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): Biosciences
Specialization (if applicable):
Profile: academic
Level and form of studies: 2nd level, full-time
Kind of subject: obligatory
Subject code W03BSS-SM2006W
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)	75				
Form of crediting (Examination / crediting with grade)	crediting with grade				
For group of courses mark (X) final course					
Number of ECTS points	3				
including number of ECTS points for practical classes (P)					
including number of ECTS points corresponding to classes that require direct participation of lecturers and other academics (BU)	1,3				

*delete as not necessary

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES
1. Knowledge of the basics of organic chemistry
2. Knowledge of the basics of biology

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SUBJECT OBJECTIVES
C1 To familiarize students with the basics of drug design.
C2 Understanding the economic aspects of drug design.
C3 Learning about targeted therapy methods.

SUBJECT EDUCATIONAL EFFECTS
relating to knowledge:
Person who passed the subject:
PEU_W01 – knows the basic principles of drug design,
PEU_W02 – is able to select the appropriate drug design technique depending on the level of knowledge about the physiological process,
PEU_W03 – has basic knowledge about the costs and time horizon of drug design,
PEU_W04 – understands the physiological and economic effects of using drugs.

relating to:
Person who passed the subject:
PEU_K01 – recognizes the importance of non-technical aspects of scientific activity

PROGRAMME CONTENT		
Lecture		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 Louyis 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 irreversivble 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 flexability.	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	Final Test	2
	Total hours	30

TEACHING TOOLS USED
N1. lecture with multimedia presentation N2. own work

EVALUATION OF SUBJECT LEARNING OUTCOMES ACHIEVEMENT

Evaluation (F – forming during semester), P – concluding (at semester end)	Learning outcomes code	Way of evaluating learning outcomes achievement
P	PEU_W01 - PEU_W04 PEU_K01	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)
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