Federal State Autonomous Educational Institution for Higher Education
PEOPLES' FRIENDSHIP UNIVERSITY OF RUSSIA named after P. Lumumba
(RUDN University)
Science faculty

educational division (faculty/institute/academy) as higher education programme developer

COURSE SYLLABUS

Fundamentals of drug design

course title

Recommended by the Didactic Council for the Education Field of:

04.04.01 «Chemistry»

field of studies / speciality code and title

The course instruction is implemented within the professional education programme of higher education:

«Fundamental and applied chemistry»

higher education programme profile/specialisation title

2023

1. COURSE GOAL(s)

The goal of the course of «Fundamentals of drug design» is in the formation of the system of knowledge about biological targets, structure-activity relationship and modern methodology for the design of medicinal substances.

2. REQUIREMENTS FOR LEARNING OUTCOMES

Mastering the discipline "Fundamentals of drug design" expects students to acquire the following competences /competences in part.

Table 2.1. List of competences that students acquire through the course study

Competence code	**Competence descriptor**	**Competence formation indicators** (within this course)
M-PC-1-s	The ability to plan work and choose adequate methods for solving research problems in the chosen field of chemistry, chemical technology or sciences related to chemistry	M-PC-1-s-1. Draws up a general research plan and detailed plans for individual stages
		M-PC-1-s-2. Selects experimental and computational-theoretical methods for solving the problem based on the available material and time resources
M-PC-2-s	Ability to conduct patent information research in the chosen field of chemistry and/or related sciences	M-PC-2-s-1. Searches for specialized information in patent information databases
		M-PC-2-s-2. Analyzes and summarizes the results of a patent search on the subject of the project in the selected field of chemistry (chemical technology)

3. COURSE IN HIGHER EDUCATION PROGRAMME STRUCTURE

The course refers to the elective component of (B1) block of the higher educational programme curriculum.

Within the higher education programme students also master other (modules) and / or internships that contribute to the achievement of the expected learning outcomes as results of the course study.

Table 3.1. The list of the higher education programme components/disciplines that contribute to the achievement of the expected learning outcomes as the course study results

Competence code	**Competence descriptor**	**Previous courses/modules***	**Subsequent courses/modules***
M-PC-1-s	The ability to plan work and choose adequate methods for solving research problems in the chosen field of chemistry, chemical technology or sciences related to chemistry	Theoretical organic chemistry Methods of organic chemistry Domino reactions in the synthesis of heterocycles Molecular spectral analysis Methodology for working with the database Fundamentals of	Undergraduate practice

Competence code	Competence descriptor	Previous courses/modules*	Subsequent courses/modules*
		biotechnology Experimental research methods in the chemistry research Research work	
M-PC-2-s	Ability to conduct patent information research in the chosen field of chemistry and/or related sciences	Theoretical organic chemistry Methods of organic chemistry Domino reactions in the synthesis of heterocycles Molecular spectral analysis Methodology for working with the database Fundamentals of biotechnology Experimental research methods in the chemistry research Research work	Undergraduate practice

* To be filled in according to the competence matrix of the higher education programme.

4. COURSE WORKLOAD AND ACADEMIC ACTIVITIES

The total workload of the course is 3 credits.

Table 4.1. Types of academic activities during the periods of higher education programme mastering (full-time training)

Type of academic activities		Total academic hours	Semester(-s)			
			1	2	3	4
Contact academic hours		36			36	
including:						
Lectures (**LC**)		36			36	
Lab Works (**LW**)						
Seminars (workshops/tutorials) (S)						
Self-studies		*54*			54	
Evaluation and assessment (exam/passing/failing grade)		*18*			*18*	
Course workload	academic hours_	**108**			**108**	
	credits	**3**			**3**	

5. COURSE CONTENTS

Table 5.1. Course contents and academic activities types

Course module title	Course module contents (topics)	Academic* activities types
Section 1. Introduction. Methodological bases for the creation of drugs.	Theme 1.1. Sciences related to the creation and study of drugs. Classification of drugs. Pharmacokinetics and pharmacodynamics. Activity and selectivity of drugs. Absorption, distribution, metabolism and excretion of the drug.	LC
	Theme 1.2. Stages of drug development. Preclinical developments and clinical trials. Strategies for finding the leader connection. The general scheme for creating a drug based on continuous bioscreening. Fragment-oriented design. Ligand- and structure-oriented design. Virtual bioscreening. "*De novo*" design.	LC
Section 2. Targets of drug action. Techniques for modifying the structure of the leader compound.	Theme 2.1. The main types of biomolecules - targets of drug action. General ideas about the spatial structure of proteins and nucleic acids. Three-dimensional models of protein molecules. Protein Data Bank database. Types of biotarget–ligand interaction. Pharmacophore. Lipophilicity.	LC
	Theme 2.2. Modification of functional groups. Homologization. Restriction of conformational mobility and cyclo-chain transformations. Isosteres and bioisosteres. Privileged structures. Peptidomimetics. Structural modifications to increase oral bioavailability. Lipinsky's rule. The principle of prodrugs. Feedback in the regulation of biosynthesis. The principle of antimetabolites in the speculative design of drugs. Sulfonamide antibiotics. Antifolates in cancer therapy.	LC
Section 3. Design of drugs acting on biological membranes.	Theme 3.1. The structure of biological membranes. Detergents, ionophores, channel-forming compounds as antimicrobials and antiseptics.	LC
	Theme 3.2. The mechanism of nerve impulse conduction. Drugs for anesthesia. Local anesthetics.	LC
Section 4. Design of drugs acting on protein molecules.	Theme 4.1. Medicinal substances - enzyme inhibitors: irreversible, reversible competitive and allosteric. Penicillins are bacterial transpeptidase inhibitors. β-lactamase inhibitors. Organophosphorus compounds are nerve poisons and acetylcholinesterase reactivators. HIV protease inhibitors.	LC
	Theme 4.2. Receptors. Classification of receptors. Agonists, partial agonists and antagonists. Affinity. Techniques for creating agonists and antagonists. acetylcholine receptors. Amino acids and biogenic amines as receptor ligands.	LC

* - to be filled in only for **full** -time training: *LC - lectures; LW - lab work; S - seminars.*

6. CLASSROOM EQUIPMENT AND TECHNOLOGY SUPPORT REQUIREMENTS

Table 6.1. Classroom equipment and technology support requirements

Type of academic activities	**Classroom equipment**	**Specialised educational / laboratory equipment, software, and materials for course study** (if necessary)
Lecture	A lecture hall for lecture-type classes, equipped with a set of specialised furniture; board (screen) and technical means of multimedia presentations.	
Self-studies	A classroom for independent work of students (can be used for seminars and consultations), equipped with a set of specialised furniture and computers with access to the electronic information and educational environment.	

* The premises for students' self-studies are subject to **MANDATORY** mention

7. RESOURCES RECOMMENDED FOR COURSE STUDY

Main readings:

1. Patrick G.L. An Introduction to Medicinal Chemistry. Oxford: Oxford University Press, 2005.

2. The Practice of Medicinal Chemistry, Edited by Camille Georges Wermuth. Academic Press, London, 2008.

Additional readings:

1. Ленинджер Альберт Л. Основы биохимии : В 3-х т. Т. 1 / А.Л. Ленинджер ; Пер. с англ. В.В.Борисова и др.; Под ред. В.А.Энгельгардта, Я.М.Варшавского. - М. : Мир, 1985. - 365 с.

2. Ленинджер Альберт Л. Основы биохимии : В 3-х т. Т. 2 / А.Л. Ленинджер ; Пер. с англ. М.Г.Дуниной и др.; Под ред. В.А.Энгельгардта, Я.М.Варшавского. - М. : Мир, 1985. - 355 с.

3. Ленинджер Альберт Л. Основы биохимии : В 3-х т. Т. 3 / А.Л. Ленинджер ; Пер. с англ. В.Г.Горбулева и др.; Под ред. В.А.Энгельгардта, Я.М.Варшавского. - М. : Мир, 1985. - 324 с.

4. Основы дизайна и химии лекарств и их наноформ / А.Т. Солдатенков. - Ханой : Знания, 2014. - 281 с.

5. Химические основы жизнеспособности и здоровья человека: Научно-учебное издание / А.Т. Солдатенков. - Ханой : Изд-во Знание, 2013. - 432 с.

Internet sources

1. Electronic libraries (EL) of RUDN University and other institutions, to which university students have access on the basis of concluded agreements:

- RUDN Electronic Library System (RUDN ELS) http://lib.rudn.ru/MegaPro/Web
- EL "University Library Online" http://www.biblioclub.ru
- EL "Yurayt" http://www.biblio-online.ru
- EL "Student Consultant" www.studentlibrary.ru
- EL "Lan" http://e.lanbook.com/
- EL "Trinity Bridge"

- Journal "Nature Biotechnology": https://www.nature.com/nbt/

2. Databases and search engines:

- Yandex search engine https://www.yandex.ru/
- Google search engine https://www.google.ru/
- abstract database SCOPUS http://www.elsevierscience.ru/products/scopus/
- database Reaxys https://www.reaxys.com/#/search

Training toolkit for self- studies to master the course:*

1. The set of lectures on the course "Fundamentals of drug design".

* The training toolkit for self- studies to master the course is placed on the course page in the university telecommunication training and information system under the set procedure.

8. ASSESSMENT TOOLKIT AND GRADING SYSTEM* FOR EVALUATION OF STUDENTS' COMPETENCES LEVEL UPON COURSE COMPLETION

The assessment toolkit and the grading system* to evaluate the competences formation level (competences in part) upon the course study completion are specified in the Appendix to the course syllabus.

* The assessment toolkit and the grading system are formed on the basis of the requirements of the relevant local normative act of RUDN University (regulations / order).

DEVELOPERS:

Associate Professor of Organic Chemistry Department		**N. E. Golantsov**
Position, Department	Signature	name and surname

HEAD OF EDUCATIONAL DEPARTMENT:

Organic Chemistry Department		**L. G. Voskressensky**
Name of Department	Signature	name and surname

HEAD
OF HIGHER EDUCATION PROGRAMME:

Dean of Science faculty, Head of the Department of Organic Chemistry		**L. G. Voskressensky**
Position, Department	Signature	name and surname