

Course title in English	Application of multidimensional NMR spectroscopy in determining the structure, stereochemistry and conformation of organic compounds
Course title in Polish	Zastosowanie wielowymiarowej spektroskopii NMR w ustalaniu struktury, stereochemii i konformacji związków organicznych
Course code	
Type of course	Lecture/Seminar
Level of course	PhD
Year of study	1-4
Semester/trimester	1/3/5/7
Number of hours/credits allocated	30/2
Name of lecturer	Dr hab. Zbigniew Kaczyński, prof. UG
Objective of the course (expected learning outcomes and competences to be acquired)	<u>Knowledge</u>: The student acquires the foundations necessary for the interpretation of MS, IR, ^1H and ^{13}C NMR spectra of moderately complex molecules; learns quantum-mechanical models used to describe the phenomenon of rotation, oscillation and radiation scattering; gains basic knowledge of conformational testing of biomolecules; can present current directions of development of spectroscopic methods. <u>Skills</u>: The student acquires the ability to identify and determine the structure (hydrogen bonds, stereochemistry, etc.) of compounds with masses up to ~ 1000 D based on the interpretation of their spectra (set of spectra) ^1H and ^{13}C NMR, 1D and 2D NMR; can learn independently and use sources of information. <u>Social competence</u>: The student understands the need for further education in the "information" society of the 21st century; he learns to reach for knowledge; understands the need for ethics, honoring copyright, etc.
Prerequisites	-
Course contents	1. ^1H NMR, theory; instrument and measurement; chemical shift; spin-spin coupling; protons on heteroatoms; exchangeable protons; spin-spin heteroatomic couplings; chemical vs magnetic

	equality; spin systems AB-AX, ABC-AMX, chirality; geminal, vicinal and long-range linkages; uncoupling of spins; NOE. 2. ^{13}C NMR, theory; instrument and measurement; chemical shift; DEPT. 3. Correlation (2D-) NMR, COSY, TOCSY, HMQC, HMBC, NOESY, ROESY, INADEQUATE. A PhD student will acquire the ability to freely use the NMR technique to solve the topology and spatial structure of systems with atomic masses up to 2000 Da (peptides, polysaccharides, steroids etc.)
Recommended reading	1. Collective under ed. W. Zieliński i A. Rajca: Metody spektroskopowe ich zastosowanie do identyfikacji związków organicznych, WNT W-wa 1995, 2000. 2. R.M. Silverstein, F.X. Webster, D.J. Kiemle: Spektroskopowe metody identyfikacji związków organicznych, PWN W-wa 2007
Teaching methods	• lecture with multimedia presentation, • auditorium exercises with elements of the seminar individually and / or in small teams: exercises and spectroscopic mini-projects, analysis / interpretation of spectra / spectra sets combined with discussion.
Assessment methods	Doing assignments throughout the course, final exam
Language of instruction	Polish