FACULTY of CHEMISTRY

SUBJECT CARD

Name Of Subject In Polish	Racjonalne Projektowanie Leków
Name Of Subject In English	Rational Drug Design
Main Field Of Study (If Applicable):	Biotechnology And Chemistry
Specialization (If Applicable):	Bioinformatics, Medicinal Chemistry
Profile:	Academic
Level And Form Of Studies:	2nd Level, Full-Time
Kind Of Subject:	Obligatory
Subject Code	BTC024014
Group Of Courses	NO

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of organized classes in University (ZZU)	30				
Number of hours of total student workload (CNPS)	90				
Form of crediting	crediting with grade				
For group of courses mark (X) final course					
Number of ECTS points	3				
including number of ECTS points for practical (P) classes					
including number of ECTS points for direct teacher-student contact (BK) classes	1				

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. Basic knowledge in organic chemistry
2. Basic knowledge in biochemistry

SUBJECT OBJECTIVES

C1 Basics of drug design
C2 Economical aspects of dryg design

SUBJECT EDUCATIONAL EFFECTS

relating to knowledge:
PEK_W01 – knows basic methods of drug design
PEK_W02 – can apply appropriate drug design method depending on the state of the knowledge on
        physiological process
PEK_W03 – has basic knowledge on consts and timing of drug design
PEK_W04 – understand physiological and economical aspects of dryg application.
relating to skills:
PEK_U01 – can propose a methodology of drug design for particular medical problem

PROGRAMME CONTENT

Lectures		Number of hours
Lec 1	**Economics of drug design and development.** Cost and time required to introduce new drug to the market. Generic drugs. Globalization.	2
Lec 2	**Randomized screening**. Historical perspective. Illustration of the opinion of L. Pasteur „Fortune favors prepared minds". Case studies.	2

Lec 3	**Natural products as a source of drugs.** History of the discovery of aspirin, morphine, artemisinin, quinine, penicillin and taxol. Current trends in natural drug research.	2
Lec 4	**Choice of the target.** HIV as an example for choice of the target for drug design.	2
Lec 5	**Theory of structural analogy.** Historical perspective (sulfonamides). Direct similarity versus topological one with analogs of morphine and anti-influenza drugs as examples.	2
Lec 6	**Theory of structural analogy.** Chemical outlook, trics and "magic methods". Peptidomimetics.	2
Lec 7	**Covalent drugs.** Overview of functional groups able for irreversible bonding with proteins. Techniques of design of covalent drugs. Case studies.	2
Lec 8	**Transition-state analogues.** Techniques used for the identification of transition state. Pauling's theory of the course of enzymatic reaction. Construction of transition-state analogues. Computer-aided techniques.	2
Lec 9	**Topological conformity.** Antagonists and agonists. Natural peptides as scaffolds.	2
Lec 10	**QSAR models.** Analysis of inhibitory activity using Hansh and Wilson models.	2
Lec 11	**Three-dimensional structure of receptors as a basis for drug design.** **Construction of p**harmacophore. Computer-aided methods for drug design – QSAR and molecular modeling. Receptor flexibility.	2
Lec 12	**Selective complexation enzyme inhibitors.** The analysis of forces governing the ligand-protein binding.	2
Lec 13	**Structure-based drug design**. The use of protein crystal structure and molecular modelling tools for drug design.	2
Lec 14	**Drug targeting and delivery.** Prodrugs. Engineered metabolic activation. Targeted enzyme prodrug therapy.	2
Lec 15	Test	2
	Total hours	30

TEACHING TOOLS USED

N1. Lecture with multimedia presentation
N2. Own work

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT

Evaluation (F – forming (during semester), P – concluding (at semester end)	Educational effect number	Way of evaluating educational effect achievement
P (lecture)	PEK_W01, PEK_W02, PEK_W03, PEK_W04, PEK_U01	test

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

[1]   K. M. Merz, Drug Design, structure and Ligand-Based Approaches, Cambridge University Press, 2010
[2]   Medicinal Chemistry and Drug Design, Intech (open access), 2012

SECONDARY LITERATURE:

[1]   Design of Drugs: Basic Principles and applications, ed. J. H. Poupaert, Marcel Dekker, 2002
[2]   The Organic Chemistry of Drug Design and Drug Action, Academic Press, 2004
[3]   Virtual Screening. ed. M. O. Taha, Intech (open access), 2012
[4]   Drug Development – A Case study Based Insight intor Modern Startegies, Intech (open access), 2011

SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)
Łukasz Berlicki, lukasz.berlicki@pwr.edu.pl