · Lecture with multimedia presentation, A. Final evaluation, in accordance with the UG study regulations • In the auditorium classes students will learn lectures - exam, combined interpretation of the mass, IR, <sup>1</sup>H and <sup>13</sup>C auditorium classes – course credit with a grade NMR spectra of compounds of M.W. up to ~300 D **B.** Assessment methods by solving problems designated by the teacher (in-Lecture class on the board and in a group-/home-work. written exam, 5-10 tasks to solve, including spectra with medium degree of difficulty Auditorium classes • 4-5 obligatory 10 minutes tests from previously trained material current knowledge control based on spectroscopic problems previously given for practice by the teacher quizzes on the fastest correct solution of spectroscopic problems given by the teacher during seminars C. The basic criteria for evaluation or exam requirements Lecture: • pass the written exam 91-100%: 5.0 81-90%: 4.5 71-80%: 4.0 61-70%: 3.5 51-60%: 3.0 Less than 51% 2.0 Auditorium classes: • completed all tests, additional problems and quizzes 91-100%: 5.0 81-90%: 4.5 71-80%: 4.0 61-70%: 3.5



51-60%: 3.0 Less than 51% 2.0

## D. Method of verification of the established effects of education

#### Lecture:

- A written exam consisting of 5-10 problems covering the topics presented during the lecture and auditorium classes. Passed classes tests (see below) is prerequisite.
- Attendance at lectures are not obligatory (although presence is recommended), and the lack of knowledge resulting from the absence may be made up on the basis of other students' notes and literature.

#### Auditorium classes:

• Attendance, active participation, completed tests.

### Required courses and introductory requirements

Organic and physical chemistry

#### Aims of education

- Presenting the physical basics of the interactions of electromagnetic radiation with matter and the theoretical basis of spectroscopic methods to students
- Familiarize the students with the fundamentals of mass spectrometry (MS), oscillation spectroscopy (IR) and 1D and 2D nuclear magnetic resonance (NMR) spectroscopy;
- Familiarize the students with interpretation of MS, IR and NMR spectra of compounds up to ~ 300 D to identify the topology, hydrogen bonds, stereochemistry, dynamics etc. including the advantages and disadvantages of the used methods.

#### **Course contents**

**A**. Topics of the lecture: The properties of the electromagnetic radiation and its interactions with molecular systems: absorption, emission, dispersion. Overview of techniques: MS, IR, and NMR, including 2D NMR methods such as: COSY, TOCSY, HSQC/HMQC, NOESY; spin systems analysis, identification of molecules up to ~ 300 D; configuration, conformation, dynamic of the molecules; integrated usage of the spectroscopic methods; elements of conformational analysis of biomolecules.

**B.** Auditorium classes: Interpretation of the spectra; practical use of spectroscopic methods in structural and dynamics studies of molecules up to ~300D; to familiarize of the students with the probability of several different solutions of the same problem and verification of the correct solution; learning of the correct description of the spectra; to know the disadvantages and advantages of the particular spectroscopic methods, complementarity of the spectroscopic methods.

## **Bibliography of literature**

## A. Literature required to pass the course

- Collective red.. W. Zieliński i A. Rajca: Metody spektroskopowe ich zastosowanie do identyfikacji związków organicznych, WNT W-wa 1995, 2000.
- R.M. Silverstein, F.X. Webster, D.J. Kiemle: Spectrometric Identification of Organic Compounds, John Wiley & Sons, 2005, 2014.
- Internet: independent study, verified by the teacher.

### **B.** Extracurricular readings

- S. Płaziak: Spektrometria masowa związków organicznych, Wydaw. Naukowe UAM Poznań 1997
- R.A.W. Johnstone, M.E. Rose: Mass spectrometry for chemists and biochemists. Cambridge University, 1982, 1996
- Z. Kęcki: Podstawy spektroskopii molekularnej, PWN Warszawa 1998.
- I.Z. Siemion: Biostereochemia, PWN Warszawa 1985.
- K. Wüthrich: NMR in biological research: peptides and proteins, North-Holland, Amsterdam 1976.

### Knowledge

Students know theoretical basis for spectroscopic methods utilized in identification of simple organic compounds

Students know the advantages and disadvantages of spectroscopic methods

Students have basic knowledge about conformational analysis of biomolecules using spectroscopic methods

Students can present the current trends in the development of spectroscopic methods



## Skills

Students are able to interpret MS, IR, NMR spectra of simple organic compounds, Students have skills of drawing correct conclusions based on available data.

# Social competence

Individually and/or in a team-work:

- -Students can establish and realize a defined action plan setting priorities for its implementation.
- -Students can identify their level of knowledge and skills and understand the necessity of life-long learning in chemical spectroscopy and personal development.

### Contact

**2** +48 58 523 50 37

e-mail: s.rodziewicz-motowidlo@ug.edu.pl