COURSE DESCRIPTION CARD - SYLLABUS

Course name

Advanced methods of molecular modeling

Course

Field of study

Bioinformatics

Year/Semester

2/4

Area of study (specialization)

-

Profile of study

general academic

Level of study

Second-cycle studies

Course offered in

Polish

Form of study

full-time

Requirements

elective

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:

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Faculty of Chemical Technology

Berdychowo 4, 60-965 Poznan

Responsible for the course/lecturer:

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 advanced molecular modeling methods. The specific goals are to familiarize students with the methods of

construction and modification of multiparticulates, as well as to perform an energy balance for systems with different properties.

Course-related learning outcomes

Knowledge

K_W03 the graduate knows and understands in detail the issues of selected sciences useful for modeling biological processes P7U_W

K_W04 the graduate knows and understands the methods, techniques and tools used in the process of solving complex bioinformatics tasks, mainly of an engineering nature P7U_W

K_W09 the graduate knows and understands detailed issues in the field of modeling and analysis of biological systems based on solid theoretical foundations P7U_W

Skills

K_U01 the graduate is able to fluently use and integrate information obtained from literature and electronic sources, in Polish and English, to interpret and critically evaluate it P7U_U

K_U02 the graduate is able to draw conclusions, clearly formulate and exhaustively justify his opinions on the basis of data from various sources P7U_U

K_U06 the graduate is able, under the supervision of a research tutor, to plan and perform research tasks using analytical, simulation and experimental methods P7U_U

Social competences

K_K01 the graduate is ready to learn, inspire and organize the learning process of others throughout life P7U_K

K_K03 the graduate is ready to define priorities for the implementation of a task defined by himself or other P7U_K

K_K08 the graduate is ready to systematically update his knowledge in the field of biology and computer science and to see the possibilities of its practical application P7U_K

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 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: energetic foundations of multi-order structures (interactions between functional groups and key structural parameters), creation of a solvation monolayer and modeling of interactions with macromolecules (determining interactions on the example of a biomolecule-water), the use of modeling methods for the analysis and interpretation of real structures (analysis of IR spectra), simulation of the polymerization process (definition of monomers, the course of the process of combining mers and its structural and energetic consequences).

In addition, classes regarding the practical knowledge of the basic principles of molecular modeling will be carried out - the conformational search function as a tool for automated analysis of conformational isomers, selection of paraters and potential problems in multi-molecular systems, interpretation of spectra using prognostic models as a quick tool for structure analysis, polymerization process and structure-energy relationship for polymer systems.

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/tutorials, preparation for tests/exam) [1]	20	0,5

[1] delete or add other activities as appropriate