

PROGRAM OF STUDIES

| | |
|-----------------------------|------------------------------------------------|
| FACULTY: | CHEMISTRY |
| MAIN FIELD OF STUDY: | BIOSCIENCES |
| BRANCH OF SCIENCE: | natural sciences |
| DISCIPLINES: | D1 chemical sciences (major discipline) |
| EDUCATION LEVEL: | second-level studies (3-semester) |
| FORM OF STUDIES: | full-time studies |
| PROFILE: | general academic |
| LANGUAGE OF STUDY: | English |

Content:

1. Assumed learning outcomes – attachment no. 1 to the program of studies
2. Program of studies description – attachment no. 2 to the program of studies

Resolution no. ... of the Senate of Wrocław University of Science and Technology

In effect since **2024/2025**

ASSUMED LEARNING OUTCOMES

FACULTY: Chemistry
MAIN FIELD OF STUDY: BIOSCIENCES
EDUCATION LEVEL: second-level studies
PROFILE: general academic

Location of the main-field-of study:

Branch of science: **natural sciences** Discipline: **chemical sciences**

Explanation of the markings:

Reference to PRK characteristics:

P7U – universal first-degree characteristics corresponding to education at the second-level studies - 7 PRK level

P7S – second degree characteristics corresponding to education at the second-level studies - 7 PRK level

after the underscore:

W – category "knowledge" (extension: G = depth and scope, K = context),

U – category "skills" (extension: W = use of knowledge, K = communication, O = work organization, U = learning),

K – category "social competences" (extension: K = critical assessment, O = responsibility, R = professional role),

INŻ – learning outcomes leading to obtaining engineering competences.

Symbols of main field of study learning outcomes at the second cycle of studies for BIOSCIENCES (bs)

before the underscore:

K – directional learning outcomes,

2 – second cycle of studies

A – general academic profile

bs – direction code,

after the underscore:

W – knowledge category, **U** – skills category, **K** – social competence category

| Main field of study learning outcomes | Description of learning outcomes for the main-field-of study BIOSCIENCES After completion of studies, the graduate: | Reference to PRK characteristics | | |
|---------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------|-------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
| | | Universal first degree characteristics (U) | Second degree characteristics typical for qualifications obtained in higher education (S) | |
| | | | Characteristics for qualifications on 6 / 7* levels of PRK | Characteristics for qualifications on 6 and 7 levels of PRK, enabling acquiring engineering competences |
| KNOWLEDGE (W) | | | | |
| K2Abs_W01 | Possesses in-depth knowledge of mathematics enabling understanding, quantitative description and/or modeling of chemical and/or biotechnological processes | P7U_W | P7S_WG | P7S_WG_INŽ |
| K2Abs_W02 | Has structured and theoretically based the knowledge of advanced methods used in the identification and characterization of biomolecules and the organization of a research laboratory | P7U_W | P7S_WG | |
| K2Abs_W03 | Knows the principles of formulating hypotheses, building models and formulating theories in the context of the concepts of development of biotechnology and chemistry | P7U_W | P7S_WG | |
| K2Abs_W04 | Knows the concepts and principles of intellectual property protection, patent protection and copyright in the context of the preparation of master thesis | P7U_W | P7S_WK | |
| K2Abs_W05 | Has in-depth knowledge of chemistry necessary to perform chemical analyses, illustrating them with chemical reactions. Recognizes and explains the accompanying physicochemical phenomena | P7U_W | P7S_WG | |
| K2Abs_W06 | Possesses based knowledge enabling the description and characterization of modern instrumental analytical and/or computational methods. | P7U_W | P7S_WG | |
| K2Abs_W07 | Has extended knowledge of the structure of matter and its mathematical description. Explains the laws important in structure identification | P7U_W | P7S_WG | |
| K2Abs_W08 | Knows the postulates of quantum mechanics and the mathematical bases of computational methods of quantum chemistry and molecular mechanics | P7U_W | P7S_WG | |
| K2Abs_W09 | Knows the concepts of molecular mechanics and dynamics. | P7U_W | P7S_WG | |

| | | | | |
|-------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------|------------------|------------|
| K2Abs_W10 | Has knowledge of mathematics to the extent necessary to design and drug analysis. Knows the theoretical basis of computational methods and computer techniques used in drug design | P7U_W | P7S_WG | P7S_WG_INŽ |
| K2Abs_W11 | Has knowledge of mathematics, numerical and computational methods on the level of molecular modeling and correlating the obtained results with experimental and observational data | P7U_W | P7S_WG | |
| K2Abs_W12 | Knows the theoretical foundations of the functioning of appropriate scientific equipment in the field of drug analysis | P7_UW | P7S_WG | |
| K2Abs_W13 | Knows the physicochemical basis of techniques used in designing of new materials for biotechnology, nanomedicine and pharmacy | P7U_W | P7S_WG | |
| K2Abs_W14 | Knows informatic tools useful in biological research. | P7U_W | P7S_WG | |
| K2Abs_W15 | Has structured, theoretically based knowledge in area biopharmaceuticals | P7U_W | P7S_WG | |
| K2Abs_W16 | Understands the economic, legal and ethical conditions of professional activity | P7U_W | P7S_WK | P7S_WK_INŽ |
| K2Abs_W17 | Has in-depth knowledge of mathematical and IT tools enabling understanding, quantitative description, modeling and design of materials or engineering objects or chemical/biotechnological processes. | P7U_W | P7S_WG | P7S_WG_INŽ |
| K2Abs_W18 | Has in-depth knowledge of exact and natural sciences as well as engineering and technology, allowing the use of methods and concepts necessary to describe materials, chemical or biotechnological processes. | P7U_W | P7S_WG | P7S_WG_INŽ |
| SKILLS (U) | | | | |
| K2Abs_U01 | Selects and applies mathematical methods in planning and analysis of the experiments | P7U_UW | P7S_UW | P7S_UW_INŽ |
| K2Abs_U02 | Selects and is able to use appropriate methods, techniques and research tools within the appropriate field of study necessary to explain the given problem | P7U_UW | P7S_UW | |
| K2Abs_U03 | Uses computer software to prepare results and statistically analyze the experimental data | P7U_UW | P7S_UW | P7S_UW_INŽ |
| K2Abs_U04 | Uses acquired knowledge in chemistry to related fields of science and scientific disciplines. Demonstrates the ability to work in interdisciplinary teams | P7U_UW | P7S_UO | |
| K2Abs_U05 | Is able to develop research results, critically analyze them and formulate the conclusions | P7U_UW | P7S_UW | |
| K2Abs_U06 | Is able to present the results of own research in the form of a written study | P7U_UW | P7S_UW P7S_UK | |
| K2Abs_U07 | Is able to present the goals and results of scientific work in the form of an oral presentation using modern techniques of communication | P7U_UW | P7S_UW P7S_UK | |

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|-------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------|------------------|------------|
| K2Abs_U08 | Is able to plan experiments and perform basic analyzes using appropriate instrumental equipment and evaluate the results of the experiments. Possesses ability to make theoretical calculations and use available software to simulate the experiment | P7U_UW | P7S_UW | |
| K2Abs_U09 | Is able to use selected the programs that implement quantum chemical computational methods | P7U_UW | P7S_UW | |
| K2Abs_U10 | Is able to apply methods of molecular mechanics and dynamics to solve chemical problems and use algorithms of differentiation, integration and trajectory analysis | P7U_UW | P7S_UW | |
| K2Abs_U11 | Is able to efficiently use modern informatic tools for solving problems in the field of biological and chemical sciences | P7U_UW | P7S_UW | |
| K2Abs_U12 | Is able to use basic methods of quantum chemistry to describe the structure and physicochemical properties of molecules | P7U_UW | P7S_UW | |
| K2Abs_U13 | Is able to write programs or scripts solving numerical problems in the area of computational chemistry and engineering sciences | P7U_UW | P7S_UW | P7S_UW_INŽ |
| K2Abs_U14 | can use a foreign language at level B2+ of the Common European Framework of Reference for Languages | P7U_U | P7U_UK | |
| K2Abs_U15 | is able to independently plan and implement continuous own education in the field of chemical engineering and related sciences; is able to pass on his knowledge to others | P7U_U | P7U_UU | |
| SOCIAL COMPETENCES (K) | | | | |
| K2Abs_K01 | is ready to critically evaluate his knowledge and received content. | P7U_K | P7S_KK | |
| K2Abs_K02 | understands the need for entrepreneurial thinking and action and is aware of the need to act in the public interest. | P7U_K | P7S_KO | |
| K2Abs_K03 | understands the need to take initiatives, inspire and organize activities for the benefit of the socio-economic environment. | P7U_K | P7S_KO | |
| K2Abs_K04 | is ready to cooperate responsibly in a group, performing role taking into account the needs of the team (and/or social needs) | P7U_K | P7S_KR | |
| K2Abs_K05 | is ready to comply with the principles of professional ethics and respect the law, including copyright. | P7U_K | P7S_KR | |
| K2Abs_K06 | recognizes the importance and understands the non-technical aspects and consequences of scientific and engineering activities, including their impact on the environment, as well as the associated responsibilities. | P7U_K | P7S_KK P7S_KO | |
| K2Abs_K07 | is aware of the social role of a technical university graduate and the need to maintain the ethos of the engineering profession. | P7U_K | P7S_KR | |
| K2Abs_K08 | is ready to recognize the importance of knowledge in solving problems in the field of study and related sciences; recognizes the need to seek expert opinion when difficulties arise in solving problems. | P7U_K | P7S_KK | |

DESCRIPTION OF THE PROGRAM OF STUDIES

| | |
|------------------------------------------------------------------------------|-----------------------------------|
| Main field of study: Biosciences | Profile: general academic |
| Level of studies: 2 nd level studies (3 sem. magisterskie) | Form of studies: full-time |

1. General description

| | |
|--------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 1.1 Number of semesters: 3 | 1.2 Total number of ECTS points necessary to complete studies at a given level: 90 |
| 1.3 Total number of hours: 1095 MDC 1110 BII | 1.4 Prerequisites (particularly for second-level studies): are set out in the Order-"The conditions and procedures for recruitment" in the Technical University of Wrocław |
| 1.5 Upon completion of studies graduate obtains professional degree of: magister inżynier | 1.6 Graduate profile, employability: |

| | |
|--|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p><i>The graduate has mastered theory and practice in the use of modern methods of medicinal chemistry, theoretical and computational chemistry and bioinformatics tools enabling: drug design, structural and spectroscopic analysis and insight into the dynamics of processes occurring at the molecular level in macromolecules. The graduate knows the basics of bioinformatics data analysis, machine learning, data mining and big data science, and also has in-depth programming skills in Python and is prepared to work in IT companies, the pharmaceutical industry and in research laboratories.</i></p> |
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¹BU – number of ECTS points assigned to hours of classes requiring direct participation of academic teachers and other persons conducting classes

²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

| | |
|---------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <p>1.7 Possibility of continuing studies:</p> <p>Eligibility to apply for admission to a doctoral school, non-degree postgraduate programmes</p> | <p>1.8 Indicate connection with University's mission and its development strategy:</p> <p><i>The mission and strategy of Wrocław University of Science and Technology were defined in the document entitled: "Strategy of Wrocław University of Science and Technology 2023-2030". The second-cycle study program in Biosciences fits into the key areas of the strategy and the overarching strategic goals both in the area of education, scientific research and cooperation with the environment. It is also consistent with the mission of "creating and transmitting knowledge that responds to new challenges and opportunities emerging before society, economy and civilization. The study program is consistent with the strategic goals by: (1) developing creative skills in the nature of scientific work through an increased number of classes related to the completion of a diploma thesis, (2) a large share (over 50%) of active classes, such as laboratories, exercises, seminars and projects, (3) ensuring a balance between the general and specialized knowledge, (4) providing students with knowledge and skills covering the latest achievements of science and technology in the field of bioinformatics and medicinal chemistry, (5) developing social competences, with particular emphasis on the development of teamwork skills, (6) developing the ability to work using the project method in the IT and (bio-)chemical laboratories.</i></p> |
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2. Detailed description

2.1 Total number of learning outcomes in the program of study: W (knowledge) =18, U (skills) = 15, K (competences) = 8
W + U + K = 41

2.2 For the main field of study assigned to more than one discipline - the number of learning outcomes assigned to the discipline:

D1 (major) (this number must be greater than half the total number of learning outcomes)

2.3 For the main field of study assigned to more than one discipline - percentage share of the number of ECTS points for each discipline:

D1 100% ECTS points

2.4a. For the general academic profile of the main field of study – the number of ECTS points assigned to the classes related to the University's academic activity in the discipline or disciplines to which the main field of study is assigned – DN (must be greater than 50% of the total number of ECTS points from 1.2)

| Specialization | Total number of ECTS points |
|----------------------------|-----------------------------|
| <i>Bioinformatics</i> | 73 |
| <i>Medicinal Chemistry</i> | 73 |

2.4b. For the practical profile of the main field of study - the number of ECTS points assigned to the classes shaping practical skills (must be greater than 50% of the total number of ECTS points from 1.2)

2.5 Concise analysis of compliance of the assumed learning outcomes with the needs of the labor market

The needs of the labor market in the field of Biosciences are indirectly presented in this Study Program under the heading Profile of the graduate, employment opportunities. The preparation of graduates listed there is reflected, among others, in the following learning outcomes: (1) Is able to conduct scientific experiments, develop and interpret their results and relate them to appropriate theories or scientific hypotheses, (2) Using techniques appropriate to the field studied, I can characterize in terms of properties physicochemical and biological biological systems using both quantum chemistry and molecular modeling tools as well as selected experimental methods, (3) Has in-depth knowledge of quantum chemistry, molecular dynamics and molecular modeling, (4) Has in-depth programming skills in Python and knows the operating system Linux,

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⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

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(5) Has practical knowledge of various methods of bioinformatic data analysis in contemporary research in the field of exact and natural sciences, (6) Is aware of the importance and understanding of non-technical aspects and effects of scientific and engineering activities, including their impact on the environment, and as well as the associated responsibilities.

The expected learning outcomes meet the current needs of the biotechnology industry, including companies and workplaces dealing with the design, synthesis and development of biologically active substances technology, the pharmaceutical industry, as well as the IT sector.

2.6 The total number of ECTS points that a student must obtain in classes requiring direct participation of academic teachers or other persons conducting classes and students (enter the sum of ECTS points for subjects/ groups of classes marked with the BU¹ code)

| Specialization | Total number of ECTS points (BU) |
|----------------------------|----------------------------------|
| <i>Bioinformatics</i> | 50,5 |
| <i>Medicinal Chemistry</i> | 49,5 |

2.7. Total number of ECTS points, which student has to obtain from basic sciences classes

| | BII | MDC |
|-----------------------------------------------|----------|----------|
| Number of ECTS points for obligatory subjects | 3 | 3 |
| Number of ECTS points for optional subjects | 4 | 2 |
| Total number of ECTS points | 7 | 5 |

2.8. Total number of ECTS points, which student has to obtain from practical classes, including project and laboratory classes (enter total number of ECTS points for subjects/group of classes denoted with code P)

| | BII | MDC |
|-----------------------------------------------|-----------|-----------|
| Number of ECTS points for obligatory subjects | 10 | 10 |
| Number of ECTS points for optional subjects | 53 | 50 |
| Total number of ECTS points | 63 | 60 |

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⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

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2.9. Minimum number of ECTS points, which student has to obtain doing education blocks offered as part of University-wide classes or other main field of study (enter number of ECTS points for subjects/group of classes denoted with code O)

8 ECTS points

2.10. Total number of ECTS points, which student may obtain doing optional blocks (min. 30% of total number of ECTS points)

70 ECTS points

3. Description of the process leading to learning outcomes acquisition:

Verification and assessment of learning outcomes with reference to courses or groups of courses throughout the entire education cycle takes place in relation to the information contained in the subject cards (syllabuses).

The student acquires knowledge and skills by participating in theoretical and practical classes, which are largely based on the results of scientific research conducted by academic teachers - course tutors conducting classes with students. The basis of teaching and learning process are laboratory, seminar and project courses. Education in the field of studies is conducted in accordance with the principle of increasing the complexity of theoretical and practical tasks set for students. Modern teaching methods are implemented in the teaching practice, thanks to which the students' activity during the classes increases. Theoretical courses in the form of lectures and seminars are supplemented with project and laboratory classes, which include, among others: computer modelling and design, as well as conducting scientific research. The program is complemented by humanities and foreign language courses. The course (study programme) ends with a master thesis preparation and its defence checking the student's theoretical knowledge.

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⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

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4. List of education blocks:

4.1. List of obligatory blocks:

4.1.1 List of general education blocks

4.1.1.1 Liberal-managerial subjects block (min. ECTS points):

| No. | Subject group of classes code | Name of Subject/group of classes (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of Subject/g group of courses | Way ³ of crediting | Subject/group of classes | | | |
|-----|-------------------------------|---------------------------------------------------------------------------|------------------------|----|-----|----|-----|------------------------|-----------------|------|-----------------------|-------------------------|-------------------------|-------------------------------------------------|-------------------------------|-------------------------------|-----------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | University -wide ⁴ | Concerning scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| | | | | | | | | | | | | | | | | | | | |
| | | Total | | | | | | | | | | | | | | | | | |

4.1.1.2 Foreign languages block (min. ECTS points):

| No. | Subject group of classes code | Name of Subject/group of classes (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of Subject/g group of courses | Way ³ of crediting | Subject/group of classes | | | |
|-----|-------------------------------|---------------------------------------------------------------------------|------------------------|----|-----|----|-----|------------------------|-----------------|------|-----------------------|-------------------------|-------------------------|-------------------------------------------------|-------------------------------|-------------------------------|-----------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | University -wide ⁴ | Concerning scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| | | | | | | | | | | | | | | | | | | | |
| | | Total | | | | | | | | | | | | | | | | | |

4.1.1.3 Sporting classes block (0 ECTS points):

| No. | Subject group of classes code | Name of Subject/group of classes (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of Subject/g group of courses | Way ³ of crediting | Subject/group of classes | | | |
|-----|-------------------------------|---------------------------------------------------------------------------|------------------------|----|-----|----|-----|------------------------|-----------------|------|-----------------------|-------------------------|-------------------------|-------------------------------------------------|-------------------------------|-------------------------------|-----------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | University -wide ⁴ | Concerning scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| | | | | | | | | | | | | | | | | | | | |
| | | Total | | | | | | | | | | | | | | | | | |

¹BU – number of ECTS points assigned to hours of classes requiring direct participation of academic teachers and other persons conducting classes

²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

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4.1.1.4 Information technologies block (min. ECTS points):

| No. | Subject group of classes code | Name of Subject/group of classes (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of Subject/group of courses | Way ³ of crediting | Subject/group of classes | | | |
|-----|-------------------------------|-----------------------------------------------------------------------------------|------------------------|----|-----|----|-----|------------------------|-----------------|------|-----------------------|-------------------------|-------------------------|-----------------------------------------------|-------------------------------|------------------------------|-----------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | University-wide ⁴ | Concerning scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| | | | | | | | | | | | | | | | | | | | |
| | | Total | | | | | | | | | | | | | | | | | |

Altogether for general education blocks

| Total number of hours | | | | | Total number of ZZU hours | Total number of CNPS hours | Total number of ECTS points | Total number of ECTS points for DN classes ⁵ | Number of ECTS points for BU classes ¹ |
|-----------------------|----|-----|----|-----|---------------------------|----------------------------|-----------------------------|---------------------------------------------------------|---------------------------------------------------|
| lec | cl | lab | pr | sem | | | | | |
| | | | | | | | | | |

¹BU – number of ECTS points assigned to hours of classes requiring direct participation of academic teachers and other persons conducting classes

²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

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4.1.2 List of basic sciences blocks

4.1.2.1 Mathematics block

| No. | Subject group of classes code | Name of Subject/group of classes (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of Subject/group of courses | Way ³ of crediting | Subject/group of classes | | | |
|-------|-------------------------------|---------------------------------------------------------------------------|------------------------|----|-----|----|-----|------------------------|-----------------|------|-----------------------|-------------------------|-------------------------|-----------------------------------------------|-------------------------------|------------------------------|-----------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | University-wide ⁴ | Concerning scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| Total | | | | | | | | | | | | | | | | | | | |

4.1.2.2 Physics block

| No. | Subject group of classes code | Name of Subject/group of classes (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of Subject/group of courses | Way ³ of crediting | Subject/group of classes | | | |
|-------|-------------------------------|---------------------------------------------------------------------------|------------------------|----|-----|----|-----|------------------------|-----------------|------|-----------------------|-------------------------|-------------------------|-----------------------------------------------|-------------------------------|------------------------------|-----------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | University-wide ⁴ | Concerning scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| Total | | | | | | | | | | | | | | | | | | | |

4.1.2.3 Chemistry block

BII i MDC

| No. | Subject group of classes code | Name of Subject/group of classes (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of Subject/group of courses | Way ³ of crediting | Subject/group of classes | | | |
|--------------|-------------------------------|---------------------------------------------------------------------------|------------------------|----|-----|----|-----|-----------------------------------------------------------------------------------------|-----------------|-----------|-----------------------|-------------------------|-------------------------|-----------------------------------------------|-------------------------------|------------------------------|-----------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | University-wide ⁴ | Concerning scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| 1. | W03BSS-SM2001W | Theoretical chemistry | 2 | | | | | K2Abs_W01 K2Abs_W02 K2Abs_W07 K2Abs_W08 K2Abs_W11 K2Abs_W17 K2Abs_K01 | 30 | 75 | 3 | 3 | 1,3 | T/Z | E | | DN | | PD |
| Total | | | 2 | | | | | | 30 | 75 | 3 | 3 | 1,3 | | 1 | | | | |

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²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

Altogether for basic sciences blocks:

| | Total number of hours | | | | | Total number of ZZU hours | Total number of CNPS hours | Total number of ECTS points | Total number of ECTS points for DN classes ⁵ | Number of ECTS points for BU classes ¹ |
|-----|-----------------------|---|---|---|---|---------------------------|----------------------------|-----------------------------|---------------------------------------------------------|---------------------------------------------------|
| | w | ć | l | p | s | | | | | |
| BII | 2 | | | | | 30 | 120 | 3 | 3 | 1,3 |
| MDC | 2 | | | | | 30 | 120 | 3 | 3 | 1,3 |

¹BU – number of ECTS points assigned to hours of classes requiring direct participation of academic teachers and other persons conducting classes

²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

4.1.3 List of the main field of study blocks

4.1.3.1 Obligatory main field of study blocks

| No. | Subject group of classes code | Name of Subject group of classes (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of Subject/g roup of courses | Way ³ of crediting | Subject/group of classes | | | |
|-----|-------------------------------|-----------------------------------------------------------------------------------|------------------------|----|-----|----|-----|---------------------------------------------------------------------------------------------------------------------------------------------|-----------------|------|-----------------------|-------------------------|-------------------------|------------------------------------------------|-------------------------------|-------------------------------|------------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | University -wide ⁴ | Concerni ng scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| 1 | W03BSS-SM2001L | Theoretical chemistry | | | 2 | | | K2Abs_U03 K2Abs_U04 K2Abs_U05 K2Abs_U09 K2Abs_U12 K2Abs_K08 | 30 | 50 | 2 | 2 | 1,4 | T | Z | | DN | P | K |
| 2 | W03BSS-SM2001C | Theoretical chemistry | | 1 | | | | K2Abs_U02 K2Abs_U12 | 15 | 50 | 2 | 2 | 0,7 | T/Z | Z | | DN | P | K |
| 3 | W03BSS-SM2006W | Rational drug design | 2 | | | | | K2Abs_W02 K2Abs_W05 K2Abs_W06 K2Abs_W10 K2Abs_W12 K2Abs_W13 K2Abs_W14 K2Abs_W15 K2Abs_W18 K2Abs_K01 K2Abs_K06 | 30 | 75 | 3 | 3 | 1,3 | T/Z | Z | | DN | | K |
| 4 | W03BSS-SM2007W | Molecular modeling | 1 | | | | | K2Abs_W09 K2Abs_W11 K2Abs_W14 K2Abs_W17 | 15 | 50 | 2 | 2 | 0,65 | T/Z | E | | DN | | K |
| 5 | W03BSS-SM2007L | Molecular modeling. | | | 2 | | | K2Abs_U13 K2Abs_U10 K2Abs_U05 | 30 | 50 | 2 | 2 | 1,4 | T | Z | | DN | P | K |
| 6 | W03BSS-SM2007S | Molecular modeling.. | | | | | 1 | K2Abs_U07 | 15 | 25 | 1 | 1 | 0,7 | T/Z | Z | | DN | P | K |
| 7 | W03BSS-SM2008L | Retrieval of scientific and technical information | | | 1 | | | K2Abs_U05 K2Abs_K05 | 15 | 25 | 1 | | 0,7 | T | Z | | | P | K |

¹BU – number of ECTS points assigned to hours of classes requiring direct participation of academic teachers and other persons conducting classes

²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

| | | | | | | | | | | | | | | | | | | |
|--------------|----------------|--------------------------------------------|----------|----------|----------|--|----------|---------------------------------------------------------------|------------|------------|-----------|-----------|-------------|-----|----------|--|-----------|---|
| 8 | W03BSS-SM2013W | Machine learning for chemistry and biology | 2 | | | | | K2Abs_W01 K2Abs_W14 K2Abs_W08 K2Abs_W09 K2Abs_K01 | 30 | 50 | 2 | | 1,3 | T/Z | E | | | K |
| 9 | W03BSS-SM2013L | Machine learning for chemistry and biology | | | 2 | | | K2Abs_U02 K2Abs_U11 K2Abs_K02 K2Abs_K04 K2Abs_K05 | 30 | 50 | 2 | | 1,4 | T | Z | | P | K |
| Total | | | 5 | 1 | 7 | | 1 | | 210 | 425 | 17 | 12 | 9,55 | | 2 | | 10 | |

Altogether (for main field of study blocks):

| | Total number of hours | | | | | Total number of ZZU hours | Total number of CNPS hours | Total number of ECTS points | Total number of ECTS points for DN classes ⁵ | Number of ECTS points for BU classes ¹ |
|---------|-----------------------|---|---|---|---|---------------------------|----------------------------|-----------------------------|---------------------------------------------------------|---------------------------------------------------|
| | w | ć | l | p | s | | | | | |
| BII MDC | 5 | 1 | 7 | | 1 | 210 | 425 | 17 | 12 | 9,55 |

¹BU – number of ECTS points assigned to hours of classes requiring direct participation of academic teachers and other persons conducting classes

²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

4.2 List of optional blocks

4.2.1 List of general education blocks

4.2.1.1 Liberal-managerial subjects blocks (min. 5 ECTS points):

| No. | Subject group of classes code | Name of Subject group of classes (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of Subject/g group of courses | Way ³ of crediting | Subject/group of classes | | | |
|-------|-------------------------------|-----------------------------------------------------------------------------------|------------------------|----|-----|----|-----|--------------------------------------------------|-----------------|------|-----------------------|-------------------------|-------------------------|-------------------------------------------------|-------------------------------|------------------------------|-----------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | University-wide ⁴ | Concerning scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| 1 | W03-SM2002BH | Managerial course I | 1 | | | | | K2Abt_W16 K2Abs_K02 K2Abs_K03 K2Abs_K07 | 15 | 60 | 2 | | 0,65 | T/Z | Z | O | | | KO |
| 2 | W03-SM2001BH | Managerial course II | 2 | | | | | K2Abt_W16 K2Abs_K02 K2Abs_K03 K2Abs_K07 | 30 | 90 | 3 | | 1,3 | T/Z | Z | O | | | KO |
| Total | | | 3 | | | | | | 45 | 150 | 5 | | 1,95 | | | | | | |

4.2.1.2 Foreign languages block (min. 3 ECTS points):

| No. | Subject group of classes code | Name of Subject group of classes (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of Subject/g group of courses | Way ³ of crediting | Subject/group of classes | | | |
|-------|-------------------------------|-----------------------------------------------------------------------------------|------------------------|----|-----|----|-----|--------------------------------------------------|-----------------|------|-----------------------|-------------------------|-------------------------|-------------------------------------------------|-------------------------------|------------------------------|-----------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | University-wide ⁴ | Concerning scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| 1 | SJO-SM0004 | Foreign language I | | 1 | | | | K2Abs_U14 K2Abs_U15 K2Abs_K01 K2Abs_K04 | 15 | 30 | 1 | | 0,6 | T/Z | Z | O | | P | KO |
| 2 | SJO-SM0003 | Foreign language II | | 3 | | | | K2Abs_U14 K2Abs_U15 K2Abs_K01 K2Abs_K04 | 45 | 60 | 2 | | 1,8 | T/Z | Z | O | | P | KO |
| Total | | | | 4 | | | | | 60 | 90 | 3 | | 2,4 | | | | | 3 | |

¹BU – number of ECTS points assigned to hours of classes requiring direct participation of academic teachers and other persons conducting classes

²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

Altogether for general education blocks:

| | Total number of hours | | | | | Total number of ZZU hours | Total number of CNPS hours | Total number of ECTS points | Total number of ECTS points for DN classes ⁵ | Number of ECTS points for BU classes ¹ |
|-----|-----------------------|---|---|---|---|---------------------------|----------------------------|-----------------------------|---------------------------------------------------------|---------------------------------------------------|
| | w | é | l | p | s | | | | | |
| BII | 3 | 4 | | | | 105 | 240 | 8 | | 4,35 |
| MDC | 3 | 4 | | | | 105 | 240 | 8 | | 4,35 |

¹BU – number of ECTS points assigned to hours of classes requiring direct participation of academic teachers and other persons conducting classes

²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

4.2.2 List of basic sciences blocks

4.2.2.1 Mathematics block

BII

| No. | Subject group of classes code | Name of Subject group of classes (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of Subject/g roup of courses | Way ³ of crediting | Subject/group of classes | | | |
|--------------|-------------------------------|-----------------------------------------------------------------------------------|------------------------|----|-----|----|-----|----------------------------------------------------------------------------|-----------------|------------|-----------------------|-------------------------|-------------------------|------------------------------------------------|-------------------------------|-------------------------------|------------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | University -wide ⁴ | Concerni ng scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| 1 | W03BSS-SM2002W | Molecular dynamics | 2 | | | | | K2Abs_W03 K2Abs_W07 K2Abs_W09 K2Abs_W11 K2Abs_W18 K2Abs_K01 | 30 | 100 | 4 | 4 | 1,3 | T/Z | Z | | DN | | PD |
| Total | | | 2 | | | | | | 30 | 100 | 4 | 4 | 1,3 | | | | | | |

MDC

| No. | Subject group of classes code | Name of Subject group of classes (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of Subject/g roup of courses | Way ³ of crediting | Subject/group of classes | | | |
|--------------|-------------------------------|-----------------------------------------------------------------------------------|------------------------|----------|-----|----|-----|------------------------|-----------------|-----------|-----------------------|-------------------------|-------------------------|------------------------------------------------|-------------------------------|-------------------------------|------------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | University -wide ⁴ | Concerni ng scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| 1 | W03BSS-SM2017C | Introductory statistics | | 1 | | | | K2Abs_U03 | 15 | 50 | 2 | | 0,7 | T/Z | Z | | | P | PD |
| Total | | | | 1 | | | | | 15 | 50 | 2 | | 0,7 | | | | | 2 | |

4.2.2.2 Physics block (min. ECTS points):

| No. | Subject group of classes code | Name of Subject group of classes (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of Subject/g roup of courses | Way ³ of crediting | Subject/group of classes | | | |
|--------------|-------------------------------|-----------------------------------------------------------------------------------|------------------------|----|-----|----|-----|------------------------|-----------------|------|-----------------------|-------------------------|-------------------------|------------------------------------------------|-------------------------------|-------------------------------|------------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | University -wide ⁴ | Concerni ng scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| Total | | | | | | | | | | | | | | | | | | | |

¹BU – number of ECTS points assigned to hours of classes requiring direct participation of academic teachers and other persons conducting classes

²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

4.2.2.3 Chemistry block (min. ECTS points):

| No. | Subject group of classes code | Name of Subject group of classes (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of Subject/group of courses | Way ³ of crediting | Subject/group of classes | | | |
|-----|-------------------------------|---------------------------------------------------------------------------|------------------------|----|-----|----|-----|------------------------|-----------------|------|-----------------------|-------------------------|-------------------------|-----------------------------------------------|-------------------------------|------------------------------|-----------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | University-wide ⁴ | Concerning scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| | | | | | | | | | | | | | | | | | | | |
| | | Total | | | | | | | | | | | | | | | | | |

Altogether for basic sciences blocks:

| | Total number of hours | | | | | Total number of ZZU hours | Total number of CNPS hours | Total number of ECTS points | Total number of ECTS points for DN classes ⁵ | Number of ECTS points for BU classes ¹ |
|-----|-----------------------|----|-----|----|-----|---------------------------|----------------------------|-----------------------------|---------------------------------------------------------|---------------------------------------------------|
| | lec | cl | lab | pr | sem | | | | | |
| BII | 2 | | | | | 30 | 100 | 4 | 4 | 1,3 |
| MDC | | 1 | | | | 15 | 50 | 2 | 0 | 0,7 |

¹BU – number of ECTS points assigned to hours of classes requiring direct participation of academic teachers and other persons conducting classes

²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

4.2.3 List of main-field of study blocks

4.2.3.1 Diploma profile block (min. 29. ECTS points):

| No. | Subject group of classes code | Name of Subject/group of classes (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of Subject/group of courses | Way ³ of crediting | Subject/group of classes | | | |
|--------------|-------------------------------|-----------------------------------------------------------------------------------|------------------------|----|-----------|----|----------|-----------------------------------------------------------------------------------------|-----------------|------------|-----------------------|-------------------------|-------------------------|-----------------------------------------------|-------------------------------|---------------------------------|------------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | Univer- sity- wide ⁴ | Concerni ng scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| 1 | W03W03-SM2053S | Graduation proseminar | | | | | 1 | K2Abs_U08 K2Abs_U14 K2Abs_K01 K2Abs_K07 | 15 | 25 | 1 | 1 | 0,7 | T/Z | Z | | DN | P | K |
| 2 | W03W03-SM2054D | Graduate laboratory I | | | 4 | | | K2Abs_U02 K2Abs_U05 K2Abs_U14 K2Abs_K01 K2Abs_K05 K2Abs_K07 | 60 | 150 | 6 | 6 | 3 | T | Z | | DN | P | K |
| 3 | W03W03-SM2055D | Graduate laboratory II | | | 14 | | | K2Abs_U02 K2Abs_U05 K2Abs_U14 K2Abs_U06 K2Abs_K01 K2Abs_K05 K2Abs_K07 | 210 | 500 | 20 | 20 | 9,5 | T | Z | | DN | P | K |
| 4 | W03W03-SM2056S | Graduation seminar | | | | | 1 | K2Abs_U05 K2Abs_U07 K2Abs_K01 K2Abs_K06 K2Abs_K07 K2Abs_K08 | 15 | 50 | 2 | 2 | 0,7 | T/Z | Z | | DN | P | K |
| Total | | | | | 18 | | 2 | | 300 | 725 | 29 | 29 | 13,9 | | | | | 29 | |

¹BU – number of ECTS points assigned to hours of classes requiring direct participation of academic teachers and other persons conducting classes

²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

4.2.3.2 Optional courses block

| No. | Subject group of classes code | Name of Subject/group of classes (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of Subject/group of courses | Way ³ of crediting | Subject/group of classes | | | |
|--------------|-------------------------------|-----------------------------------------------------------------------------------|------------------------|----|-----|----|-----|------------------------|-----------------|------|-----------------------|-------------------------|-------------------------|-----------------------------------------------|-------------------------------|------------------------------|-----------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | University-wide ⁴ | Concerning scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| 1 | W03BSS-SM20BW | Elective course* | 2 | | | | | K2Abt_W02 K2Abt_K01 | 30 | 50 | 2 | | 1,3 | T/Z | Z | | | | K |
| Total | | | | | | | | | | | | | | | | | | | |

List of elective course

| No. | Subject group of classes code | Name of Subject group of classes (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of Subject/group of courses | Way ³ of crediting | Subject/group of classes | | | |
|-----|-------------------------------|-----------------------------------------------------------------------------------|------------------------|----|-----|----|-----|------------------------|-----------------|------|-----------------------|-------------------------|-------------------------|-----------------------------------------------|-------------------------------|------------------------------|-----------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | University-wide ⁴ | Concerning scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| 1 | W03BSS-SM2101w | Medicinal and biological chemistry | 2 | | | | | | 30 | 50 | 2 | | 1,3 | T/Z | Z | | | | K |
| 2 | W03BSS-SM2102w | Methodology of experimental research | 2 | | | | | | 30 | 50 | 2 | | 1,3 | T/Z | Z | | | | K |
| 3 | W03BSS-SM2103w | Bioprocess project | 2 | | | | | | 30 | 50 | 2 | | 1,3 | T/Z | Z | | | | K |
| 4 | W03BSS-SM2104w | Advanced polymers for chemical and medical applications | 2 | | | | | | 30 | 50 | 2 | | 1,3 | T/Z | Z | | | | K |

¹BU – number of ECTS points assigned to hours of classes requiring direct participation of academic teachers and other persons conducting classes

²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

Altogether for blocks:

| | Total number of hours | | | | | Total number of ZZU hours | Total number of CNPS hours | Total number of ECTS points | Total number of ECTS points for DN classes ⁵ | Number of ECTS points for BU classes ¹ |
|-----|-----------------------|----|-----|----|-----|---------------------------|----------------------------|-----------------------------|---------------------------------------------------------|---------------------------------------------------|
| | lec | cl | lab | pr | sem | | | | | |
| BII | 2 | | 18 | | 2 | 330 | 775 | 31 | 29 | 15,2 |
| MDC | 2 | | 18 | | 2 | 330 | 775 | 31 | 29 | 15,2 |

¹BU – number of ECTS points assigned to hours of classes requiring direct participation of academic teachers and other persons conducting classes

²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

4.2.4 List of specialization blocks

4.2.4.1 Specialization subjects blocks

BII Bioinformatics (min. 27 ECTS points):

| No. | Subject group of classes code | Name of Subject/group of courses (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of Subject/group of courses | Way ³ of crediting | Subject/group of classes | | | |
|-----|-------------------------------|-----------------------------------------------------------------------------------|------------------------|----|-----|----|-----|---------------------------------------------------------------|-----------------|------|-----------------------|-------------------------|-------------------------|-----------------------------------------------|-------------------------------|---------------------------------|------------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | Univer- sity- wide ⁴ | Concerni ng scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| 1 | W03BSS-SM2002L | Molecular dynamics | | | 2 | | | K2Abs_U02 K2Abs_U03 K2Abs_U06 K2Abs_U10 K2Abs_K08 | 30 | 50 | 2 | 2 | 1,4 | T | Z | | DN | P | S |
| 2 | W03BSS-SM2004W | Bioinformatics | 2 | | | | | K2Abs_W14 | 30 | 75 | 3 | 3 | 1,3 | T/Z | E | | DN | | S |
| 3 | W03BSS-SM2004L | Bioinformatics. | | | 2 | | | K2Abs_U11 | 30 | 50 | 2 | 2 | 1,4 | T | Z | | DN | P | S |
| 4 | W03BSS-SM2003L | Networks and workstations with UNIX system | | | 2 | | | K2Abs_U13 | 30 | 50 | 2 | | 1,4 | T | Z | | | P | S |
| 5 | W03BSS-SM2005L | Applied informatics | | | 4 | | | K2Abs_U13 K2Abs_U11 K2Abs_K08 | 60 | 100 | 4 | 4 | 2,8 | T | Z | | DN | P | S |
| 6 | W03BSS-SM2010P | Advanced bioinformatics | | | | 3 | | K2Abs_K04 K2Abs_U11 K2Abs_U13 | 45 | 75 | 3 | 3 | 2,25 | | Z | | DN | P | S |
| 7 | W03BSS-SM2011W | Bionanotechnology | 2 | | | | | K2Abs_W07 K2Abs_W09 K2Abs_W11 K2Abs_W13 K2Abs_W18 | 30 | 50 | 2 | 2 | 1,3 | T/Z | E | | DN | | S |
| 8 | W03BSS-SM2011S | Bionanotechnology. | | | | | 1 | K2Abs_U07 K2Abs_K07 | 15 | 25 | 1 | 1 | 0,7 | T/Z | Z | | DN | P | S |
| 9 | W03BSS-SM2012L | Advanced programming and numerical methods | | | 3 | | | K2Abs_W17 K2Abs_K04 | 45 | 75 | 3 | 3 | 2,1 | T | Z | | DN | P | S |

¹BU – number of ECTS points assigned to hours of classes requiring direct participation of academic teachers and other persons conducting classes

²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

| | | | | | | | | | | | | | | | | | | | |
|-------|----------------|-------------------------------------------|----------|--|-----------|----------|----------|---------------------------------------------------------------|------------|------------|-----------|-----------|-------------|-----|----------|--|----|-----------|---|
| | | | | | | | | K2Abs_U11 K2Abs_U13 | | | | | | | | | | | |
| 10 | W03BSS-SM2009L | Data mining | | | 1 | | | K2Abs_U02 K2Abs_K05 | 15 | 25 | 1 | 1 | 0,7 | T | Z | | DN | P | S |
| 11 | W03BSS-SM2014W | Computational genomics | 1 | | | | | K2Abs_W02 K2Abs_W14 K2Abs_W17 | 15 | 25 | 1 | 1 | 0,65 | T/Z | E | | DN | | S |
| 12 | W03BSS-SM2014L | Computational genomics. | | | 1 | | | K2Abs_U01 K2Abs_K07 | 15 | 25 | 1 | 1 | 0,7 | T | Z | | DN | P | S |
| 13 | W03BSS-SM2015L | Molecular engineering in genomic analyses | | | 3 | | | K2Abs_W06 K2Abs_U02 K2Abs_U03 K2Abs_U05 K2Abs_U08 | 45 | 50 | 2 | 2 | 2,1 | T | Z | | DN | P | S |
| Total | | | 5 | | 18 | 3 | 1 | | 405 | 675 | 27 | 25 | 18,8 | | 3 | | | 21 | |

¹BU – number of ECTS points assigned to hours of classes requiring direct participation of academic teachers and other persons conducting classes

²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

MDC Medicinal chemistry (min 29 ECTS points)

| No. | Subject group of classes code | Name of Subject/group of courses (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of Subject/group of courses | Way ³ of crediting | Subject/group of classes | | | |
|-----|-------------------------------|-----------------------------------------------------------------------------------|------------------------|----|-----|----|-----|---------------------------------------------------------------|-----------------|------|-----------------------|-------------------------|-------------------------|-----------------------------------------------|-------------------------------|-------------------------------|------------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | Unive-rsity-wide ⁴ | Concerni-ng scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| 1. | W03BSS-SM2020W | Spectroscopic methods in medicinal chemistry | 2 | | | | | K2Abs_W02 K2Abs_W06 K2Abs_W13 | 30 | 50 | 2 | 2 | 1,3 | T/Z | E | | DN | | S |
| 2. | W03BSS-SM2020L | Spectroscopic methods in medicinal chemistry | | | 2 | | | K2Abs_U02 K2Abs_U08 K2Abs_K08 | 30 | 50 | 2 | 2 | 1,4 | T | Z | | DN | P | S |
| 3. | W03BSS-SM2021W | Metabolomics | 1 | | | | | K2Abs_W06 K2Abs_W07 K2Abs_K01 | 15 | 50 | 2 | 2 | 0,65 | T/Z | Z | | DN | | S |
| 4. | W03BSS-SM2021L | Metabolomics | | | 2 | | | K2Abs_W14 K2Abs_U03 K2Abs_K06 | 30 | 50 | 2 | 2 | 1,4 | T | Z | | DN | P | S |
| 5. | W03BSS-SM2018W | Crystallography and structure of solids | 2 | | | | | K2Abs_W02 K2Abs_W06 K2Abs_W07 K2Abs_W18 K2Abs_K01 | 30 | 50 | 2 | 2 | 1,3 | T/Z | Z | | DN | | S |
| 6. | W03BSS-SM2018C | Crystallography and structure of solids | | 1 | | | | K2Abs_U01 K2Abs_U02 | 15 | 25 | 1 | 1 | 0,7 | T/Z | Z | | DN | P | S |
| 7. | W03BSS-SM2019W | Analytical methods in drug design and technology | 1 | | | | | K2Abs_W02 K2Abs_W06 | 15 | 50 | 2 | 2 | 0,65 | T/Z | Z | | DN | | S |
| 8. | W03BSS-SM2019L | Analytical methods in drug design and technology. | | | 2 | | | K2Abs_U01 K2Abs_U03 K2Abs_U08 | 30 | 50 | 2 | 2 | 1,4 | T | Z | | DN | P | S |
| 9. | W03BSS-SM2016L | Isolation and identification of bioproducts | | | 2 | | | K2Abs_U02 K2Abs_U03 K2Abs_W05 K2Abs_K08 | 30 | 50 | 2 | 2 | 1,4 | T | Z | | DN | P | S |
| 10. | W03BSS-SM2022W | Medicinal natural products | 1 | | | | | K2Abs_W03 K2Abs_W12 K2Abs_W15 | 15 | 50 | 2 | 2 | 0,65 | T/Z | E | | DN | | S |

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³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

| | | | | | | | | | | | | | | | | | | | |
|--------------|----------------|-----------------------------------------------|-----------|----------|-----------|--|--|---------------------------------------------------------------|------------|------------|-----------|-----------|-------------|-----|----------|--|----|-----------|---|
| 11. | W03BSS-SM2022L | Medicinal natural products. | | | 2 | | | K2Abs_U02 K2Abs_K04 | 30 | 50 | 2 | 2 | 1,4 | T | Z | | DN | P | S |
| 12. | W03BSS-SM2023W | Modern pharmaceuticals and biopharmaceuticals | 2 | | | | | K2Abs_W02 K2Abs_W07 K2Abs_W12 K2Abs_W06 K2Abs_K01 | 30 | 50 | 2 | 2 | 1,3 | T/Z | E | | DN | | S |
| 13. | W03BSS-SM2023L | Modern pharmaceuticals and biopharmaceuticals | | | 2 | | | K2Abs_U02 K2Abs_U05 K2Abs_K05 K2Abs_K08 | 30 | 50 | 2 | 2 | 1,4 | T | Z | | DN | P | S |
| 14. | W03BSS-SM2024L | Multistep organic synthesis | | | 4 | | | K2Abs_U02 K2Abs_U04 K2Abs_U05 K2Abs_K08 | 60 | 75 | 3 | 3 | 2,8 | T | Z | | DN | P | S |
| 15. | W03BSS-SM2025W | Inorganic drugs | 1 | | | | | K2Abs_W02 K2Abs_W03 | 15 | 25 | 1 | 1 | 0,65 | T/Z | Z | | DN | | S |
| Total | | | 10 | 1 | 16 | | | | 405 | 725 | 29 | 29 | 18,4 | | 3 | | | 16 | |

Altogether for specialization blocks:

| | Total number of hours | | | | | Total number of ZZU hours | Total number of CNPS hours | Total number of ECTS points | Total number of ECTS points for DN classes ⁵ | Number of ECTS points for BU classes ¹ |
|-----|-----------------------|----|-----|----|-----|---------------------------|----------------------------|-----------------------------|---------------------------------------------------------|---------------------------------------------------|
| | lec | cl | lab | pr | sem | | | | | |
| BII | 5 | | 18 | 3 | 1 | 405 | 675 | 27 | 25 | 18,8 |
| MDC | 10 | 1 | 16 | | | 405 | 725 | 29 | 29 | 18,4 |

¹BU – number of ECTS points assigned to hours of classes requiring direct participation of academic teachers and other persons conducting classes

²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

4.3 Training block - concerning principles of training crediting – attachment no.

Not applicable

Opinion of the Advisory Faculty Council concerning the rules of crediting training block

| Name of training | | | |
|-----------------------|---------------------------------------------------|-------------------------|------|
| Number of ECTS points | Number of ECTS points for BU ¹ classes | Training crediting mode | Code |
| | | | |
| Training duration | | Training objective | |
| | | | |

4.4 „Diploma dissertation” block

| Type of diploma dissertation | Licencjat / inżynier / magister / magister inżynier* | |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------|----------------------------------------------------------------------|
| Number of diploma dissertation semesters | Number of ECTS points | Code |
| 3 | 29 | W03W03-SM2053S W03W03-SM2054D W03W03-SM2055D W03W03-SM2056S |
| Character of diploma dissertation | | |
| Thesis of the second cycle (master) should have traits of scientific, experimental or theoretical, with a primary or practical. Work should lead to new results of original research or technical and technological solutions, and its presentation in the form of written work should include the results and show the knowledge and skills of the author, including but not limited to: (1)The ability to formulate objectives and research questions; (2)Ability to use literature and other sources of knowledge ;(3)The ability to plan and carry out research and other activities to achieve its objectives and problems; (4)Ability to correctly interpret the results; (5)Ability to use precise and clear language and the proper matching of the images presented to illustrate the problem. | | |
| Number of BU ¹ ECTS points | 13,9 | |

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⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

5. Ways of verifying assumed learning outcomes

| Form of classes | Ways of verifying assumed learning outcomes |
|----------------------|-------------------------------------------------------------|
| lecture | e.g. examination, progress/final test |
| class | e.g. progress/final test |
| laboratory | e.g. pretest, report from laboratory |
| project | e.g. project defence |
| seminar | e.g. participation in discussion, topic presentation, essay |
| diploma dissertation | prepared diploma dissertation |

6. Range of diploma examination

BII

1. General aspects of biotechnology.
2. Drug design methods
3. Bioinformatics - selected issues

MDC

1. General aspects of medicinal chemistry.
2. Methods of drug design and synthesis
3. Biological chemistry - selected issues

7. Requirements concerning deadlines for crediting subject/groups of subject for all courses in particular blocks

Each course should be passed in accordance with the study plan. If it is necessary to repeat a course, it should be completed in the next semester in which it is offered.

***T/Z** Remote form of classes requires Dean's approved, but cannot exceed 75 % of ECTS points.

T/Z option is accepted only for lectures, exercises and seminars

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³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

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8. Plan of studies (attachment no. 4)

Approved by faculty student government legislative body:

.....
Date

.....
name and surname, signature of student representative

.....
Date

.....
Dean's signature

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²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

PLAN OF STUDIES

| | |
|-----------------------------|------------------------------------------|
| FACULTY: | Chemistry |
| MAIN FIELD OF STUDY: | BIOSCIENCES |
| EDUCATION LEVEL: | second-level studies (3-semester) |
| FORM OF STUDIES: | full-time studies |
| PROFILE: | general academic |
| SPECIALIZATION: | Bioinformatics |
| LANGUAGE OF STUDY: | English |

In effect since **2024/2025**

Plan of studies structure (optionally)

1) in ECTS point layout

(space for scheme of plan)

2) in hourly layout

(space for scheme of plan)

¹BU – number of ECTS points assigned to hours of classes requiring direct participation of academic teachers and other persons conducting classes

²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

2nd LEVEL STUDIES (MASTER LEVEL STUDIES) (3 sem)**Field of study: BIOSCIENCES****Specialization: Bioinformatics**

Specialization subjects

Obligatory subjects

Optional subjects

| Sem. | I | II | III |
|-------|-----------------------------------------------------------|------------------------------------------------------------------|-------------------------------------------------------------------|
| Godz. | 24h / 30ECTS / 2E | 26h / 30ECTS / 2E | 24h/ 30 ECTS /2E |
| 26 | | Rational drug design 2w (3ECTS) | |
| 25 | | | |
| 24 | Elective course 2w(2ECTS) | Molecular modeling 1w+2l+1s (2+2+1) ECTS | Machine learning for chemistry and biology 2w+2l (2+2) ECTS |
| 23 | | | |
| 22 | Theoretical chemistry 2w +1c +2l (3 +2 + 2) ECTS | | |
| 21 | | | |
| 20 | | Retrieval of scientific and technical information 1l (1 ECTS) | Computational genomics 1w+1l (1+1) ECTS |
| 19 | | Data mining 1l (1ECTS) | |
| 18 | | Advanced bioinformatics 3p (3 ECTS) | Molecular engineering in genomic analyses 3l (2 ECTS) |
| 17 | Molecular dynamics 2w +2l (4 + 2) ECTS | | |
| 16 | | | |
| 15 | | Bionanotechnology 2w + 1s (2 + 1) ECTS | Graduate laboratory II 14l (20 ECTS) |
| 14 | | | |
| 13 | Networks and workstations with UNIX system 2l (2 ECTS) | | |
| 12 | | Advanced programming and numerical methods 3l (3 ECTS) | |
| 11 | Bioinformatics 2w +2l (3 + 2) ECTS | | |
| 10 | | | |
| 9 | | Managerial course II 2w (3 ECTS) | |
| 8 | | | |
| 7 | Applied informatics 4l (4 ECTS) | Foreign language II 3c (2 ECTS) | |
| 6 | | | |
| 5 | | | |
| 4 | | Graduate laboratory I 4l (6 ECTS) | |
| 3 | Managerial course I 1w (2 ECTS) | | |
| 2 | Foreign language I 1c (1 ECTS) | | |
| 1 | Graduation proseminar 1s (1 ECTS) | | Graduation seminar 1s (2 ECTS) |
| Sem. | I | II | III |

1. Set of obligatory and optional subjects and groups of classes in semestral arrangement

Semester 1

Obligatory subjects / groups of classes Number of ECTS points 7

| No. | Subject / groups of classescode | Name of subject / groups of classes (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of subject / groups of classes | Way ³ of crediting | Subject / groups of classes | | | |
|--------------|---------------------------------|--------------------------------------------------------------------------------------|------------------------|----------|----------|----|-----|-----------------------------------------------------------------------------------------|-----------------|------------|-----------------------|-------------------------|-------------------------|--------------------------------------------------|-------------------------------|------------------------------|-----------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | University-wide ⁴ | Concerning scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| 1 | W03BSS-SM2001W | Theoretical chemistry | 2 | | | | | K2Abs_W01 K2Abs_W02 K2Abs_W07 K2Abs_W08 K2Abs_W11 K2Abs_W17 K2Abs_K01 | 30 | 75 | 3 | 3 | 1,3 | T/Z | E | | DN | | PD |
| 2 | W03BSS-SM2001L | Theoretical chemistry | | | 2 | | | K2Abs_U03 K2Abs_U04 K2Abs_U05 K2Abs_U09 K2Abs_U12 K2Abs_K08 | 30 | 50 | 2 | 2 | 1,4 | T | Z | | DN | P | K |
| 3 | W03BSS-SM2001C | Theoretical chemistry | | 1 | | | | K2Abs_U02 K2Abs_U12 | 15 | 50 | 2 | 2 | 0,7 | T/Z | Z | | DN | P | K |
| Total | | | 2 | 1 | 2 | | | | 75 | 175 | 7 | 7 | 3,4 | | 1 | | | 4 | |

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³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

Specialization subjects: *Bioinformatics*
Number of ECTS points 17

| No. | Subject / groups of classescode | Name of subject / groups of classes (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of subject / groups of classes | Way ³ of crediting | Subject / groups of classes | | | |
|--------------|---------------------------------|--------------------------------------------------------------------------------------|------------------------|----|-----------|----|-----|----------------------------------------------------------------------------|-----------------|------------|-----------------------|-------------------------|-------------------------|--------------------------------------------------|-------------------------------|------------------------------|-----------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | University-wide ⁴ | Concerning scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| 1 | W03BSS-SM2002W | Molecular dynamics | 2 | | | | | K2Abs_W03 K2Abs_W07 K2Abs_W09 K2Abs_W11 K2Abs_W18 K2Abs_K01 | 30 | 100 | 4 | 4 | 1,3 | T/Z | Z | | DN | | PD |
| 2 | W03BSS-SM2002L | Molecular dynamics | | | 2 | | | K2Abs_U02 K2Abs_U03 K2Abs_U06 K2Abs_U10 K2Abs_K08 | 30 | 50 | 2 | 2 | 1,4 | T | Z | | DN | P | S |
| 3 | W03BSS-SM2004W | Bioinformatics | 2 | | | | | K2Abs_W14 | 30 | 75 | 3 | 3 | 1,3 | T/Z | E | | DN | | S |
| 4 | W03BSS-SM2004L | Bioinformatics. | | | 2 | | | K2Abs_U11 | 30 | 50 | 2 | 2 | 1,4 | T | Z | | DN | P | S |
| 5 | W03BSS-SM2003L | Networks and workstations with UNIX system | | | 2 | | | K2Abs_U13 | 30 | 50 | 2 | | 1,4 | T | Z | | | P | S |
| 6 | W03BSS-SM2005L | Applied informatics | | | 4 | | | K2Abs_U13 K2Abs_U11 K2Abs_K08 | 60 | 100 | 4 | 4 | 2,8 | T | Z | | DN | P | S |
| Total | | | 4 | | 10 | | | | 210 | 425 | 17 | 15 | 9,6 | | 1 | | | 10 | |

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²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

Optional subjects / groups of classes 6 ECTS points

| No. | Subject / groups of classescode | Name of subject / groups of classes (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of subject / groups of classes | Way ³ of crediting | Subject / groups of classes | | | |
|--------------|---------------------------------|--------------------------------------------------------------------------------------|------------------------|----------|-----|----|----------|--------------------------------------------------|-----------------|------------|-----------------------|-------------------------|-------------------------|--------------------------------------------------|-------------------------------|------------------------------|-----------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | University-wide ⁴ | Concerning scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| 1 | SJO-SM0004 | Foreign language I | | 1 | | | | K2Abs_U14 K2Abs_U15 K2Abs_K01 K2Abs_K04 | 15 | 30 | 1 | | 0,6 | T/Z | Z | O | | P | KO |
| 2 | W03-SM2002BH | Managerial course I | 1 | | | | | K2Abt_W16 K2Abs_K02 K2Abs_K03 K2Abs_K07 | 15 | 60 | 2 | | 0,65 | T/Z | Z | O | | | KO |
| 3 | W03W03-SM2053S | Graduation proseminar | | | | | 1 | K2Abs_U08 K2Abs_U14 K2Abs_K01 K2Abs_K07 | 15 | 25 | 1 | 1 | 0,7 | T/Z | Z | | DN | P | K |
| 4 | W03BSS-SM20BW | Elective course* | 2 | | | | | K2Abt_W02 K2Abt_K01 | 30 | 50 | 2 | | 1,3 | T/Z | Z | | | | K |
| Total | | | 3 | 1 | | | 1 | | 75 | 165 | 6 | 1 | 3,25 | | | | | 2 | |

Altogether in semester

| Total number of hours | | | | | Total number of ZZU hours | Total number of CNPS hours | Total number of ECTS points | Total number of ECTS points for DN classes ⁵ | Number of ECTS points for BU classes ¹ |
|-----------------------|----------|-----------|----------|----------|---------------------------|----------------------------|-----------------------------|---------------------------------------------------------|---------------------------------------------------|
| lec | cl | lab | pr | sem | | | | | |
| 9 | 2 | 12 | 0 | 1 | 360 | 765 | 30 | 23 | 16,25 |

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²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

Semester 2

Obligatory subjects / groups of classes

Number of ECTS points 9

| No. | Subject / groups of classescode | Name of subject / groups of classes (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of subject / groups of classes | Way ³ of crediting | Subject / groups of classes | | | |
|--------------|---------------------------------|--------------------------------------------------------------------------------------|------------------------|----|----------|----|----------|---------------------------------------------------------------------------------------------------------------------------------------------|-----------------|------------|-----------------------|-------------------------|-------------------------|--------------------------------------------------|-------------------------------|------------------------------|-----------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | University-wide ⁴ | Concerning scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| 1 | W03BSS-SM2008L | Retrieval of scientific and technical information | | | 1 | | | K2Abs_U05 K2Abs_K05 | 15 | 25 | 1 | | 0,7 | T | Z | | | P | K |
| 2 | W03BSS-SM2007W | Molecular modeling | 1 | | | | | K2Abs_W09 K2Abs_W11 K2Abs_W14 K2Abs_W17 | 15 | 50 | 2 | 2 | 0,65 | T/Z | E | | DN | | K |
| 3 | W03BSS-SM2007L | Molecular modeling. | | | 2 | | | K2Abs_U13 K2Abs_U10 K2Abs_U05 | 30 | 50 | 2 | 2 | 1,4 | T | Z | | DN | P | K |
| 4 | W03BSS-SM2007S | Molecular modeling.. | | | | | 1 | K2Abs_U07 | 15 | 25 | 1 | 1 | 0,7 | T/Z | Z | | DN | P | K |
| 5 | W03BSS-SM2006W | Rational drug design | 2 | | | | | K2Abs_W02 K2Abs_W05 K2Abs_W06 K2Abs_W10 K2Abs_W12 K2Abs_W13 K2Abs_W14 K2Abs_W15 K2Abs_W18 K2Abs_K01 K2Abs_K06 | 30 | 75 | 3 | 3 | 1,3 | T/Z | Z | | DN | | K |
| Total | | | 3 | | 3 | | 1 | | 105 | 225 | 9 | 8 | 4,75 | | 1 | | | 4 | |

¹BU – number of ECTS points assigned to hours of classes requiring direct participation of academic teachers and other persons conducting classes

²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

Specialization subjects: *Bioinformatics*
Number of ECTS points 10

| No. | Subject / groups of classescode | Name of subject / groups of classes (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of subject / groups of classes | Way ³ of crediting | Subject / groups of classes | | | |
|--------------|---------------------------------|--------------------------------------------------------------------------------------|------------------------|----|----------|----------|----------|---------------------------------------------------------------|-----------------|------------|-----------------------|-------------------------|-------------------------|--------------------------------------------------|-------------------------------|-------------------------------|-----------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | University -wide ⁴ | Concerning scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| 1 | W03BSS-SM2012L | Advanced programming and numerical methods | | | 3 | | | K2Abs_W17 K2Abs_U11 K2Abs_U13 K2Abs_K04 | 45 | 75 | 3 | 3 | 2,1 | T | Z | | DN | P | S |
| 2 | W03BSS-SM2011W | Bionanotechnology | 2 | | | | | K2Abs_W07 K2Abs_W09 K2Abs_W11 K2Abs_W13 K2Abs_W18 | 30 | 50 | 2 | 2 | 1,3 | T/Z | E | | DN | | S |
| 3 | W03BSS-SM2011S | Bionanotechnology. | | | | | 1 | K2Abs_U07 K2Abs_K07 | 15 | 25 | 1 | 1 | 0,7 | T/Z | Z | | DN | P | S |
| 4 | W03BSS-SM2010P | Advanced bioinformatics | | | | 3 | | K2Abs_U11 K2Abs_U13 K2Abs_K04 | 45 | 75 | 3 | 3 | 2,25 | | Z | | DN | P | S |
| 5 | W03BSS-SM2009L | Data mining | | | 1 | | | K2Abs_U02 K2Abs_K05 | 15 | 25 | 1 | 1 | 0,7 | T | Z | | DN | P | S |
| Total | | | 2 | | 4 | 3 | 1 | | 150 | 250 | 10 | 10 | 7,05 | | 1 | | | 8 | |

¹BU – number of ECTS points assigned to hours of classes requiring direct participation of academic teachers and other persons conducting classes

²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

Optional subjects / groups of classes 11 ECTS points

| No. | Subject / groups of classescode | Name of subject / groups of classes (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of subject / groups of classes | Way ³ of crediting | Subject / groups of classes | | | |
|--------------|---------------------------------|--------------------------------------------------------------------------------------|------------------------|----------|----------|----|-----|----------------------------------------------------------------------------|-----------------|------------|-----------------------|-------------------------|-------------------------|--------------------------------------------------|-------------------------------|------------------------------|-----------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | University-wide ⁴ | Concerning scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| 1 | SJO-SM0003 | Foreign language II | | 3 | | | | K2Abs_U14 K2Abs_U15 K2Abs_K01 K2Abs_K04 | 45 | 60 | 2 | | 1,8 | T/Z | Z | O | | P | KO |
| 2 | W03-SM2001BH | Managerial course II | 2 | | | | | K2Abt_W16 K2Abs_K02 K2Abs_K03 K2Abs_K07 | 30 | 90 | 3 | | 1,3 | T/Z | Z | O | | | KO |
| 3 | W03W03-SM2054D | Graduate laboratory I | | | 4 | | | K2Abs_U02 K2Abs_U05 K2Abs_U14 K2Abs_K01 K2Abs_K05 K2Abs_K07 | 60 | 150 | 6 | 6 | 3 | T | Z | | DN | P | K |
| Total | | | 2 | 3 | 4 | | | | 135 | 300 | 11 | 6 | 6,1 | | | | | 8 | |

Altogether in semester

| Total number of hours | | | | | Total number of ZZU hours | Total number of CNPS hours | Total number of ECTS points | Total number of ECTS points for DN classes ⁵ | Number of ECTS points for BU classes ¹ |
|-----------------------|----|-----|----|-----|---------------------------|----------------------------|-----------------------------|---------------------------------------------------------|---------------------------------------------------|
| lec | cl | lab | pr | sem | | | | | |
| 7 | 3 | 11 | 3 | 2 | 390 | 775 | 30 | 24 | 17,9 |

¹BU – number of ECTS points assigned to hours of classes requiring direct participation of academic teachers and other persons conducting classes

²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject / group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

Semester 3

Obligatory subjects / groups of classes Number of ECTS points 4

| No. | Subject / groups of classescode | Name of subject / groups of classes (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of subject / groups of classes | Way ³ of crediting | Subject / groups of classes | | | |
|--------------|---------------------------------|--------------------------------------------------------------------------------------|------------------------|----|----------|----|-----|-----------------------------------------------------------------------------------------|-----------------|------------|-----------------------|-------------------------|-------------------------|--------------------------------------------------|-------------------------------|------------------------------|-----------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | University-wide ⁴ | Concerning scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| 1 | W03BSS-SM2013W | Machine learning for chemistry and biology | 2 | | | | | K2Abs_W01 K2Abs_W14 K2Abs_W08 K2Abs_W09 K2Abs_K01 | 30 | 50 | 2 | | 1,3 | T/Z | E | | | | K |
| 2 | W03BSS-SM2013L | Machine learning for chemistry and biology | | | 2 | | | K2Abs_U01 K2Abs_U02 K2Abs_U04 K2Abs_U11 K2Abs_K02 K2Abs_K04 K2Abs_K05 | 30 | 50 | 2 | | 1,4 | T | Z | | | P | K |
| Total | | | 2 | | 2 | | | | 60 | 100 | 4 | | 2,7 | | 1 | | | 2 | |

¹BU – number of ECTS points assigned to hours of classes requiring direct participation of academic teachers and other persons conducting classes

²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

Specialization subjects: *Bioinformatics*
Number of ECTS points 4

| No. | Subject / groups of classescode | Name of subject / groups of classes (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of subject / groups of classes | Way ³ of crediting | Subject / groups of classes | | | |
|--------------|---------------------------------|--------------------------------------------------------------------------------------|------------------------|----|----------|----|-----|---------------------------------------------------------------|-----------------|------------|-----------------------|-------------------------|-------------------------|--------------------------------------------------|-------------------------------|------------------------------|-----------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | University-wide ⁴ | Concerning scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| 1 | W03BSS-SM2014W | Computational genomics | 1 | | | | | K2Abs_W02 K2Abs_W14 K2Abs_W17 | 15 | 25 | 1 | 1 | 0,65 | T/Z | E | | DN | | S |
| 2 | W03BSS-SM2014L | Computational genomics. | | | 1 | | | K2Abs_U01 K2Abs_K07 | 15 | 25 | 1 | 1 | 0,7 | T | Z | | DN | P | S |
| 3 | W03BSS-SM2015L | Molecular engineering in genomic analyses | | | 3 | | | K2Abs_W06 K2Abs_U02 K2Abs_U03 K2Abs_U05 K2Abs_U08 | 45 | 50 | 2 | 2 | 2,1 | T | Z | | DN | P | S |
| Total | | | 1 | | 4 | | | | 75 | 100 | 4 | 4 | 3,45 | | 1 | | | 3 | |

¹BU – number of ECTS points assigned to hours of classes requiring direct participation of academic teachers and other persons conducting classes

²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

Optional subjects / groups of classes
22 ECTS points

| No. | Subject / groups of classes code | Name of subject / groups of classes (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of subject / groups of classes | Way ³ of crediting | Subject / groups of classes | | | |
|--------------|-------------------------------------|--------------------------------------------------------------------------------------|------------------------|----|-----------|----|----------|-----------------------------------------------------------------------------------------|-----------------|------------|-----------------------|-------------------------|-------------------------|--------------------------------------------------|-------------------------------|------------------------------|-----------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | University-wide ⁴ | Concerning scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| 1 | W03W03-SM2055D | Graduate laboratory II | | | 14 | | | K2Abs_U02 K2Abs_U05 K2Abs_U14 K2Abs_U06 K2Abs_K01 K2Abs_K05 K2Abs_K07 | 210 | 500 | 20 | 20 | 9,5 | T | Z | | DN | P | K |
| 2 | W03W03-SM2056S | Graduation seminar | | | | | 1 | K2Abs_U05 K2Abs_U07 K2Abs_K01 K2Abs_K06 K2Abs_K07 K2Abs_K08 | 15 | 50 | 2 | 2 | 0,7 | T/Z | Z | | DN | P | K |
| Total | | | | | 14 | | 1 | | 225 | 550 | 22 | 22 | 10,2 | | | | | 22 | |

Altogether in semester

| Total number of hours | | | | | Total number of ZZU hours | Total number of CNPS hours | Total number of ECTS points | Total number of ECTS points for DN classes ⁵ | Number of ECTS points for BU classes ¹ |
|-----------------------|----|-----------|----|----------|---------------------------|----------------------------|-----------------------------|---------------------------------------------------------|---------------------------------------------------|
| lec | cl | lab | pr | sem | | | | | |
| 3 | | 20 | | 1 | 360 | 750 | 30 | 26 | 16,35 |

¹BU – number of ECTS points assigned to hours of classes requiring direct participation of academic teachers and other persons conducting classes

²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject / group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

2. Set of examinations in semestral arrangement

| Subject / groups of classes code | Names of subjects / groups of classes ending with examination | Semester |
|----------------------------------|---------------------------------------------------------------|----------|
| W03BSS-SM2001W | Theoretical chemistry | 1 |
| W03BSS-SM2004W | Bioinformatics | |
| W03BSS-SM2007W | Molecular modeling | 2 |
| W03BSS-SM2011W | Bionanotechnology | |
| W03BSS-SM2014W | Computational genomics | 3 |
| W03BSS-SM2013W | Machine learning for chemistry and biology | |

3. Numbers of allowable deficit of ECTS points after particular semesters

| Semester | Allowable deficit of ECTS points after semester |
|----------|-------------------------------------------------|
| 1 | 15 |
| 2 | 15 |
| 3 | 0 |

¹BU – number of ECTS points assigned to hours of classes requiring direct participation of academic teachers and other persons conducting classes

²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

Opinion of student government legislative body

.....

Date

.....

Name and surname, signature of student representative

.....

Date

.....

Dean's signature

¹BU – number of ECTS points assigned to hours of classes requiring direct participation of academic teachers and other persons conducting classes

²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

PLAN OF STUDIES

| | |
|-----------------------------|------------------------------------------|
| FACULTY: | Chemistry |
| MAIN FIELD OF STUDY: | BIOSCIENCES |
| EDUCATION LEVEL: | second-level studies (3-semester) |
| FORM OF STUDIES: | full-time studies |
| PROFILE: | general academic |
| SPECIALIZATION: | Medicinal Chemistry |
| LANGUAGE OF STUDY: | English |

In effect since **2024/2025**

Plan of studies structure (optionally)

1) in ECTS point layout

(space for scheme of plan)

2) in hourly layout

(space for scheme of plan)

¹BU – number of ECTS points assigned to hours of classes requiring direct participation of academic teachers and other persons conducting classes

²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

2nd LEVEL STUDIES (MASTER LEVEL STUDIES) (3 sem)

Field of study: BIOSCIENCES

Specialization: Medicinal Chemistry

Specialization subjects

Obligatory subjects

Optional subjects

| Sem. | I | II | III |
|-------|------------------------------------------------------------|------------------------------------------------------------------|--------------------------------------------------------------|
| Godz. | 24h / 30 ECTS / 2E | 25h / 30 ECTS / 3E | 24h / 30 ECTS / 1E |
| 25 | | Rational drug design 2w (3ECTS) | |
| 24 | Elective course | | Multistep organic synthesis |
| 23 | 2w (2 ECTS) | Molecular modeling E | 4l (3 ECTS) |
| 22 | Theoretical chemistry E | 1w+2l+1s (2+2+1) ECTS | |
| 21 | 2w +1c+2l (3+2+2) ECTS | | Inorganic drugs 1w (1 ECTS) |
| 20 | | | Machine learning for chemistry and biology 2w+2l E |
| 19 | | Retrieval of scientific and technical information 1l (1 ECTS) | (2+2) ECTS |
| 18 | | Metabolomics 2l (2 ECTS) | |
| 17 | Isolation and identification of bioproducts 2l (2 ECTS) | | |
| 16 | | Medicinal natural products E | |
| 15 | Introductory statistics 1c (2 ECTS) | 1w +2l (2 +2) ECTS | Graduate laboratory II 14l (20 ECTS) |
| 14 | Crystallography and structure of solids 2w +1c | | |
| 13 | (2+1) ECTS | Modern pharmaceuticals and biopharmaceuticals E | |
| 12 | | 2w+2l (2+2) ECTS | |
| 11 | Analytical methods in drug design and technology 1w +2l | | |
| 10 | (2+2) ECTS | Managerial course II | |
| 9 | | 2w (3 ECTS) | |
| 8 | Spectroscopic methods in medicinal chemistry E | | |
| 7 | 2w +2l (2+2) ECTS | Foreign language II 3c (2 ECTS) | |
| 6 | | | |
| 5 | | | |
| 4 | Metabolomics 1w (2 ECTS) | Graduate laboratory I 4l (6 ECTS) | |
| 3 | Managerial course I 1w (2 ECTS) | | |
| 2 | Foreign language I 1c (1 ECTS) | | |
| 1 | Graduation proseminar 1s (1 ECTS) | | Graduation seminar 1s (2 ECTS) |
| Sem. | I | II | III |

1. Set of obligatory and optional subjects and groups of classes in semestral arrangement

Semester 1

Obligatory subjects / groups of classes Number of ECTS points 7

| No. | Subject / groups of classes code | Name of subject / groups of classes (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of subject / groups of classes | Way ³ of crediting | Subject / groups of classes | | | |
|--------------|-------------------------------------|-----------------------------------------------------------------------------------------|------------------------|----------|----------|----|-----|-----------------------------------------------------------------------------------------|-----------------|----------|-----------------------|-------------------------|-------------------------|--------------------------------------------------|-------------------------------|------------------------------|-----------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | University-wide ⁴ | Concerning scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| 1 | W03BSS-SM2001W | Theoretical chemistry | 2 | | | | | K2Abs_W01 K2Abs_W02 K2Abs_W07 K2Abs_W08 K2Abs_W17 K2Abs_W11 K2Abs_K01 | 30 | 75 | 3 | 3 | 1,3 | T/Z | E | | DN | | PD |
| 2 | W03BSS-SM2001L | Theoretical chemistry | | | 2 | | | K2Abs_U03 K2Abs_U04 K2Abs_U05 K2Abs_U09 K2Abs_U12 K2Abs_K08 | 30 | 50 | 2 | 2 | 1,4 | T | Z | | DN | P | K |
| 3 | W03BSS-SM2001C | Theoretical chemistry | | 1 | | | | K2Abs_U02 K2Abs_U12 | 15 | 50 | 2 | 2 | 0,7 | T/Z | Z | | DN | P | K |
| Total | | | 2 | 1 | 2 | | | 75 | 175 | 7 | 7 | 3,4 | | 1 | | | 4 | | |

¹BU – number of ECTS points assigned to hours of classes requiring direct participation of academic teachers and other persons conducting classes

²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject / group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

Specialization subjects: Medicinal Chemistry Number of ECTS points 17

| No. | Subject / groups of classescode | Name of subject / groups of classes (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of subject / groups of classes | Way ³ of crediting | Subject / groups of classes | | | |
|--------------|---------------------------------|--------------------------------------------------------------------------------------|------------------------|----------|----------|----|-----|---------------------------------------------------------------|-----------------|------------|-----------------------|-------------------------|-------------------------|--------------------------------------------------|-------------------------------|------------------------------|-----------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | University-wide ⁴ | Concerning scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| 1 | W03BSS-SM2021W | Metabolomics | 1 | | | | | K2Abs_W02 K2Abs_W06 K2Abs_W13 K2Abs_K01 | 15 | 50 | 2 | 2 | 0,65 | T/Z | Z | | DN | | S |
| 2 | W03BSS-SM2020W | Spectroscopic methods in medicinal chemistry | 2 | | | | | K2Abs_U02 K2Abs_U08 | 30 | 50 | 2 | 2 | 1,3 | T/Z | E | | DN | | S |
| 3 | W03BSS-SM2020L | Spectroscopic methods in medicinal chemistry | | | 2 | | | K2Abs_W02 K2Abs_W06 K2Abs_W13 K2Abs_K08 | 30 | 50 | 2 | 2 | 1,4 | T | Z | | DN | P | S |
| 4 | W03BSS-SM2019W | Analytical methods in drug design and technology | 1 | | | | | K2Abs_W02 K2Abs_W06 | 15 | 50 | 2 | 2 | 0,65 | T/Z | Z | | DN | | S |
| 5 | W03BSS-SM2019L | Analytical methods in drug design and technology. | | | 2 | | | K2Abs_U01 K2Abs_U03 K2Abs_U08 | 30 | 50 | 2 | 2 | 1,4 | T | Z | | DN | P | S |
| 6 | W03BSS-SM2018W | Crystallography and structure of solids | 2 | | | | | K2Abs_W02 K2Abs_W06 K2Abs_W07 K2Abs_W18 K2Abs_K01 | 30 | 50 | 2 | 2 | 1,3 | T/Z | Z | | DN | | S |
| 7 | W03BSS-SM2018C | Crystallography and structure of solids | | 1 | | | | K2Abs_U01 K2Abs_U02 | 15 | 25 | 1 | 1 | 0,7 | T/Z | Z | | DN | P | S |
| 8 | W03BSS-SM2017C | Introductory statistics | | 1 | | | | K2Abs_U03 | 15 | 50 | 2 | | 0,7 | T/Z | Z | | | P | PD |
| 9 | W03BSS-SM2016L | Isolation and identification of bioproducts | | | 2 | | | K2Abs_U02 K2Abs_U03 K2Abs_W05 K2Abs_K08 | 30 | 50 | 2 | 2 | 1,4 | T | Z | | DN | P | S |
| Total | | | 6 | 2 | 6 | | | | 210 | 425 | 17 | 15 | 9,5 | | 1 | | | 9 | |

¹BU – number of ECTS points assigned to hours of classes requiring direct participation of academic teachers and other persons conducting classes

²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

Optional subjects / groups of classes 6 ECTS points

| No. | Subject / groups of classescode | Name of subject / groups of classes (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of subject / groups of classes | Way ³ of crediting | Subject / groups of classes | | | |
|--------------|---------------------------------|--------------------------------------------------------------------------------------|------------------------|----------|-----|----|----------|--------------------------------------------------|-----------------|------------|-----------------------|-------------------------|-------------------------|--------------------------------------------------|-------------------------------|------------------------------|-----------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | University-wide ⁴ | Concerning scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| 1 | SJO-SM0004 | Foreign language I | | 1 | | | | K2Abs_U14 K2Abs_U15 K2Abs_K01 K2Abs_K04 | 15 | 30 | 1 | | 0,6 | T/Z | Z | O | | P | KO |
| 2 | W03-SM2002BH | Managerial course I | 1 | | | | | K2Abt_W16 K2Abs_K02 K2Abs_K03 K2Abs_K07 | 15 | 60 | 2 | | 0,65 | T/Z | Z | O | | | KO |
| 3 | W03W03-SM2053S | Graduation proseminar | | | | | 1 | K2Abs_U08 K2Abs_U14 K2Abs_K01 K2Abs_K07 | 15 | 25 | 1 | 1 | 0,7 | T/Z | Z | | DN | P | K |
| 4 | W03BSS-SM20BW | Elective course* | 2 | | | | | K2Abt_W02 K2Abt_K01 | 30 | 50 | 2 | | 1,3 | T/Z | Z | | | | K |
| Total | | | 3 | 1 | | | 1 | | 75 | 165 | 6 | 1 | 3,25 | | | | | 2 | |

Altogether in semester

| Total number of hours | | | | | Total number of ZZU hours | Total number of CNPS hours | Total number of ECTS points | Total number of ECTS points for DN classes ⁵ | Number of ECTS points for BU classes ¹ |
|-----------------------|----------|----------|----|----------|---------------------------|----------------------------|-----------------------------|---------------------------------------------------------|---------------------------------------------------|
| lec | cl | lab | pr | sem | | | | | |
| 11 | 4 | 8 | | 1 | 360 | 765 | 30 | 23 | 16,15 |

¹BU – number of ECTS points assigned to hours of classes requiring direct participation of academic teachers and other persons conducting classes

²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

Semester 2

Obligatory subjects / groups of classes Number of ECTS points 9

| No. | Subject / groups of classescode | Name of subject / groups of classes (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of subject / groups of classes | Way ³ of crediting | Subject / groups of classes | | | |
|--------------|---------------------------------|--------------------------------------------------------------------------------------|------------------------|----|----------|----|----------|---------------------------------------------------------------------------------------------------------------------------------------------|-----------------|------------|-----------------------|-------------------------|-------------------------|--------------------------------------------------|-------------------------------|------------------------------|-----------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | University-wide ⁴ | Concerning scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| 1 | W03BSS-SM2008L | Retrieval of scientific and technical information | | | 1 | | | K2Abs_W09 K2Abs_W11 K2Abs_W14 K2Abs_K05 | 15 | 25 | 1 | | 0,7 | T | Z | | | P | K |
| 2 | W03BSS-SM2007W | Molecular modeling | 1 | | | | | K2Abs_W17 K2Abs_U13 K2Abs_U10 K2Abs_U05 | 15 | 50 | 2 | 2 | 0,65 | T/Z | E | | DN | | K |
| 3 | W03BSS-SM2007L | Molecular modeling. | | | 2 | | | K2Abs_U07 | 30 | 50 | 2 | 2 | 1,4 | T | Z | | DN | P | K |
| 4 | W03BSS-SM2007S | Molecular modeling.. | | | | | 1 | K2Abs_W09 K2Abs_W11 K2Abs_W14 | 15 | 25 | 1 | 1 | 0,7 | T/Z | Z | | DN | P | K |
| 5 | W03BSS-SM2006W | Rational drug design | 2 | | | | | K2Abs_W02 K2Abs_W05 K2Abs_W06 K2Abs_W10 K2Abs_W12 K2Abs_W13 K2Abs_W14 K2Abs_W15 K2Abs_W18 K2Abs_K01 K2Abs_K06 | 30 | 75 | 3 | 3 | 1,3 | T/Z | Z | | DN | | K |
| Total | | | 3 | | 3 | | 1 | | 105 | 225 | 9 | 8 | 4,75 | | 1 | | | 4 | |

¹BU – number of ECTS points assigned to hours of classes requiring direct participation of academic teachers and other persons conducting classes

²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject / group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

Specialization subjects: Medicinal Chemistry
Number of ECTS points 10

| No. | Subject / groups of classes code | Name of subject / groups of classes (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of subject / groups of classes | Way ³ of crediting | Subject / groups of classes | | | |
|--------------|-------------------------------------|-----------------------------------------------------------------------------------------|------------------------|----|----------|----|-----|----------------------------------------------------------------------------|-----------------|------------|-----------------------|-------------------------|-------------------------|--------------------------------------------------|-------------------------------|------------------------------|-----------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | University-wide ⁴ | Concerning scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| 1 | W03BSS-SM2023W | Modern pharmaceuticals and biopharmaceuticals | 2 | | | | | K2Abs_W02 K2Abs_W07 K2Abs_W12 K2Abs_W18 K2Abs_W06 K2Abs_K01 | 30 | 50 | 2 | 2 | 1,3 | T/Z | E | | DN | | S |
| 2 | W03BSS-SM2023L | Modern pharmaceuticals and biopharmaceuticals | | | 2 | | | K2Abs_U02 K2Abs_U05 K2Abs_K05 K2Abs_K08 | 30 | 50 | 2 | 2 | 1,4 | T | Z | | DN | P | S |
| 3 | W03BSS-SM2022W | Medicinal natural products | 1 | | | | | K2Abs_W03 K2Abs_W12 K2Abs_W15 K2Abs_W18 | 15 | 50 | 2 | 2 | 0,65 | T/Z | E | | DN | | S |
| 4 | W03BSS-SM2022L | Medicinal natural products. | | | 2 | | | K2Abs_U02 K2Abs_K04 | 30 | 50 | 2 | 2 | 1,4 | T | Z | | DN | P | S |
| 5 | W03BSS-SM2021L | Metabolomics | | | 2 | | | K2Abs_W14 K2Abs_U03 K2Abs_K06 | 30 | 50 | 2 | 2 | 1,4 | T | Z | | DN | P | S |
| Total | | | 3 | | 6 | | | | 135 | 250 | 10 | 10 | 6,15 | | 2 | | | 6 | |

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²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject / group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

Optional subjects / groups of classes 11 ECTS points

| No. | Subject / groups of classescode | Name of subject / groups of classes (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of subject / groups of classes | Way ³ of crediting | Subject / groups of classes | | | |
|--------------|---------------------------------|--------------------------------------------------------------------------------------|------------------------|----------|----------|----|-----|----------------------------------------------------------------------------|-----------------|------------|-----------------------|-------------------------|-------------------------|--------------------------------------------------|-------------------------------|------------------------------|-----------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | University-wide ⁴ | Concerning scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| 1 | SJO-SM0003 | Foreign language II | | 3 | | | | K2Abs_U14 K2Abs_U15 K2Abs_K01 K2Abs_K04 | 45 | 60 | 2 | | 1,8 | T/Z | Z | O | | P | KO |
| 2 | W03-SM2001BH | Managerial course II | 2 | | | | | K2Abt_W16 K2Abs_K02 K2Abs_K03 K2Abs_K07 | 30 | 90 | 3 | | 1,3 | T/Z | Z | O | | | KO |
| 3 | W03W03-SM2054D | Graduate laboratory I | | | 4 | | | K2Abs_U02 K2Abs_U05 K2Abs_U14 K2Abs_K01 K2Abs_K05 K2Abs_K07 | 60 | 150 | 6 | 6 | 3 | T | Z | | DN | P | K |
| Total | | | 2 | 3 | 4 | | | | 135 | 300 | 11 | 6 | 6,1 | | | | | 8 | |

Altogether in semester

| Total number of hours | | | | | Total number of ZZU hours | Total number of CNPS hours | Total number of ECTS points | Total number of ECTS points for DN classes ⁵ | Number of ECTS points for BU classes ¹ |
|-----------------------|----------|-----------|----|----------|---------------------------|----------------------------|-----------------------------|---------------------------------------------------------|---------------------------------------------------|
| lec | cl | lab | pr | sem | | | | | |
| 8 | 3 | 13 | | 1 | 375 | 775 | 30 | 24 | 17 |

¹BU – number of ECTS points assigned to hours of classes requiring direct participation of academic teachers and other persons conducting classes

²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

Semester 3

Obligatory subjects / groups of classes

Number of ECTS points 4

| No. | Subject / groups of classescode | Name of subject / groups of classes (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of subject / groups of classes | Way ³ of crediting | Subject / groups of classes | | | |
|--------------|---------------------------------|--------------------------------------------------------------------------------------|------------------------|----|----------|----|-----|-----------------------------------------------------------------------------------------|-----------------|------------|-----------------------|-------------------------|-------------------------|--------------------------------------------------|-------------------------------|------------------------------|-----------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | University-wide ⁴ | Concerning scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| 1 | W03BSS-SM2013W | Machine learning for chemistry and biology | 2 | | | | | K2Abs_W01 K2Abs_W14 K2Abs_W08 K2Abs_W09 K2Abs_K01 | 30 | 50 | 2 | | 1,3 | T/Z | E | | | | K |
| 2 | W03BSS-SM2013L | Machine learning for chemistry and biology | | | 2 | | | K2Abs_U01 K2Abs_U02 K2Abs_U04 K2Abs_U11 K2Abs_K02 K2Abs_K04 K2Abs_K05 | 30 | 50 | 2 | | 1,4 | T | Z | | | P | K |
| Total | | | 2 | | 2 | | | | 60 | 100 | 4 | | 2,7 | | 1 | | | 2 | |

¹BU – number of ECTS points assigned to hours of classes requiring direct participation of academic teachers and other persons conducting classes

²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject / group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

Specialization subjects: Medicinal chemistry Number of ECTS points 4

| No. | Subject / groups of classescode | Name of subject / groups of classes (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of subject / groups of classes | Way ³ of crediting | Subject / groups of classes | | | |
|--------------|---------------------------------|--------------------------------------------------------------------------------------|------------------------|----|----------|----|-----|--------------------------------------------------|-----------------|------------|-----------------------|-------------------------|-------------------------|--------------------------------------------------|-------------------------------|------------------------------|-----------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | University-wide ⁴ | Concerning scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| 1 | W03BSS-SM2025W | Inorganic drugs | 1 | | | | | K2Abs_W02 K2Abs_W03 | 15 | 25 | 1 | 1 | 0,65 | T/Z | Z | | DN | | S |
| 2 | W03BSS-SM2024L | Multistep organic synthesis | | | 4 | | | K2Abs_U02 K2Abs_U04 K2Abs_U05 K2Abs_K08 | 60 | 75 | 3 | 3 | 2,8 | T | Z | | DN | P | S |
| Total | | | 1 | | 4 | | | | 75 | 100 | 4 | 4 | 3,45 | | 1 | | | 3 | |

Optional subjects / groups of classes 22 ECTS points

| No. | Subject / groups of classescode | Name of subject / groups of classes (denote group of courses with symbol GK) | Weekly number of hours | | | | | Learning effect symbol | Number of hours | | Number of ECTS points | | | Form ² of subject / groups of classes | Way ³ of crediting | Subject / groups of classes | | | |
|--------------|---------------------------------|--------------------------------------------------------------------------------------|------------------------|----|-----------|----|----------|-----------------------------------------------------------------------------------------|-----------------|------------|-----------------------|-------------------------|-------------------------|--------------------------------------------------|-------------------------------|------------------------------|-----------------------------------------------|------------------------|-------------------|
| | | | lec | cl | lab | pr | sem | | ZZU | CNPS | Total | DN ⁵ classes | BU ¹ classes | | | University-wide ⁴ | Concerning scientific activities ⁵ | Practical ⁶ | Type ⁷ |
| 1 | W03W03-SM2055D | Graduate laboratory II | | | 14 | | | K2Abs_U02 K2Abs_U05 K2Abs_U14 K2Abs_U06 K2Abs_K01 K2Abs_K05 K2Abs_K07 | 210 | 500 | 20 | 20 | 9,5 | T | Z | | DN | P | K |
| 2 | W03W03-SM2056S | Graduation seminar | | | | | 1 | K2Abs_U05 K2Abs_U07 K2Abs_K01 K2Abs_K06 K2Abs_K07 K2Abs_K08 | 15 | 50 | 2 | 2 | 0,7 | T/Z | Z | | DN | P | K |
| Total | | | | | 14 | | 1 | | 225 | 550 | 22 | 22 | 10,2 | | | | | 22 | |

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³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

Altogether in semester

| Total number of hours | | | | | Total number of ZZU hours | Total number of CNPS hours | Total number of ECTS points | Total number of ECTS points for DN classes ⁵ | Number of ECTS points for BU classes ¹ |
|-----------------------|----|-----|----|-----|---------------------------|----------------------------|-----------------------------|---------------------------------------------------------|---------------------------------------------------|
| lec | cl | lab | pr | sem | | | | | |
| 3 | | 20 | | 1 | 360 | 750 | 30 | 26 | 16,35 |

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³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

2. Set of examinations in semestral arrangement

| Subject / groups of classes code | Names of subjects / groups of classes ending with examination | Semester |
|-------------------------------------|---------------------------------------------------------------|----------|
| W03BSS-SM2001W | Theoretical chemistry | 1 |
| W03BSS-SM2020W | Spectroscopic methods in medicinal chemistry | |
| W03BSS-SM2007W | Molecular modeling | 2 |
| W03BSS-SM2022W | Medicinal natural products | |
| W03BSS-SM2023W | Modern pharmaceuticals and biopharmaceuticals | |
| W03BSS-SM2013W | Machine learning for chemistry and biology | 3 |

3. Numbers of allowable deficit of ECTS points after particular semesters

| Semester | Allowable deficit of ECTS points after semester |
|----------|-------------------------------------------------|
| 1 | 15 |
| 2 | 15 |
| 3 | 0 |

¹BU – number of ECTS points assigned to hours of classes requiring direct participation of academic teachers and other persons conducting classes

²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject / group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

Opinion of student government legislative body

.....

Date

.....

Name and surname, signature of student representative

.....

Date

.....

Dean's signature

¹BU – number of ECTS points assigned to hours of classes requiring direct participation of academic teachers and other persons conducting classes

²Traditional – enter T, remote – enter Z

³Exam – enter E, crediting – enter Z. For the group of classes – after the letter E or Z - enter in brackets the final subject form (lec, cl, lab, pr, sem)

⁴University-wide subject /group of classes – enter O

⁵DN - number of ECTS points assigned to the classes related to the University's academic activity in the discipline/disciplines to which the main field of study is assigned

⁶Practical subject / group of classes – enter P. For the group of classes – in brackets enter the number of ECTS points assigned to practical courses

⁷KO – general education courses, PD – basic sciences courses, K – main field of study courses, S – specialization courses

KARTY PRZEDMIOTÓW

FACULTY OF CHEMISTRY

SUBJECT CARD**Name of subject in Polish** **Zaawansowana Bioinformatyka****Name of subject in English** **Advanced bioinformatics****Main field of study (if applicable):** **Biosciences****Specialization (if applicable):** **Bioinformatics****Profile:** **academic****Level and form of studies:** **2nd level, full-time****Kind of subject:** **obligatory****Subject code** W03BSS-SM2010P**Group of courses** NO

| | Lecture | Classes | Laboratory | Project | Seminar |
|----------------------------------------------------------------------------------------------------------------------------------|---------|---------|------------|----------------------|---------|
| Number of hours of organized classes in University (ZZU) | | | | 30 | |
| Number of hours of total student workload (CNPS) | | | | 60 | |
| Form of crediting (Examination / crediting with grade) | | | | crediting with grade | |
| For group of courses mark (X) final course | | | | | |
| Number of ECTS points | | | | 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) | | | | 1 | |

*delete as not necessary

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. Knowledge of biological basis related to bioinformatics
2. Proficiency in use of online bioinformatics databases of sequences, genes, genomes etc.
3. Proficiency with use of Unix systems, ability to work in the command line
4. Ability to solve algorithmic problems and automating computing tasks with use of a programming language like Python

SUBJECT OBJECTIVES

- C1 Gain of the skills necessary to use remote computing facilities ("cloud computing" services), including preparation and configuration of system images packaged with necessary software to be run on such services;
- C2 Gain of the skills necessary to document and archive the team work on the process of creation, testing and development of specialized software and workflows to process bioinformatical data sets, with use of interactive Jupyter notebooks, version control systems and online repositories;
- C3 Gain of the skills necessary to perform data processing, analysis and interpretation of the results of new generation sequencing experiments, including quality control and filtering (trimming), mapping on reference genomes, analysis and visualization;
- C4 Gain of the skill necessary to use GNU R package with selected Bioconductor modules to perform typical bioinformatics analyses and visualization of experimental results.

SUBJECT EDUCATIONAL EFFECTS

Relating to skills:

PEU_U01 Students can prepare and configure system images with software packages and services required to run bioinformatics related computation, data processing and analysis on remote computing facilities (“cloud computing”).

PEU_U02 Students can document and archive the performed analysis workflows and results and developed software codes using version control systems, online repositories and interactive notebooks.

PEU_U03 Students can perform full analysis of NGS sequencing results, from the initial data processing to mapping on the reference genomes, visualization and interpretation

PEU_U04 Students can use the GNU R system and Bioconductor libraries to perform typical analyses of experimental data sets available online, and to visualize the results.

Relating to social competences:

PEU_K01 Students can work in teams to solve problems and improve proposed solutions

PEU_K02 Students can communicate and describe the workflow and results of typical data analyses performed in bioinformatics.

PROGRAMME CONTENT

| Project | | Number of hours |
|---------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------|
| Proj 1 | Introductory classes: the form and organization of the classes, didactic materials, requirements for the final grade | 2 |
| Proj 2 | Documentation and archiving of the performed analyses, workflows and developed software: <ul style="list-style-type: none"> • Version control system git and online repositories (github, gitlab etc.). Team working practices. • Documentation of the work using interactive Jupyter notebooks • Markdown syntax | 2 |
| Proj 3 | Project 1: Cloud computing <ul style="list-style-type: none"> • Preparation of system images for remote execution using Docker. Configuring network services and permanent storage. Simple servers of Jupyter, ssh, sshfs. • Preparation and configuration of Docker system image with all services needed to run the GALAXY environment. • Preparation and configuration of Docker system image with Jupyter or JupyterLab server, Jupyter R kernel, R system and selected Bioconductor modules. • Depositing of the results (Dockerfiles, notebooks) in a git repository. Working in teams to test solutions and solve problems. | 4 |
| Proj 4 | Project 2: Analysis of NGS sequencing data using the GALAXY platform <ul style="list-style-type: none"> • Different sequencing platforms and their relation to the results and their analysis • Characteristics of NGS data: read quality Q, FASTQ format variants, sequencing depth, filtering of low quality results. • Initial data processing (trimming). • Mapping results on the reference genome; analysis and visualization of results. | 10 |

| | | |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------|
| Proj 5 | Project 3: Analysis of experimental data sets using GNU R and Bioconductor <ul style="list-style-type: none"> • Introduction to use of the GNU R system: data types, plotting and visualization • Selected Bioconductor modules and functions • Characteristics of experimental data depending on the platform, required processing • Analysis of example data sets | 10 |
| Proj 6 | Students presentations of their projects | 2 |
| | Total hours | 30 |
| TEACHING TOOLS USED | | |
| <p>N1. Instructions and video recording for self-study prior to the relevant classes (the “reverse classroom” approach).</p> <p>N2. Multimedia presentations and live demonstration how to use software.</p> <p>N3. Problem solving – individual and in teams – with the help of the tutor and using online resources.</p> <p>N4. Use of specialized software for performing typical analyses of bioinformatics data sets .</p> <p>N5. Students presentations of their work, solved problems and results.</p> | | |

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 | | | | | | | | | | | | |
|----------------------------------------------------------------------------|---------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------|-------|-----------|-----|-----------|-----|-----------|-----|-----------|-----|---------|-----|
| F1 | PEU_U01, PEU_U02, PEU_K01 | Project 1 score | | | | | | | | | | | | |
| F2 | PEU_U03, PEU_K02 | Project 2 score | | | | | | | | | | | | |
| F3 | PEU_U04, PEU_K02 | Project 3 score | | | | | | | | | | | | |
| P = F1 + F2 + F3 | | <table style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: left;">Score</th> <th style="text-align: left;">Grade</th> </tr> </thead> <tbody> <tr> <td>50-59,99%</td> <td>3,0</td> </tr> <tr> <td>60-69,99%</td> <td>3,5</td> </tr> <tr> <td>70-79,99%</td> <td>4,0</td> </tr> <tr> <td>80-89,99%</td> <td>4,5</td> </tr> <tr> <td>90-100%</td> <td>5,0</td> </tr> </tbody> </table> | Score | Grade | 50-59,99% | 3,0 | 60-69,99% | 3,5 | 70-79,99% | 4,0 | 80-89,99% | 4,5 | 90-100% | 5,0 |
| Score | Grade | | | | | | | | | | | | | |
| 50-59,99% | 3,0 | | | | | | | | | | | | | |
| 60-69,99% | 3,5 | | | | | | | | | | | | | |
| 70-79,99% | 4,0 | | | | | | | | | | | | | |
| 80-89,99% | 4,5 | | | | | | | | | | | | | |
| 90-100% | 5,0 | | | | | | | | | | | | | |
| PRIMARY AND SECONDARY LITERATURE | | | | | | | | | | | | | | |

PRIMARY LITERATURE:

Due to rapid progress of the relevant technologies, the best sources of information are the online learning resources and software documentation:

- [1] <https://git-scm.com/doc>
- [2] <https://docs.docker.com>
- [3] <https://docs.jupyter.org>
- [4] <https://training.galaxyproject.org>
- [5] <https://cran.r-project.org/doc/manuals>
- [6] <https://bioconductor.org/help>
- [7] Relevant articles on <https://wikipedia.org>

SECONDARY LITERATURE:

- [1] „Next-generation sequencing : current technologies and applications”, ed. Xu, Jianping; Caister Academic Press, Norfolk 2014. ISBN 978-1-908230-33-1
https://omnis-pwr.primo.exlibrisgroup.com/permalink/48OMNIS_TUR/d7ok8p/alma9960747679207668
(mostly of historical interest due to rapid progress of NGS technology and software, but it does introduce the basic background and concepts)
- [2] <https://socviz.co/gettingstarted.html> (Introduction to RMarkdown as a tool to document an analysis workflow and results using the R system)

SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)

Paweł Kędzierski, pawel.kedzierski@pwr.edu.pl

FACULTY OF CHEMISTRY

SUBJECT CARD**Name of subject in Polish** Zaawansowane programowanie i metody numeryczne**Name of subject in English** Advanced programming and numerical methods**Main field of study (if applicable):** Biosciences**Specialization (if applicable):** Bioinformatics**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-SM2012L**Group of courses** ~~YES~~ / ~~NO~~*

| | Lecture | Classes | Laboratory | Project | Seminar |
|----------------------------------------------------------------------------------------------------------------------------------|---------|---------|----------------------|---------|---------|
| Number of hours of organized classes in University (ZZU) | | | 45 | | |
| Number of hours of total student workload (CNPS) | | | 75 | | |
| Form of crediting (Examination / crediting with grade) | | | Crediting with grade | | |
| For group of courses mark (X) final course | | | | | |
| Number of ECTS points | | | 3 | | |
| including number of ECTS points for practical classes (P) | | | 3 | | |
| including number of ECTS points corresponding to classes that require direct participation of lecturers and other academics (BU) | | | 2,1 | | |

*delete as not necessary

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. Knowledge of basics of any programming language
- 2.
- 3.

SUBJECT OBJECTIVES

C1 Familiarizing students with good practices in programming

C2 Teaching students the construction of algorithms

C3 Familiarizing students with numerical recipes

SUBJECT EDUCATIONAL EFFECTS

relating to skills:

PEU_U01 Student is able to apply a random number generator in Monte Carlo algorithms

PEU_U02 Student is able to design and implement an algorithm for different sorting algorithms

PEU_U03 Student is able to develop the code for numerical integration of Newton equations of motion

...

relating to social competences:

PEU_K01 Student is able to work in team

PROGRAMME CONTENT

| Laboratory | | Number of hours |
|-------------------|----------------------------------------------------------------------------------------|------------------------|
| Lab 1 | Organization of course and conditions for passing the course. Programming environment. | 3 |
| Lab 2 | Random number generators. | 3 |
| Lab 3 | Numerical integration of functions. | 3 |
| Lab 4 | Interpolation and extrapolation. | 9 |
| Lab 5 | Numerical analysis of functions. | 12 |
| Lab 6 | Monte Carlo methods. | 12 |
| Lab 7 | End credit | 3 |
| Total hours | | 45 |

TEACHING TOOLS USED

- N1.Multimedia presentation
- N2.Specialized computer software
- N3.Gamification

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 |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------|--------------------------------------------------------|
| P | PEU_W01-W03 PEU_U01-U03, PEU_K01 | Final assignment (max 100 pts) |
| P 2.0, when (F1+F2) < 50% points 3.0, when (F1+F2) = 51-59% points 3.5, when (F1+F2) = 60-69% points 4.0, when (F1+F2) = 70-79% points 4.5, when (F1+F2) = 80-89% points 5.0, when (F1+F2) = 90-99% points 5.5, when (F1+F2) = 100% points | | |

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

[1] "Numerical Recipes in C: The art of scientific computing" W. Press, S. Teukolsky, W. Vetterling, B. Flannery, Cambridge University Press, 1988-1992, ISBN 0521 431085

SECONDARY LITERATURE:**SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)**

Bartłomiej Szyja, PhD, DSc, Eng. b.m.szyja@pwr.edu.pl

| FACULTY of CHEMISTRY | | | | | |
|----------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------|---------|----------------------|---------|---------|
| SUBJECT CARD | | | | | |
| Name of subject in Polish | Metody Analityczne w Projektowaniu i Technologii Wytwarzania Leku | | | | |
| Name of subject in English | Analytical Methods in Drug Design and Technology | | | | |
| 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-SM2019W, W03BSS-SM2019L | | | | | |
| 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 | X | | | | |
| 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. Principles of organic chemistry, theoretical and practical.
2. Basic knowledge on chromatographic and spectroscopic methods.
3. Knowledge in the field of basis of analytical chemistry is recommended.

SUBJECT OBJECTIVES

- C1 To acquaint student with the theoretical and practical aspects of good laboratory practice (GLP) and good manufacture practice (GMP).
- C2 Gaining of the knowledge on the modern chromatographic techniques and their applications in drug design and technological process of drugs production.
- C3 Acquaintance with the different technological concepts of application of spectroscopic methods in drugs design and quality control in the production system.
- C4 Expanding the knowledge in the field of electrochemical methods applications in the design

of biologically active compounds and the production procedures of them.
C5 Acquaintance with the different concepts in the field of mixed analytical methods.

SUBJECT EDUCATIONAL EFFECTS

relating to knowledge:

Student, who has completed the course:

PEU_W01 – has knowledge on good laboratory practice (GLP) rules, good manufacture practice (GMP) rules, and validation procedures necessary to be used in analytical methods,

PEU_W02 – has knowledge about the modern chromatographic, spectroscopic, electrochemical and mixed analytical techniques and their applications in drug design and technological process of drugs production,

PEU_W03 – can define the advantages and disadvantages of the analytical techniques, the sensitivity level of each of them.

relating to skills:

Student, who has completed the course:

PEU_U01 – has skills of use chromatographic techniques for separation of a mixture of different compounds, to detect them, do interpretation of the results and prepare the report according to GLP,

PEU_U02 – has knowledge about using different types of spectrometric instruments, and about the parameters of the sample ready to analyze,

PEU_U03 – has skills to do the analysis of the biologically active compounds using electrochemical methods, do interpretation of the results and prepare the report according to GLP,

PEU_U04 – has skills to detect the biologically active compounds in a drug formulation using physical and physicochemical methods.

PROGRAMME CONTENT

| | Lecture | Number of hours |
|-------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------|
| Lec 1 | Introduction to analytical techniques as tools for drug design and production. Good practice rules in analytical chemistry. Error estimation in analytical methods used in drugs design and technology. | 2 |
| Lec 2 | Validation techniques. Pharmacopoeias. GLP, GMP and drugs production normalization rules. | 2 |
| Lec 3 | Chromatographic techniques in drugs design and control of production process. Solving of popular troubles. | 2 |
| Lec 4 | Spectroscopic techniques in drugs design and control of production process. | 2 |
| Lec 5 | Mixed advanced analytical techniques as a tool in drugs design and control of their activity. | 2 |
| Lec 6 | The electrochemical methods in drug design and technology. | 2 |
| Lec 7 | Methods of the analysis of solid state drug formulation ingredients - powders and granules. | 2 |
| Lec 8 | Novel advanced applications in quality control systems in the pharmaceutical industry. | 1 |
| | Total hours | 15 |

| Laboratory | | Number of hours |
|------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------|
| Lab 1 | Safety rules in the laboratory of organic chemistry, good laboratory practice and the rules of the reports preparation. | 2 |
| Lab 2 | HPLC technique – a scheme of the procedure of a sample preparation. Preparation of a sample to HPLC analysis. | 2 |
| Lab 3 | HPLC – the equipment scheme. The analysis of biologically active components of a pharmaceutical formulation. Gas chromatography equipment and the procedure of analysis. Detection techniques. | 2 |
| Lab 4 | GC analysis - diagram of API separation procedure. Sample preparation for GC analysis. | 2 |
| Lab 5 | GC-MS – the equipment diagram. Chromatographic analysis and interpretation of the results. | 2 |
| Lab 6 | Turbidimetry – the analytical method useful to drug design and quality control of it using microplates reader. | 4 |
| Lab 7 | Comparison of thermostability and photostability of the active substance in solid, semi-solid and liquid pharmaceutical formulations. | 4 |
| Lab 8 | Potentiometry – the method used for potentiometric titration of the biologically active molecules possessing positive or negative charge. Application of potentiometric titration to pH-metric analysis. | 4 |
| Lab 9 | UV-Vis spectrophotometry – principles of the method and procedure of measurement. The quality analysis of a pharmaceutical formulation. | 4 |
| Lab 10 | Infrared spectroscopy (FT-IR) of a biologically active compound. Sample preparation and spectrum collection. | 4 |
| | Total hours | 30 |

TEACHING TOOLS USED

N1 Multimedial presentation.

N2 Performing experiments with different laboratory equipment and instruments.

N3 Preparation of report including analysis and interpretation of obtained results.

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 |
|----------------------------------------------------------------------------|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------|
| F1 | PEU_W01 – PEU_W03 | grades for the short queries in the topics of the laboratory experiments. |
| F2 | PEU_U01 – PEU_U4 | grades for reports on the experiments conducted. |
| P1 (laboratory) | | Average from N grades for the queries (F1) and N for the reports on the experiments conducted (F2) $P1 = \Sigma (F1+F2)/N$ |
| P2 (lecture) | PEU_W01– PEU_W03 | Final test. |

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

- [1] J. Ermer, J.H.McB. Miller, Method Validation in Pharmaceutical Analysis. A Guide to Best Practice. Wiley-VCH, Weinheim. 2005.
- [2] Farmakopea Polska, Urząd Rejestracji Leków, Wyrobów Medycznych i Produktów Biobójczych, Warszawa.
- [3] W. Jennings, E. Mittlefehldt, P. Stremple, Analytical Gas Chromatography. 2nd Ed. Academic Press, 1997.
- [4] R.P.W. Scott, Tandem Techniques. John Wiley & Sons, 1997.
- [5] M.S. Lee, Integrated Strategies in Drug Discovery Using Mass Spectrometry. John Wiley & Sons, 2005.
- [6] A.J. Bard, R.L. Faulkner, Electrochemical Methods. Fundamental and Applications. John Wiley & Sons, 2001.

SECONDARY LITERATURE:

- [1] D.M. Bliesner, Validating Chromatographic Methods. A Practical Guide. John Wiley & Sons, 2006.
- [2] P.A. Christensen and A. Hamnett, Techniques and Mechanisms in Electrochemistry. Kluwer Academic Press, 1994.
- [3] AC Moffat, MD Osselton, B Widdop, Clarke's analysis of drugs and poisons. Pharmaceutical Press, 2005.
- [4] F.A. Settle, Handbook of Instrumental Techniques for Analytical Chemistry. Prentice-Hall Inc., 1997.

SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)

dr hab. inż. Izabela Pawlaczyk-Graja, prof. uczelni izabela.pawlaczyk@pwr.edu.pl

FACULTY OF CHEMISTRY

SUBJECT CARD**Name of subject in Polish** Informatyka stosowana**Name of subject in English** Applied informatics**Main field of study (if applicable):** Biosciences**Specialization (if applicable):** Bioinformatics**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-SM2005L**Group of courses** ~~YES~~ / ~~NO~~*

| | Lecture | Classes | Laboratory | Project | Seminar |
|----------------------------------------------------------------------------------------------------------------------------------|---------|---------|----------------------|---------|---------|
| Number of hours of organized classes in University (ZZU) | | | 60 | | |
| Number of hours of total student workload (CNPS) | | | 100 | | |
| Form of crediting (Examination / crediting with grade) | | | Crediting with grade | | |
| For group of courses mark (X) final course | | | | | |
| Number of ECTS points | | | 4 | | |
| including number of ECTS points for practical classes (P) | | | 4 | | |
| including number of ECTS points corresponding to classes that require direct participation of lecturers and other academics (BU) | | | 2,8 | | |

*delete as not necessary

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. None

SUBJECT OBJECTIVES

C1 Familiarizing students with basics of Unix environment

C2 Teaching students the basic algorithms and numerical methods

C3 Familiarizing students with concepts of procedural and object-oriented programming

SUBJECT EDUCATIONAL EFFECTS

...

relating to skills:

PEU_U01 Student is able to use a programming environment to develop a program

PEU_U02 Student is able to design and implement an algorithm for the common numerical methods

PEU_U03 Student is able to effectively use the procedural and object-oriented methods in programming

...

relating to social competences:

PEU_K01 – uznaje znaczenie wiedzy w rozwiązywaniu problemów informatycznych

| PROGRAMME CONTENT | | |
|-----------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------|------------------------|
| Laboratory | | Number of hours |
| Lab 1 | Organization of course and conditions for passing the course. Basic Unix commands. | 4 |
| Lab 2 | BASH scripting. Resource management. Queueing systems | 8 |
| Lab 3 | Using the programming environment. Writing and executing programs. Conditional expressions. Loops. | 8 |
| Lab 4 | Simple and complex types of data. Objects. Functions and methods. | 8 |
| Lab 5 | Commonly used numerical algorithms. | 16 |
| Lab 6 | Applications of programming in biochemistry and biotechnology | 12 |
| Lab 7 | End credit | 4 |
| | Total hours | 60 |
| TEACHING TOOLS USED | | |
| N1.Multimedia presentation N2.Specialized computer software N3.Gamification | | |

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 |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------|--------------------------------------------------------|
| F1 | PEU_W01-W03, PEU_K01 | Partial tests (max 4 pts) |
| P1 | PEU_U01-U03, PEU_K01 | Final assignment (max 6 pts) |
| P (F1+P1) 2.0, if P < 50% pts 3.0, if P = 51-59% pts 3.5, if P = 60-69% pts 4.0, if P = 70-79% pts 4.5, if P = 80-89% pts 5.0, if P = 90-99% pts 5.5, if P = 100% pts | | |

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

[1] "Python Programming for Biology: Bioinformatics and Beyond", Tim J. Stevens, Wayne Boucher, Cambridge University Press; 1 edition (April 6, 2015) ISBN-13: 978-0521720090

[2]

[3]

[4]

SECONDARY LITERATURE:

[1]

[2]

[3]

SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)

Bartłomiej Szyja, PhD, DSc, Eng. b.m.szyja@pwr.edu.pl

| | | | | | |
|---------------------------------------------|--------------------------------|--|--|--|--|
| FACULTY OF CHEMISTRY | | | | | |
| SUBJECT CARD | | | | | |
| Name of subject in Polish | Bioinformatyka | | | | |
| Name of subject in English | Bioinformatics | | | | |
| Main field of study (if applicable): | Biosciences | | | | |
| Specialization (if applicable): | Bioinformatics | | | | |
| Profile: | academic | | | | |
| Level and form of studies: | 2nd level, full-time | | | | |
| Kind of subject: | obligatory | | | | |
| Subject code | W03BSS-SM2004W, W03BSS-SM2004L | | | | |
| Group of courses | NO | | | | |

| | Lecture | Classes | Laboratory | Project | Seminar |
|----------------------------------------------------------------------------------------------------------------------------------|-------------|---------|----------------------|---------|---------|
| Number of hours of organized classes in University (ZZU) | 30 | | 30 | | |
| Number of hours of total student workload (CNPS) | 75 | | 50 | | |
| Form of crediting (Examination / crediting with grade) | Examination | | crediting with grade | | |
| For group of courses mark (X) final course | | | | | |
| Number of ECTS points | 3 | | 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) | 1,3 | | 1,4 | | |

*delete as not necessary

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. Knowledge of basics concepts and vocabulary of biology, biochemistry and genetics
2. Ability to use computer, Internet and command line (shell) interface
3. Fluent command of English language

SUBJECT OBJECTIVES

- C1 Teaching the retrieval of specific information from databases of biosequences, genes, genomes, structures, protein families and other biochemistry and medicine related databases.
- C2 Understanding of various sequence similarity measures and their interpretation required to perform comparative analysis of multiple sequences.
- C3 Ability to search for homologous sequences, creation and use of sequence similarity profiles and to analyze relations between sequences.
- C4 Ability to build and evaluate protein models using contemporary structure prediction methods.
- C5 Ability to automate typical bioinformatics analyzes and searches using self programmed scripts using specialized libraries.

SUBJECT EDUCATIONAL EFFECTS

Relating to knowledge:

PEU_W01 Knowledge on the availability and scope of information available in databases of sequences, sequence families, genes, genomes, biochemical and medicinal databases.

PEU_W02 Knowledge on the theoretical foundations of methods employed to compare sequences and analyze their features and function, necessary to evaluate the statistical significance of the results.

PEU_W03 Knowledge on the theoretical foundations of methods used for comparative analyzes, their advantages, disadvantages and scope

PEU_W04 Knowledge of the contemporary methods of structure prediction

Relating to skills:

PEU_U01 Ability to construct complex queries against the databases of sequence, gene, genome, biochemical and medicinal information to retrieve the specific data or sequences

PEU_U02 Ability to search sequence databases for similar sequences, including searches with similarity profiles, to identify homologs

PEU_U03 Ability to calculate, edit and employ multiple sequence alignments to recognize features, functions, structure and phylogenesis and other comparative analyzes of biosequence database

PEU_U04 Ability to automate common bioinformatics tasks and analyses using scripting programming languages and specialized libraries

PROGRAMME CONTENT

| | Lecture | Number of hours |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------|
| Lec 1 | Bioinformatics databases | 2 |
| Lec 2 | Efficient use of databases: annotations, organization of information, complex queries against specified record fields. | 2 |
| Lec 3 | Similarity and homology. Evaluation and interpretation of sequence similarity and of its statistical significance. | 2 |
| Lec 4 | Methods of sequence alignments. Theoretical basis of methods of similarity-based database searches. | 2 |
| Lec 5 | Approaches to multiple sequence alignment problem. | 2 |
| Lec 6 | Similarity profiles as representation of sequence similarity and features. Families of sequences and databases of families of homologs. Database queries using similarity profiles. | 2 |
| Lec 7 | Introduction to Bayesian statistics and interpretation of information encoded in biological sequences | 2 |
| Lec 8 | Hidden Markov Models, machine learning methods and stochastic optimization approaches – applications in bioinformatics. | 2 |
| Lec 9 | Theoretical models and calculation of evolutionary distances. | 2 |
| Lec 10 | Methods of molecular phylogenetic analysis: inferring relations and mutation history among related sequences | 2 |
| Lec 11 | Structure prediction methods, model evaluation and optimization | 2 |
| Lec 12 | Automation of common bioinformatics tasks and analyses: bioinformatics programming APIs and libraries | 2 |
| Lec 13 | Automation of sequence analysis, structure prediction and other tasks | 2 |

| | | |
|-------------------|------------------------------------------------------------------------------------------------------------------------------------|------------------------|
| Lec 14 | Contemporary research, analytic and diagnostic techniques. | 4 |
| | Total hours | 30 |
| Laboratory | | Number of hours |
| Lab 1 | Introduction to course topics, organization of the lab, required software. Introduction to NCBI databases and the Entrez System | 2 |
| Lab 2 | Complex queries. Available sequence, gene, genome and secondary databases. Different search engines. | 2 |
| Lab 3 | Uniprot KB, Protein Data Bank, Brenda Enzymes and a selection of other databases related to biochemistry and medicine. | 2 |
| Lab 4 | Individual task #1 | 2 |
| Lab 5 | Searching for similar sequences using BLAST variants. Interpretation of results. | 2 |
| Lab 6 | Searching for remote homology using similarity profiles | 2 |
| Lab 7 | Individual task #2 | 2 |
| Lab 8 | Calculation, analysis, verification and visualization of multiple sequence alignments | 2 |
| Lab 9 | Use of Python scripting language and Biopython library for automation of database queries and calculations | 2 |
| Lab 10 | Phylogenetic analysis | 2 |
| Lab 11 | Statistical evaluation of results using bootstrap analysis | 2 |
| Lab 12 | Individual task #3 | 2 |
| Lab 13 | Protein structure prediction based on templates. | 2 |
| Lab 14 | Ab initio protein structure prediction. Evaluation of models. | 2 |
| Lab 15 | Individual task #4 | 2 |
| | Total hours | 30 |

TEACHING TOOLS USED

- N1. Lecture with multimedia presentation
N2. Problem solving
N3. Use of specialized software
N4. Preparation of reports of individual tasks, with analysis of results

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 |
|----------------------------------------------------------------------------|------------------------|-------------------------------------------------|
| F1_Lab | PEU_U01 | Individual task #1 |
| F2_Lab | PEU_U02 | Individual task #2 |
| F3_Lab | PEU_U03, PEU_U05 | Individual task #3 |
| F4_Lab | PEU_U04, PEU_U05 | Individual task #4 |
| P_Lecture: grade based on exam score | | Score Grade |
| P_Lab: grade based on total score | | 50-59,99% 3,0 |
| F1_Lab+F2_Lab+F3_Lab+F4_Lab | | 60-69,99% 3,5 |
| | | 70-79,99% 4,0 |
| | | 80-89,99% 4,5 |
| | | 90-100% 5,0 |

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

- [1] S.Q. Ye, Bioinformatics. A practical approach, Chapman & Hall/CRC, 2008
- [2] I. Eidhammer, I. Johanssen, W.R. Taylor, Protein Bioinformatics - an algorithmic approach to sequence and structure analysis, Wiley, 2004
- [3] P.E. Bourne & H. Weissig (ed.), Structural Bioinformatics, Wiley, 2003
- [4] A.D. Baxevanis, B.F.F. Oullette, Bioinformatics, Wiley, 2001

SECONDARY LITERATURE:

- [1] The National Center for Biotechnology Information (NCBI) Handbook:
<https://www.ncbi.nlm.nih.gov/books/NBK21101/>
- [2] Documentation of used WWW services (available online)
- [3] <http://www.ncbi.nlm.nih.gov/guide/training-tutorials/>

SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)

Paweł Kędzierski, Pawel.Kedzierski@pwr.edu.pl

FACULTY OF CHEMISTRY

SUBJECT CARD**Name of subject in Polish** Bionanotechnologia**Name of subject in English** Bionanotechnology**Main field of study (if applicable):** Biosciences**Specialization (if applicable):** Bioinformatics**Profile:** academic**Level and form of studies:** 2nd level**Kind of subject:** obligatory**Subject code** W03BSS-SM2011W, W03BSS-SM2011S**Group of courses** NO

| | Lecture | Classes | Laboratory | Project | Seminar |
|---------------------------------------------------------------------------------|----------------|----------------|-------------------|----------------|----------------------|
| Number of hours of organized classes in University (ZZU) | 30 | | | | 15 |
| Number of hours of total student workload (CNPS) | 50 | | | | 25 |
| Form of crediting | Examination | | | | crediting with grade |
| For group of courses mark (X) final course | | | | | |
| Number of ECTS points | 2 | | | | 1 |
| including number of ECTS points for practical (P) classes | | | | | 1 |
| including number of ECTS points for direct teacher-student contact (BK) classes | 1,3 | | | | 0,7 |

**PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER
COMPETENCES**

1. Basic knowledge of physical chemistry (1st level)
2. Basic knowledge of biochemistry (1st level)
3. Basic knowledge of molecular dynamics (2nd level)

| SUBJECT OBJECTIVES | |
|---------------------------|------------------------------------------------------------------------------------------------------------------------|
| C1 | Principles underlying the functioning of molecular machines in biology |
| C2 | Basic knowledge about methods utilized in bionanotechnology to design, synthesize and analyze bionanomachines |
| C3 | Practical knowledge on how to perform basic molecular dynamics (MD) simulations to solve problems in bionanotechnology |
| C4 | Basic knowledge on the recent achievements in bionanotechnology |

SUBJECT EDUCATIONAL EFFECTS

Relating to knowledge:

PEU_W01 – Basic concepts of nanobiotechnology and bionanotechnology

PEU_W02 – Principles of functioning of molecular machines in biology

PEU_W03 – Basic knowledge on experimental methods used in design, synthesis and analysis in bionanotechnology

PEU_W04 – Basic knowledge on experimental methods used in structural investigation in bionanotechnology

PEU_W05 – Basic techniques in designing synthetic bionanomachines

PEU_W06 – Basic principles of functioning of bionanomachines

PEU_W07 – Basic knowledge on molecular modelling tools used in designing bionanomachines

PEU_W08 - Basic knowledge on the recent achievements in modern bionanotechnology

Relating to skills:

PEU_U01 – Practical knowledge on how to prepare input files and how to perform minimization and MD of nanopore

PEU_U02 – Practical knowledge of performing basic MD simulations of DNA within the nanopore

PEU_U03 – Practical knowledge on how to prepare and present a seminar on the last achievements in bionanotechnology

| PROGRAMME CONTENT | | |
|----------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----|
| Form of classes - lecture | | Nu |
| Lec1 | Basic concepts. Nonotechnology, biotechnology, bionanotechnology, nanobiotechnology. Feynman's idea. Top-down and bottom-up approaches. Milestone achievements in bionanotechnology. Nanobiotechnology/bionanotechnology in electronics, informatics, energetics, army, agriculture and food technology – examples. | 2 |
| Lec2 | How do molecular machines work in biology?: Properties of particles at macro- and nano-levels. Bionanomolecules in water environment – hydrophobic effect. Proteins as a structural material in bionanotechnology. Limitations of natural bionanomolecules. | 2 |
| Lec3 | Methods in bionanotechnology: to design, synthesize and analyze. Rekombinant DNA technology. DNA cloning. PCR method. Protein synthesis in vitro. Directed mutagenesis. Fusion and chimeric proteins. Monoclonal antibodies. | 2 |
| Lec4 | Methods in bionanotechnology: to design, synthesize and analyze – part 2 . X-ray and NMR methods to investigate structure of biomolecules. Electron spectroscopy methods: TEM, SEM, tomography. AFM method. Molecular modelling as a tool to obtain information on structure and dynamics of biomolecule. | 2 |
| Lec5 | Design of nanomachines. Methods used in bionanomachines design: sequential covalent bond formation, polymerization, self-organization and aggregation. Protein folding. Role of chaperones in folding. Proteins stable in high temperatures. How to make a protein more rigid? How to introduce a disorder in a protein? Symmetric and quasi-symmetric complexes. | 2 |
| Lec6 | Functional aspects of biomolecules. Energy transfer in natural bionanomachines. Electron transfer in natural bionanomachines. Light-driven molecular bionanomachines. Charge transfer in biosystems. How do enzymes work? Methods to control bionanomachines – allosteric regulation and covalent modification. | 2 |

| | | |
|------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------|
| Lec7 | Design of bionanomachines. De novo protein design. Enzyme design based on molecular modelling methods. Design of biosystems having specific spectral properties. PNA (Peptide Nucleic Acid) vs. DNA. | 2 |
| Lec8 | Exam | 2 |
| Lab1 | DNA sequencing using MD – part 1. Construction of a crystal membrane of Si ₃ N ₄ . Synthetic nanopore in Si ₃ N ₄ .membrane. | 2 |
| Lab2 | DNA sequencing using MD – part 2. Calibration of force field to reproduce experimental value of dielectric constant. | 2 |
| Lab3 | DNA sequencing using MD – part 3. Solvation of a nanopore. | 2 |
| Lab4 | DNA sequencing using MD – part 4. Energy minimization. Molecular dynamics under constant pressure. Measuring ionic current in nanopores. | 2 |
| Lab5 | DNA sequencing using MD – part 5. Simulating the process of DNA transport through a nanopore. | 2 |
| Lab6 | DNA sequencing using MD – part 6. Ionic current in nanopores in the presence of DNA. Comparison of ionic current with/without DNA in the system. | 2 |
| Lab7 | DNA sequencing using MD – part 7. Transporting DNA through nanopore – MD simulation. Transporting ubiquitin through nanopore – MD simulation. | 2 |
| | Total hours | 30 |

| | | |
|----------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------|
| Form of classes - seminar | | Nu |
| Se1-15 | Students in the form of oral contribution present and discuss the late achievements and trends in bionanotechnology based on the most recent scientific literature. The list of possible topics is upgraded every year due to the very rapid progress in this field. | 15 |
| | Total hours | 15 |

| TEACHING TOOLS USED | |
|----------------------------|--------------------------------------|
| N1 | Lecture with multimedia presentation |
| N2 | Practical usage of software |
| N3 | Preparation of reports |
| N4 | Seminar presentation |

| EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT | | |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------|--------------------------------------------------|
| Evaluation F – forming (during semester), C – concluding (at semester end) | Educational effect number | Way of evaluating educational effect achievement |
| F1 (lecture) | PEU_W01 – PEU_W07 | Written exam |
| F2 (lecture) | PEU_U01 – PEU_U02 | Report |
| P (seminar) | PEU_U03, PEU_K01 | Seminar presentation |
| <p>P (lecture) = 3.0 if (F1 + F2) = 50-60% max. no of poins. 3.5 if (F1 + F2) = 61-70% max. no of poins. 4.0 if (F1 + F2) = 71-80% max. no of poins. 4.5 if (F1 + F2) = 81-90% max. no of poins. 5.0 if (F1 + F2) = 91-99% max. no of poins. 5.5 if (F1 + F2) = 100% max. no of poins.</p> | | |

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

[1] D.S. Goodsell “*Bionanotechnology: Lessons from nature*” Plenty of room for biology at the bottom: An introduction to bionanotechnology”, Wiley-Liss, 2004.

SECONDARY LITERATURE:

[1] *Bionanotechnology: Proteins to Nanodevices*, Eds. V. Renugopalakrishnan, R.V.Lewis, Springer, 2006.

[2] *Nanobiotechnology: Concepts, Applications and Perspectives*, Eds. C.M.Niemeyer, C.A.Mirkin, Wiley-VCH, 2004.

[3] *Nanobiotechnology II: More Concepts and Applications*, Eds. C.M.Niemeyer, C.A.Mirkin, Wiley-VCH, 2007.

[4] E. Gazit “Plenty of room for biology at the bottom: An introduction to bionanotechnology”, Imperial College Press, 2007.

SUBJECT SUPERVISOR

(NAME AND SURNAME, E-MAIL ADDRESS)

prof. dr hab. Tadeusz Andruniów, tadeusz.andruniow@pwr.wroc.pl

FACULTY OF CHEMISTRY

SUBJECT CARD**Name of subject in Polish** Genomika obliczeniowa**Name of subject in English** Computational genomics**Main field of study (if applicable):** Biosciences**Specialization (if applicable):** Bioinformatics**Profile:** academic**Level and form of studies:** 2nd level, full-time**Kind of subject:** obligatory**Subject code** W03BSS-SM2014W, W03BSS-SM2014L**Group of courses** NO

| | Lecture | Classes | Laboratory | Project | Seminar |
|----------------------------------------------------------------------------------------------------------------------------------|-------------|---------|----------------------|---------|---------|
| Number of hours of organized classes in University (ZZU) | 15 | | 15 | | |
| Number of hours of total student workload (CNPS) | 25 | | 25 | | |
| Form of crediting (Examination / crediting with grade) | Examination | | crediting with grade | | |
| For group of courses mark (X) final course | | | | | |
| Number of ECTS points | 1 | | 1 | | |
| including number of ECTS points for practical classes (P) | | | 1 | | |
| including number of ECTS points corresponding to classes that require direct participation of lecturers and other academics (BU) | 0,65 | | 0,7 | | |

*delete as not necessary

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. Basic bioinformatics, genetics and molecular biology knowledge
2. Basic knowledge of computer science
3. Specialized English

SUBJECT OBJECTIVES

- C1 Teaching elementary topics in genomics.
- C2 Introducing main genomics databases.
- C3 Familiarizing students with methods of sequencing, assembling and description of genomes.
- C4 Familiarizing students with comparative genomics methods and applications.
- C5 Introducing main concepts and methods used in transcriptomic research.
- C6 Teaching about practical applications of genomics research and genomic information.
- C7 Acquainting students with the ethical aspects of genomics research and the use and safety of genomic information.

SUBJECT EDUCATIONAL EFFECTS

relating to knowledge:

- PEU_W01 – knowledge of the basic concepts in genomics;
- PEU_W02 – knowledge of the content and organization of genomic databases;
- PEU_W03 – knowledge of the genome mapping, sequencing, assembly and description methods;
- PEU_W04 – knowledge of the tools used to analyze and compare genomic sequences;
- PEU_W05 – knowledge of the methods used in transcriptomic and their applications;
- PEU_W06 – knowledge of the possible use of genomic information.

relating to skills:

- PEU_U01 – ability to search the genomic databases and retrieve information from such sources;
- PEU_U02 – ability to select appropriate methods and tools for the studied problem;
- PEU_U03 – ability to conduct basic manipulations, comparisons and analysis on genomic information;
- PEU_U04 – ability to perform the quality control and genome assembly using sequencing data;
- PEU_U05 – ability to conduct the basic analysis and visualization of transcriptomic data;
- PEU_U06 – ability to analyze the obtained results.

relating to social competences:

- PEU_K01 – awareness of the ethical aspects of genomics research and challenges associated with data protection.

PROGRAMME CONTENT

| Lecture | Number of hours |
|----------------|------------------------|
|----------------|------------------------|

| | | |
|-------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----|
| Lec 1 | Introductory lecture: the plan and content of the course and crediting rules. Introduction of the basic concepts in genomics, historical background of genomic research, applications and perspectives. | 2h |
| Lec 2 | Genomic information organization: sources of genomic information and principles of data collection and access. Introduction of genomic databases and data structure. | 2h |
| Lec 3 | Assembly of genome sequences: presentation of the gene assembly process based on homology approach and <i>de novo</i> . Introduction to the procedures and methods used for quality control and assembly of genome sequences. | 2h |
| Lec 4 | Structural genomics and description of genomes: overview of principles and methods of genome mapping including types of genomic maps. Presentation of main rules and methods of genes prediction and genome annotations. | 2h |
| Lec 5 | Functional and comparative genomics: the types of data gained from transcriptomic experiments, approach to the transcriptomic data analysis, presentation and applications. Overview of the comparative genomics methods together with applications examples. | 2h |
| Lec 6 | Experimental techniques: presentation of main experimental techniques used for the exploration of genomes including new generation techniques. Discussion of the application possibilities and the future of these field. | 2h |
| Lec 7 | Ethical aspects of genomic research: the ethical aspects of genomic research, the use of genomic information in science and other fields and challenges of data safety. Law regulations regarding the genomic information. | 2h |
| Lec 8 | Written exam | 1h |
| | Total hours | 15h |

| Laboratory | | Number of hours |
|-------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------|
| Lab 1 | Introductory classes: the program of laboratory classes, organization and rules of the computer lab. Overview of basic tools and software used during the course. Introduction to the Ensembl genome browser. | 2h |
| Lab 2 | Genomic databases: introduction to the main genomic databases, data organization and visualization. Overview of related 'omics' databases. | 2h |
| Lab 3 | Genomic databases; genome description: Practical examples reflecting the genome annotation, including analysis of known transcript or variants. The use of genomic databases as a source of information including basic comparative analysis. | 2h |
| Lab 4 | Project I: Practical individual tasks for the first report. | 2h |
| Lab 5 | Genome information analysis: Practical examples of large-scale genomic data retrieving, handling, sorting, comparing, etc., using genomic databases and online tools. | 2h |

| | | |
|-------|---------------------------------------------------------------------------------------------------------------------------------|-----|
| Lab 6 | Genome assembly: Introduction to genome sequencing data (reads) quality control and genome assembly. Practical examples. | 2h |
| Lab 7 | Transcriptomics: Practical examples of transcriptomic data analysis and methods of visualization of the results. | 2h |
| Lab 8 | Project II: Practical individual tasks for the second report. | 1h |
| | Total hours | 15h |

TEACHING TOOLS USED

- N1. Lecture
- N2. Multimedia presentation
- N3. Practical usage of databases
- N4. Practical usage of software
- N5. Tutorials with examples for analyzed problems
- N5. Solving individual tasks
- N6. Preparation of reports

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 |
|----------------------------------------------------------------------------|---------------------------------------------|-------------------------------------------------|
| P (Lecture) | PEU_W01- PEU_W06, PEU_U01, PEU_U02, PEU_K01 | Final exam |
| F1 (Laboratory) | PEU_W01-PEU_W02, PEU_U01-PEU_U03 | Report from the Individual Project I |
| F2 (Laboratory) | PEU_W01- PEU_W05, PEU_U01-PEU_U06 | Report from the Individual Project II |
| P (Laboratory) = F1+F2 | | |

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

[1] *Fundamentals of Bioinformatics and Computational Biology*, G.B. Singh, Springer-Verlag London, 2015.

[3] *Introduction to Genomics*, Lesk A. Oxford University Press, Oxford, 2017.

[2] *Big Data Analytics in Genomics*, Wong, Ka-Chun, Springer-Verlag London, 2016.

SECONDARY LITERATURE:

[1] *Comparative Gene Finding, Models, Algorithms and Implementation*, M. Axelson-Fisk, Springer-Verlag London, 2015.

[2] *Genomes*, T. A. Brown, 4th Edition, Garland Science: New York, 2017.

SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)

Renata Grzywa, PhD, renata.grzywa@pwr.edu.pl

| | | | | | |
|----------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------|----------------------|------------|---------|---------|
| FACULTY of CHEMISTRY | | | | | |
| SUBJECT CARD | | | | | |
| Name of subject in Polish | Krystalografia i struktura ciał stałych | | | | |
| Name of subject in English | Crystallography and structure of solids | | | | |
| Main field of study (if applicable): | Biosciences | | | | |
| Specialization (if applicable): | Medicinal Chemistry | | | | |
| Profile: | academic | | | | |
| Level and form of studies: | 2nd level, full-time | | | | |
| Kind of subject: | obligatory | | | | |
| Subject code | W03BSS-SM2018W, W03BSS-SM2018C | | | | |
| Group of courses | NO | | | | |
| | Lecture | Classes | Laboratory | Project | Seminar |
| Number of hours of organized classes in University (ZZU) | 30 | 15 | | | |
| Number of hours of total student workload (CNPS) | 50 | 25 | | | |
| 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 | 1 | | | |
| including number of ECTS points for practical classes (P) | | 1 | | | |
| including number of ECTS points corresponding to classes that require direct participation of lecturers and other academics (BU) | 1,3 | 0.7 | | | |

*delete as not necessary

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. General knowledge of mathematics, physics and chemistry.

SUBJECT OBJECTIVES

C1 Knowledge of the structure, symmetry and diffraction of macro-, micro- and nanocrystals.

C2 Knowledge of directions of development of crystallography.

C3 Understanding data in crystallographic papers.

SUBJECT EDUCATIONAL EFFECTS

relating to knowledge:

A person who has completed the course:

PEU_W01 has knowledge of the structure and symmetry of crystals.

PEU_W02 understands the international symbols and graphical representation of space groups and the international symbols of crystal classes.

PEU_W03 knows the relationships between a diffraction pattern and crystal structure.
 PEU_W04 has knowledge of directions of development of crystallography.
relating to skills:
 A person who has completed the course:
 PEU_U01 is able to study scientific literature on crystal structures and evaluate crystal data.
related to social competences:
 A person who has completed the course:
 PEU_K01 is able to take part in discussions on crystallographic structural studies.
 PEU_K02 understands the importance of crystallography in science and industry.

| PROGRAMME CONTENT | | |
|--------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------|
| Lecture | | Number of hours |
| Lec 1 | The historical and current definitions of crystals and crystallography. The internal structure of crystals. A crystal lattice, row lines, lattice planes, Miller symbols, a unit cell and cell types. The mosaic structure of real crystals, dislocations. | 2 |
| Lec 2, Lec 3 | The internal symmetry of crystals. Symmetry elements and operations. Relationships between the internal and external symmetry of crystals. Crystal systems vs symmetry. | 4 |
| Lec 4 | Crystal systems and cell parameters. The conventional choice of unit cells. The Bravais unit cells. | 2 |
| Lec 5 | Space groups: international symbols and graphical representations. An asymmetric unit cell. | 2 |
| Lec 6 | Relationships between the symbol of a space group and the symbol of a point group (crystal class). The types of point groups. | 2 |
| Lec 7 | Examples of crystal structures. Crystallographic databases. | 2 |
| Lec 8 | X-rays: properties and sources. Synchrotron radiation: sources of the first, second, third and fourth generations and properties. Synchrotron crystallographic studies. | 2 |
| Lec 9, Lec 10 | The directions and intensities of diffracted beams. Factors influencing the directions and intensities. The phase problem. Diffraction pattern vs internal structure and symmetry of crystals. | 4 |
| Lec 11 | Neutronography and electronography vs roentgenography. Crystallographic information files (cif). | 2 |
| Lec 12, Lec 13 | Nanocrystals. The quantitative and qualitative definition. The internal structure of nanocrystals vs macrocrystals. Defects. External appearance. Diffraction in nanocrystals vs diffraction in microcrystalline materials. The broadening and shifting of peaks in powder diffraction patterns. Apparent lattice parameters: determination and influencing factors. Properties. Synchrotron crystallographic studies of nanocrystals. | 4 |
| Lec 14 | Quasi crystals: 1D, 2D and 3D-dimensional. Internal and external structure. Diffraction. Properties. | 2 |
| Lec 15 | Crystallographic data in scientific papers. | 2 |
| Total hours | | 30 |

| Classes | | Number of hours |
|------------------------|--------------------------------------------------------------------------------------------|-----------------|
| Cl 1 | The preliminary class. | 1 |
| Cl 2 | Lattice points, row lines, lattice planes. | 1 |
| Cl 3, Cl 4, Cl 5 | Symmetry elements: an inversion center, a mirror plane, rotation axes, rotoinversion axes. | 3 |
| Cl 6, Cl 7 | Screw axes and glide planes. | 2 |
| Cl 8 | Bravais lattices. | 1 |
| Cl 9 | Partial test I | 1 |
| Cl 10, Cl 11 | Systematic absences. | 2 |
| Cl 12, Cl 13 | Crystal classes: symbols and graphical representation. | 2 |
| Cl 14 | Physical properties of crystals. | 1 |
| Cl 15 | Partial test II | 1 |
| | Total hours | 15 |

TEACHING TOOLS USED

N1. A multimedia presentation
 N2. Crystallographic models
 N3. A blackboard

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 |
|----------------------------------------------------------------------------|-------------------------------|-------------------------------------------------|
| F1 (lectures) | PEU_W01, PEU_W02, PEU_K01-K02 | partial test I |
| F2 (lectures) | PEU_K01-K02, PEU_W03, PEU_W04 | partial test II |
| F3 (classes) | PEU_W01 PEU_W02 | partial test I |
| F4 (classes) | PEU_W03, PEU_U01 | partial test II |
| $P1=(F1+F2)/2$ $P2=(F3+F4)/2$ | | |

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

- [1] P. Luger, Modern X-Ray Analysis on Single Crystals, de Gruyter, Berlin, 2014.
 [2] R. J. D. Tilley, Crystals and Crystal Structures, John Wiley & Sons Ltd, Chichester, 2006.

SECONDARY LITERATURE:

- [1] C. Giacovazzo, H. L. Monaco, G. Artioli, D. Viterbo, G. Ferraris, G. Gilli, G. Zanotti, M. Catti, Fundamentals of crystallography, C. Giacovazzo Ed., Oxford, 2011.
 [2] International Tables for Crystallography, Volume A, Springer, 2005; Wiley 2016.

SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)

team

FACULTY of Chemistry

SUBJECT CARD**Name of subject in Polish – Eksploracja Danych****Name of subject in English – Data Mining****Main field of study (if applicable): Biosciences****Specialization (if applicable): Bioinformatics****Profile: academic****Level and form of studies: 2nd level, full-time****Kind of subject: obligatory****Subject code W03BSS-SM2009L****Group of courses NO**

| | Lecture | Classes | Laboratory | Project | Seminar |
|----------------------------------------------------------------------------------------------------------------------------------|---------|---------|----------------------|---------|---------|
| Number of hours of organized classes in University (ZZU) | | | 15 | | |
| Number of hours of total student workload (CNPS) | | | 25 | | |
| Form of crediting (Examination / crediting with grade) | | | crediting with grade | | |
| For group of courses mark (X) final course | | | | | |
| Number of ECTS points | | | 1 | | |
| including number of ECTS points for practical classes (P) | | | 1 | | |
| including number of ECTS points corresponding to classes that require direct participation of lecturers and other academics (BU) | | | 0,7 | | |

*delete as not necessary

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. Computer skills
2. Knowledge of the programming basics

SUBJECT OBJECTIVES

C1 Understand the applications of data mining methods to biological data.

C2 Learn how to analyze the results of an experiment using learnt methods.

SUBJECT EDUCATIONAL EFFECTS

relating to skills:

PEU_U01 Proficiency in basic concepts of data exploration, data visualization, diverse data mining techniques, and the application of results in real-world contexts.

relating to social competences:

PEU_K01 Effective communication and the integration of data-driven insights into decision-making processes.

PROGRAMME CONTENT

| Laboratory | | Number of hours |
|------------|-----------------------------|-----------------|
| La1 | Introduction to Data Mining | 1 |

| | | |
|-------------|---------------------------------------------|----|
| La2 | Data Preparation and Cleaning | 2 |
| La3 | Data Exploration and Visualization | 2 |
| La4 | Data Mining Techniques | 2 |
| La5 | Classification Algorithms in Data Mining | 2 |
| La6 | Clustering Algorithms in Data Mining | 2 |
| La7 | Evaluation and Validation metrics | 2 |
| La8 | Knowledge evaluation – end semester project | 2 |
| Total hours | | 15 |

TEACHING TOOLS USED

- N1. Computer Lab
N2. Presentation with elements of live coding
N3. Consultations
N4. Independent additional studies

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 |
|----------------------------------------------------------------------------|------------------------------------------|-------------------------------------------------------------------------------------|
| F | PEU_W01 PEU_W02 PEU_U01 PEU_K01 | Grade based on the assessment of the final project completed during the laboratory. |
| P = F | | |

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

- [1] [Python for data analysis (1st. ed.)], McKinney Wes. 2012., O'Reilly Media, Inc.
[2] Introduction to Data Mining, Pang-Ning Tan, Michael Steinbach, Anuj Karpatne, Vipin Kumar, 2019, Pearson.
[3] The StatQuest Illustrated Guide To Machine, Josh Starmer, 2022, StatQuest Publications

SECONDARY LITERATURE:

- [1] Internet resources

SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)

Dr inż. Wojciech Wojtowicz
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| | | | | | |
|----------------------------------------------------------------------------------------------------------------------------------|---------|---------|------------|---------|---------|
| FACULTY of CHEMISTRY | | | | | |
| SUBJECT CARD | | | | | |
| Name of subject in Polish ...Leki nieorganiczne..... | | | | | |
| Name of subject in English ...Inorganic drugs..... | | | | | |
| Main field of study (if applicable):Biosciences..... | | | | | |
| Specialization (if applicable): ...Medicinal Chemistry..... | | | | | |
| Profile: academic | | | | | |
| Level and form of studies: 2nd level, full-time | | | | | |
| Kind of subject: obligatory | | | | | |
| Subject code W03BSS-SM2025W | | | | | |
| Group of courses: NO | | | | | |
| | Lecture | Classes | Laboratory | Project | Seminar |
| Number of hours of organized classes in University (ZZU) | 15 | | | | |
| Number of hours of total student workload (CNPS) | 25 | | | | |
| Form of crediting (Examination / crediting with grade) | | | | | |
| For group of courses mark (X) final course | | | | | |
| Number of ECTS points | 1 | | | | |
| including number of ECTS points for practical classes (P) | | | | | |
| including number of ECTS points corresponding to classes that require direct participation of lecturers and other academics (BU) | 0.65 | | | | |

*delete as not necessary

| |
|--------------------------------------------------------------------------|
| PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES |
| 1. Principles of inorganic chemistry. |
| 2. |
| 3. |

| |
|--------------------------------------------------------------------------------------------------------------------|
| SUBJECT OBJECTIVES |
| C1 To provide students with inorganic biologically active compounds and their influence on human metabolism. |
| C2 To provide students with issues regarding the use of inorganic compounds in the field of medicine and pharmacy. |

| |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| SUBJECT EDUCATIONAL EFFECTS |
| relating to knowledge: |
| PEU_W01 – the student has general knowledge about metal-based inorganic drugs and metal-based diagnostic agents and knows the basic concepts in the field of inorganic |

| |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <p>medicinal chemistry.</p> <p>PEU_W02 – the student knows the structure of commonly used inorganic drugs and their physicochemical properties, reactivity, and mechanism of their action.</p> <p>PEU_W03 – has general knowledge about current development directions and the latest discoveries regarding the use of inorganic compounds in therapy and diagnostics,</p> <p>PEU_W04 – can distinguish particular groups of inorganic drugs and determine their use and therapeutic effect.</p> |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|

PROGRAMME CONTENT

| Lecture | | Number of hours |
|---------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------|
| Lec 1 | Medicinal inorganic chemistry: state of the art. Classification of metal-based drugs according to their mechanisms of action (essential elements, therapeutic agents, radiopharmaceuticals, metallomics, chelation therapy, enzyme mimics, contrast agents, protein/enzyme regulators). Design of therapeutic and diagnostic agents. | 2 |
| Lec 2 | The concept of bond theory in medicinal inorganic chemistry: nomenclature, coordination geometry, chelating ligands, isomerism, kinetic and thermodynamic stability. | 2 |
| Lec 3 | Metal compounds as therapeutic agents. (antibacterial and antiviral agents, antiparasitic drugs, antiarthritic drugs, antimalarial drugs, treatment of diabetes and obesity, redox-active metal-based mediators). | 3 |
| Lec 4 | Metal-related metabolic disorders. (controversial drugs, heavy-metal poisoning, chelation therapy). | 1 |
| Lec 5 | Medical diagnostics with the use of inorganic complexes and radioisotopes (MRI, MRA, PET, SPECT). | 2 |
| Lec 6 | Discovery of cisplatin, synthesis, its mechanism of anticancer activity and the path to obtaining next generations of drugs based on platinum. | 2 |
| Lec 7 | Search for non-platinum anticancer drugs with the interesting biological properties (drugs based on: Pd, Ti, Ga, As, Ru, Bi, V, Au). | 2 |
| Lec 8 | Final test. | 1 |
| | Total hours | 15 |

TEACHING TOOLS USED

N1. Lecture with multimedia presentation.
 N2.
 N3.

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 |
|----------------------------------------------------------------------------|------------------------|-------------------------------------------------|
| P | PEU_W01-PEU_W04 | Final test |
| | | |

| | | |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--|--|
| | | |
| PRIMARY AND SECONDARY LITERATURE | | |
| <u>PRIMARY LITERATURE:</u> | | |
| [1] E. Alessio (Ed.) Bioinorganic Medicinal Chemistry, Wiley-VCH, 2011 | | |
| [2] K. A. Strohfeldt, Essentials of Inorganic Chemistry for Students of Pharmacy, Pharmaceutical Sciences and Medicinal Chemistry, Wiley, 2015, | | |
| [3] J.C. Dabrowiak Metals in Medicine. Wiley, 2009. | | |
| <u>SECONDARY LITERATURE:</u> | | |
| [4] Nicholas P. Farrell, Uses of inorganic chemistry in medicine, RSC, 1999. | | |
| [5] EudraLex, The Rules Governing Medicinal Products in the European Union, Volume 4, EU Guidelines for Good Manufacturing Practice for Medicinal Products for Human and Veterinary Use, European Commission, health and consumers directorate-general, Ref. Ares(2012)778531 - 28/06/2012. | | |
| [6] J.L.Sessler, S.R.Doctrow, T.J.McMurry, S.J.Lippard, Medicinal Inorganic Chemistry 2005. | | |
| [7] Metallopharmaceuticals I, DNA Interactions Eds. M.J. Clarke, P.J. Sadler (1999). | | |
| [8] Metallopharmaceuticals II, Diagnosis and Therapy. Eds. M.J. Clarke, P.J. Sadler (1999). | | |
| SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS) | | |
| dr hab. Rafal Petrus, rafal.petrus@pwr.edu.pl | | |
| dr inż. Magdalena Malik, magdalena.malik@pwr.edu.pl | | |

| FACULTY of CHEMISTRY | | | | | |
|----------------------------------------------------------------------------------------------------------------------------------|---------|----------------------------|------------|---------|---------|
| SUBJECT CARD | | | | | |
| Name of subject in Polish | | Wprowadzenie do Statystyki | | | |
| Name of subject in English | | Introductory Statistics | | | |
| 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-SM2017C | | | | | |
| Group of courses NO | | | | | |
| | Lecture | Classes | Laboratory | Project | Seminar |
| Number of hours of organized classes in University (ZZU) | | 15 | | | |
| Number of hours of total student workload (CNPS) | | 50 | | | |
| Form of crediting (Examination / crediting with grade) | | crediting with grade | | | |
| For group of courses mark (X) final course | | | | | |
| Number of ECTS points | | 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) | | 0.7 | | | |

*delete as not necessary

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. Basic knowledge of mathematical calculations, linear algebra.
2. Basic ability to use a spreadsheet software.

SUBJECT OBJECTIVES

- C1 Acquainting the student with the basics of descriptive statistics and possibilities of its practical usage.
- C2 Acquainting the student with possibilities of mathematical models utilization in analysis and interpretation of data.

SUBJECT EDUCATIONAL EFFECTS

relating to knowledge:

PEU_W01 Student has a basic knowledge in the area of descriptive statistics.

PEU_W02 Student has information about data analysis methods with aid of statistics.

relating to skills:

PEU_U01 Student is able to solve basic problems from the descriptive statistics field and is able to present experimental data sets in an appropriate way.

relating to social competences:

PEU_K01 Student is able to present and explain the results of the completed project.

PROGRAMME CONTENT

| Classes | | Number of hours |
|-------------|-----------------------------------------------------------------------------------|-----------------|
| CI 1 | Introduction to the basic subjects of descriptive statistics. Types of data sets. | 2 |
| CI 2 | Methods of experimental data processing and its analysis. | 2 |
| CI 3 | Numerical and graphical representation of the statistical data. | 2 |
| CI 4 | Confidence intervals and statistical hypothesis testing. Student's t-test. | 2 |
| CI 5 | Data distribution functions and its utilization. | 2 |
| CI 6 | Correlation analysis of experimental data. | 2 |
| CI 7 | Usage of ANOVA tests in data analysis. | 2 |
| CI 8 | Analysis of common errors and application of improvements. | 1 |
| Total hours | | 15 |

TEACHING TOOLS USED

N1. Multimedia presentation.

N2. Solving project tasks with mathematical and statistical calculations software.

N3. Project with usage of *Design thinking* method.

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 |
|----------------------------------------------------------------------------|------------------------------------|-------------------------------------------------|
| F1 | PEU_W01, PEU_U01 | Sprawozdanie 1 |
| F2 | PEU_W01, PEU_W02, PEU_U01 | Sprawozdanie 2 |
| F3 | PEU_W01, PEU_W02, PEU_U01, PEU_K01 | Sprawozdanie 3 |
| P = (F1 + F2 + F3) / 3 | | |

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

- [1] A. Agresti, C. A. Franklin, Statistics: the art and science of learning from data, Pearson Prentice Hall, Upper Saddle River, 2007,
[2] T. Hill. P. Lewicki, Statistic: methods and applications: a comprehensive reference for science, industry and data mining, StatSoft, Tulsa, 2006.

SECONDARY LITERATURE:

- [1] L. Rogers, D. Willoughby, Numbers: data and statistics for the non-specialist, HarperCollins Publishers, London, 2013.

SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)

dr hab. inż. Izabela Pawlaczyk-Graja, prof. uczelni izabela.pawlaczyk@pwr.edu.pl

Attachment no. 4. to the Program of Studies

| | |
|---------------------------------------------|---------------------------------------------|
| FACULTY of CHEMISTRY | |
| KARTA PRZEDMIOTU | |
| Name of subject in Polish | Izolacja i identyfikacja bioproduktów |
| Name of subject in English | Isolation and identification of bioproducts |
| Main field of study (if applicable): | Biosciences |
| Specialization (if applicable): | Medicinal Chemistry |
| Profile: | academic |
| Level and form of studies: | 2nd level |
| Kind of subject: | obligatory |
| Subject code | W03BSS-SM2016L |
| Group of courses | NO |

| | Lecture | Classes | Laboratory | Project | Seminar |
|----------------------------------------------------------------------------------------------------------------------------------|---------|---------|----------------------|---------|---------|
| Number of hours of organized classes in University (ZZU) | | | 30 | | |
| Number of hours of total student workload (CNPS) | | | 50 | | |
| Form of crediting (Examination / crediting with grade) | | | Crediting with grade | | |
| For group of courses mark (X) final course | | | | | |
| Number of ECTS points | | | 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) | | | 1,4 | | |

*delete as not necessary

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. Knowledge of organic chemistry at the university level.
2. Knowledge of analytical chemistry at the university level.
3. Proficiency in practical work in an organic chemistry laboratory.
4. Familiarity with basic techniques for identifying chemical compounds in mixtures.

SUBJECT OBJECTIVES

- C1 Familiarization with the classification of chromatographic methods.
- C2 Familiarization with the operation and software of gas chromatography.
- C3 Understanding the impact of chromatographic experiment parameters on the separation of organic compounds.
- C4 Familiarization with issues related to qualitative and quantitative analysis.
- C5 Learning methods for identifying compounds released into the environment.
- C6 Introduction to the basics of thin-layer chromatography.

SUBJECT EDUCATIONAL EFFECTS

relating to knowledge:

A person who has passed the subject:

PEU_W01 - knows the classification of chromatographic methods and the principles of chromatographic separation.

PEU_W02 - knows the types of applications of chromatographic techniques in various fields of science.

PEU_W03 - understands the operating principle of analytical equipment.

PEU_W04 - can plan a scientific experiment.

relating to skills:

A person who has passed the subject:

PEU_U01 - can perform analyses using analytical equipment.

PEU_U02 - can conduct a scientific experiment.

PEU_U03 - can determine the concentration of organic compounds in an unknown sample using analytical equipment.

PEU_U04 - can prepare a report from the experiment in the form of a scientific article.

Z zakresu kompetencji:

Osoba, która zaliczyła przedmiot:

PEU_K01 – uznaje znaczenie wiedzy w rozwiązaniu problemów w zakresie identyfikacji bioproduktów

| PROGRAMME CONTENT - laboratory | | Number of hours |
|--------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------|
| La1 | Overview of the curriculum and assessment methods. Safe working conditions in a chemical laboratory. Description of basic working tools. Proposal for a scientific project topic. | 4 |
| La2 | Gas chromatography. Preparation of a method for the initial qualitative analysis. Impact of temperature and flow on the separation of volatile organic compounds. Qualitative analysis of a natural compound solution. Quantitative analysis. Creation of a calibration curve for a natural compound. Determination of concentration in an unknown sample. | 4 |
| La3 | Implementation of a scientific project. Independent work. | 4 |
| La4 | Implementation of a scientific project. Independent work. | 4 |
| La5 | Implementation of a scientific project. Independent work. | 4 |
| La6 | Implementation of a scientific project. Independent work. | 4 |

| | | |
|-----|-----------------------------------------------------------------------------------------------------------------------------------------|----|
| La7 | Implementation of a scientific project. Independent work. | 4 |
| La8 | Final assessment class. Presentation of project results in the form of an article in the format of an international scientific journal. | 2 |
| | Total hours | 30 |

TEACHING TOOLS USED

N1 Working with a computer using scientific and patent databases.
 N2 Independent experimental work in the field of chromatographic techniques.

OCENA OSIĄGNIĘCIA PRZEDMIOTOWYCH EFEKTÓW UCZENIA SIĘ

| Evaluation (F – forming during semester), P – concluding (at semester end) | Learning outcomes code | Way of evaluating learning outcomes achievement |
|----------------------------------------------------------------------------|--------------------------------------------------------|-------------------------------------------------|
| P (laboratory) | PEU_W01- PEU_W04 PEU_U01- PEU_U04, PEU_K01 | Written assessment paper |

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

1. J.L. Anderson *et al.* *Analytical Separation Science*, vol. 3 Wiley-VCH Verlag, Weinheim, **2015**;
2. Anonymous (University of California Davis) *Thin Layer Chromatography*, LibreTexts: https://chem.libretexts.org/Core/Analytical_Chemistry/Lab_Techniques/Thin_Layer_Chromatography; ostatnia modyfikacja: **16.02.2017**
3. Lecture 3 – Thin layer chromatography | MIT 5.301 Chemistry Laboratory Techniques, IAP **2004**; access: Massachusetts Institute of Technology OpenCourseWare - <https://www.youtube.com/watch?v=EUn2skAAjHk>
4. K. Thet, N. Woo, *Gas Chromatography*. LibreTexts; https://chem.libretexts.org/Core/Analytical_Chemistry/Instrumental_Analysis/Chromatography/Gas_Chromatography
Last modification: **13.03.2015**
5. A. Wesółowska *et al.* Comparison of chemical compositions of essential oils isolated by hydrodistillation from wild thyme (*Thymus serpyllum* L.) with use of Deryng and Clevenger apparatus. *herba polonica*, **2014**, 60(2), DOI: 10.2478/hepo-2014-0006

SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)

Dr inż. Daniel Strub, daniel.strub@pwr.edu.pl

FACULTY OF CHEMISTRY

SUBJECT CARD

Name of subject in Polish Uczenie maszynowe w chemii i biologii
Name of subject in English Machine Learning for Chemistry and Biology
Main field of study (if applicable): Biosciences
Specialization (if applicable):
Profile: academic / practical*

Level and form of studies: 2nd level, full-time**Kind of subject:** obligatory**Subject code** W03BSS-SM2013W, W03BSS-SM2013L**Group of courses** NO

| | Lecture | Classes | Laboratory | Project | Seminar |
|----------------------------------------------------------------------------------------------------------------------------------|-------------|---------|-----------------------|---------|---------|
| Number of hours of organized classes in University (ZZU) | 30 | | 30 | | |
| Number of hours of total student workload (CNPS) | 50 | | 50 | | |
| Form of crediting | Examination | | 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) | 1.3 | | 1.4 | | |

*delete as not necessary

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. Fundamentals of Physical Chemistry
2. Understanding the structure of bioorganic molecules
3. Fundamentals of mathematical analysis and linear algebra
4. Pre-intermediate experience with python scripting

SUBJECT OBJECTIVES

- C1 To familiarize the students with the fundamentals of machine learning and deep learning methods.
 C2 To familiarize the students with possible applications of machine learning models in chemistry and biology.
 C3 Acquiring the ability to identify and apply the most appropriate machine learning methods to solve a given research problem or analyze data.
 C4 Learning how to evaluate the trained models and interpret their results.

SUBJECT EDUCATIONAL EFFECTS

relating to knowledge:

PEU_W01 Knows the basic strategies and algorithms of supervised and unsupervised learning.

PEU_W02 Has knowledge of common applications of machine learning methods in chemistry and biology.

PEU_W03 Is able to assess the strengths, weaknesses and limitations of individual machine learning methods in applications to various problems in the field of computational biology.

PEU_W04 Has knowledge of good practices in training machine learning models to avoid overtraining and identify potential shortcomings in the training data set.

PEU_W05 Knows various forms of representation of the structure of bioorganic molecules, including commonly used geometry formats (xyz, pdb, zmat, smiles, smarts, sdf) as well as representations dedicated to machine learning.

PEU_W06 Knows the formats and representations of data that can be used to train machine learning models.

relating to skills:

PEU_U01 Is able to effectively select and prepare a representative data set in the appropriate format for a given machine learning method.

PEU_U02 Can apply supervised learning models for data classification.

PEU_U03 Can apply unsupervised learning models for data clustering.

PEU_U04 Can conceptually/schematically describe an algorithm to solve a given research problem or data analysis problem.

PEU_U05 Can implement an algorithm to solve a given research problem or data analysis problem using the Python scripting language.

PEU_U06 Can evaluate machine learning models and interpret the results they offer.

relating to social competences:

PEU_K01 Students are able to work in a group, performing various roles, including group leader

PEU_K02 Students are aware of the social role of an MSc in Bioinformatics

PEU_K03 Students are ready to critically evaluate his knowledge and the received content

PROGRAMME CONTENT

| PROGRAMME CONTENT | | |
|-------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------|
| | Lecture | Number of hours |
| Lec 1 | Introduction to machine learning. Explanation of the term machine learning and its relation to the so-called artificial intelligence. To familiarize students with the general classification of supervised and unsupervised learning methods. An overview of the most popular applications of machine learning in science, engineering, and life sciences. | 2 |
| Lec 2 | Machine learning datasets. Data sources and representative data formats that can be used for machine learning. Sources of data errors. Good practices in data selection. | 2 |

| | | |
|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----|
| Lec 3 | Supervised learning - artificial neural networks I. A brief history of artificial neural networks and similarities to biological networks. Research directions and applications of neural networks. Linear networks. | 2 |
| Lec 4 | Supervised learning - artificial neural networks II. Training a neural network using the gradient descent method and back propagation. Rosenblatt perceptron. Multilayer and deep networks. Detailed application examples. | 2 |
| Lec 5 | Supervised learning - other methods. Support vector machines, kernel ridge regression, decision trees, random forest. | 2 |
| Lec 6 | Unsupervised learning. Description of the basic methods of unsupervised learning. Classification and grouping. Train the model to recognize features that characterize the data set. | 2 |
| Lec 7 | Structural biology I. Introduction/review of selected issues in structural biology concerning the structure and dynamics of proteins and nucleic acids. Predicting the secondary structure of peptides from sequences. | 2 |
| Lec 8 | Structural biology II. Predicting the structure of biomolecules - AlphaFold and nucleic acids. | 2 |
| Lec 9 | Machine learning models in molecular simulations I. Introduction/review of the elements of computational chemistry. Potential and free energy surfaces. Classification of various methods in computational chemistry including machine learning potentials. | 2 |
| Lec 10 | Machine learning models in molecular simulations II. Representation of the geometry/structure of molecules in machine learning. Training of models to reproduce the shape of the potential energy surface and selection of the data set. Advantages and disadvantages of neural networks and kernel ridge regression. | 2 |
| Lec 11 | Machine learning models in molecular simulations III. Learning molecular properties. Non-bonding interactions, oxidation states and electron configurations. | 2 |
| Lec 12 | Drug design. Interaction of the drug with the active site. Methods of estimating the free energy of active substance binding in the active site. | 2 |
| Lec 13 | Prediction of synthetic pathways to organic molecules. Reaxys database. SMARTS and SMILES structure formats. Approaches to prediction of organic synthesis pathways using retrosynthesis. | 2 |
| Lec 14 | Image analysis and medical applications. Examples and methods of analyzing diagnostic images using machine learning | 2 |
| Lec 15 | Revision of the most important topics presented during the lectures. Preparation for the exam, discussion and questions. | 2 |
| | Total hours | 30 |

| Laboratory | | Number of hours |
|-------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------|
| Lab 1 | Organization of work in the computer laboratory and computing center. Discussion of the principles of occupational health and safety. Account distribution and basic information about available operating systems. Reminder of elements and selected commands of the LINUX operating system. Basic information about the operating system. Using Anaconda and Jupyter Notebooks. | 2 |
| Lab 2 | Introduction to the basics of statistics using the Pandas module. Tasks: histograms, block plots, exploration of pseudo-random number generation, meshing histograms with Pandas; binomial, Poisson and normal distributions. Introduction to the SciKit-learn library in python. | 4 |

| | | |
|-------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----|
| Lab 3 | Data visualization and dimensionality reduction - introduction and exercises. Tasks: use of block charts to visualize many variables simultaneously. Correlation analysis between data based on heat maps. | 4 |
| Lab 4 | Data classification - introduction and exercises. Tasks: classification of white and red wines on the basis of physical and chemical properties. Assessment of the accuracy of the trained model. | 4 |
| Lab 5 | Regression methods - introduction and exercises. Tasks: regularization. | 4 |
| Lab 6 | Structural biology: Grouping of biomolecular structures using the DBSCAN algorithm. Sequence based peptide secondary structure prediction. | 4 |
| Lab 7 | Training models for molecular simulations based on DFT calculations - models based on kernel ridge regression (AQML) and neural networks (ANI). | 4 |
| Lab 8 | Work on individual projects. Presentation of reports on the implementation of individual projects. | 4 |
| | Total hours | 30 |

TEACHING TOOLS USED

- N1. Presentation.
N2. Problem solving in a small-group setting.
N3. Implementation of solutions to problems and realization of tasks in a computer laboratory.

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 |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------|------------------------------------------------------|
| F1 | PEU_U01-PEU_U06, PEU_K01-03 | Grading mid-term reports (max 50 points) |
| P1 | PEU_U01-PEU_U06 | Grading the final report and project (max 50 points) |
| P2 | PEU_W01-PEU_W06 | Exam grade (max 100 points) |
| P (lab classes) 2.0 if (F1+P1) < 50 points 3.0 if (F1+P1) = 50 - 59 points 3.5 if (F1+P1) = 60 - 69 points 4.0 if (F1+P1) = 70 - 79 points 4.5 if (F1+P1) = 80 - 89 points 5.0 if (F1+P1) = 90 - 97 points 5.5 if (F1+P1) = 98 - 100 points P (lecture) 2.0 if (P2) < 50 points 3.0 if (P2) = 50 - 59 points 3.5 if (P2) = 60 - 69 points 4.0 if (P2) = 70 - 79 points 4.5 if (P2) = 80 - 89 points | | |

5.0 if (P2) = 90 - 97 points
5.5 if (P2) = 98 - 100 points

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

- [1] A. Géron, Hands-on Machine Learning with Scikit-Learn, Keras, and TensorFlow: Concepts, Tools, and Techniques to Build Intelligent Systems, O'Reilly Media, Sebastopol, CA, 2020.
[2] B. Ramsunda, P. Eastman, P. Walters, V. Pande, Deep Learning for the Life Sciences, O'Reilly Media, Sebastopol, CA, 2019.

SECONDARY LITERATURE:

- [1] Lafuente D. et al., A Gentle Introduction to Machine Learning for Chemists: An Undergraduate Workshop Using Python Notebooks for Visualization, Data Processing, Analysis, and Modeling, J. Chem. Educ. 2021, 98, 2892–2898
[2] Keith J.A. et al., Combining Machine Learning and Computational Chemistry for Predictive Insights Into Chemical Systems, Chem. Rev. 2021, 121, 9816–9872.
[3] Artrith N. et al., Best practices in machine learning for chemistry, Nat. Chem. 2021, 13, 505-508.

SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)

dr inż. Rafał Szabla, rafal.szabla@pwr.edu.pl

FACULTY of CHEMISTRY

SUBJECT CARD**Name of subject in Polish** *Naturalne produkty medyczne***Name of subject in English** *Medicinal natural products***Main field of study (if applicable):** Biosciences**Specialization (if applicable):** Medicinal chemistry**Profile:** academic**Level and form of studies:** 2nd level, full-time**Kind of subject:** obligatory**Subject code:** W03BSS-SM2022W, W03BSS-SM2022L**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) | examination | | passing with a grade | | |
| For group of courses mark (X) final course | | | | | |
| Number of ECTS points | 2 | | 2 | | |
| including number of ECTS points for practical classes (P) | 0 | | 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. Knowledge in the field of general and organic chemistry.
2. Skills in basic laboratory techniques used in organic and analytical chemistry.

SUBJECT OBJECTIVES

C1 Acquiring knowledge about important groups of active compounds present in plant material – their structures, properties, isolation and identification methods, mechanism of action, activity, and sources of occurrence.

C2 Familiarizing students with methods of isolation and identification of biologically active compound products.

C3 Developing skills for selecting isolation methods for specific plant raw materials.

SUBJECT EDUCATIONAL EFFECTS

relating to knowledge:

PEU_W01 Familiarity with basic concepts in the field of phytochemistry and pharmacognosy.

PEU_W02: Understanding the chemical groups determining the therapeutic properties of plant substances and products.

PEU_W03: Knowledge of the basic chemical structures of coumarins, flavonoids, terpenoids, and alkaloids, including their actions and applications.

PEU_W04: Understanding the main biogenetic pathways and building blocks of plant secondary metabolites.

PEU_W05: Familiarity with methods for isolating biologically active compounds from plant material.

relating to skills:

PEU_U01: Safely handling tasks in organic chemistry laboratories.

PEU_U02: Properly conducting planned chemical experiments.

PEU_U03: Isolating biologically active compounds from natural materials (e.g., plants).

PEU_U04: Applying distillation and extraction techniques in the isolation of natural products.

PEU_U05: Using chromatographic methods for the purification and identification of isolated compounds.

PEU_U06: Writing a detailed report on conducted experiments, analyzing results, and drawing correct conclusions.

relating to social competences:

PEU_K01: Ability to collaborate effectively in a group during laboratory sessions.

PEU_K02: Willingness to organize one's work efficiently, critically assess acquired knowledge, and evaluate the progress of assigned tasks.

PROGRAMME CONTENT

| Lecture | | Number of hours |
|---------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------|
| Lec 1 | Development of phytochemistry and natural product chemistry. Basic concepts, the role of compounds of natural origin in modern medicine and pharmacy. Secondary metabolites. Contemporary principles of classifying plant compounds. Preliminary information, assessment criteria. | 1 |
| Lec 2 | Biogenesis and Building Blocks. Main biogenetic pathways and building blocks of plant secondary metabolites. The information will encompass elements of their biogenesis. | 2 |
| Lec 3 | Coumarins. Characteristics of coumarins as a group of compounds with diverse pharmacological actions (e.g., anticoagulant, photosensitizing effects). Properties, structure, and mechanisms of action. Plant sources. Coumarin preparations available on the Polish market. | 3 |
| Lec 4 | Flavonoids and Stilbenes. Occurrence and characteristics of polyphenolic compounds, exemplified by flavonoids and stilbenes, natural antioxidants with diverse pharmacological significance (e.g., anti-inflammatory, vasodilatory, antimicrobial, vascular-sealing effects). Structure, classification, properties, and application of polyphenolic compounds (including glycosides) in medicinal products; plant sources rich in polyphenolic compounds. Polyphenolic preparations available on the Polish | 4 |

| | | |
|-------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------|
| | market. | |
| Lec 5 | Terpenoids. Characteristics, structure, and properties of terpenoid compounds present in essential oils, used as medicinal products and dietary supplements (e.g., in digestive system disorders). Plant sources rich in essential oils. Preparations available on the Polish market. | 3 |
| Lec 6 | Alkaloids and Their Glycosides. Structure, definition, properties, and classification of alkaloids, pharmacological properties of selected alkaloids and protoalkaloids, plant sources. Selected alkaloid preparations available on the Polish market. | 2 |
| | Total hours | 15 |
| Classes | | Number of hours |
| Cl 1 | | |
| Cl 2 | | |
| Cl 3 | | |
| Cl 4 | | |
| .. | | |
| | Total hours | |
| Laboratory | | Number of hours |
| Lab 1 | Organizational activities, discussion of methods for isolating active substances from plant material, and occupational health and safety training. | 2 |
| Lab 2 | Plant fats – isolation of trimyristin from nutmeg. Determination of the saponification value. Hydrolysis of trimyristin to myristic acid. Determination of the acid value. | 4 |
| Lab 3 | Terpenes – isolation of eugenol from clove oil. | 4 |
| Lab 4-5 | The role of lycopene and β -carotene in the body – isolation of lycopene and β -carotene from tomatoes and carrots. Application of column chromatography for product separation. | 8 |
| Lab 6 | Steroids - isolation of cholesterol from egg yolk. | 4 |
| Lab 7-8 | Triterpene alcohols – isolation of betulin from birch bark. Continuous extraction. Passing grade colloquium. | 8 |
| | Total hours | 30 |
| Project | | Number of hours |
| Proj 1 | | |
| Proj 2 | | |
| Proj 3 | | |
| Proj 4 | | |
| ... | | |
| | Total hours | |
| Seminar | | Number of hours |

| | | |
|------------|-------------|--|
| Semin 1 | | |
| Semin 2 | | |
| Semin 3 | | |
| ... | | |
| | Total hours | |

TEACHING TOOLS USED

- N1. Lecture with audiovisual aids.
N2. Laboratory classes – conducting experiments.

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 |
|----------------------------------------------------------------------------|---------------------------------------|-----------------------------------------------------------------------------------------------------------------------|
| P (lecture) | PEU_W01- PEU_W05 | examination |
| F1 (laboratory) | PEU_U01 - PEU_U06, PEU_K01- K02 | passing with a grade |
| F2 (laboratory) | PEU_U01 - PEU_U06, PEU_K01- K02 | Assessment of the correctness of experiment execution and preparation of a report after completing laboratory classes |
| P (laboratory) = F1 + F2; F1 – 60%; F2 – 40% | | |

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

[1] J. Sołoducho, J. Cabaj, *Medicinal natural products*, <http://zasobynauki.pl/>

SECONDARY LITERATURE:

[1] P.M. Dewick, *Medicinal natural products*, Wiley 2009

SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)

Joanna Cabaj, joanna.cabaj@pwr.edu.pl

| 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 | | Activiti 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 |

| FACULTY of CHEMISTRY | | | | | |
|----------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------|---------|----------------------|---------|---------|
| SUBJECT CARD | | | | | |
| Name of subject in Polish | Nowoczesne Leki i Biofarmaceutyki | | | | |
| Name of subject in English | Modern Pharmaceuticals and Biopharmaceuticals | | | | |
| 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-SM2023W, W03BSS-SM2023L | | | | | |
| Group of courses NO | | | | | |
| | Lecture | Classes | Laboratory | Project | Seminar |
| Number of hours of organized classes in University (ZZU) | 30 | | 30 | | |
| Number of hours of total student workload (CNPS) | 50 | | 50 | | |
| Form of crediting (Examination / crediting with grade) | Exam | | 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) | 1,3 | | 1,4 | | |

*delete as not necessary

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. Principles of organic chemistry, theoretical and practical.
2. Basic knowledge on biochemistry.
3. Knowledge in the field of basis of analytical chemistry is recommended.

SUBJECT OBJECTIVES

- C1 Acquaintance with the knowledge on the distribution of medicinal products and medical devices on basic groups, according to their mechanism of action on the human body.
- C2 Acquaintance with issues of the elementary production processes units in the area of pharmaceutical technology and biopharmacy.
- C3 Acquaintance with the generally applicable operating in the pharmaceutical industry and related sectors quality standards, concerning the manufacturing process and the final product, including the ways of managing waste and REACH requirements.

SUBJECT EDUCATIONAL EFFECTS

Relating to knowledge:

PEU_W01 – has knowledge on the distribution of medicines and medical products on the basic groups,

PEU_W02 – has knowledge on the methods of obtaining biologically active substances and the elementary production processes units in the area of pharmaceutical technology and biopharmacy,

PEU_W03 – can define the various forms of medicines and medical devices, and has knowledge on the technology of receiving them,

PEU_W04 – has knowledge on the generally applicable operating in the pharmaceutical industry and related sectors quality standards, concerning the manufacturing process and the final product, taking into account REACH directive.

Relating to skills:

PEU_U01 – has skills in the qualitative and quantitative analysis of a pharmaceutical formulation, due to the principles of proper samples preparation, precision and repetition in measurements and proper interpretation of the results,

PEU_U02 – has the ability to prepare simple biopharmaceutical preparation,

PEU_U03 – has skills in working in accordance with the principles of good laboratory practice (GLP), in the interpretation of the results of analyzes, error assessment, and the preparation of a laboratory report.

Relating to social competences:

PEU_K01 - Student is able to interact in a group and to plan an experiment.

PEU_K02 - Student is able to discuss the quality of an experimental result.

PEU_K03 - Student works consciously and effectively in a sub-group to searches information and can subject them to critical analysis.

PROGRAMME CONTENT

| Lecture | | Number of hours |
|---------|--------------------------------------------------------------------------------------------------------------------------------------|-----------------|
| Lec1 | The modern pharmaceutical industry: key assets to scientific and medical progress. | 2 |
| Lec2 | Drug targets – the idea of „golden bullet” for proteins, carbohydrates, lipids, DNA, and RNA. | 2 |
| Lec3 | From discovery to clinical trials – the phases of pharmaceutical development. Good Clinical Practice rules (GCP) established by WHO. | 2 |
| Lec 4 | Quality assurance of pharmaceuticals and biopharmaceuticals. | 2 |
| Lec 5 | Ways of obtaining active pharmaceutical ingredients (API). | 2 |
| Lec 6 | Biotechnology-derived drug product development. | |
| Lec 7 | Biopharmaceuticals – historical perspectives and future directions. | 2 |
| Lec 8 | Biopharmaceuticals of animal and microbial origin. | |
| Lec 9 | Physical and physicochemical bases of pharmaceutical formulation. | 2 |
| Lec 10 | Pharmaceutical preformulation: types of naturally occurred excipients. Purity problem. | 2 |
| Lec 11 | Pharmaceutical preformulation: synthetic and semisynthetic excipients. | 2 |

| | | |
|-------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------|
| Lec 12 | Tablets and capsules design. Modern solid dosage systems. | 2 |
| Lec 13 | Controlled release of API from solid and semisolid formulations – bioavailability problem. | 2 |
| Lec 14 | The role of micro- and nanotechnology in pharmaceutical industry. Pharmaceutically accepted micro- and nanosystems. | 2 |
| Lec 15 | Modern control mechanisms of the pharmaceutical industry. The influence of worldwide trends on the drug regulatory system. | 2 |
| | Total hours | 30 |
| Laboratory | | Number of hours |
| Lab 1 | Safety rules in the laboratory of organic chemistry, good laboratory practice (GLP) and the rules of the reports preparation. Introduction to the separation and identification techniques of API. | 2 |
| Lab 2 | Identification and qualitative analysis of drotaverine hydrochloride in NO-SPA tablet according to Pharmacopoeia regulations. | 4 |
| Lab 3 | Suspension form of a drug for children containing ibuprophen – isolation and purification techniques of API. Analysis of the main compound. | 4 |
| Lab 4 | Three compounds drug: Etopiryna (ethenzamide + acetylsalicylic acid + caffeine) – strategies of APIs separation from a tablet form. | 4 |
| Lab 5 | Three compounds drug – analysis of the isolated APIs. | 4 |
| Lab 6 | Polymeric nanocarriers for oral delivery of lipophilic vitamins – synthesis and characterization. | 4 |
| Lab 7 | Kinetics of the release of clotrimazole from the ointment for epidermal application. | 4 |
| Lab 8 | Electrophoresis as a tool for qualitative and quantitative analysis of high-protein dietary supplement. | 4 |
| | Total hours | 30 |
| TEACHING TOOLS USED | | |
| N1 Multimedial presentations. | | |
| N2 Performing experiments with different laboratory equipment and instruments. | | |
| N3 Preparation of report including analysis and interpretation of obtained results. | | |

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 |
|-------------------------------------------------------------------------------------------------|----------------------------------------|----------------------------------------------------------|
| F1 | PEU_W01-W04, PEU_U01 – PEU_U03 | Exam - the grade for the final test of the lectures part |
| F2 | PEU_U01 – PEU_U04 PEU_K01 – PEU_K03 | grades of the laboratory experiments (reports) |
| P = the grade for the final test of the lectures part + average grade of the laboratory reports | | |
| PRIMARY AND SECONDARY LITERATURE | | |

PRIMARY LITERATURE:

- [1] House of Commons Health Committee. The Influence of the Pharmaceutical Industry. HC 42-I [Incorporating HC 1030-i-iii], Published by authority of the House of Commons London: The Stationery Office Limited. 2005.
- [2] The European Federation of Pharmaceutical Industries and Associations. The Pharmaceutical Industry in Figures. 2022.
- [3] Quality assurance of pharmaceuticals: a compendium of guidelines and related materials. Vol. 2, Good manufacturing practices and inspection. – 2nd ed. WHO Press. 2007.
- [4] Shayne Cox Gad, Pharmaceutical Manufacturing Handbook. Production and Processes. John Wiley & Sons, Inc. 2008.
- [5] Alfred Fahr, Voigt's Pharmaceutical Technology. John Willey & Sons Inc., 2018.
- [6] Introduction to Biopharmaceuticals. Montgomery County Community College, 2016.

SECONDARY LITERATURE:

- [7] EudraLex, The Rules Governing Medicinal Products in the European Union, Volume 4, EU Guidelines for Good Manufacturing Practice for Medicinal Products for Human and Veterinary Use, European Commission, health and consumers directorate-general, Ref. Ares(2012)778531 - 28/06/2012
- [8] Mark Gibson. Pharmaceutical Preformulation and Formulation Second Edition. A Practical Guide from Candidate Drug Selection to Commercial Dosage Form. Informa Healthcare USA, Inc. 2009.

SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)

dr hab. inż. Izabela Pawlaczyk-Graja, prof. uczelni izabela.pawlaczyk@pwr.edu.pl

FACULTY of Chemistry

SUBJECT CARD**Name of subject in Polish : Dynamika Molekularna****Name of subject in English : Molecular Dynamics****Main field of study (if applicable): Biosciences.....****Specialization (if applicable): Bioinformatics.....****Profile: academic****Level and form of studies: 2nd level, full-time****Kind of subject: obligatory****Subject code W03BSS-SM2002W, W03BSS-SM2002L****Group of courses NO**

| | Lectur e | Classe s | Laborator y | Projec t | Semina r |
|----------------------------------------------------------------------------------------------------------------------------------|--------------------------------|-------------|--------------------------------|-------------|-------------|
| Number of hours of organized classes in University (ZZU) | 30 | | 30 | | |
| Number of hours of total student workload (CNPS) | 100 | | 50 | | |
| Form of crediting (Examination / crediting with grade) | Credit ing with grade | | Credit ing with grade | | |
| For group of courses mark (X) final course | | | | | |
| Number of ECTS points | 4 | | 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) | 1,3 | | 1,4 | | |

*delete as not necessary

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. General Chemistry, Physics I and I
2. Algebra, Mathematical Analysis
3. Physical Chemistry

SUBJECT OBJECTIVES

- C1. Basic knowledge of statistical thermodynamics
- C2. Design of force fields and basics of molecular dynamics (MD)
- C3. Algorithms used in molecular dynamics
- C4. Preparation and running of molecular dynamics simulations

SUBJECT EDUCATIONAL EFFECTS

relating to knowledge:

- PEU_W01 – Basic concepts and laws of statistical thermodynamics
- PEU_W02 – Potential energy form for a force field and understanding the physical meaning of each term
- PEU_W03 – Methods to search for a global minimum in biological systems
- PEU_W04 – How to choose suitable algorithms for molecular dynamics simulations
- PEU_W05 – Algorithms to control temperature and pressure
- PEU_W06 – Algorithms to calculate free energy within molecular dynamics framework
- PEU_W07 – Analysis of MD results

Relating to skills:

- PEU_U01 – Practical knowledge of Linux operating system
- PEU_U02 – Practical knowledge of specific software to visualize and manipulate biomolecules
- PEU_U03 – Practical knowledge of preparing input files and run and analyze simple minimization and MD simulations
- PEU_U04 – Practical knowledge on how to prepare and run basic MD simulations for proteins

Relating to social competences:

- PEU_K01 student is ready to critically evaluate his/her knowledge and received content

PROGRAMME CONTENT

| Lectures | | Nu |
|-----------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----|
| Lec 1 | Basic concepts. Molecular mechanics vs. quantum mechanics. Limitations of molecular mechanics. How good can MD be? - comparison with experimental results. The choice of a time step in MD simulations to describe various phenomena. | 2 |
| Lec 2 | Introduction to statistical thermodynamics. Permutations and configurations. Probability theory in chemistry. Stirling approximation. Maxwell distribution. Partition function. Significance of Boltzmann distribution in chemistry. Statistical ensembles. Canonical ensemble. Canonical partition function: translational, rotational, vibrational and electronic terms. | 2 |
| Lec 3 | Introduction to statistical thermodynamics – part 2. Internal energy and partition function: translational, rotational, vibrational and electronic contributions. Heat capacity and partition function. Entropy and partition function. Boltzmann equation and canonical partition function. Residual entropy. Free energy and equilibrium constant and partition function. | 2 |
| Lec 4 | Quiz 1. Statistical thermodynamics | 2 |
| Lec 5 | Force field – part 1. Definition of force field. Potential energy in force field. Bonding and non-bonding terms of potential. Harmonic and Morse potential. Mixed terms. Point charge model. RESP procedure. Buckingham and Lennarda-Jones potentials. Combination rules to create van der Waals parameters. Scaling of non-bonding potentials. Evaluation of cpu time in calculations of various potential energy terms. | 2 |
| Lec 6 | Force field – part 2. All-atom and united-atom force fields. Transferability of force field parameters among different force fields. Accuracy of various force fields. | 2 |
| Lec 7 | Preparation of input files for MD simulations. GROMACS options. How to choose an initial structure? A choice of a force field. Phases of MD procedure: minimization, heating, equilibration and production phase. Preparation of all required input files for MD simulations. | 2 |

| | | |
|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------|
| Lec 8 | Methods of searching for global minimum in biomolecules. Methods for energy minimization. Levinthal paradox. Local and global minima in biosystems. Monte-Carlo method. Simulated annealing method. Genetic algorithm. Chain growth method. Homology modelling. Distance-geometry algorithm. Fragment-based algorithm. | 2 |
| Lec 9 | MD algorithms – part 1. Determinism. Lyapunov instability. Newton's formalism. Lagrange's formalism. Hamilton's formalism. Integer algorithms: Euler, Verlet, velocity-Verlet, leap-frog, predictor-corrector. What are the features of a good algorithm? What are the criteria of choosing an optimal algorithm? | 2 |
| Lec 10 | MD algorithms– part 2. Time step. Shake and rattle algorithms. Multiple time-step method. Liouville operator. | 2 |
| Lec 11 | MD algorithms– part 3. Periodic boundary conditions. Minimum image convention. Cut-off technique. Switching and shifting functions. Neighbor list, cell list and Verlet list methods. | 2 |
| Lec 12 | MD algorithms – part 4. Temperature and pressure in MD. Methods to control temperature in MD: stochastic, weak-coupling, strong-coupling, Nose-Hoover. Methods to control pressure in MD: volume scaling, Berendsen, Nose-Hoover and Andersen. | 2 |
| Lec 13 | Free energy in MD. Algorithms to calculate free energy in MD: thermodynamic perturbation, thermodynamic integration and linear interaction energy. Free energy of solvation. Free energy binding of inhibitor to enzyme. | 2 |
| Lec 14 | Analysis of MD results. Average quantities – temperature and pressure. Fluctuations: isobaric and isochoric heat capacity. Structural quantities: pair distribution function and static structure factor. Dynamic quantities: diffusion coefficient, velocity autocorrelation function, dynamic structure factor, MSD. Dipole autocorrelation function. | 2 |
| Lec 15 | Quiz 2. MD algorithms | 2 |
| | Total hours | 30 |

| | |
|----------------------------|----|
| Computer laboratory | Nu |
|----------------------------|----|

| | | |
|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------|
| | | |
| Lab 1 | Requirements to pass a laboratory course. | 2 |
| Lab 2 | Basic Linux commands | 2 |
| Lab 3 | Basic commands of 'vim' text editor. | 2 |
| Lab 4 | Statistical thermodynamics - solving tasks. | 2 |
| Lab 5 | Statistical thermodynamics - solving tasks. | 2 |
| Lab 6 | VMD as a tool to analyze results of MD simulations. | 2 |
| Lab 7 | VMD as a tool to analyze results of MD simulations. | 2 |
| Lab 8 | Preparation of input files to simulate 216 water molecules using GROMACS. Calculations and analysis of results. | 2 |
| Lab 9 | Preparation of input files to simulate 216 methanol molecules using GROMACS. Calculations and analysis of results. | 2 |
| Lab 10 | Preparation of input files to simulate a ribonuclease S-peptide using MD. | 2 |
| Lab 11 | Analysis of MD results for ribonuclease S-peptide in water. | 2 |
| Lab 12 | Preparation of input files for minimization procedure of BPTI protein in water. | 2 |
| Lab 13 | MD simulations of BPTI protein in water – heating, equilibration and production phases of MD. | 2 |
| Lab 14 | Trajectory analysis of MD simulations of BPTI protein in water: RMSD, RMSF, kinetic energy, temperature, pressure, Ramachandran plot, hydrogen bonds and salt bridges, density of protein and water. | 2 |
| Lab 15 | How does the change in time step, force field, deviation in Cartesian coordinates, the choice of an algorithm and van der Waals cut-off affect the physical properties of S-peptide? Analysis of the results. | 2 |
| | Total hours | 30 |

| TEACHING TOOLS USED | |
|----------------------------|--------------------------------------|
| N1 | Lecture with multimedia presentation |

| | |
|----|-------------------------------|
| N2 | Solving practice problem sets |
| N3 | Usage of software |
| N4 | Preparation of reports |

| EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT | | |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------|------------------------------------------------------|
| Evaluation F – forming (during semester), C – concluding (at semester end) | Educational effect number | Way of evaluating educational effect achievement |
| F1 | PEU_W01, PEU_K01 | Quiz 1 |
| F2 | PEU_W02 – PEU_W07, PEU_K01 | Quiz 2 |
| P (laboratory) | PEU_U01 – PEU_U05 | Report+obligatory presence at all laboratory classes |
| <p style="text-align: center;">P (lecture) = 3.0 if (F1 + F2) = 50-60% max. no of poins 3.5 if (F1 + F2) = 61-70% max. no of poins 4.0 if (F1 + F2) = 71-80% max. no of poins 4.5 if (F1 + F2) = 81-90% max. no of poins 5.0 if (F1 + F2) = 91-99% max. no of poins 5.5 if (F1 + F2) = 100% max. no of poins.</p> | | |

| PRIMARY AND SECONDARY LITERATURE |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <p><u>PRIMARY LITERATURE:</u> [1]. D. Frenkel, B. Smith “Understanding Molecular Simulation”, Academic Press, 2001. [2] J.M. Haile “Molecular Dynamics Simulation: Elementary Methods”, Wiley-Interscience, 1997.</p> <p><u>SECONDARY LITERATURE:</u> [1] M. P. Allen, D. J. Tildesley “Computer Simulation of Liquids”, Oxford University Press, 1989.</p> |

SUBJECT SUPERVISOR
(NAME AND SURNAME, E-MAIL ADDRESS)

prof. dr hab. Tadeusz Andruniów, tadeusz.andruniow@pwr.edu.pl

FACULTY OF CHEMISTRY

SUBJECT CARD**Name of subject in Polish** Inżynieria molekularna w analizach genomowych**Name of subject in English** Molecular engineering in genomic analyses**Main field of study (if applicable):** Biosciences**Specialization (if applicable):** Bioinformatics**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-SM2015L**Group of courses** ~~YES~~ / NO*

| | Lecture | Classes | Laboratory | Project | Seminar |
|----------------------------------------------------------------------------------------------------------------------------------|---------|---------|----------------------|---------|---------|
| Number of hours of organized classes in University (ZZU) | | | 45 | | |
| Number of hours of total student workload (CNPS) | | | 50 | | |
| Form of crediting (Examination / crediting with grade) | | | crediting with grade | | |
| For group of courses mark (X) final course | | | | | |
| Number of ECTS points | | | 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) | | | 2.1 | | |

*delete as not necessary

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. The knowledge of basic molecular biology and genetic engineering.
2. The knowledge of the basic laboratory skills.
3. The ability of the basic laboratory calculations including calculations of mass and molar concentrations

SUBJECT OBJECTIVES

- C1 Familiarization with analytical DNA techniques used in biotechnology, medicine, agriculture, archaeology and others.
- C2 Ability to isolate genetic material.
- C3 Familiarization with techniques used for detection of polymorphisms within genomic sequences.
- C4 Familiarization with techniques used for editing of nucleotide sequence.
- C5 Familiarization with techniques used for gene/genomes structure analysis.
- C6 Familiarization with analysis of genes expression and their function.

SUBJECT EDUCATIONAL EFFECTS**Relating to knowledge:**

A student who has completed the course:

| | |
|----------------------------|------------------------------------------------------------------------------------------------------------|
| PEU_W01 | – knows basic molecular tools and techniques used for obtainment and analysis of DNA |
| PEU_W02 | – knows basic techniques of isolation, amplification and biochemical/biophysical description of DNA |
| PEU_W03 | – knows techniques used for analysis of gene and genomes sequences |
| PEU_W04 | – knows techniques used for analysis of gene expression and function |
| PEU_W05 | – know the possible applications of genetic engineering in biotechnology, medicine, agriculture and others |
| PEU_W06 | – know techniques of DNA sequence editing |
| Relating to skills: | |
| PEU_U01 | – can isolate genetic material from various sources |
| PEU_U02 | – can plan restriction reaction and perform |
| PEU_U03 | – can perform agarose gel electrophoresis and can interpret obtained results |
| PEU_U04 | – can design primers and PCR program for enhancement of desired genome fragment |
| PEU_U05 | – can use bioinformatics tools to compare genomic sequences |

| PROGRAMME CONTENT | | |
|----------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------|
| Laboratory | | Number of hours |
| Lab 1 | Introduction, Health and Safety training, discussion on form of crediting of the course and the general introduction of the objective of this course. | 6 |
| Lab 2 | Isolation of the genetic material from the chick epithelium. | 6 |
| Lab 3 | Polymorphism of the gene coding for alcohol dehydrogenase ADH3 | 6 |
| Lab 4 | Analysis of the insertion-deletion polymorphism of the gene coding for angiotensin convertase ACE. | 6 |
| Lab 5 | The use of a single-nucleotide polymorphism to predict bitter-tasting ability | 6 |
| Lab 6 | Analysis of the meat product authenticity. | 6 |
| Lab 7 | Detection of the transgenic soya beans in the food products /Analysis of the polymorphism of insertion of Alu element. | 6 |
| Lab 8 | Test | 3 |
| | Total hours | 45 |
| TEACHING TOOLS USED | | |
| N1. | Short introduction | |
| N2. | Multimedia presentation | |
| N3. | Realisation of the laboratory protocol | |
| N4. | Calculations, problem solving | |
| N5. | Preparation of the final assessment | |
| N6. | Bioinformatics software | |

EVALUATION OF SUBJECT LEARNING OUTCOMES ACHIEVEMENT

| Evaluation (F – forming during | Learning outcomes code | Way of evaluating learning outcomes achievement |
|------------------------------------------|------------------------|-------------------------------------------------|
|------------------------------------------|------------------------|-------------------------------------------------|

| | | |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| semester), P – concluding (at semester end) | | |
| F1 (laboratory) | PEK_U01- PEK_U05 | Written end-course examination and/or short question quiz at the beginning of the laboratory (according to teacher instructions presented during introduction laboratory) |
| F2 (laboratory) | PEK_U01- PEK_U05 | Written assessment from the performer work |
| F3 (laboratory) | PEK_U01- PEK_U05 | Activity and involvement during classes |
| <p>P (laboratory) = $0,8 \cdot F1 + 0,15 \cdot F2 + 0,05 \cdot F3$ Attendance every class and submission of all the assessment is necessary to pass the course.</p> <p>P (laboratory) = 3,0 if $(0,8 \cdot F1 + 0,15 \cdot F2 + 0,05 \cdot F3) = 60,0 - 70,0$ points 3,5 if $(0,8 \cdot F1 + 0,15 \cdot F2 + 0,05 \cdot F3) = 70,1 - 75,0$ points 4,0 if $(0,8 \cdot F1 + 0,15 \cdot F2 + 0,05 \cdot F3) = 75,1 - 80,0$ points 4,5 if $(0,8 \cdot F1 + 0,15 \cdot F2 + 0,05 \cdot F3) = 80,1 - 85,0$ points 5,0 if $(0,8 \cdot F1 + 0,15 \cdot F2 + 0,05 \cdot F3) = 85,1 - 90,0$ points 5,5 if $(0,8 \cdot F1 + 0,15 \cdot F2 + 0,05 \cdot F3) = 90,1 - 100,0$ points</p> | | |

| |
|-------------------------------------------------------------------------------------------------------------------------|
| PRIMARY AND SECONDARY LITERATURE |
| <u>PRIMARY LITERATURE:</u> |
| [1] Brown, T.A. <i>Gene Cloning and DNA Analysis: An Introduction</i> . John Wiley & Sons, 7 th edition |
| [2] Experiment manuals available on the course-specific website only to qualified students |
| <u>SECONDARY LITERATURE:</u> |
| [1] Voet, D., Voet, J.G. <i>Biochemistry</i> Wiley & Sons, Inc., 4 th edition |
| [2] Brown, T.A. <i>Genomy</i> PWN 2018 |
| [3] Węgleński, P. <i>Genetyka molekularna</i> PWN 2012 |
| [4] Berg, J.M., Tymoczko, J.L., Stryer, L. <i>Biochemia</i> PWN 2018 |
| [5] Berg, J.M., Tymoczko, J.L., Stryer, L. <i>Biochemistry</i> W.H. Freeman and Co., New York – 9 th edition |
| [6] http://www.blackwellpublishing.com/genecloning/ |
| SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS) |
| Prof. Andrzej Ożyhar, DSc, PhD, Eng andrzej.ozyhar@pwr.edu.pl |

*delete if not necessary

| FACULTY OF CHEMISTRY | | | | | |
|----------------------------------------------------------------------------------------------------------------------------------|-------------|--------------------------------|----------------------|---------|----------------------|
| SUBJECT CARD | | | | | |
| Name of subject in Polish | | Modelowanie molekularne | | | |
| Name of subject in English | | Molecular modeling | | | |
| Main field of study (if applicable): Biosciences | | | | | |
| Specialization (if applicable): | | | | | |
| Profile: | | academic | | | |
| Level and form of studies: | | 2nd level, full-time | | | |
| Kind of subject: | | obligatory | | | |
| Subject code W03BSS-SM2007W, W03BSS-SM2007L, W03BSS-SM2007S | | | | | |
| Group of courses NO | | | | | |
| | Lecture | Classes | Laboratory | Project | Seminar |
| Number of hours of organized classes in University (ZZU) | 15 | | 30 | | 15 |
| Number of hours of total student workload (CNPS) | 50 | | 50 | | 25 |
| Form of crediting (Examination / crediting with grade) | Examination | | crediting with grade | | crediting with grade |
| For group of courses mark (X) final course | | | | | |
| Number of ECTS points | 2 | | 2 | | 1 |
| including number of ECTS points for practical classes (P) | | | | | |
| including number of ECTS points corresponding to classes that require direct participation of lecturers and other academics (BU) | 1,3 | | 1,4 | | 0,7 |

*delete as not necessary

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. Basic knowledge of atomic and molecular structure concepts
2. Basic knowledge of analytic geometry
3. Basic knowledge of computer science
4. Basic knowledge of organic chemistry

SUBJECT OBJECTIVES

- C1 Teaching construction of 3-D molecular models
 C2 Teaching applications of quantum chemistry methods
 C3 Teaching elementary concepts of the theory of intermolecular interactions
 C4 Teaching modeling techniques of molecular aggregates
 C5 Teaching modeling chemical reactions

SUBJECT EDUCATIONAL EFFECTS**Relating to knowledge:**

- PEU_W01 – knowledge of construction of 3-dimensional molecular models and their transformations
 PEU_W02 – knowledge of elementary molecular modeling methods and limits of their applications.
 PEU_W03 – knowledge of major components of intermolecular interaction energy
 PEU_W04 – knowledge of modeling drugs and biocatalysts

| | |
|---------------------------------------------------------------------------------------------------|--|
| Relating to skills: | |
| PEU_U01 – ability of construction of 3-D molecular model starting from assumed hybridization type | |
| PEU_U02 – ability to predict molecular structure and properties | |
| PEU_U03 – ability to predict possible structures of molecular aggregates | |
| PEU_U04 – ability to analyse protein-ligand interactions | |
| PEU_U05 – ability to model dynamic properties of molecular aggregates | |

PROGRAMME CONTENT

| Lecture | | Number of hours |
|------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------|
| Lec 1 | Basic concepts. Interdisciplinary character of molecular modeling. Typical molecular modeling tasks. Molecular structure sources. Algorithms used in construction of 3-D molecular models with examples. Hybridization. Coordinate transformations. Basic concepts of molecular graphics. Visualization techniques. Literature review. | 2 |
| Lec 2 | Basic concepts of quantum chemistry. Review of quantum chemistry computational methods. Hueckel Molecular Orbitals and <i>ab initio</i> methods. Theoretical prediction of physical properties and structures. | 2 |
| Lec 3 | Construction of molecular models – exercises and test | 2 |
| Lec 4 | Basic concepts of the theory of intermolecular interactions. Perturbation theory. Characteristics of major components of intermolecular interaction components. | 2 |
| Lec 5 | Hydrogen bonding. Molecular charge distribution and electrostatic models. Force fields. | 2 |
| Lec 6 | Predicting properties and structure of molecular aggregates – exercises and test. | 2 |
| Lec 7 | Modeling interactions in receptors and enzyme active centers. Drug design techniques. Molecular dynamic. Homology modeling. | 2 |
| Lec 8 | Analysis of enzyme catalytic activity and biocatalyst design. | 1 |
| | Total hours | 15 |
| Laboratory | | Number of hours |
| Lab 1 | Introduction and lab organization. Editing of molecular structures. | 2 |
| Lab 2 | Force field parametrization of arbitral organic molecules: initial topology, atom types and non-bonding parameters | 2 |
| Lab 3 | Force field parametrization of arbitral organic molecules: optimization of atomic charges | 2 |
| Lab 4 | Force field parametrization of arbitral organic molecules: bonding parameters | 2 |
| Lab 5 | Computational task #1. | 2 |
| Lab 6 | Preparing molecular dynamics simulations | 2 |
| Lab 7 | Preparing molecular dynamics simulations | 2 |
| Lab 8 | Analysis of molecular dynamics trajectories | 2 |
| Lab 9 | Computational task #2. | 2 |
| Lab 10 | Introduction to hybrid QM/MM modeling | 2 |

| | | |
|----------------------------|-----------------------------------------------------------|------------------------|
| Lab 11 | Modeling energy profile of a reaction using QM/MM methods | 2 |
| Lab 12 | Computational task #3. | 2 |
| Lab 13 | Receptor-ligand docking and virtual screening | 2 |
| Lab 14 | Quantum mechanical calculation of interaction energies | 2 |
| Lab 15 | Computational task #4 | 2 |
| | Total hours | 30 |
| Seminar | | Number of hours |
| Se1 | Student's presentations of selected topics | 1 |
| Se2 | | 2 |
| Se3 | | 2 |
| Se4 | | 2 |
| Se5 | | 2 |
| Se6 | | 2 |
| Se7 | | 2 |
| Se8 | | 2 |
| | Total hours | 15 |
| TEACHING TOOLS USED | | |
| N1 | Lecture with multimedia presentation | |
| N2 | Solving problems | |
| N3 | Use of software | |
| N4 | Student multimedia presentation | |
| N5 | Preparing report | |

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 |
|-----------------------------------------------------------------------------------|---------------------------------------------|--------------------------------------------------------------|
| F_Lec1 | PEU_W01, PEU_W02, PEU_U01 | Test with problem solving |
| F_Lec2 | PEU_W02, PEU_W03, PEU_W04, PEU_U01, PEU_U03 | Test with problem solving |
| F_Lab1 | PEU_W04, PEU_U05 | Computational task #1 |
| F_Lab2 | PEU_W01, PEU_W04, PEU_U01, PEU_U04 | Computational task #2 |
| F_Lab3 | PEU_W04, PEU_U03, PEU_U04 | Computational task #3 |
| F_Lab4 | PEU_W04, PEU_U02 | Computational task #4 |
| P_lecture = F_Lec1+F_Lec2 or final exam | | Score Grade |
| P_lab = F_Lab1+F_Lab2+F_Lab3+F_Lab4 | | 50-59,99% 3,0 |
| | | 60-69,99% 3,5 |
| | | 70-79,99% 4,0 |
| | | 80-89,99% 4,5 |
| | | 90-100% 5,0 |
| P_seminar | | Preparation and presentation of seminar on individual topic; |

Active participation in discussion of presentations
of other students

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

- [1] L. Piel, Quantum Chemistry Ideas, Elsevier, 2010
- [2] A.R. Leach, Molecular Modeling: Principles and Applications, (2-nd Ed), Prentice Hall, 2001
- [3] H.D. Hotje, Molecular modeling. Basic principles and applications, (3-rd Ed), Wiley, 2008
- [4] T. Schlick, Molecular modeling and simulation, Springer, 2002.

SECONDARY LITERATURE:

- [1] F. Jensen, Introduction to computational chemistry, Wiley, 2006 (2-nd Ed)
- [2] J.M. Goodman, Chemical Applications of Molecular Modeling, RSC, 1999.
- [3] J.P. Doucet, J. Weber, Computer-Aided Molecular Design, 1996, Academic Press, 1996
- [4] G.H. Grant, W.G. Richards, Computational chemistry, Oxford Sci. Publ., 1995

SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)

Paweł Kędzierski, Pawel.Kedzierski@pwr.edu.pl

| FACULTY of CHEMISTRY | | | | | |
|----------------------------------------------------------------------------------------------------------------------------------|---------|---------|-----------------------|---------|---------|
| SUBJECT CARD | | | | | |
| Name of subject in Polish ...Wieloletapowa synteza organiczna | | | | | |
| Name of subject in EnglishMultistep organic synthesis.... | | | | | |
| Main field of study (if applicable): ...BIOSCIENCES.... | | | | | |
| Specialization (if applicable): ...Medicinal chemistry | | | | | |
| Profile: academic | | | | | |
| Level and form of studies: 2nd level, | | | | | |
| Kind of subject: obligatory | | | | | |
| Subject code ... W03BSS-SM2024L | | | | | |
| Group of courses YES/ NO* | | | | | |
| | Lecture | Classes | Laboratory | Project | Seminar |
| Number of hours of organized classes in University (ZZU) | | | 60 | | |
| Number of hours of total student workload (CNPS) | | | 75 | | |
| Form of crediting (Examination / crediting with grade) | | | crediting with grade) | | |
| For group of courses mark (X) final course | | | | | |
| Number of ECTS points | | | 3 | | |
| including number of ECTS points for practical classes (P) | | | 3 | | |
| including number of ECTS points corresponding to classes that require direct participation of lecturers and other academics (BU) | | | 2,8 | | |

*delete as not necessary

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. Knowledge and skills at the level of completing the "Fundamentals of organic chemistry - laboratory" course or equivalent
2. Basic knowledge of English at a communicative level

SUBJECT OBJECTIVES

- C1 Acquires students' proficiency in laboratory work using advanced experimental techniques of organic synthesis.
- C2 Ability to practically use various transformation methods in multi-stage synthesis - creating new C-C bonds, transformations on functional groups
- C3 Ability to perform a complex synthetic sequence based on literature data.

SUBJECT EDUCATIONAL EFFECTS

relating to skills:

PEU_U01 – is able to carry out a multi-stage synthesis of an organic compound,

PEU_U02 – knows how to use scientific literature and chemical databases

PEU_U03 – is able to select the conditions for various transformations and plan methods of isolating and purifying products,

PEU_U04 – is able to independently interpret the results, measure basic physicochemical constants, interpret spectroscopic spectra of organic compounds

relating to social competences:

PEU_K01 – knows English at a communicative level, is able to keep a laboratory journal in English

PROGRAMME CONTENT

| Lecture | | Number of hours |
|------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------|
| Lec 1 | | |
| Lec 2 | | |
| Lec 3 | | |
| Lec 4 | | |
| Lec 5 | | |
| | | |
| | Total hours | |
| Classes | | Number of hours |
| Cl 1 | | |
| Cl 2 | | |
| Cl 3 | | |
| Cl 4 | | |
| .. | | |
| | Total hours | |
| Laboratory | | Number of hours |
| Lab 1 | Information on how to conduct and pass exercises and keep a laboratory journal. Basic equipment (glass and metal) and laboratory operations. Work safety in the laboratory: harmful, flammable substances, etc. Synthesis planning - using literature and databases. | 4 |
| Lab 2 | Carrying out one-step syntheses requiring selective reduction of the C=O and C=C bonds - procedures to be selected by the lecturer (from a prepared script) | 4 |
| Lab 3 | | 4 |
| Lab 4 | | 4 |
| Lab 5 | | 4 |
| Lab 6 | Carrying out a one-step synthesis requiring selective oxidation - procedure to be selected by the instructor (from a prepared script) | 4 |
| Lab 7 | | 4 |
| Lab 8 | Conducting a 3- and 4-step synthesis of a compound with known biological | 4 |

| | | |
|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---|
| Lab 9 | activity, including both the formation of new C-C bonds and transformations on various functional groups. Purification, identification and characterization of products - measurement of physico-chemical constants. Calculations of the yield at individual stages and total yield. Interpretation of the results. | 4 |
| Lab 10 | | 4 |
| Lab 11 | | 4 |
| Lab 12 | | 4 |
| Lab 13 | | 4 |
| Lab 14 | | 4 |
| Lab 15 | Settlement of laboratory equipment and laboratory notes. | 4 |
| | Total hours | |

| Project | | Number of hours |
|----------------|-------------|------------------------|
| Proj 1 | | |
| Proj 2 | | |
| Proj 3 | | |
| Proj 4 | | |
| ... | | |
| | Total hours | |

| Seminar | | Number of hours |
|----------------|-------------|------------------------|
| Semin 1 | | |
| Semin 2 | | |
| Semin 3 | | |
| ... | | |
| | Total hours | |

| TEACHING TOOLS USED | | |
|--------------------------------------------------------------------------------------------------------------|--|--|
| N1. Discussion of the experiment: planning the equipment, techniques used and subsequent stages of synthesis | | |
| N2. Carrying out experiments independently | | |
| N3. Preparing a report in a laboratory journal (in English) | | |

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 |
|-----------------------------------------------------------------------------------|--------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| P | PEU_U01- PEU_U04 PEU_K01 | Independent synthesis of given products, measurement of physical and chemical constants for product characterization, preparing a report in the laboratory book in English. |

| PRIMARY AND SECONDARY LITERATURE |
|-----------------------------------------|
|-----------------------------------------|

PRIMARY LITERATURE:

- [1] R. Siedlecka, Multistep organic synthesis. Laboratory course for students of medicinal chemistry, Wrocław, 2020;
- [2] A. Mucha, R. Siedlecka, Multistep organic synthesis. Practical course, Wrocław, 2010;
- [3] A. I. Vogel, Preparatyka organiczna, WNT, Warszawa, 2006;
- [4] Bazy danych: Beilstein, Chemical Abstracts, Current Contents.

SECONDARY LITERATURE:

- [1] J. Gawroński, K. Gawrońska, K. Kacprzak, M. Kwit, Współczesna synteza organiczna, PWN, Warszawa, 2004
- [2] L.-T. Ho, *Tactics of Organic Synthesis*, J. Wiley, New York, 1994

SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)

Dr hab. inż. Renata Siedlecka, renata.siedlecka@pwr.edu.pl

FACULTY Chemistry

SUBJECT CARD**Name of subject in Polish: Sieci i stacje robocze z systemem unix****Name of subject in English: Networks and workstations with unix system****Main field of study (if applicable): Biosciences****Specialization (if applicable): Bioinformatics****Profile: academic / practical*****Level and form of studies: 2nd level, full-time****Kind of subject: obligatory****Subject code W03BSS-SM2003L****Group of courses NO**

| | Lecture | Classes | Laboratory | Project | Seminar |
|----------------------------------------------------------------------------------------------------------------------------------|---------|---------|----------------------|---------|---------|
| Number of hours of organized classes in University (ZZU) | | | 30 | | |
| Number of hours of total student workload (CNPS) | | | 50 | | |
| Form of crediting (Examination / crediting with grade) | | | crediting with grade | | |
| For group of courses mark (X) final course | | | | | |
| Number of ECTS points | | | 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) | | | 1,4 | | |

*delete as applicable

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. English - basic level
2. Basic computer skills

SUBJECT OBJECTIVES

C1 Learning the mechanisms of unix system, and rules of computer network based on the internet protocol

C2 Developing skills for using unix systems at unassisted administration level

SUBJECT EDUCATIONAL EFFECTS

relating to skills:

PEU_U01 Student can run programs from the command line, to perform various file operations, and use a text editor

PEU_U02 Student can use documentation for programs, available in unix system

PEU_U03 Student can write an inittab file and simple scripts responsible for initial system configuration, check the consistency of a filesystem and attach it to the directory tree

PEU_U04 Student can add and remove user accounts, change passwords and assign users to groups, can write session scripts (bash shell)

PEU_U05 Student can assign the network address to network interface, build the routing table, create local list of address-name relationships and prepare the system for using the DNS service

PEU_U06 Student can use network services of remote terminal, copying files between systems and electronic mail, can make them available for remote users and limit this remote access to specific addresses.

PEU_U07 Student can run local and remote graphical applications in the X window system

PROGRAMME CONTENT

| Laboratory | | Number of hours |
|------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------|
| Lab 1 | Programs and processes. Parent and child processes, system mechanisms for running programs and process termination. Signals. User's and group's identifiers - introduction of mechanisms regulating access rights to various system resources. | 2 |
| Lab 2 | Files and file types: normal, directories, special (character and block devices), files representing communication channels (sockets and named pipes). Normal pipes and their similarity to files. The notion of a filesystem, hard and symbolic links. Review of programs for various file operations, including short introduction to the vi editor. | 2 |
| Lab 3 | Running the linux kernel under control of the QEMU emulator. Creation of a file representing hard disk, partitioning and creation of filesystem. Archives created with the tar program. Installation of minimal set of programs, needed for running the system. | 2 |
| Lab 4 | Duties of the program running with process identifier equal to 1. Configuration of the init program (implementation: sysvinit) - the inittab file. Review of tasks performed at the system's initialization stage. | 2 |
| Lab 5 | Checking of filesystems' consistency and attaching filesystems to the directory tree. Mount and umount programs, the /etc/fstab file. Shared libraries. | 2 |
| Lab 6 | User accounts - entries in the /etc/passwd file, relationship of names with user identifiers, home directories, encryption and storing of passwords. System and personal session scripts. Creation of groups (the /etc/group file). Programs: su and newgrp. | 2 |
| Lab 7 | IP address, address' class, structure of an address within given network segment (network mask). Assignment of IP address to the network interface, with the ifconfig program. The loopback interface. Creation of the routing table with the route program. | 2 |
| Lab 8 | Internet names, name-address relationship. Methods of translating names to addresses and addresses to names: local list in the /etc/hosts file and the DNS network service. | 2 |
| Lab 9 | TCP and UDP transport protocols. The notion of network socket. Assignment of network services to port numbers (/etc/services file). Rules of making services available by the inetd program. | 2 |
| Lab 10 | Limiting remote access to network services – mechanisms and configuration of the TCP wrappers software (tcpd program and library code) by access control lists in /etc/hosts.allow and /etc/hosts.deny files. | 2 |
| Lab 11 | Working in a remote system - services of remote terminal (telnet and ssh) and file transfer (ftp, scp, sftp). Reasons for using encrypted communication channels. | 2 |

| | | |
|--------|--------------------------------------------------------------------------------------------------------------------------------------------------------------|----|
| Lab 12 | Electronic mail - MTA and MUA programs, running an MTA program (smail) and using the mutt mail client (MUA). Basic rules for securing the mail server (MTA). | 2 |
| Lab 13 | The WWW server - basic configuration of the boa program, creation of simplest WWW pages in the HTML language. Text WWW browser - lynx. | 2 |
| Lab 14 | The X window system - graphical environment with client-server architecture. | 2 |
| Lab 15 | Crediting | 2 |
| | Total hours | 30 |

TEACHING TOOLS USED

- N1. Demonstration
N2. Practical exercises, under teacher's control
N3. Practical exercises, with a simple problem to be solved single-handedly by the student

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT

| Evaluation (F – forming (during semester), P – concluding (at semester end)) | Educational effect number | Way of evaluating educational effect achievement |
|-----------------------------------------------------------------------------------------------------------------------------------|---------------------------|---------------------------------------------------|
| F1 | PEU_U01-U07 | practical exercises (up to 25 points) |
| P1 | PEU_U02-U06 | written test (up to 75 points) |
| F2 | PEU_U02-U06 | outstanding knowledge or skills (up to 10 points) |
| $C = F1 + P1 + F2$ 50 ≤ C < 60 3.0 60 ≤ C < 70 3.5 70 ≤ C < 80 4.0 80 ≤ C < 90 4.5 90 ≤ C < 100 5.0 C ≥ 100 5.5 | | |

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

[1] Aeleen Frisch, UNIX: administracja systemu, O'Reilly & Associates, wydawnictwo RM, Warszawa 1997

SECONDARY LITERATURE:

[1] Craig Hunt, TCP/IP : administracja sieci. wydawnictwo RM, Warszawa 2003

SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)

dr hab. inż. Krzysztof Strasburger, e-mail: krzysztof.strasburger@pwr.edu.pl, strasbur@chkw386.ch.pwr.wroc.pl

Attachment no. 4. to the Program of Studies

| | | | | | |
|----------------------------------------------------------------------------------------------------------------------------------|---------|-----------------------|----------------------|---------|---------|
| FACULTY of Chemistry | | | | | |
| SUBJECT CARD | | | | | |
| Name of subject in Polish: | | Praca dyplomowa I | | | |
| Name of subject in English: | | Graduate laboratory I | | | |
| Main field of study (if applicable): | | | | | |
| Specialization (if applicable): | | | | | |
| Profile: | | academic | | | |
| Level and form of studies: | | 2nd level, full-time | | | |
| Kind of subject: | | obligatory | | | |
| Subject code W03W03-SM1054D, W03W03-SM2054D | | | | | |
| Group of courses | | NO | | | |
| | Lecture | Classes | Laboratory | Project | Seminar |
| Number of hours of organized classes in University (ZZU) | | | 60 | | |
| Number of hours of total student workload (CNPS) | | | 150 | | |
| Form of crediting (Examination / crediting with grade) | | | crediting with grade | | |
| For group of courses mark (X) final course | | | | | |
| Number of ECTS points | | | 6 | | |
| including number of ECTS points for practical classes (P) | | | 6 | | |
| including number of ECTS points corresponding to classes that require direct participation of lecturers and other academics (BU) | | | 3 | | |

*delete as not necessary

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

- 1.
- 2.

SUBJECT OBJECTIVES

C1 Developing the ability to select and analyze sources of knowledge, including scientific literature

C2 Developing the ability to create a written study on the topic of the diploma thesis

C3 Expanding the skills of planning and conducting scientific work

SUBJECT EDUCATIONAL EFFECTS

In relation to knowledge:

PEU_W01 – knows the types of sources of scientific and professional knowledge,

PEU_W02 – has in-depth knowledge of the topic of the diploma thesis

In relation to skills:

PEU_U01 – is able to collect information useful for learning about a specific issue and preparing for the completion of a diploma thesis
 PEU_U02 – is able to critically analyze the collected information in a form written on a selected scientific or practical issue.
 PEU_U03 – (optional) is able to plan and carry out experiments/design work as well as develop the results and draw conclusions from their achievements and plan further work
 In relation to social competences:
 PEU_K01 – is ready to critically evaluate knowledge obtained from various sources
 PEU_K02 – is ready to comply with the principles of professional ethics and respect copyrights

PROGRAMME CONTENT

| Laboratory | | Number of hours |
|-------------------|-----------------------------------------------------------------------------------------------------------------|------------------------|
| Lab 1- Lab15 | Individual student work on a selected topic according to the schedule agreed with the diploma thesis supervisor | 60 |
| Total hours | | 60 |

TEACHING TOOLS USED

N1. consultations

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 |
|-----------------------------------------------------------------------------------|-------------------------------------------------------------|-------------------------------------------------------------------------------|
| P | PEU_W01 – PEU_W02 PEU_U01 – PEU_U03 PEU_K01 – PEU_K02 | assessment of student work based on progress in completing the diploma thesis |

PRIMARY AND SECONDARY LITERATURE

Scientific and professional literature indicated by the course tutor and/or found by the student.

SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)

Supervisors of individual diploma thesis topics
 Subject card preparation:
 Piotr Rutkowski, piotr.rutkowski@pwr.edu.pl

Attachment no. 4. to the Program of Studies

| | | | | | |
|----------------------------------------------------------------------------------------------------------------------------------|---------|------------------------|----------------------|---------|---------|
| FACULTY of Chemistry | | | | | |
| SUBJECT CARD | | | | | |
| Name of subject in Polish: | | Praca dyplomowa II | | | |
| Name of subject in English: | | Graduate laboratory II | | | |
| Main field of study (if applicable): | | | | | |
| Specialization (if applicable): | | | | | |
| Profile: | | academic | | | |
| Level and form of studies: | | 2nd level, full-time | | | |
| Kind of subject: | | obligatory | | | |
| Subject code W03W03-SM1055D, W03W03-SM2055D | | | | | |
| Group of courses | | NO | | | |
| | Lecture | Classes | Laboratory | Project | Seminar |
| Number of hours of organized classes in University (ZZU) | | | 210 | | |
| Number of hours of total student workload (CNPS) | | | 500 | | |
| Form of crediting (Examination / crediting with grade) | | | crediting with grade | | |
| For group of courses mark (X) final course | | | | | |
| Number of ECTS points | | | 20 | | |
| including number of ECTS points for practical classes (P) | | | 20 | | |
| including number of ECTS points corresponding to classes that require direct participation of lecturers and other academics (BU) | | | 9,5 | | |

*delete as not necessary

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1.

SUBJECT OBJECTIVES

C1 implementation of a research project

C2 written preparation of the diploma thesis

SUBJECT EDUCATIONAL EFFECTS

In relation to knowledge:

PEU_W01 – knows the types of sources of scientific and professional knowledge

PEU_W02 – has advanced knowledge of the topic of the diploma thesis

In relation to skills:

PEU_U01– is able to carry out experiments / develop a project in accordance with the developed work plan

PEU_U02 – is able to compare information obtained from sources of knowledge with the results of research, verify the results of own research, draw conclusions and plan further work

PEU_U03 – is able to develop the results of his/her work on a selected topic and present them in the form of a diploma thesis

In relation to social competences:

PEU_K01 – is ready to critically evaluate the obtained results of research work on a selected topic

PEU_K02 – is ready to comply with the principles of professional ethics and respect copyrights

PROGRAMME CONTENT

| Laboratory | | Number of hours |
|-------------------|-----------------------------------------------------------------------------------------------------------------|------------------------|
| Lab 1- Lab15 | Individual student work on a selected topic according to the schedule agreed with the diploma thesis supervisor | 210 |
| | Total hours | 210 |

TEACHING TOOLS USED

N1. consultations

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 |
|-----------------------------------------------------------------------------------|----------------------------------------------------------------------|-------------------------------------------------------------------------------|
| P | PEU_W01 – PEU_W02 PEU_U01 – PEU_U03 PEU_K01 – PEU_K02 | assessment of student work based on progress in completing the diploma thesis |

PRIMARY AND SECONDARY LITERATURE

Scientific and professional literature indicated by the course tutor and/or found by the student.

SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)

Supervisors of individual diploma thesis topics
Subject card preparation:
Piotr Rutkowski, piotr.rutkowski@pwr.edu.pl

Attachment no. 4. to the Program of Studies

| | | | | | |
|----------------------------------------------------------------------------------------------------------------------------------|---------|-----------------------|------------|---------|----------------------|
| FACULTY of Chemistry | | | | | |
| SUBJECT CARD | | | | | |
| Name of subject in Polish: | | Proseminarium | | | |
| Name of subject in English: | | Graduation proseminar | | | |
| Main field of study (if applicable): | | | | | |
| Specialization (if applicable): | | | | | |
| Profile: | | academic | | | |
| Level and form of studies: | | 2nd level, full-time | | | |
| Kind of subject: | | obligatory | | | |
| Subject code W03W03-SM1053S, W03W03-SM2053S | | | | | |
| Group of courses | | NO | | | |
| | Lecture | Classes | Laboratory | Project | Seminar |
| Number of hours of organized classes in University (ZZU) | | | | | 15 |
| Number of hours of total student workload (CNPS) | | | | | 25 |
| Form of crediting (Examination / crediting with grade) | | | | | crediting with grade |
| For group of courses mark (X) final course | | | | | |
| Number of ECTS points | | | | | 1 |
| including number of ECTS points for practical classes (P) | | | | | 1 |
| including number of ECTS points corresponding to classes that require direct participation of lecturers and other academics (BU) | | | | | 0,7 |

*delete as not necessary

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

- 1.
- 2.
- 3.

SUBJECT OBJECTIVES

C1
C2

SUBJECT EDUCATIONAL EFFECTS

In relation to knowledge:

PEU_W01 – has knowledge of research topics related to the studied field of study conducted in organizational units of the Faculty of Chemistry

In relation to skills:

PEU_U01 – can take an active part in discussions on scientific topics

In relation to social competences:
 PEU_K01 – is aware of the need to improve their competences in the field of research within the field of study

PROGRAMME CONTENT

| Seminar | | Number of hours |
|----------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------|
| Semin 1-15 | Discussion of the topics of diploma theses by employees of the Faculty's units conducting research related to the field of study; Presentation of research and analytical laboratories in the Faculty's units; Discussion of the rules for selecting the topics of diploma theses and the rules for implementing/passing the "Diploma Thesis" courses | 15 |
| | Total hours | 15 |

TEACHING TOOLS USED

- N1. Presentation
- N2. Discussion
- N3. Consultations

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 |
|-----------------------------------------------------------------------------------|-------------------------------|-----------------------------------------------------------------------------------------------------|
| P | PEU_W01 PEU_U01 PEU_K01 | Attendance at classes, participation in discussions - assessed by the people conducting the classes |

PRIMARY AND SECONDARY LITERATURE

N/A

SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)

Chairman of the study program committee

Attachment no. 4. to the Program of Studies

| | | | | | |
|----------------------------------------------------------------------------------------------------------------------------------|---------------------------------|---------|------------|---------|---------|
| FACULTY of Chemistry | | | | | |
| SUBJECT CARD | | | | | |
| Name of subject in Polish: | Przedmiot kierunkowy wybieralny | | | | |
| Name of subject in English: | Elective course | | | | |
| Main field of study (if applicable): | | | | | |
| Specialization (if applicable): | | | | | |
| Profile: | academic | | | | |
| Level and form of studies: | 2nd level, full-time | | | | |
| Kind of subject: | elective | | | | |
| Subject code | | | | | |
| Group of courses | NO | | | | |
| | Lecture | Classes | Laboratory | Project | Seminar |
| Number of hours of organized classes in University (ZZU) | 30 | | | | |
| Number of hours of total student workload (CNPS) | 25 | | | | |
| Form of crediting (Examination / crediting with grade) | Zaliczenie na ocenę | | | | |
| For group of courses mark (X) final course | | | | | |
| Number of ECTS points | 2 | | | | |
| including number of ECTS points for practical classes (P) | | | | | |
| including number of ECTS points corresponding to classes that require direct participation of lecturers and other academics (BU) | 1,3 | | | | |

*delete as not necessary

| |
|--------------------------------------------------------------------------|
| PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES |
| 1. |
| 2. |
| 3. |

| |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| SUBJECT OBJECTIVES |
| C1 Familiarizing the student with advanced issues in the field of chemical sciences (including biotechnology) and/or materials engineering and/or chemical engineering (including chemical technology) |
| SUBJECT EDUCATIONAL EFFECTS |
| In relation to knowledge: PEU_W01 – Knows and is able to describe the basic phenomena and processes occurring in the life cycle of devices, objects and technical systems. |

PEU_W02 – has in-depth knowledge of development trends and new achievements in the field of chemical engineering and technology and related sciences
 In relation to social competences:
 PEU_K01 – is ready to critically evaluate the knowledge acquired and the content received
 PEU_K02 – is aware of the role of a technical university graduate and the need to maintain the ethos of the engineering profession

PROGRAMME CONTENT

| Lecture | | Number of hours |
|------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------|
| Lec 1- Lec 15 | To familiarize students with advanced concepts, theories describing phenomena, operations and processes occurring in living and inanimate systems, as well as with the latest trends in chemical sciences, chemical engineering and related sciences. Issues presented in an elective subject, depending on the field studied, may include, among others: <ul style="list-style-type: none"> - adsorbents in environmental protection and industry - alternative and renewable energy sources, renewable raw materials in industry, recycling technologies - technical security - medical and pharmaceutical chemistry - chemistry of coordination compounds - chemistry of fragrance compounds - physical chemistry of chemical processes and products - chemistry, engineering and technology of materials (polymer, carbon, ceramic, metallic) and composites - technologies of dispersed systems - catalysts and catalysis in industry - instrumental methods in chemistry - physicochemical description of simple and complex systems - from the borderline of biology and medicine, describing the biological and biochemical basis of the functioning of organisms, including chemical and biochemical processes at the cellular and molecular level - industrial aspects of biotechnology - recycling of precious metals - issues of technological process and quality management, principles of investing and operating chemical technologies - modern chemical technologies - biotechnology development trends - basics of spectroscopic methods, - bioelectrochemical systems - issues related to sustainable development - characteristics of the biotechnology and chemical industry in Poland and in the world | 30 |
| | Total hours | 30 |

TEACHING TOOLS USED

N1. Presentation
 N2. Discussion

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 |
| P | PEU_W01- PEU_W02 PEU_K01- PEU_K02 | Writing test (to pass minimum 50% of points) |
| PRIMARY AND SECONDARY LITERATURE | | |
| [1] Literature is provided during the first classes by the teachers of the elective subject | | |
| SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS) | | |
| Chairman of study program committee | | |

FACULTY OF CHEMISTRY

SUBJECT CARD**Name of subject in Polish** Racjonalne projektowanie leków**Name of subject in English** Rational drug design**Main field of study (if applicable):** Biosciences**Specialization (if applicable):****Profile:** academic**Level and form of studies:** 2nd level, full-time**Kind of subject:** obligatory**Subject code** W03BSS-SM2006W**Group of courses** NO

| | Lecture | Classes | Laboratory | Project | Seminar |
|----------------------------------------------------------------------------------------------------------------------------------|----------------------|---------|------------|---------|---------|
| Number of hours of organized classes in University (ZZU) | 30 | | | | |
| Number of hours of total student workload (CNPS) | 75 | | | | |
| Form of crediting (Examination / crediting with grade) | crediting with grade | | | | |
| For group of courses mark (X) final course | | | | | |
| Number of ECTS points | 3 | | | | |
| including number of ECTS points for practical classes (P) | | | | | |
| including number of ECTS points corresponding to classes that require direct participation of lecturers and other academics (BU) | 1,3 | | | | |

*delete as not necessary

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. Knowledge of the basics of organic chemistry
2. Knowledge of the basics of biology

SUBJECT OBJECTIVES

C1 To familiarize students with the basics of drug design.

C2 Understanding the economic aspects of drug design.

C3 Learning about targeted therapy methods.

SUBJECT EDUCATIONAL EFFECTS

relating to knowledge:

Person who passed the subject:

PEU_W01 – knows the basic principles of drug design,

PEU_W02 – is able to select the appropriate drug design technique depending on the level of knowledge about the physiological process,

PEU_W03 – has basic knowledge about the costs and time horizon of drug design,

PEU_W04 – understands the physiological and economic effects of using drugs.

relating to:

Person who passed the subject:

PEU_K01 – recognizes the importance of non-technical aspects of scientific activity

| PROGRAMME CONTENT | | |
|--------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------|
| | Lecture | Number of hours |
| Lec 1 | Economics of drug design and development. Cost and time required to introduce new drug to the market. Generic drugs. Globalization. | 2 |
| Lec 2 | Randomized screening. Historical perspective. Illustration of the opinion of Louyis Pasteur „Fortune favors prepared minds”. Case studies. | 2 |
| Lec 3 | Natural products as a source of drugs. History of the discovery of aspirin, morphine, artemisinin, quinine, penicillin and taxol. Current trends in natural drug research. | 2 |
| Lec 4 | Choice of the target. HIV as an example for choice of the target for drug design. | 2 |
| Lec 5 | Theory of structural analogy. Historical perspective (sulfonamides). Direct similarity versus topological one with analogs of morphine and anti-influenza drugs as examples. | 2 |
| Lec 6 | Theory of structural analogy. Chemical outlook, tricks and “magic methods”. Peptidomimetics. | 2 |
| Lec 7 | Covalent drugs. Overview of functional groups able for irreversivble bonding with proteins. Techniques of design of covalent drugs. Case studies. | 2 |
| Lec 8 | Transition-state analogues. Techniques used for the identification of transition state. Pauling's theory of the course of enzymatic reaction. Construction of transition-state analogues. Computer-aided techniques. | 2 |
| Lec 9 | Topological conformity. Antagonists and agonists. Natural peptides as scaffolds. | 2 |
| Lec 10 | QSAR models. Analysis of inhibitory activity using Hansh and Wilson models. | 2 |
| Lec 11 | Three-dimensional structure of receptors as a basis for drug design. Construction of pharmacophore. Computer-aided methods for drug design – QSAR and molecular modeling. Receptor flexibility. | 2 |
| Lec 12 | Selective complexation enzyme inhibitors. The analysis of forces governing the ligand-protein binding. | 2 |
| Lec 13 | Structure-based drug design. The use of protein crystal structure and molecular modelling tools for drug design. | 2 |
| Lec 14 | Drug targeting and delivery. Prodrugs. Engineered metabolic activation. Targeted enzyme prodrug therapy. | 2 |
| Lec 15 | Final Test | 2 |
| | Total hours | 30 |

TEACHING TOOLS USED

N1. lecture with multimedia presentation
N2. own work

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 |
|----------------------------------------------------------------------------|------------------------------|-------------------------------------------------|
| P | PEU_W01 - PEU_W04 PEU_K01 | Test |

PRIMARY AND SECONDARY LITERATURE**PRIMARY LITERATURE:**

- [1] K. M. Merz, Drug Design, structure and Ligand-Based Approaches, Cambridge University Press, 2010
- [2] Medicinal Chemistry and Drug Design, Intech (open access), 2012

SECONDARY LITERATURE:

- [1] Design of Drugs: Basic Principles and applications, ed. J. H. Poupaert, Marcel Dekker, 2002
- [2] The Organic Chemistry of Drug Design and Drug Action, Academic Press, 2004
- [3] Virtual Screening. ed. M. O. Taha, Intech (open access), 2012
- [4] Drug Development – A Case study Based Insight into Modern Strategies, Intech (open access), 2011

SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)

Prof. dr hab. Łukasz Berlicki, lukasz.berlicki@pwr.edu.pl

| FACULTY OF CHEMISTRY | | | | | |
|----------------------------------------------------------------------------------------------------------------------------------------|---------|---------|----------------------|---------|---------|
| SUBJECT CARD | | | | | |
| Name of subject in Polish <i>Informacja naukowa i techniczna</i> | | | | | |
| Name of subject in English <i>Retrieval of scientific and technical information</i> | | | | | |
| Main field of study (if applicable): <i>Biosciences</i> | | | | | |
| Specialization (if applicable): <i>Bioinformatics, Medicinal Chemistry</i> | | | | | |
| 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-SM2008L | | | | | |
| Group of courses NO | | | | | |
| | Lecture | Classes | Laboratory | Project | Seminar |
| Number of hours of organized classes in University (ZZU) | | | 15 | | |
| Number of hours of total student workload (CNPS) | | | 25 | | |
| Form of crediting (Examination / crediting with grade) | | | Crediting with grade | | |
| For group of courses mark (X) final course | | | | | |
| Number of ECTS points | | | 1 | | |
| including number of ECTS points for practical classes (P) | | | 1 | | |
| including number of ECTS points corresponding to classes that require direct participation of lecturers and other academics (BU) | | | 0,7 | | |

*delete as not necessary

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. Basic knowledge of information technology

SUBJECT OBJECTIVES

- C1 Acquainting with the selected topics regarding the scientific literature
- C2 Acquainting with the literature databases
- C3 Acquainting with the factographic databases in the fields of chemistry and biotechnology
- C4 Acquainting with the research funding
- C5 Acquainting with the selected topics of ethics in science

SUBJECT EDUCATIONAL EFFECTS

relating to skills:

- PEU_U01 Student is able to develop the complex search queries for literature databases
- PEU_U02 Student is able to develop the complex search queries for factographic databases
- PEU_U03 Student is able to find job and internship calls
- PEU_U04 Student is able to find active grants regarding the selected topic
- PEU_U05 Student is able to detect the plagiarism

relating to social competences:

- PEU_K01 Student appreciates the necessity of the assessment of the quality and credibility of

the scientific information
 PEU_K02 Student is able to follow the code of ethics in science and to respect the copyright policies

PROGRAMME CONTENT

| Lecture | | Number of hours |
|-------------------|----------------------------------------------------------------------------------|------------------------|
| Lec 1 | | |
| Lec 2 | | |
| Lec 3 | | |
| Lec 4 | | |
| Lec 5 | | |
| | | |
| | Total hours | |
| Classes | | Number of hours |
| Cl 1 | | |
| Cl 2 | | |
| Cl 3 | | |
| Cl 4 | | |
| .. | | |
| | Total hours | |
| Laboratory | | Number of hours |
| Lab 1 | Structure and preparation of scientific articles | 2 |
| Lab 2 | Current Contents literature database and building of search queries | 2 |
| Lab 3 | Web of Science literature database and Journal Citation Reports | 2 |
| Lab 4 | Preparation of grant proposals and searching for grants, internships and patents | 2 |
| Lab 5 | Analysis of structural data from Cambridge Structural Database | 2 |
| Lab 6 | Reaxys-Beilstein and Scifinder-Chemical Abstracts databases | 2 |
| Lab 7 | Searching for job offers and preparation of academic resume | 2 |
| Lab 8 | Code of ethics in science | 1 |
| | Total hours | 15 |
| Project | | Number of hours |
| Proj 1 | | |
| Proj 2 | | |
| Proj 3 | | |
| Proj 4 | | |
| ... | | |
| | Total hours | |
| Seminar | | Number of |

| | | hours |
|---------|-------------|-------|
| Semin 1 | | |
| Semin 2 | | |
| Semin 3 | | |
| ... | | |
| | Total hours | |

TEACHING TOOLS USED

- N1. Lecture with multimedia presentation
 N2. Problem solving
 N3. Problem solving with the 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 |
|---------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------|-------------------------------------------------|
| F | PEU_U01-PEU_U05 PEU_K01, PEU_K02 | Final report (max 100 points) |
| P = 3,0 (F=50-60 points) 3,5 (F=61-70 points) 4,0 (F=71-80 points) 4,5 (F=81-90 points) 5,0 (F=91-95 points) 5,5 (F=96-100 points) | | |

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

- [1] D. Ridley, Finding scientific information – information retrieval, Wiley, 2002
 [2] D. Lindsay, Scientific writing = thinking in words, CSIRO Publishing, 2011
 [3] M. Carter, Designing Science Presentations. A Visual Guide to Figures, Papers, Slides, Posters, and More, Academic Press 2013

SECONDARY LITERATURE:

- [1] On Being a Scientist: A Guide to Responsible Conduct in Research: Third Edition, 2009, The National Academies Press

SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)

Dr inż. Edyta Dyguda-Kazimierowicz, Edyta.Dyguda@pwr.edu.pl

Attachment no. 4. to the Program of Studies

| | |
|---------------------------------------------|---------------------------------------|
| FACULTY of Chemistry | |
| SUBJECT CARD | |
| Name of subject in Polish: | Seminarium dyplomowe |
| Name of subject in English: | Graduation seminar |
| Main field of study (if applicable): | |
| Specialization (if applicable): | |
| Profile: | academic |
| Level and form of studies: | 2nd level, full-time |
| Kind of subject: | obligatory |
| Subject code: | W03W03-SM1056S, W03W03-SM2056S |
| Group of courses: | NO |

| | Lecture | Classes | Laboratory | Project | Seminar |
|----------------------------------------------------------------------------------------------------------------------------------|---------|---------|------------|---------|----------------------|
| Number of hours of organized classes in University (ZZU) | | | | | 15 |
| Number of hours of total student workload (CNPS) | | | | | 50 |
| Form of crediting (Examination / crediting with grade) | | | | | crediting with grade |
| For group of courses mark (X) final course | | | | | |
| Number of ECTS points | | | | | 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) | | | | | 0,7 |

*delete as not necessary

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

n/a

SUBJECT OBJECTIVES

C1 development of students' social competences in presenting the results of their diploma thesis, initiating discussions and actively participating in them

SUBJECT EDUCATIONAL EFFECTS

relating to knowledge:

PEU_W01 – has in-depth knowledge of the topic of the diploma thesis

relating to skills:

PEU_U01 – is able to collect and verify information necessary to learn about the selected research topic
 PEU_U02 – is able to draw conclusions from the results of one's own research in relation to literature sources
 PEU_U03 – is able to publicly present the results of his research and defend them during public discussion
 PEU_U04 – is able to transfer knowledge to others
relating to social competences:
 PEU_K01 – is aware of the importance of knowledge, including its critical analysis
 PEU_K02 – is ready to deepen knowledge and skills, and, if necessary, use the help of experts

| PROGRAMME CONTENT | | |
|--------------------------|--------------------------------------------------------------------------|------------------------|
| Seminar | | Number of hours |
| Se 1 | Discussion of the diploma process in the field of study | 1 |
| Se 2 – Se 15 | Presenting a multimedia presentation and participating in the discussion | 14 |
| | Total hours | 15 |

| TEACHING TOOLS USED |
|---------------------------------------------------------|
| N1. Presentation N2. Discussion N3. Consultations |

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 |
|-----------------------------------------------------------------------------------|---------------------------------------------------|------------------------------------------------------------------|
| P | PEU_W01 PEU_U01 – PEU_U04 PEU_K01 – PEU_K02 | assessment based on the presentation and activity in discussions |

| PRIMARY AND SECONDARY LITERATURE |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| N/A |
| SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS) |
| Chairman of the program committee for the relevant field of study Card preparation: Piotr Rutkowski, piotr.rutkowski@pwr.edu.pl |

| FACULTY of CHEMISTRY | | | | | |
|----------------------------------------------------------------------------------------------------------------------------------|---------|---------|------------|---------|---------|
| SUBJECT CARD | | | | | |
| Name of subject in Polish Metody spektroskopowe w chemii medycznej | | | | | |
| Name of subject in English Spectroscopic methods in medicinal chemistry | | | | | |
| Main field of study (if applicable): Biosciences | | | | | |
| Specialization (if applicable): Medicinal chemistry | | | | | |
| Profile: academic | | | | | |
| Level and form of studies: 2nd level, | | | | | |
| Kind of subject: obligatory | | | | | |
| Subject code W03BSS-SM2020W, W03BSS-SM2020L | | | | | |
| Group of courses NO | | | | | |
| | Lecture | Classes | Laboratory | Project | Seminar |
| Number of hours of organized classes in University (ZZU) | 30 | | 30 | | |
| Number of hours of total student workload (CNPS) | 50 | | 50 | | |
| Form of crediting (Examination / crediting with grade) | Ex | | crediting | | |
| 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) | 1,3 | | 1,4 | | |

*delete as not necessary

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. Knowledge of general chemistry.
2. Basic knowledge of physical chemistry.
3. Basic knowledge of organic chemistry.
4. Basic skills in the field of physicochemical and mathematical calculations.
5. Basic knowledge of spectroscopic techniques used in structural analysis.

SUBJECT OBJECTIVES

- C1 Acquiring knowledge about spectroscopic analysis methods
- C2 Acquiring knowledge about methods of interpreting one-dimensional magnetic resonance spectra.
- C3 Acquiring knowledge about methods of interpreting two-dimensional magnetic resonance spectra.
- C4 Acquiring knowledge on how to interpret FT-IR spectra and mass spectrometry spectra.
- C5 Practical knowledge of selected applications of mass spectrometry and magnetic resonance.

SUBJECT EDUCATIONAL EFFECTS

relating to knowledge:

PEU_W01 Has knowledge of spectroscopic analysis methods

PEU_W02 Has knowledge of the use of spectroscopy in analysis

PEU_W03 Has knowledge of the use of spectroscopic methods and medical diagnostics

relating to skills:

PEU_U01 Is able to prepare material for analysis

PEU_U02 Is able to assess what methods to solve the current problem

PEU_U03 Is able to analyze spectroscopic data

relating to social competences:

Z zakresu kompetencji społecznych:

PEU_K01 Ma świadomość powiązań pomiędzy różnymi obszarami nauk chemicznych i/lub technicznych oraz ich aspekty praktyczne.

PROGRAMME CONTENT

| Lecture | | Number of hours |
|------------|-----------------------------------------------------------------|-----------------|
| Lec 1 | Introduction in spectroscopic methods | 2 |
| Lec 2 | IR spectroscopy – theoretical background and applications | 2 |
| Lec 3 | Raman spectroscopy - introduction | 2 |
| Lec 4 | Raman spectroscopy - applications | 2 |
| Lec 5 | Mass spectrometry - introduction | 2 |
| Lec 6 | Mass spectrometry – types of ionization | 2 |
| Lec 7 | Mass spectrometry - analizators | 2 |
| Lec 8 | Mass spectrometry – fragmentation and interpretation of spectra | 2 |
| Lec 9 | UV-Vis and CD spectroscopy | 2 |
| Lec 10 | NMR spectroscopy – theoretical background | 2 |
| Lec 11 | NMR spectroscopy – chemical shift | 2 |
| Lec 12 | NMR spectroscopy – coupling constant | 2 |
| Lec 13 | 2D NMR spectroscopy | 2 |
| Lec 14 | 2D NMR spectroscopy | 2 |
| Lec 15 | EPR spectroscopy | 2 |
| | Total hours | 30 |
| Laboratory | | Number of hours |
| Lab 1 | Introduction in spectroscopic methods | 2 |
| Lab 2 | IR spectroscopy – interpretation of spectra | 2 |
| Lab 3 | Raman spectroscopy | 2 |
| Lab 4 | Raman spectroscopy | 2 |
| Lab 5 | Mass spectrometry – introduction | 2 |

| | | |
|--------|--------------------------------------------------|----|
| Lab 6 | Mass spectrometry – fragmentation | 2 |
| Lab 7 | Mass spectrometry - interpretation of spectra | 2 |
| Lab 8 | Mass spectrometry – interpretation of spectra | 2 |
| Lab 9 | NMR spectroscopy – the principles | 2 |
| Lab 10 | NMR spectroscopy – interpretation of 1D spectra | 2 |
| Lab 11 | NMR spectroscopy – interpretation of 2D spectra | 2 |
| Lab 12 | NMR spectroscopy – spectra simulations | 2 |
| Lab 13 | NMR spectroscopy – spectra simulations | 2 |
| Lab 14 | UV-Vis spectroscopy - applications | 2 |
| Lab 15 | CD spectroscopy – interpretation and simulations | 2 |
| | Total hours | 30 |

TEACHING TOOLS USED

- N1. Problem lectures – multimedia presentations
 N2. Laboratory – problematic issues (multimedia presentations)
 N3. Laboratory - solving practical examples, drawing structures and spectra and performing calculations on a multimedia board
 N4. Own work – preparation for partial tests
 N5. Own work – consultations with the teacher

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 |
|----------------------------------------------------------------------------|-------------------------|-------------------------------------------------|
| P1 (lecture) | PEU_W01-W03, PEU_K01 | examination |
| F2 (laboratory) | PEU_UO1-UO2 | test |
| P (1 laboratory) = arithmetic mean of test grades | | |

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

- [1] K. Pigoń, Z. Ruziewicz, Chemia fizyczna t 2 Fizykochemia molekularna, Wyd. PWN, Warszawa 2007
 [2] P.W. Atkins, Chemia fizyczna, PWN 2001
 [3] R. M. Silverstein, F. X. Webster, D. J. Kiemle, Spektroskopowe metody identyfikacji związków organicznych PWN, Wraszawa 2007.
 [4] D. A. Skoog, D. M. West, F. J. Holler, S. R. Crouch, Podstawy chemii analitycznej 2, PWN, Warszawa 2007.
 [5] Z. Kęcki, Podstawy spektroskopii molekularnej, Wyd. PWN, Warszawa 1992.

SECONDARY LITERATURE:

- [1] A. Cygański, Metody spektroskopowe w chemii analitycznej. WNT Warszawa, 2009
 [2] J. Demichowicz-Pigoniowa, Chemia fizyczna t 3, Obliczenia fizykochemiczne, PWN, Warszawa 2010
 [3] J. Najbar, A. Turek, Fotochemia i spektroskopia optyczna, PWN, Warszawa 2009.

[4] P. Suppan, Chemia i światło, PWN, Warszawa 1997.

[5] W. Zieliński, A. Rajca, Metody spektroskopowe i ich zastosowanie do identyfikacji związków organicznych, WNT, Warszawa 2000

SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)

Prof Rafal Latajka, rafal.latajka@pwr.edu.pl

| FACULTY OF CHEMISTRY | | | | | |
|----------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------|----------------------|----------------------|---------|---------|
| SUBJECT CARD | | | | | |
| Name of subject in Polish | Chemia Teoretyczna | | | | |
| Name of subject in English | Theoretical Chemistry | | | | |
| Main field of study (if applicable): | Biosciences | | | | |
| Specialization (if applicable): | | | | | |
| Profile: | academic | | | | |
| Level and form of studies: 2nd level, full-time | | | | | |
| Kind of subject: obligatory | | | | | |
| Subject code | W03BSS-SM2001W, W03BSS-SM2001C, W03BSS-SM2001L | | | | |
| Group of courses | NO | | | | |
| | Lecture | Classes | Laboratory | Project | Seminar |
| Number of hours of organized classes in University (ZZU) | 30 | 15 | 30 | | |
| Number of hours of total student workload (CNPS) | 100 | 50 | 50 | | |
| Form of crediting (Examination / crediting with grade) | Exam | crediting with grade | crediting with grade | | |
| For group of courses mark (X) final course | | | | | |
| Number of ECTS points | 3 | 2 | 2 | | |
| including number of ECTS points for practical classes (P) | | 2 | 2 | | |
| including number of ECTS points corresponding to classes that require direct participation of lecturers and other academics (BU) | 1,3 | 0,7 | 1,4 | | |

*delete as not necessary

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. General Chemistry and Physics
2. Linear algebra and mathematical analysis
3. Fundamentals of physical and quantum chemistry

SUBJECT OBJECTIVES

- C1 To acquaint students with fundamentals of molecular quantum mechanics.
- C2 To acquaint students with modern methods of theoretical description of the electronic structure of atoms and molecules and to acquire the ability to apply these methods to determine the electronic structure and properties of molecular systems.
- C3. Acquiring the ability to apply methods of theoretical chemistry to prediction and interpretation of selected spectral and thermodynamical properties of molecular systems.

SUBJECT EDUCATIONAL EFFECTS**related to knowledge:**

Upon finishing the course, a student:

PEU_W01 - understands the problems and shortcomings of classical physics in the microscopic description,

PEU_W02 - knows the postulates of quantum mechanics and elements of the operator calculus,

PEU_W03 - can write the Schrödinger equation (SE) for model systems and for any molecular system,

PEU_W04 - knows the solutions of SE for the free particle, particle in model systems and for the hydrogen atom; understands the interpretation of these solutions,

PEU_W05 - knows the basic approximations used in the description of the electronic structure of molecular systems: the Born-Oppenheimer approximation and the basics of the variational and perturbational methods,
 PEU_W06 - knows the basics of the theory of molecular orbitals,
 PEU_W07 - has a basic knowledge of the solutions of the Hartree-Fock and Hartree-Fock-Roothan equations,
 PEU_W08 - has basic knowledge of the theory of electron correlation and methods of its calculation (configuration interaction method, many-body perturbation theory, density functional theory),
 PEU_W09 - has a basic knowledge of the theory of intermolecular interactions.

related to skills:

Upon finishing the course, a student:

PEU_U01 - can plan, carry out and interpret the results of calculations of the electronic structure of molecules within HF approximation and using selected methods taking into account electron correlation,
 PEU_U02 - can predict the equilibrium structure of molecules,
 PEU_U03 - can predict and interpret spectra of electronic states of molecules,
 PEU_U04 - can interpret spectroscopic measurements based on quantum-chemical calculations,
 PEU_U05 - can analyze the mechanisms of chemical reactions based on the results of quantum-chemical calculations.

related to social competences:

PEU_K01 student is ready to critically evaluate his/her knowledge and received content

PROGRAMME CONTENT

| Lecture | | Number of hours |
|----------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------|
| Lec 1 | Introduction to molecular quantum mechanics. Discussion of postulates of non-relativistic quantum mechanics. Definition of a wave function and its probabilistic interpretation. Definition of operators representing mechanical observables and elements of operator algebras. Time-dependent and time-independent Schrödinger's equation. | 2 |
| Lec 2 | Free particle and particle in model potentials. Solving the Schrödinger equation for a free particle, particle in a box and in a harmonic potential. | 2 |
| Lec 3 | Hydrogen atom. Solving the Schrödinger equation for a rigid rotator and hydrogen-like atoms. | 2 |
| Lec 4 | Molecular Hamiltonian. Separation of the electronic and nuclear degrees of freedom. The adiabatic approximation and the Born-Oppenheimer approximation. The harmonic approximation. Normal modes analysis and interpretation of absorption spectra in the infrared range. | 2 |
| Lec 5 | Approximate methods of solving the Schrödinger equation I. Variation calculus and its applications to model problems. Rayleigh-Ritz method. Molecular orbitals theory. Hückel method and its illustrative applications. | 2 |
| Lec 6 | Approximate methods of solving the Schrödinger equation II. A time-independent perturbation theory. Perturbation in two-state and multi-state systems. Perturbation theory for degenerate reference states. | 2 |
| Lec 7 | Wave functions for many-electron systems. Symmetry of the wave function. A determinantal wave function. The Slater-Condon rules. General expressions for matrix elements between Slater's determinants. | 2 |
| Lec 8 | The Hartree-Fock method. The self-consistent field method. The Hartree-Fock-Roothan method. The charge density and matrix elements of the Fock operator. | 2 |

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| Lec 9 | Molecular orbitals. Elements of point group theory. Symmetry and nomenclature of molecular orbitals. Molecular orbitals diagrams for diatomic and polyatomic molecules. Walsh diagrams. | 2 |
| Lec 10 | Electronic correlation I. Limitations of the Hartree-Fock method. Definition and methods for determining the electron correlation. The configuration interaction method. | 2 |
| Lec 11 | Electronic correlation II. The Møller-Plesset perturbation theory. Elements of the coupled clusters method. | 2 |
| Lec 12 | The density functional theory. One-particle density matrix and pair-density matrix. The Hohenberg-Kohn theorems. The Kohn-Sham method. | 2 |
| Lec 13 | The interaction of matter with electromagnetic radiation. The fate of molecules in electronically excited states. Photochemical and photophysical processes in molecular systems. Jabłoński diagram. Absorption and fluorescence spectra in the UV and visible range. Fine structure of absorption and fluorescence spectra | 2 |
| Lec 14 | Processes of nonradiative deactivation of excited states. Fermi's golden rule. Selection rules. Internal conversion. Conical intersections. Intersystem crossings. Excitation energy transfer - Förster's and Dexter's mechanisms. Natural and artificial light-harvesting systems. Photosynthesis. | 2 |
| Lec 15 | Intermolecular interactions. The theory of intermolecular interactions. Hydrogen bond. Secondary structure of molecular systems, conformational analysis. | 2 |
| | Total hours | 30 |
| Classes | | Number of hours |
| Cl 1 | Syllabus. Operator calculus. Elements of linear algebra. Examining the properties of operators, operator eigenproblem. | 2 |
| Cl 2 | Solutions to the Schrödinger equation for model problems. | 2 |
| Cl 3 | Simple applications of the variational principle to model problems. | 2 |
| Cl 4 | Simple applications of the Rayleigh-Schrödinger perturbation theory to model problems. | 2 |
| Cl 5 | Calculations of the electronic structure in the Hückel method for selected molecules I. The π -electronic approximation and basic assumptions of the Hückel method for unsaturated hydrocarbons. Eigenproblem solution. Determination of molecular orbital coefficients for simple molecules. | 2 |
| Cl 6 | Calculations of the electronic structure in the Hückel model for selected molecules II. Own problem in matrix form. Hamiltonian diagonalization and interpretation of eigenvalue and eigenvector spectra. Bond density and order matrix and population analysis. | 2 |
| Cl 7 | Hartree-Fock method I. Slater-Condon rules. Solving problems within the Hartree-Fock method. | 2 |
| Cl 8 | Review and Test. | 1 |
| | Total hours | 15 |
| Laboratory | | Number of hours |
| Lab 1 | Work organization in a computer lab and a computing center. Discussing the principles of health and safety at work. Distribution of accounts and basic information about available operating systems. | 2 |
| Lab 2 | Elements of the LINUX system I. Basic information about the operating system. Selected BASH shell commands. | 2 |

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| Lab 3 | Elements of the LINUX system II. Support for selected text editors. Simple BASH shell scripts. | 2 |
| Lab 4 | Selected electronic structure calculation packages. Preparation of batch files. Calculations of the electronic structure of atoms using the restricted and unrestricted Hartree-Fock method (HF). Structure of output files and interpretation of the results of calculations. | 2 |
| Lab 5 | Representation of the structure of molecular systems. Orthogonal coordinates and internal coordinates on the example of Z-matrix. | 2 |
| Lab 6 | Accuracy of computational chemistry methods. Selection of the basis functions. Comparison of the accuracy of selected ab initio methods and density functional theory methods. Validation of electronic structure calculation methods. | 2 |
| Lab 7 | Optimization of equilibrium geometry of molecules and analysis of normal-mode vibrations. Discussion of gradient geometry optimization algorithms. Calculations of the harmonic frequencies' spectrum. Analysis of normal coordinates. Prediction and interpretation of infrared spectra. | 2 |
| Lab 8 | Molecular orbital theory. Determination of potential energy curves for diatomic molecules in the HF method. Determination and interpretation of molecular orbital and Walsh diagrams. Charge-density population analysis. | 2 |
| Lab 9 | Configuration interaction method. Calculation of electronic states' spectra using the configuration interaction method with single (CIS) and double excitations (CISD). Size-extensivity and size-consistency of the CI method. Project I. Calculations of the electronic states spectra and their interpretation for selected polyatomic molecules. | 2 |
| Lab 10 | Project I. Calculations of the molecular structure and thermodynamical properties | 2 |
| Lab 11 | Mechanisms of chemical reactions. Location of transition state geometry. | 2 |
| Lab 12 | Project II – Calculations of electronic states spectra and their interpretation for selected polyatomic molecules. | 2 |
| Lab 13 | Work on individual projects I. | 2 |
| Lab 14 | Work on individual projects II. | 2 |
| Lab 15 | Work on individual projects III. | 2 |
| | Total hours | 30 |
| TEACHING TOOLS USED | | |
| N1. Lecture at the blackboard N2. Multimedia presentation N3. Implementation of tasks / projects in the computer lab N4. Personal computers / resources of the computing center / specialized 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 |
|----------------------------------------------------------------------------|------------------------|-------------------------------------------------|
| P | PEU_Lec01- | Final exam |

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|---------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|----------------------------|
| | PEU_Lec15, PEU_K01 | |
| F1 | PEU_CI01- PEU_CI08, PEU_K01 | Home assignments and test. |
| F2 | PEU_La1- PEU_La15, PEU_K01 | Individual projects |
| P | | |
| PRIMARY AND SECONDARY LITERATURE | | |
| <u>PRIMARY LITERATURE:</u> | | |
| [1] | Engel, T., Reid, P., Quantum Chemistry and Spectroscopy, 3rd ed. ed. Pearson, Boston, 2013 | |
| [2] | L. Piela, "Ideas of Quantum Chemistry" 3rd Edition, Elsevier, 2019 | |
| [3] | D. O. Hayward, "Quantum Mechanics for Chemists", RSC, 2002 | |
| <u>SECONDARY LITERATURE:</u> | | |
| [1] | R. W. Góra, teaching materials for the course: "Theoretical chemistry", 2019 | |
| SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS) | | |
| Robert Góra, robert.gora@pwr.edu.pl | | |