

#### POZNAN UNIVERSITY OF TECHNOLOGY

EUROPEAN CREDIT TRANSFER AND ACCUMULATION SYSTEM (ECTS)

### **COURSE DESCRIPTION CARD - SYLLABUS**

Course name

Geometric biocrystallography [S1Bioinf1>BKG]

Course

Field of study Year/Semester

Bioinformatics 3/5

Area of study (specialization) Profile of study

general academic

Level of study Course offered in

first-cycle polish

Form of study Requirements

full-time elective

**Number of hours** 

Lecture Laboratory classes Other (e.g. online)

30 30

Tutorials Projects/seminars

0 0

Number of credit points

4,00

Coordinators Lecturers

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# **Prerequisites**

The student should have knowledge of the basics of inorganic and organic chemistry, mathematics and physics. The student should be able to obtain information from literature, databases and other properly selected sources

# Course objective

The aim of the course is to learn the basics of crystallography as a scientific field with tools and methods for determining the molecular structure of biologically active molecules. Students will learn basic information about crystalline bodies, gain knowledge of the hierarchy of intermolecular interactions and their role in shaping structures. In addition, they will learn the skills of determining the relationship between the structural structure of a solid and its physicochemical properties.

### Course-related learning outcomes

#### Knowledge:

The graduate knows and understands:

K\_W04 issues in the field of chemistry useful for the formulation and solving of simple bioinformatics tasks, covering the basic concepts and laws of chemistry, organic chemistry and biochemistry

K\_W19 techniques and methods for the identification of biomolecules and biologically active compounds

#### Skills:

The graduate is able to:

K\_U01 obtain information from literature, databases and other properly selected sources, also in English K\_U04 use analytical methods for the quantitative and qualitative determination of biochemical compounds, evaluate their suitability

K\_U05 use basic techniques and laboratory tools to solve problems in the field of bioinformatics, biotechnology and related disciplines, assess their usefulness

K\_U07 under the supervision of a research tutor, use analytical, simulation and experimental methods to formulate and solve research tasks

#### Social competences:

The graduate is ready to:

K\_K01 learning throughout life and improving one"s competences

K\_K03 determining priorities for the implementation of a task defined by himself or others

# Methods for verifying learning outcomes and assessment criteria

Learning outcomes presented above are verified as follows:

Learning outcomes presented above are verified as follows:

The knowledge acquired during the lectures is verified by an exam held after the end of the lecture cycle.

The skills acquired in the laboratories are verified on an ongoing basis - short tests.

#### Programme content

- Application of biocrystallography, perspectives and directions of its development
- Symmetry in the world of crystals and molecules
- Definition of a crystal, unit cell, basic tetrahedron
- Crystallographic geometry: open and closed symmetry, point and space groups, Bravaise cells, parameters describing crystal structures
- Rules for joining symmetry elements, Becke"s degrees of symmetry
- Types of chemical bonds and interactions, coordination polyhedron, crystal types and coordination number
- Orientation and texture in solids and methods of their determination
- Determination of Miller indices of planes and directions, including proteins and nucleic acids
- Protein crystallization process
- Determination and modeling of protein and nucleic acid structures
- Elements of crystallochemistry, structure and classification of protein roll and types of structure of nucleic acids
- The phenomenon of polymorphism of crystalline compounds and the influence on the physicochemical properties
- Relationships between the supermolecular structure and macroscopic properties of biomaterials
- X-ray diffraction on a crystal structure, Bragg diffraction conditions. X-ray diffraction methods. Location and intensity of diffraction reflections.
- Qualitative and quantitative analysis by X-ray diffraction method, application of the PDF-4 database in the identification analysis

### **Teaching methods**

- 1. Lecture: multimedia presentations illustrated with examples given on the blackboard.
- 2. Laboratories: practical classes, individual and team work.

### **Bibliography**

#### Basic

- 1. J. Dereń, J. Haber, R. Pampuch, Chemia ciała stałego, PWN 1975.
- 2. Ch. A. Wert, R. M. Thomson, Fizyka ciała stałego, PWN 1974.
- 3. W. Przygocki, A Włochowicz, Uporządkowanie makrocząsteczek w polimerach i włóknach, WNT 2006.

Additional 1. Von Meerssche, J.Feneau-Dupont, Krystalografia i chemia strukturalna, PWN, 1984.

# Breakdown of average student's workload

|  | Hours | ECTS |
|--|-------|------|
| Total workload   | 100   | 4,00 |
| Classes requiring direct contact with the teacher  | 60    | 2,50 |
| Student's own work (literature studies, preparation for laboratory classes/tutorials, preparation for tests/exam, project preparation) | 40    | 1,50 |