COURSE DESCRIPTION CARD - SYLLABUS

Course name
Physical Chemistry

Course

Field of study	Year/Semester
Pharmaceutical Engineering	2/4
Area of study (specialization)	Profile of study
-	general academic
Level of study	Course offered in
First-cycle studies	polish
Form of study	Requirements
full-time	compulsory

Number of hours

Lecture	Laboratory classes	Other (e.g. online)
30	30	0
Tutorials	Projects/seminars	
0	0	

Number of credit points
5

Lecturers

Responsible for the course/lecturer:	Responsible for the course/lecturer:
prof. dr. hab. Franciszek Główka	

Prerequisites
Mastery of general chemistry, matemathics, and physics.

Course objective
The aim of the course is to teach students the fundamentals of thermodynamics, kinetics, molecular spectroscopy, physical methods for investigating medicinal substances as well as the basic aspects of molecular modeling and drug design. Providing the foundation for understanding drug pharmacokinetics, modern analytical methods, the problems of chemical technology of medicinal products and pharmaceutical engineering.

Course-related learning outcomes
Knowledge
1. Student knows the fundamentals of thermodynamics, kinetics, and catalysis of chemical processes (K_W11).
2. Student knows the fundamentals of pharmacokinetics (K_W1).
3. Student has ordered general knowledge in the field of quantum mechaniscs and physical methods for

examining medicinal substances chemistry. Student knows the principles of molecular modeling and rational drug design (K_W24).
4. Student has ordered knowledge on the colligative properties of solutions, ionic equilibria, potentiometry, emulsions, viscosity of coloids and polymers. Student performs calculations of selected physicochemical parameters (K_W5).
5. Student knows the significance of dipole moment, pKa, logP, and logD for the fate of drugs 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

3. 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:
METHODS FOR VERIFYING LEARNING OUTCOMES

Knowledge, points 1, 3, 4: Entrance quiz and oral answers during laboratory classes, tests, exam.
Knowledge, points 2, 5: Tests, exam.
Skills, point 1: Observation of a student during the lab (performance of the task), assessment of the report from the experiment.
Skills, point 2: Entrance quiz and oral answer during laboratory classes, evaluation of the report from the experiment, tests, exam.
Social competences, point 1: Observation of a student during the lab classes (task completion).

ASSESSMENT CRITERIA

After each part of lectures, i.e. I - elements of thermodynamics, II - kinetics with the elements of pharmacokinetics, III - fundamentals of molecular spectroscopy and drug design, a test is carried out. The test may consist of closed single and multiple choice electronic questions (OpenOLAT) and/or open questions in writing. Obtaining at least 60% of the total number of points is required to pass the test.

During calculations, students are assessed for their ability to solve the calculation exercise on his/her own and for knowledge of the theory related to a given issue.

During each laboratory class, the students are assessed for the preparation of a theory (written entrance quiz or test), performance of the lab experiment and the way of presenting the results in the form of a report. The final grade of the classes is the arithmetic mean.

The condition of passing the classes is attending them, demonstrating the ability to solve calculation exercises (obtaining positive grades and making up unsatisfactory grades), demonstrating knowledge of theoretical issues concerning the experimental part of the classes, and obtaining credit for all the lab reports.

The course ends with an exam, consisting of single or multiple-choice closed questions in an electronic form (OpenOLAT) and/or open questions in writing, which covers the material realized during lectures and lab classes. Obtaining at least 60% of the total number of points is required to pass the exam. The exam can be taken by students who have completed the classes and tests according to the course schedule.

Programme content

LECTURES

1. Elements of thermodynamics:

Expansion work, internal energy, the first law of thermodynamics. Enthalpy. Heat capacity of the system. Heat of chemical reaction, heat of formation, heat of combustion. Hess's law and Kirchoff's laws. Entropy. Reversible and irreversible processes, the second law of thermodynamics. Free energy and free enthalpy (Gibbs energy). Chemical potential. Dependence of equilibrium constants on temperature and pressure, van't Hoff isobar and isotherm. The third law of thermodynamics.

2. Chemical kinetics with the elements of pharmacokinetics:

The concept of the rate, order, and molecularity of a chemical reaction. Determination of the reaction order. Zero-, first- and second-order reactions, second-order autocatalytic reaction. Reaction rate constant. Drug half-life t0.5 and shelf-life t0.1. Influence of temperature on a reaction rate, Arrhenius equation, activation energy. Homogeneous catalysis. Kinetics of enzymatic reactions according to the Michaelis-Menten model. The fate of drugs in the body (LADME). The concept of a compartment. Pharmacokinetic parameters. Determination of pharmacokinetic equations to describe changes in drug concentration in blood and the amount of drug in urine after a single intravenous and oral dose in a single-compartment model. Bateman's equation.

3. Fundamentals of molecular spectroscopy and drug design:

Electromagnetic radiation and its characteristics. Energy of molecules. Wave-corpuscular duality, wave function, Schrödinger equation. Heisenberg uncertainty principle. Light absorption. Electrical properties of molecules and their effect on the biological activity of substances. Refraction. Optical rotatory dispersion, circular birefringence, circular dichroism. Lasers. Nuclear magnetic resonance. Electron paramagnetic resonance. Amorphous and crystalline solids, polymorphism. X-ray diffraction. Molecular modeling methods. Rational drug design. The importance of pKa, logP and logD for the fate of the drug in the body. SAR and QSAR. Descriptors.

LABORATORY CLASSES - calculation part:
Properties of solutions. Ionic equilibria. Colloidal systems. Surface phenomena. Kinetics.

LABORATORY CLASSES - experimental part:
Determination of pKa of acetylsalicylic acid by potentiometric titration and determination of the solubility product of a sparingly soluble calcium salt.
Determination of the rate constant and thermodynamic parameters of acetylsalicylic acid hydrolysis.
Preparation and determination of emulsion types. Determination of the molecular weight of a polymer by viscometric method. Determination of the isoelectric point of gelatin.
Adsorption of acetaminophen on activated charcoal.

Teaching methods

LECTURES: Multimedia presentation, illustrated with examples on the board.

LABORATORY CLASSES - calculation part: Discussion on the calculation exercise solutions.

LABORATORY CLASSES - experimental part: Performing experiments under the supervision of the assistant - experimental exercises.

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

Breakdown of average student's workload

	Hours	ECTS
Total workload	135	5,0
Classes requiring direct contact with the teacher	75	2,8
Student's own work (literature studies, preparation for laboratory classes, preparation for tests/exam, reports preparation) [1]	60	2,2

[1] delete or add other activities as appropriate