

Course title Wybrane aspekty analizy biomolekuł / Selected aspects of biomolecular analysis		ECTS code 13.3.0925	
Name of unit administrating study Faculty of Chemistry			
Studies			
Field of study	Type	Form	
Chemistry	Master	Full-time studies	
Dr hab. Sylwia Rodziewicz-Motowidło, prof. UG			
Forms of classes, the realization and number of hours		ECTS credits	
A. Forms of classes, in accordance with the UG Rector's regulations Auditorium classes		classes 30 hours consultation 2 hours student's own work 18 hours TOTAL: 50 hours - 2 ECTS	
B. The realization of activities classes in the didactic room			
Number of hours Seminars 30 hours			
The academic cycle Second year, winter semester			
Type of course obligatory		Language of instruction Polish	
Teaching methods Discussion		Form and method of assessment and basic criteria for evaluation or examination requirements	
		A. Final evaluation, in accordance with the UG study regulations Course completion (with a grade)	
		B. Assessment methods determining the final grade based on partial grades received during the semester test	
		C. The basic criteria for evaluation or exam requirements A. Method of passing • Credit with grade B. Forms of getting credit - three partial colloquia covering the scope of material carried out at each class; for some peptide and protein classes - written colloquium with open questions, - determining the final grade based on three partial grades received during the semester. C. Basic criteria • a positive assessment is at least 51% of points possible to obtain from each of the three partial written tests covering the scope of material carried out during the exercises; the final grade will be their arithmetic average, • any negative partial assessment can be improved on the basis of an additional test from material covering the scope of exercises (each time min 51% of points possible).	
Required courses and introductory requirements Formal requirements, organic chemistry, biochemistry, physical chemistry, chemical spectroscopy			

Prerequisites, basic knowledge of the chemistry of sugars and polysaccharides, amino acids, peptides and proteins, preliminary information on spectroscopic methods of studying the structure of simple organic compounds

Aims of education

1. Getting to know of students with all issues listed in the content of the exercises,
2. Getting to know of students with methods of spectroscopic analysis of 1D, 2D NMR spectra of peptides, proteins, derivatives of monosaccharides, oligo- and polysaccharides,
3. introduction to the issues of: determining the structure of first level mono-, oligo- and polysaccharides (bacterial) - components of biomolecules, chemical methods, mass spectrometry (EI MS, CI MS, MALDI TOF MS) and NMR,
4. introduction into the principles of interpretation of the following spectra: ¹H, ¹³C NMR, homo- and heterocorrelation and MS of their simple sugars and native bacterial polysaccharides,
5. acquaintance with the methods of determining the structure of the first year and second row Peptides and proteins based on 1D, 2D NMR spectra,
6. familiarizing students with the procedure for preparing a peptide or protein sample for NMR spectra measurements.

Course contents

Problems of auditorium exercises:

Part I (Structural analysis of monosaccharides) will cover such issues as: Interpretation of ¹H and ¹³C NMR spectra and NMR spectra of homo- and heterocorrelation sugar derivatives; 2D NMR methods in the analysis of monosaccharides and their derivatives;

Part II - Brief characteristics of selected biomolecules containing sugar fragments. Determination of the first order structure the oligo- and polysaccharide part of biologically active compounds. Sugar and methylation analysis - interpretation of mass spectra (EI MS, CI MS) of acetyl derivatives and acetyl derivatives of partially methylated alditols. The use of MALDI TOF MS to determine the molecular weight of glycoconjugates. Interpretation of NMR spectra of polysaccharides on the example of bacterial antigens (¹H and ¹³C NMR spectra, homo- and heterocorrelation NMR spectra).

Part III (Structural analysis of peptides) covers such issues as: History of nuclear magnetic resonance applied to peptides and proteins, method of preparing a peptide or protein sample for NMR studies, advantages and disadvantages of NMR technique applied to peptides and proteins, interpretation of TOCSY spectra, NOESY, COSY peptides, determining the spatial structure of peptides using CSI (chemical shift index) data - coupling constants and NOE effects, interpretation of 1D NMR spectra of temperature peptides to determine temperature coefficients.

Bibliography of literature

A. Literature required for the final passing of the class (passing test):

Part I. Zieliński W., Rajca A. (red) Spectroscopic methods and their application to the identification of organic compounds, WNT, Warsaw, 1995.

Johnstone R. A. W., Rose M. E. Mass Spectrometry, PWN, Warsaw, 2001.

Silverstein R. M., Webster F. X., Kiemle D. J. Spectroscopic methods for identification of organic compounds, PWN, Warsaw, 2007.

Part II Silverstein R. M., Webster F. X., Kiemle D. J. Spectroscopic methods for identification of organic compounds, PWN, Warsaw, 2007.

Johnstone R. A. W., Rose M. E. Mass Spectrometry, PWN, Warsaw, 2001.

Zieliński W., Rajca A. (ed.) Spectroscopic methods and their application to the identification of organic compounds, WNT, Warsaw, 1995.

Wiśniewski A., Madaj J. Basics of sugar chemistry, AGRA-ENVIRO Lab., Poznań - Gdańsk, 1997.

E. de Hoffman, J. Charette, V. Stroobant, Mass Spectrometry, WNT, Warsaw 1998.

Part III Silverstein R. M., Webster F. X., Kiemle D. J. Spectroscopic methods for identification of organic compounds, PWN, Warsaw, 2007.

Johnstone R. A. W., Rose M. E. Mass Spectrometry, PWN, Warsaw, 2001.

E. de Hoffman, J. Charette, V. Stroobant, Mass Spectrometry, WNT, Warsaw 1998.

Knowledge

1. describes the basic methods used to determine the structure of simple sugars
2. knows the procedure for determining the structure of first order bacterial oligosaccharides and polysaccharides,
3. characterizes primary and secondary fragmentation rules in alditol derivative mass spectrometry
4. distinguishes the ranges of chemical shifts in ^1H and ^{13}C NMR of atoms of specific moieties from polymer sugar residues,
5. identifies the anomeric configuration based on ^1H and ^{13}C NMR spectra and HSQC,
6. recognizes sugar residue protons (COSY, TOCSY spectra) and ^{13}C nuclei conjugated with them (HSQC spectrum),
7. understands literature on selected issues of mass spectrometry and NMR in the native language, and uncomplicated texts on this subject in English,
8. lists and describes the basic parameters for describing NMR spectra of peptides and proteins,
9. characterizes processes occurring in peptides and proteins using NMR technique.

Skills

1. determines the structure of monosaccharides based on NMR spectra,
2. determines the configuration of the simple sugar derivative based on the ^1H NMR spectrum,
3. can explain the rules of primary and secondary fragmentation in alditola derivative mass spectrometry and on this basis draws conclusions about the structure of monosaccharide residues and the position of their glycosylation in the polysaccharide,
4. predicts the structure of bacterial polysaccharide or its fragments based on ^1H and ^{13}C NMR spectra and correlation spectra (COSY, TOCSY, HSQC),
5. determines the chemical shifts for individual amino acids in the peptide based on the 2D NMR spectrum,
6. determines the amino acid sequence of the peptide based on the 2D NMR spectrum,
7. determines the secondary structure of the peptide based on the calculated CSI, NOE correlation signals and coupling constants.

Social competence

1. understands the need for further learning;
2. Appreciates the need for teamwork skills through discussion and consultation,
3. discusses when determining the structure of biomolecules, giving substantive arguments,
4. shows creativity in solving structural problems,
5. maintains criticism when analyzing the results and drawing conclusions,
6. is active in deepening knowledge and understands the need for continuous learning.