

FACULTY of CHEMISTRY

**SUBJECT CARD****Name of subject in Polish** Metody spektroskopowe w chemii medycznej**Name of subject in English** Spectroscopic methods in medicinal chemistry**Main field of study (if applicable):** Biosciences**Specialization (if applicable):** Medicinal chemistry**Profile:** academic**Level and form of studies:** 2nd level,**Kind of subject:** obligatory**Subject code** W03BSS-SM2020W, W03BSS-SM2020L**Group of courses** NO

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of organized classes in University (ZZU)	30		30		
Number of hours of total student workload (CNPS)	50		50		
Form of crediting (Examination / crediting with grade)	Ex		crediting		
For group of courses mark (X) final course					
Number of ECTS points	2		2		
including number of ECTS points for practical classes (P)			2		
including number of ECTS points corresponding to classes that require direct participation of lecturers and other academics (BU)	1,3		1,4		

\*delete as not necessary

**PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES**

1. Knowledge of general chemistry.
2. Basic knowledge of physical chemistry.
3. Basic knowledge of organic chemistry.
4. Basic skills in the field of physicochemical and mathematical calculations.
5. Basic knowledge of spectroscopic techniques used in structural analysis.

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**SUBJECT OBJECTIVES**

C1 Acquiring knowledge about spectroscopic analysis methods

C2 Acquiring knowledge about methods of interpreting one-dimensional magnetic resonance spectra.

C3 Acquiring knowledge about methods of interpreting two-dimensional magnetic resonance spectra.

C4 Acquiring knowledge on how to interpret FT-IR spectra and mass spectrometry spectra.

C5 Practical knowledge of selected applications of mass spectrometry and magnetic resonance.

SUBJECT EDUCATIONAL EFFECTS		
relating to knowledge:		
PEU_W01 Has knowledge of spectroscopic analysis methods		
PEU_W02 Has knowledge of the use of spectroscopy in analysis		
PEU_W03 Has knowledge of the use of spectroscopic methods and medical diagnostics		
relating to skills:		
PEU_U01 Is able to prepare material for analysis		
PEU_U02 Is able to assess what methods to solve the current problem		
PEU_U03 Is able to analyze spectroscopic data		
relating to social competences:		
Z zakresu kompetencji społecznych:		
PEU_K01 Ma świadomość powiązań pomiędzy różnymi obszarami nauk chemicznych i/lub technicznych oraz ich aspekty praktyczne.		
PROGRAMME CONTENT		
Lecture		Number of hours
Lec 1	Introduction in spectroscopic methods	2
Lec 2	IR spectroscopy – theoretical background and applications	2
Lec 3	Raman spectroscopy - introduction	2
Lec 4	Raman spectroscopy - applications	2
Lec 5	Mass spectrometry - introduction	2
Lec 6	Mass spectrometry – types of ionization	2
Lec 7	Mass spectrometry - analizators	2
Lec 8	Mass spectrometry – fragmentation and interpretation of spectra	2
Lec 9	UV-Vis and CD spectroscopy	2
Lec 10	NMR spectroscopy – theoretical background	2
Lec 11	NMR spectroscopy – chemical shift	2
Lec 12	NMR spectroscopy – coupling constant	2
Lec 13	2D NMR spectroscopy	2
Lec 14	2D NMR spectroscopy	2
Lec 15	EPR spectroscopy	2
	Total hours	30
Laboratory		Number of hours
Lab 1	Introduction in spectroscopic methods	2
Lab 2	IR spectroscopy – interpretation of spectra	2
Lab 3	Raman spectroscopy	2
Lab 4	Raman spectroscopy	2
Lab 5	Mass spectrometry – introduction	2

Lab 6	Mass spectrometry – fragmentation	2
Lab 7	Mass spectrometry - interpretation of spectra	2
Lab 8	Mass spectrometry – interpretation of spectra	2
Lab 9	NMR spectroscopy – the principles	2
Lab 10	NMR spectroscopy – interpretation of 1D spectra	2
Lab 11	NMR spectroscopy – interpretation of 2D spectra	2
Lab 12	NMR spectroscopy – spectra simulations	2
Lab 13	NMR spectroscopy – spectra simulations	2
Lab 14	UV-Vis spectroscopy - applications	2
Lab 15	CD spectroscopy – interpretation and simulations	2
	Total hours	30

### TEACHING TOOLS USED

- N1. Problem lectures – multimedia presentations  
 N2. Laboratory – problematic issues (multimedia presentations)  
 N3. Laboratory - solving practical examples, drawing structures and spectra and performing calculations on a multimedia board  
 N4. Own work – preparation for partial tests  
 N5. Own work – consultations with the teacher

### EVALUATION OF SUBJECT LEARNING OUTCOMES ACHIEVEMENT

Evaluation (F – forming during semester), P – concluding (at semester end)	Learning outcomes code	Way of evaluating learning outcomes achievement
P1 (lecture)	PEU_W01-W03, PEU_K01	examination
F2 (laboratory)	PEU_UO1-UO2	test
P (1 laboratory) = arithmetic mean of test grades		

### PRIMARY AND SECONDARY LITERATURE

#### **PRIMARY LITERATURE:**

- [1] K. Pigoń, Z. Ruziewicz, Chemia fizyczna t 2 Fizykochemia molekularna, Wyd. PWN, Warszawa 2007
- [2] P.W. Atkins, Chemia fizyczna, PWN 2001
- [3] R. M. Silverstein, F. X. Webster, D. J. Kiemle, Spektroskopowe metody identyfikacji związków organicznych PWN, Wraszawa 2007.
- [4] D. A. Skoog, D. M. West, F. J. Holler, S. R. Crouch, Podstawy chemii analitycznej 2, PWN, Warszawa 2007.
- [5] Z. Kęcki, Podstawy spektroskopii molekularnej, Wyd. PWN, Warszawa 1992.

#### **SECONDARY LITERATURE:**

- [1] A. Cygański, Metody spektroskopowe w chemii analitycznej. WNT Warszawa, 2009
- [2] J. Demichowicz-Pigoniowa, Chemia fizyczna t 3, Obliczenia fizykochemiczne, PWN, Warszawa 2010
- [3] J. Najbar, A. Turek, Fotochemia i spektroskopia optyczna, PWN, Warszawa 2009.

[4] P. Suppan, Chemia i światło, PWN, Warszawa 1997.

[5] W. Zieliński, A. Rajca, Metody spektroskopowe i ich zastosowanie do identyfikacji związków organicznych, WNT, Warszawa 2000

**SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)**

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