Approved by: ……..

Dean

Date.....

SOFIA UNIVERSITY "ST. KLIMENT OHRIDSKI"

Faculty: .....Chemistry and Pharmacy…….....

Subject area: *(code and name)*

C	H	L	3	8	2	4	1	3

.....**Pharmacy**.....

Master Program: *(code and name)*

C	H	L	3	8	2	4	1	3

.....**Pharmacy**.....

C U R R I C U L U M

Course:

C	1	6	5

(code and name) ***Physical Chemistry with Colloid Chemistry 1***

Lecturer: Assoc. Prof. Konstantin Balashev, Assoc. Prof. Galia Madjarova

Teaching assistant:

Academic work	Components	Acad. hours
In-class work	Lectures	30
	Seminars	
	Practical exercises (school internships)	30
Total in-class work		**60**
Out-of-class work	Topical writing /Course paper	
	Presentation	
	Scientific essay	
	Course project	30
	Field trip	
	Independent literature research	35
	Student teaching	
Total out-of-class work		**65**
TOTAL ACADEMIC WORK		**125**
ECTS credits in-class work		2.4
ECTS credits out-of-class work		2.6
TOTAL ECTS CREDITS		**5**

№	Grade components[1]	% of the grade
1.	Workshops {search of information and group discussions of presentations and topical writings)	
2.	Participation in topical discussions during the classes	10
3.	Demonstrations in class	
4.	Field trip attendance	
5.	Portfolio	
6.	Quizzes throughout the semester	15
7.	Course project	15
8.	Homeworks/mid-term test	
9.		
10.		
11.		
12.	Final exam	60

Outline of the course:

The concepts and methods of Physical Chemistry and their application in Pharmacy and Medicine are presented in the course of Physical and Colloid Chemistry.

The first general part includes basic approaches: molecular, kinetic and thermodynamic, to describe the properties of homogeneous and heterogeneous single-component and multi-component physicochemical systems.

The Laboratory practicum introduces students to some important physicochemical measurements and calculation of molecular properties.

The program is approved by the Department Council of the Department of Physical Chemistry (№ 11/26.11.2012) and by the Faculty Council of the Faculty of Chemistry and Pharmacy (№ ..... / .....)

Preliminary requirements:

Course in General and Inorganic Chemistry

Compulsory completion of the Lab practicum and submission of protocols after each exercise.

The first 12 hours of the Lab course cannot be completed after the week to which the particular exercise is assigned. The first part of the practicum ends with a written course project.

Key competences acquired:

Students should acquire fundamental knowledge in the field of Physical Chemistry and use them in subsequent courses for theoretical and experimental characterization of substances and materials with application in pharmacy.

[1] Depending on the course specificity and on the requirements of the teacher, other types of activity can be added or the unnecessary ones can be removed.

Lessons plan

№	Topic:	Acad. hours
	Lectures	
	MOLECULAR AND KINETIC APPROACHES	
1	**Theoretical methods to describe molecules and bio objects**. Molecular mechanical models and force fields. Classical approaches. Simulations of biosystems. Enzyme reactions, steric energy and selectivity. Activation energy.	3
2	**Molecular characteristics of the bio objects**. Optimum geometry. Connection between electronic configurations, stability and properties of the molecules. Bond order and atomic charge. Structure-properties relationship.	3
3	**Pharmacophores**. Types of pharmacophores. Structure-based approaches to drug design.	2
4	**Electric properties of the molecules.** Dipole moment, polarizability and hyperpolarizability. Relation to molecular refraction and permittivity. Electrostatic potential.	2
5	**Non-covalent interactions.** Origin, types and evaluation. Systems with hydrogen bond. Hydrophobic interactions. Molecular aggregates. Supramolecular structure of the macromolecules. Solvation models and effects.	2
6	**Molecular - kinetic theory of gases.** Ideal gas. Pressure, mean free path and number of collisions. Ideal gas in a force field. Transport phenomena in the ideal gas. Real gases.	2
II	**THERMODYNAMIC APPROACH**	
7	**Fluids.** Characteristics in terms of their molecular structure. Transport phenomena in liquids. Viscosity. Liquid crystals. Physical state of biological systems.	2
8	**Energy balance of the processes.** First law of thermodynamics. Application to a single-component homogeneous system – the ideal gas.	2
9	**Spontaneity and equilibrium processes**. Second law of thermodynamics. Entropy. Application to a single-component homogeneous system – the ideal gas.	2
10	**Characterization of the direction of the processes and of equilibrium in non-isolated systems**. Helmholtz Energy and Gibbs Energy. Application to single-component homogeneous systems - ideal gas, real gas, liquid, and solid. Application of the first and second laws of thermodynamics to a single-component heterogeneous system. Liquid-vapor phase equilibrium.	2

11	**Thermodynamic treatment of multicomponent systems.** Chemical potentials. Equilibrium conditions in multi-component heterogeneous systems. Phase equilibrium.	1
12	**Binary liquid solutions**. Classification. Ideal solutions. Perfect and dilute solutions. Colligative properties. Raoult's law. Relative reduction of the vapor pressure over a solution of a non-volatile substance. Temperature rise and temperature drop. Applications. Osmotic pressure and tonicity. Real solutions. Completely miscible liquids. Liquid solutions of limited miscibility. Separation of components by distillation.	3
13	**Distribution of drug substances in heterogeneous multi-component systems.** Lipophilicity and hydrophilicity.	1
14	**Chemical equilibrium.** Chemical equilibrium in isolated systems. Application of the first and second laws of thermodynamics to chemical reactions. Third thermodynamic law. Use of the three thermodynamic laws for calculation of the equilibrium constant. Study of some biochemical equilibrium reactions.	2
15	**Thermodynamics of drug-macromolecule interaction**. Patterns of interaction. Interaction of medicinal substances with tissue and plasma proteins.	1
	Seminars/Practical exercises	
1.	Organization of the exercises. Computer simulations of biomolecules: lipids, amino acids, DNA.	3
2.	Geometry and electronic structure of the molecule. Molecular reactivity.	
3	Calculation of the dipole moment and polarizability. Electrostatic potential. Determination of the physicochemical quantities by measuring the molecular refraction.	3
4.	Solvent effects: changes in the geometry, electron density distribution and electric characteristics; energy of solvation	3
5.	Presentations of experimental results. Graphical determination of the constants in linear and nonlinear functions. Study of the mutual solubility in a three-component system. Gibbs diagram.	3
6.	Calorimetric determination of the heat of neutralization.	3
7.	Determination of the molecular weight of dilute aqueous solutions of a non-volatile component by measuring the decrease of the crystallization temperature.	3
8.	Methods for preparation of isotonic solutions. Problems solving.	3
9.	Determination of the equilibrium constant of a homogeneous reaction in solution.	3
10.	Water and lipid solubility. Distribution of benzoic acid.	3

Topics Covered on the Final Exam

№	Topic
1	**Theoretical methods to describe molecules and bio species.**
2	**Molecular characteristics of the bio species.**
3	**Pharmacophores.**
4.	**Electric properties of the molecules.**
5.	**Non-covalent interactions.**
6.	**Molecular - kinetic theory of gases.**
7.	**Fluids.**
8.	**Energy balance of the processes.**
9.	**Spontaneity and equilibrium processes.**
10.	**Characterize the direction of the processes and equilibrium in non-isolated systems.**
11.	**Thermodynamic treatment of multicomponent systems.**
12.	**Binary liquid solutions.**
13.	**Distribution of drug substances in heterogeneous multi-component systems.**
14.	**Chemical equilibrium.**
15.	**Thermodynamics of drug-macromolecule interaction**.

Bibliography

Main sources:

1. I. Panayotov "Introduction to Biophysical Chemistry", Univ. Press, 2007 (in Bulgarian language).

2. P. J. Sinko, Martin's Physical Pharmacy and Pharmaceutical Sciences, Kluwer, 2011

3. G. W. Castellan," Physical Chemistry", 3rd ed., 1987

4. V. Ruseva, Tz. Zhivkova, "Physical Chemistry. Guide for Students of Pharmacy", Med. Press "Arso" Sofia, 2004. (in Bulgarian language).

5. N. Rangelova, S. Chalyovska, M. Nedyalkov, J. Petrov, M. Kaisheva, "Guidance of Physical and Colloid Chemistry, Uni. Press St. Kl. Ohridski, Sofia, 1997. (in Bulgarian language).

Additional sources:

1. M. Jackson, Molecular and Cellular Biophysics, Cambridge University Press, 2006

2. K. A. Connors, S. Mecozzi, Thermodynamics of Pharmaceutical Systems, Wiley, 2010

3. Lecture notes and supporting materials given by lecturers.