



## COURSE DESCRIPTION CARD - SYLLABUS

Course name

Basic molecular modeling

### Course

Field of study

Bioinformatics

Area of study (specialization)

-

Level of study

Second-cycle studies

Form of study

full-time

Year/Semester

2/3

Profile of study

general academic

Course offered in

Polish

Requirements

compulsory

### Number of hours

Lecture

15

Laboratory classes

15

Other (e.g. online)

0

Tutorials

0

Projects/seminars

0

### Number of credit points

2

### Lecturers

Responsible for the course/lecturer:

dr inż. Łukasz Ławniczak

Responsible for the course/lecturer:

e-mail: lukasz.lawniczak@put.poznan.pl

phone +48 61 665 35 34

Faculty of Chemical Technology

Berdychowo 4, 60-965 Poznan

### Prerequisites

At the beginning of the course, the student should have basic knowledge regarding the structure of organic compounds (e.g. hydrocarbon structures, functional groups) and their properties (e.g. interactions between particular groups, structure-properties relationship). In addition, the student should be able to obtain information from the indicated sources and be aware of the need to develop their competences.

### Course objective

The aim is to ensure that students acquire basic theoretical and practical knowledge in the field of molecular modeling of simple organic compounds and biomolecules. The specific goals are to familiarize



students with the software used to analyze and evaluate the structural and physicochemical properties of simple and complex molecules.

### Course-related learning outcomes

#### Knowledge

K\_W02 graduate knows and understands complex physicochemical and biochemical processes, including the principles of proper selection of materials, raw materials, apparatus and equipment for their implementation and characterization of products

K\_W03 to a deeper extent, the issues in selected sciences useful for modeling of biological processes

K\_W04 methods, techniques and tools used in the process of solving complex bioinformatics tasks, mainly of engineering character

#### Skills

K\_U01 the graduate can fluently use and integrate information from literature and electronic sources, in Polish and English, interpret and critically evaluate them

K\_U02 The graduate is able to draw conclusions, clearly formulate and fully justify his/her opinions on the basis of data from various sources

K\_U04 The graduate is able to use advanced techniques and computer tools to solve biological problems, and to assess their usefulness

#### Social competences

K\_K01 the graduate is ready to learn throughout life, inspire and organize the learning process of others

K\_K03 the graduate is ready to determine priorities in order to accomplish a task defined by him/herself or others

K\_K06 take responsibility for assessing risks arising from the applied research techniques and for creating safe working conditions

### Methods for verifying learning outcomes and assessment criteria

Learning outcomes presented above are verified as follows:

#### Lecture:

After the end of the lecture series, the knowledge of students will be verified based on a written exam with 5 open questions regarding theoretical and practical issues. A passing grade is obtained when the number of points is greater than 50% of the accepted maximum.

#### Laboratories:

During the series of laboratory classes, the knowledge of students will be verified based on through the implementation of program tasks. At the end of the series of laboratory classes, a practical test will be conducted on the knowledge of molecular modeling methods, covering three tasks. A passing grade is obtained when the number of points is greater than 50% of the accepted maximum.



## Programme content

The course covers the following theoretical issues: basic geometric parameters and the distribution of atoms in space, types of models (projections), isomerism and types of isomers (constitutional, geometric, optical, conformational), the influence of conformation on the energy of the molecule (geometric optimization), and the effect of hydrogen bonds in chemical structures (inregardiongon practical knowledge in the field of basic principles of molecular modeling will be carried out - spatial manipulation of models of molecules with specific structural parameters in two and three dimensions, basic techniques of molecule structure, modeling and measurement of structural parameters, building multifunctional molecules, minimizing the energy of a molecule or particle system in a vacuum.

## Teaching methods

The lecture includes a multimedia presentation of the discussed content and involving students in scientific discussions.

Laboratories include training in occupational health and safety, the use of basic laboratory equipment, basic methods of analysis and purification of organic compounds as well as practical implementation of syntheses along with keeping a laboratory journal.

## Bibliography

### Basic

1. J. Clayden, N. Greeves, S. Warren, P. Wothers, *Chemia organiczna*, tom I, II i III, WNT, Warszawa 2009.
2. J. Gawroński, K. Gawrońska, K. Kacprzak, M. Kwit, *Współczesna synteza organiczna*, PWN, Warszawa

### Additional

1. J. Skarżewski - *Wprowadzenie do syntezy organicznej*, PWN, Warszawa 1999
2. M.B. Smith, J. March, *Advanced Organic Chemistry, Reaction, Mechanism and Structure*, J.Wiley & Sons, New Jersey 2007
3. A.I. Vogel, *Preparatyka organiczna*, WNT, Warszawa 2006

## Breakdown of average student's workload

	Hours	ECTS
Total workload	50	2,0
Classes requiring direct contact with the teacher	30	1,5
Student's own work (literature studies, preparation for laboratory classes, preparation for tests) <sup>1</sup>	20	0,5

<sup>1</sup> delete or add other activities as appropriate