



Subject card

Subject name and code	Methods of Structural Analysis, PG_00054717						
Field of study	Biotechnology						
Date of commencement of studies	October 2022		Academic year of realisation of subject		2024/2025		
Education level	first-cycle studies		Subject group		Obligatory subject group in the field of study Subject group related to scientific research in the field of study		
Mode of study	Full-time studies		Mode of delivery		at the university		
Year of study	3		Language of instruction		Polish		
Semester of study	5		ECTS credits		3.0		
Learning profile	general academic profile		Assessment form		assessment		
Conducting unit	Department of Organic Chemistry -> Faculty of Chemistry						
Name and surname of lecturer (lecturers)	Subject supervisor		prof. dr hab. inż. Maria Milewska				
	Teachers		prof. dr hab. inż. Maria Milewska dr hab. inż. Witold Przychodzeń dr hab. inż. Teresa Olszewska dr inż. Monika Gensicka-Kowalewska				
Lesson types and methods of instruction	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	30.0	0.0	15.0	0.0	0.0	45
	E-learning hours included: 0.0						
Learning activity and number of study hours	Learning activity	Participation in didactic classes included in study plan		Participation in consultation hours		Self-study	SUM
	Number of study hours	45		5.0		25.0	75
Subject objectives	A main goal is to teach students basic spectroscopic methods including: NMR, IR, UV, and MS, and their application in the analysis of the structure of organic compounds						
Learning outcomes	Course outcome		Subject outcome		Method of verification		
	K6_U01		Student is able to apply knowledge of the basics of physical, organic chemistry and mathematics to analyze spectroscopic spectra		[SU3] Assessment of ability to use knowledge gained from the subject		
	K6_U02		The student is able to apply knowledge of general, physical and quantum chemistry to predict the physical and chemical properties of biomolecules and organic compounds		[SU2] Assessment of ability to analyse information		
	K6_W09		The student has knowledge of the basics of spectroscopic methods; knows and understands the principle of operation and application of the most important spectroscopic methods to analyze the structure of organic compounds		[SW1] Assessment of factual knowledge		

Subject contents	Principles of spectroscopy electromagnetic radiation, energy levels in molecules, absorption of radiation, line shape, selection rules, application of the Fourier transformation in spectroscopy. NMR magnetic properties of atomic nuclei, the chemical shift, the spin-spin coupling, diamagnetic anisotropy of molecules, interpretation of the proton NMR spectra, spin systems, the Karplus equation, dynamic effects, NOE, the Fourier transformation (FT-NMR), two-dimensional spectra (2D-NMR), basics of ^{19}F and ^{13}C NMR, elements of NMR of other nuclei. Infrared spectroscopy (IR) harmonic and anharmonic oscillator, vibrations of multiatom molecules, the normal vibrations, transition probability, group frequencies, measurements of the IR spectra, interpretation of the IR spectra, hydrogen bonds in the IR spectroscopy, the Raman spectroscopy. Mass spectroscopy (MS) physical basis of the MS spectroscopy, methods of sample ionization including electro- ant thermospray, ion types in MS, determination of molecular mass and molecular formula, fragmentation of molecules. Electronic spectra (UV-vis) electronic levels, spectrometers, selection rules, band shape, simple chromophores, aromatic chromophores, influence of substituents, steric effects, solvent effects.											
Prerequisites and co-requisites	1. Knowledge of theoretical basis of spectroscopy 2. Knowledge of structures of organic compounds 3. Knowledge of nomenclature of organic compounds											
Assessment methods and criteria	<table><tr><th>Subject passing criteria</th><th>Passing threshold</th><th>Percentage of the final grade</th></tr><tr><td>Midterm colloquium H and C NMR, IR, MS, UV</td><td>60.0%</td><td>50.0%</td></tr><tr><td>teoretical colloquium</td><td>60.0%</td><td>50.0%</td></tr></table>	Subject passing criteria	Passing threshold	Percentage of the final grade	Midterm colloquium H and C NMR, IR, MS, UV	60.0%	50.0%	teoretical colloquium	60.0%	50.0%		
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Midterm colloquium H and C NMR, IR, MS, UV	60.0%	50.0%										
teoretical colloquium	60.0%	50.0%										
Recommended reading	Basic literature	1. R. M. Silverstein, F. X. Webster, D. J. Kiemle "Spektroskopowe metody identyfikacji związków organicznych", PWN, Warszawa, 2007. 2. "Spektroskopowe metody badania struktury związków organicznych", praca zbiorowa red. A. Rajca, WNT, Warszawa, 1996 lub 2000. 3. R. M. Silverstein, G. C. Bassler "Spektroskopowe metody identyfikacji związków organicznych", PWN, Warszawa, 1970. 4. L. K. Kazicyna, N. B. Kuplarska "Metody spektroskopowe wyznaczania struktury związków organicznych", PWN, Warszawa, 1974 5. J. B. Lambert, H. F. Shurvell, D. A. Lightner, R. G. Cooks "Organic Structural Spectroscopy" Prentice-Hall, Inc., 1998										

	Supplementary literature	1. R. A.W. Johnstone, M. E. Rose "Spektrometria mas podręcznik dla chemików i biochemików", PWN, Warszawa, 2001. 2. A. Zschunke "Spektroskopia magnetycznego rezonansu jądrowego w chemii organicznej", PWN Warszawa, 1976. 3. Z. Kęcki "Podstawy spektroskopii molekularnej", PWN, Warszawa, 1972. 4. H. Günther, "Spektroskopia magnetycznego rezonansu jądrowego", PWN, Warszawa, 1983. 5. M. Gensicka-Kowalewska, M.J. Milewska, Podstawy metod badań struktury związków organicznych w zadaniach", Wydawnictwo PG, Gdańsk, 2024
	eResources addresses	Uzupełniające Adresy na platformie eNauczanie: METODY BADAŃ STRUKTURALNYCH - Moodle ID: 40851 https://enauczanie.pg.edu.pl/moodle/course/view.php?id=40851
Example issues/ example questions/ tasks being completed	1. The pair of protons at C-3 of cis-1,2-dichlorocyclopropane are diastereotopic. Explain. 2. Characterize the indicated protons as being homotopic, enantiotopic, or diastereotopic ; magnetically equivalent or nonequivalent.. For example: 1-fluoro-1-iodoethene 3. Write out the rotamers of 2-chloroethanol. What is the spin notation at slow rotation for each rotamer and at fast rotation for the average?	
Work placement	Not applicable	

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