

FACULTY of CHEMISTRY

SUBJECT CARD**Name of subject in Polish** METABOLOMIKA**Name of subject in English** METABOLOMICS**Main field of study (if applicable):** BIOSCIENCES**Specialization (if applicable):** MEDICINAL CHEMISTRY**Profile:** academic / ~~practical~~***Level and form of studies:** ~~1st/ 2nd level, uniform magister studies*~~, full-time / ~~part-time~~***Kind of subject:** obligatory / ~~optional~~ / ~~university-wide~~***Subject code** W03BSS-SM2021W, W03BSS-SM2021L**Group of courses** NO

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of organized classes in University (ZZU)	15		30		
Number of hours of total student workload (CNPS)	50		50		
Form of crediting (Examination / crediting with grade)	Crediting with grade		Crediting with grade		
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)	0,65		1,4		

*delete as not necessary

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. Basic knowledge of biochemistry.
2. The ability to search for scientific information in magazines.
3. The ability to work in a group.
4. The ability to use remote work tools.
5. Knowledge of English.

SUBJECT OBJECTIVES

- C1. To familiarize students with metabolomics and the practical possibilities of its use in medicine and biotechnology.
- C2. To familiarize students with the use of modern chemical diagnostic methods in medicine and analytical methods of NMR spectroscopy and mass spectrometry.
- C3. To familiarize students with methods of preparing biological samples for analysis; safety rules.

- C4. Familiarizing students with scientific literature and the ability to interpret results and develop research protocols.
- C5. To familiarize students with the elements of chemometrics and statistics.
- C6. To familiarize students with metabolomics databases.
- C7. To familiarize students with ethical problems in science - metabolomics.

SUBJECT EDUCATIONAL EFFECTS

relating to knowledge:

- PEU_W01 – knows what metabolomics is and knows the scope of its applicability.
- PEU_W02 – is able to interpret data on metabolites based on metabolomic pathways.
- PEU_W03 – knows what chemometrics is and knows the basic methods of data analysis.
- PEU_W04 – knows how to use databases.
- PEU_W05 – knows what NMR spectroscopy and MS spectrometry are and knows how they can be used in metabolomics research.
- PEU_W06 – knows the procedures for preparing biological material for a specific measurement method.

relating to skills:

- PEU_U01 – can read chemometric and statistical data.
- PEU_U02 – is able to assign the appropriate sample preparation procedure to the appropriate measurement method.
- PEU_U03 – is able to construct complex questions in factual databases and search for and analyze professional literature.
- PEU_U04 – can look for relationships between biochemical pathways based on metabolomics data.
- PEU_U05 – knows bioinformatics tools intended for the analysis of metabolomics data.
- PEU_U06 – is able to work in the laboratory with biological material.
- PEU_U07 – is able to use appropriate laboratory techniques for use in metabolomics.
- PEU_K01 – jest gotów do krytycznej oceny posiadanej wiedzy

PROGRAMME CONTENT

Lecture		Number of hours
Lec 1	General presentation of the subject's characteristics - assumptions, goals, possibilities <i>General overview of the subject, definitions of assumptions and goals of metabolomics</i>	1
Lec 2	Methods of sample preparation for metabolomics analysis. <i>Discussion of the preparation of various types of samples for analysis.</i> <i>Discussion of the preparation of samples of biofluids, muscle tissue, feces, filamentous fungi and bacteria.</i>	2

Lec 3	Application of MS mass spectrometry in metabolomics. <i>Discussion of the basics and principles of operation of a mass spectrometer coupled with liquid chromatography.</i>	2
Lec 4	Application of nuclear magnetic resonance (NMR) spectrometry in metabolomics <i>Discussion of the basics and principles of operation of nuclear magnetic resonance spectroscopy.</i>	2
Lec 5	Application of chemometric and statistical methods in metabolomics. <i>Introduction to statistical and chemometric methods used in metabolomics, familiarization with the interpretation of results.</i>	2
Lec 6	Bioinformatics tools <i>Metabolomics analysis programs will be discussed, e.g. the MetPa program, along with the determination of disturbed metabolic pathways.</i>	2
Lec 7	Application of metabolomics methods in medical diagnostics <i>Discussion of the use of metabolomics methods in metabolomic, medical and biotechnological discrimination.</i>	4
	Total hours	15

Laboratory		Number of hours
Lab 1	Presentation of the general characteristics of the subject - literature review <i>Discussion of basic concepts and definitions. Scope of applicability of metabolomics research. Methods used</i>	1
Lab 2	Application of NMR spectroscopy in metabolomics – literature review <i>Discussion of the principles of NMR spectroscopy, processing and interpretation of spectra, search for biomarkers</i>	5
Lab 3	Application of MS mass spectrometry in metabolomics – a literature review <i>Discussion of the principles of MS mass spectrometry, processing and interpretation of spectra, search for biomarkers</i>	5
Lab 4	Application of statistical and chemometric methods in metabolomics – literature review <i>Discussion of statistical and chemometric methods (PCA, PLS-DA, OPLS-DA) used in metabolomics, interpretation of the obtained data, search for a panel of biomarkers.</i>	4
Lab 5	Discussion of the operation of the instruments, preparation of NMR and MS spectra <i>Presentation of the NMR and MS instrument with a discussion of the measurements. Demonstration of important individual measurement steps.</i>	2
Lab 6	Preparation of biofluid samples for analysis (e.g. blood and milk - commercial material of animal origin) with and without extraction of metabolites and NMR spectra <i>Preparation of biofluids along with individual stages of metabolite extraction. Influence of sample preparation/extraction conditions on the results obtained. Sample preparation - with and without metabolite</i>	3

	<i>extraction. Differences in the sample preparation process</i>	
Lab 7	Preparation of muscle and liver tissue for analysis (model purchased material - pork) along with preparation of NMR and MS spectra. <i>Preparation of muscle and liver tissue along with individual stages of metabolite extraction. Influence of sample preparation/extraction conditions on the results obtained.</i>	3
Lab 8	Analysis of the obtained spectra for the determination of selected metabolites. Presentation of spectra with discussion of metabolites and their interpretation. <i>The use of computer programs for visualization of NMR and MS spectra along with their discussion</i>	4
Lab 9	Application of statistical, chemometric and bioinformatic tools to analyze results, discriminant analysis <i>Application of computer programs for statistical, chemometric and bioinformatic analysis of the obtained results - comparative and discriminatory studies.</i>	3
	Total hours	30

TEACHING TOOLS USED
N1. Multimedia presentations at lecture. N2. Film screenings. N3. Instruments of the metabolomic laboratory (homogenizer, centrifuge, etc.) N4. Computer software

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
Lecture		
P	PEU_W01-PEU_W06, PEU_K01	kolokwium
Laboratory		
F1	PEU_U01- PEU_U07	Report on laboratory classes
F2		Activities during classes
P		$P = 70\%F1 + 30\%F2$

PRIMARY AND SECONDARY LITERATURE
PRIMARY LITERATURE: [1] Spectroscopic methods and their application to the identification of organic compounds, edited by Wojciech Zieliński and Andrzej Rajca; [author] Roman Mazurkiewicz [et al.] [2] Statistics and chemometrics in analytical chemistry, James Miller, Miller Jane [3] Materials from the lecture [4] scientific journals containing information related to the subject [5] knowledge found on websites. SECONDARY LITERATURE: [1] William J Griffiths, NMR spectroscopy, Basic principles, concepts, and applications in chemistry, Secodn Edition, H Guenter, JOOHN WILEY & SONS [2] Metabolomics, Methods and Protocols, Wolfram Weckwerth, HUMANA PRESS; [3] Metabolomics, Metabonomics and Metabolite Profiling, William J. Griffiths, RSC Publishing [4] Mass Spectrometry, Juergen H Gross, Springer SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS) prof. dr hab. Piotr Mlynarz, piotr.mlynarz@pwr.edu.pl