COURSE DESCRIPTION CARD - SYLLABUS

Course name
Fundamentals of physicochemical methods for drug testing - spectroscopic techniques and molecular modelling [S1IFar2>PFMBLtsimm]

Course

Field of study
Pharmaceutical Engineering

Year/Semester
3/6

Area of study (specialization)
–

Profile of study
general academic

Level of study
first-cycle

Course offered in
Polish

Form of study
full-time

Requirements
elective

Number of hours

Lecture
0

Laboratory classes
0

Other
0

Tutorials
15

Projects/seminars
0

Number of credit points

1,00

Coordinators

Lecturers

Prerequisites

Mastery of general chemistry, matemathics, and physics at a high school level.

Course objective

The aim of the course is to familiarize students with the basics of molecular spectroscopy and physical methods for investigating medicinal substances as well as the basic aspects of molecular modeling and drug design. Providing the basis for understanding modern analytical methods.

Course-related learning outcomes

Knowledge:
1. Student has general knowledge in the field of quantum mechanics and physical methods of investigating medicinal substances. The student knows the basic principles of molecular modeling and rational drug design [K_W24].
2. Student knows the significance of dipole moment, pKa, logP and logD for the fate of the drug in the body [K_W7].

Skills:
1. Student uses a specific equipment and research apparatus in determining selected physicochemical

parameters, elaborates the experiment report [K_U8].
2. Student uses a correct chemical and pharmaceutical terminology in the field of physical chemistry [K_U3].

Social competences:
1. The student is able to interact and work in a group of 3-4 people to carry out a specific experiment [K_K2].

Methods for verifying learning outcomes and assessment criteria

Learning outcomes presented above are verified as follows:

During the classes the student is obliged to be familiar with the theory related to the discussed issue and to actively participate in the discussion and solving of problem exercises. The preparation of theoretical issues and student activity are assessed on the basis of an oral answer.
The course ends with a test consisting of single or multiple-choice closed questions in an electronic form (OpenOLAT) and open questions in writing, which include the material realized during the classes. Obtaining at least 60% of the total number of points is pass the test. (stationary or remote form depending on the epidemiological situation).

Programme content

The program covers the following topics:
1. Electromagnetic radiation and its characteristics. Quantum mechanics.
2. Polarization, dipole moment, polarizability.
3. Electrical properties of molecules and biological activity.
4. Refraction.
5. Methods for studying the optical activity of chemical compounds.
6. Emission spectra of chemical compounds.
7. Generation and analysis of NMR and EPR spectra.
8. Crystal structure analysis.
9. Molecular modeling.
10. Descriptors.

Course topics

Electromagnetic radiation and its features. Quantum mechanics. Heisenberg uncertainty principle. Application of the Lambert-Beer equation. Polarization, dipole moment, polarizability. Electrical properties of the molecule versus biological activity. Refraction. Methods for testing the optical activity of chemical compounds. Emission spectra of chemical compounds. Formation and analysis of NMR and EPR spectra. Lasers. Crystal structure analysis, Bragg's law. Molecular modeling. Lipinski's rule. SAR and QSAR. Descriptors.

Teaching methods

Multimedia presentation, illustrated with examples on the board, combined with the problems solving with the active participation of students.

Bibliography

Basic:
1. P.W. Atkins, Chemia fizyczna, Wydawnictwo Naukowe PWN, 2007.
2. P.W. Atkins, Podstawy chemii fizycznej, Wydawnictwo Naukowe PWN, 2009.
3. T.W. Hermann (ed.), Chemia fizyczna, Wydawnictwo Lekarskie PZWL, 2007

Additional:
1. F. Główka (ed.) Farmacja fizyczna. Ćwiczenia laboratoryjne dla studentów farmacji i analityki medycznej , Wydawnictwo Naukowe Uniwersytetu Medycznego im. Karola Marcinkowskiego w Poznaniu, 2015.
2. A.G. Whittaker, A.R. Mount, M.R. Heal, Chemia fizyczna, Wydawnictwo Naukowe PWN, 2003.
3. N.K. Pandit Introduction to the Pharmaceutical Sciences, Lippincott Williams & Wilkins, 2007.

Breakdown of average student's workload

	Hours	ECTS
Total workload	30	1,00
Classes requiring direct contact with the teacher	15	0,50
Student's own work (literature studies, preparation for laboratory classes/ tutorials, preparation for tests/exam, project preparation)	15	0,50