

FACULTY of CHEMISTRY					
<b>SUBJECT CARD</b>					
<b>Name of subject in Polish</b> METABOLOMIKA					
<b>Name of subject in English</b> METABOLOMICS					
<b>Main field of study (if applicable):</b> BIOSCIENCES					
<b>Specialization (if applicable):</b> MEDICINAL CHEMISTRY					
<b>Profile:</b> academic / <del>practical</del> *					
<b>Level and form of studies:</b> <del>1st/ 2nd level, uniform magister studies*</del> , full-time / <del>part-time</del> *					
<b>Kind of subject:</b> obligatory / <del>optional</del> / <del>university-wide</del> *					
<b>Subject code</b> W03BSS-SM2021W, W03BSS-SM2021L					
<b>Group of courses</b> 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	<b>General presentation of the subject's characteristics - assumptions, goals, possibilities</b> <i>General overview of the subject, definitions of assumptions and goals of metabolomics</i>	1
Lec 2	<b>Methods of sample preparation for metabolomics analysis.</b> <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	<b>Application of MS mass spectrometry in metabolomics.</b> <i>Discussion of the basics and principles of operation of a mass spectrometer coupled with liquid chromatography.</i>	2
Lec 4	<b>Application of nuclear magnetic resonance (NMR) spectrometry in metabolomics</b> <i>Discussion of the basics and principles of operation of nuclear magnetic resonance spectroscopy.</i>	2
Lec 5	<b>Application of chemometric and statistical methods in metabolomics.</b> <i>Introduction to statistical and chemometric methods used in metabolomics, familiarization with the interpretation of results.</i>	2
Lec 6	<b>Bioinformatics tools</b> <i>Metabolomics analysis programs will be discussed, e.g. the MetPa program, along with the determination of disturbed metabolic pathways.</i>	2
Lec 7	<b>Application of metabolomics methods in medical diagnostics</b> <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	<b>Presentation of the general characteristics of the subject - literature review</b> <i>Discussion of basic concepts and definitions. Scope of applicability of metabolomics research. Methods used</i>	1
Lab 2	<b>Application of NMR spectroscopy in metabolomics – literature review</b> <i>Discussion of the principles of NMR spectroscopy, processing and interpretation of spectra, search for biomarkers</i>	5
Lab 3	<b>Application of MS mass spectrometry in metabolomics – a literature review</b> <i>Discussion of the principles of MS mass spectrometry, processing and interpretation of spectra, search for biomarkers</i>	5
Lab 4	<b>Application of statistical and chemometric methods in metabolomics – literature review</b> <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	<b>Discussion of the operation of the instruments, preparation of NMR and MS spectra</b> <i>Presentation of the NMR and MS instrument with a discussion of the measurements. Demonstration of important individual measurement steps.</i>	2
Lab 6	<b>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</b> <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	<b>Preparation of muscle and liver tissue for analysis (model purchased material - pork) along with preparation of NMR and MS spectra.</b> <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	<b>Analysis of the obtained spectra for the determination of selected metabolites.</b> <b>Presentation of spectra with discussion of metabolites and their interpretation.</b> <i>The use of computer programs for visualization of NMR and MS spectra along with their discussion</i>	4
Lab 9	<b>Application of statistical, chemometric and bioinformatic tools to analyze results, discriminant analysis</b> <i>Application of computer programs for statistical, chemometric and bioinformatic analysis of the obtained results - comparative and discriminatory studies.</i>	3
	<b>Total hours</b>	<b>30</b>

#### 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

<b>Evaluation</b> (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		Activiti during classes
P		P = 70%F1 + 30%F2

<b>PRIMARY AND SECONDARY LITERATURE</b>
<b>PRIMARY LITERATURE:</b> [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.
<b>SECONDARY LITERATURE:</b> [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
<b>SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)</b>
<b>prof. dr hab. Piotr Mlynarz, piotr.mlynarz@pwr.edu.pl</b>