COURSE DESCRIPTION CARD - SYLLABUS

Course name
Basic molecular modeling [S1Bioinf1>MMOL]

Course

Field of study
Bioinformatics

Year/Semester
4/7

Area of study (specialization)
–

Profile of study
general academic

Level of study
first-cycle

Course offered in
polish

Form of study
full-time

Requirements
compulsory

Number of hours

Lecture
15

Laboratory classes
15

Other (e.g. online)
0

Tutorials
0

Projects/seminars
0

Number of credit points

2,00

Coordinators

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Lecturers

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_W04 the graduate knows and understands issues in the field of chemistry useful for formulating and solving simple bioinformatics tasks, including the basic concepts and laws of chemistry, organic chemistry and biochemistry

K_W08 the graduate knows and understands selected groups of bioactive compounds, their biochemical properties and the effect on cells and living organisms P6U_W
K_W12 the graduate knows and understands the basic methods, techniques and tools used in the process of solving bioinformatics tasks, mainly of an engineering nature P6U_W

Skills:
K_U01 the graduate is able to obtain information from literature, databases and other properly selected sources, also in English P6U_U
K_U02 the graduate is able to integrate and interpret the obtained information as well as to draw conclusions and formulate and justify their opinions. P6U_U
K_U06 the graduate is able to use basic techniques and IT tools to solve biological problems, evaluate their usefulness P6U_U

Social competences:
K_K01 the graduate is ready for lifelong learning and improving his competences P6U_K
K_K03 the graduate is ready to define priorities for the implementation of a task defined by himself or others P6U_K
K_K06 the graduate is ready to take responsibility for the safety of his own work and that of others; taking appropriate actions in emergency states P6U_K

Methods for verifying learning outcomes and assessment criteria

Learning outcomes presented above are verified as follows:

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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 sthrough 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 (inregardingon 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	2,00
Classes requiring direct contact with the teacher	30	1,50
Student's own work (literature studies, preparation for laboratory classes/ tutorials, preparation for tests/exam, project preparation)	20	0,50