COURSE DESCRIPTION CARD - SYLLABUS

Course name
Molecular modeling of biomolecules [S2Bioinf2>MMB]

Course

Field of study
Bioinformatics

Year/Semester
1/2

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
30

Laboratory classes
30

Other
0

Tutorials
0

Projects/seminars
0

Number of credit points

5,00

Coordinators

dr inż. Łukasz Ławniczak
lukasz.lawniczak@put.poznan.pl

dr hab. inż. Mariusz Sandomierski prof. PP
mariusz.sandomierski@put.poznan.pl

Lecturers

Prerequisites

At the beginning of the course, the student should have basic knowledge in the field of molecular modeling (e.g. creating simple and complex molecule models, geometric optimization) and structure- energy relations (e.g. the influence of conformational changes and hydrogen bonds on the energy of the system). In addition, the student should have practical skills in using molecular modeling software acquired during the first-cycle studies.

Course objective

The aim is to ensure that students acquire theoretical and practical knowledge in the field of molecular modeling of biological macromolecules. The specific goals are to familiarize students with the methods of construction and modification of complex biomolecules, as well as the possibility of predicting their properties using in silico methods.

Course-related learning outcomes

Knowledge:
- knows and understands in-depth issues in the field of mathematical methods, statistics, optimization and artificial intelligence useful for modeling and analyzing biological processes
- knows and understands the methods, techniques and tools used in the process of solving complex bioinformatics tasks, mainly of an engineering nature
- knows and understands detailed issues in the field of modeling and analysis of biological systems based on solid theoretical foundations
- knows and understands detailed issues in the field of structural bioinformatics based on solid theoretical foundations

Skills:
- is able to proficiently use and integrate information obtained from literature and electronic sources, in Polish and English, evaluate, critically analyze, synthesize and creatively interpret it
- is able to draw conclusions, clearly formulate and comprehensively justify his/her opinions based on data from various sources
- is able to apply knowledge of biochemistry and related sciences to solve bioinformatics problems
- is able to plan and carry out research tasks, including engineering ones, under the supervision of a research supervisor, using analytical, simulation and experimental methods
- is able to use mathematical methods (including statistical ones) and specialist techniques and IT tools to describe processes and analyze biological data

Social competences:
- is ready to define priorities for the implementation of a task defined by himself or others and to take action to implement the tasks in an entrepreneurial manner
- is ready to define priorities for the implementation of a task defined by himself or others and to take action to implement the tasks in an entrepreneurial manner

Methods for verifying learning outcomes and assessment criteria

Learning outcomes presented above are verified as follows:

Formative assessment:
Lecture
Each subsequent lecture will begin with a brief summary of the topics covered in the previous lecture, along with a brief discussion regarding the understanding and application of this knowledge. This will allow students to assess whether they have learned the material.
Laboratories
During the series of laboratory classes, the knowledge of the students will be verified by completing program tasks. Each time, elements that appeared in previous classes will be repeated, which will allow the students to analyze of the degree to which they have mastered them.
Summative assessment:
Lecture
After the end of the lecture series, the knowledge of students will be verified based on a written examination with 10 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
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 will discuss the principles of molecular modeling of biomolecules.

Course topics

The course covers the following theoretical issues: structures of biocompounds (order, stabilization by bonds), formation of biopolymer structures (monomer structures, influence on the conformation of biological oligo- and polymers), computer-aided analysis of infrared spectra (analysis and interpretation of model and real results), practical application of periodic box functions (simulation of the behavior of compounds in the environment of a solvent). Further discussed topics include the basics of

supramolecular chemistry, macrostructures, biopolymers and computer-assisted interpretation of spectral analyses.
In addition, classes regarding the practical knowledge of the principles of molecular modeling will be carried out - analysis of key geometric parameters in advanced biomolecule structures, differences resulting from the level of molecular modeling in the context of macrostructures and multiparticulates, use of computer simulations and experimental data for structural analysis, the interaction of macrobiomolecules with selected compounds with a significant biological role, issues associated with multi-molecule systems, use of databases for rapid construction of biomolecules.

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	125	5,00
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)	65	2,50