COURSE DESCRIPTION CARD - SYLLABUS

Course name
Basic molecular modeling [S2Bioinf1>MMOL]

Course

Field of study
Bioinformatics

Year/Semester
2/3

Area of study (specialization)
–

Profile of study
general academic

Level of study
second-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_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:

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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