Документ подписан простой электронной подписью Информация о владельце:

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**RUDN** University

# **Faculty of Science**

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

COURSE SYLLABUS
Modern organic synthesis and pharmacology
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:

«Bioenergies and Biorefineries»

higher education programme profile/specialisation title

## 1. COURSE GOAL

The goal of the course "Modern organic synthesis and pharmacology" is to familiarize with the basic concepts of Green Chemistry principles in modern organic chemistry. To introduce students to Alternative Synthetic Pathways. To define the applicability limits and the existing methods problems.

# 2. REQUIREMENTS FOR LEARNING OUTCOMES

Mastering the course "Modern organic synthesis and pharmacology" is aimed at the development of the following competences:

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

Competence code	Competence descriptor	Competence formation indicators (within this course)
	Ability to analyze, interpret and generalize the results of experimental and	GPC-2.1 Ability to carry out a critical analysis of the results of own experimental and computational-theoretical works and to interpret them correctly
GPC-2		GPC-2.2. Ability to formulate summary and conclusions based on the results of the analysis of literature data, own experimental and computational-theoretical works in the chosen field of chemistry or related sciences
PC-1	plan and to choose adequate methods for solving research problems in the chosen field	PC-1.1. Ability to prepare a general plan of research and detailed plans for individual stages; PC-1.2. Ability to select experimental and calculation-theoretical methods for solving the problems based on the available material and time resources

## 3. COURSE IN HIGHER EDUCATION PROGRAMME STRUCTURE

The course "Modern organic synthesis and pharmacology" refers to the **variable** 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	Competence	Previous	Subsequent
code	descriptor	courses/modules*	courses/modules*
GPC-2	Ability to analyze,		Actual problems of modern
	interpret and		chemistry
	generalize the results		Bioproducts, Biomaterials and
	of experimental and		Biorefineries
	computational-		Advanced Organic Synthesis

Competence	Competence	Previous	Subsequent
code	descriptor	courses/modules*	courses/modules*
	theoretical work in the chosen field of chemistry or related sciences.		Catalyst (nanomaterials) design and applications Catalysis: from Basic principles to applications. Homogeneous, Heterogeneous, PhotoCatalysis, Biocatalysis, Electrocatalysis Experimental lab 1: Flow synthesis and alternative technologies Experimental lab 2: Biorefineries and Bioproducts Experimental lab 3: Advanced Organic Synthesis Student Scientific-Research work Pre-graduation practical training
PC-1	Ability to develop a work plan and to choose adequate methods for solving research problems in the chosen field of chemistry, chemical technology or sciences related to chemistry		Advanced Organic Synthesis Catalyst (nanomaterials) design and applications Experimental lab 1: Flow synthesis and alternative technologies Experimental lab 2: Biorefineries and Bioproducts Experimental lab 3: Advanced Organic Synthesis Emerging contaminants: from fate to environmental remediation The methods of working with databases Student Scientific-Research work Pre-graduation practical training

<sup>\*</sup> 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 "Modern organic synthesis and pharmacology" is 4 credits (144 academic hours).

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

	Total		Training	modules	
Type of academic activities	academic hours	1	2	3	4
Contact academic hours	27	27			

Type of academic activities		Total		Training	modules	
		academic	1	2	3	4
including:						
Lectures (LC)		18	18			
Lab work (LW)		9	9			
Seminars (workshops/tutorials) (	S)					
Self-studies		108	108			
Evaluation and assessment (exam/passing/failing grade)		9	9			
Course workload	academic hours	144	144			
	credits	4	4			

# 5. COURSE MODULES AND CONTENTS

Table 5.1. Course contents and academic activities types

Course module title	Course module contents (topics)	Academic activities types
Module 1. Pharmacology	Topic 1.1 Introduction to Pharmacology	LC
	Topic 1.2 Physicochemical properties of Active	LC
	Pharmaceutical Ingredients (APIs). Ionization of	
	pharma compounds. Acidic APIs. Basic APIs.	
	Isoelectric point. pKa and pKb. Partition	
	coefficient.	
	Topic 1.3 Pharmacokinetics and	LC, LW
	pharmacodynamics: Concepts and examples.	
	Pharmacokinetics: Absorption and distribution of	
	APIs. Bioavailability. Pharmacodynamics.	
	Pharmacological receptors. Agonist and antagonist molecules. APIs classification:	
	antagonist molecules. APIs classification: structural specific and nonspecific APIs	
	Topic 1.4 Structural characteristics of APIs and	LC, LW
	Pharmacological action. Stereoisomerism. Optic,	LC, LW
	geometric and conformational isomers and	
	pharmacological action. Chemical Isostery.	
	Concept. Bioisosterism. Classic and non classic	
	bio-isosterism	
	Topic 1.5 Rational design of APIs.	LC, LW
	Pharmacological design. Pharmacomodulation.	·
	QSAR methods for pharma design. Hammet	
	equation. Taft equation. Hansch method. Method	
	of Free-Wilson. QSAR-3D methodologies.	
	Examples.	
	Topic 1.6 Metabolic pathways of APIs. Definition	LC, LW
	of toxicology. Basic principles of toxicology.	
	Synergism, potentiation and antagonism. Dose-	
	response relationships. Xenobiotics and	
	endogenous substances. Examples. Pharma	
	metabolism. Metabolic reactions (Phase I, Phase	
	II). Metabolic routes. Examples for common	

Course module title	Course module contents (topics)	Academic activities types
	pharmaceuticals.	
Module 2. Pharma synthesis	Topic 2.1 Green metrics and Green Chemistry in Pharma	
5,5	Introduction and applications of fundamental green metrics into modern synthesis; solvent selections and applications of sustainable solvent	LC, LW
	systems in modern approaches to organic synthesis and catalysis. Atom economy. E-factor. Functional Oriented Synthesis (FOS).	
	Topic 2.2 Real examples of application of Green Chemistry principles I in Pharma synthesis:  Synthesis of Sildenafil (Viagra®, Pfizer),	
	Synthesis of Talampanel (LY300164, Lilly Research Laboratories, Green Chemistry Award 1999), Synthesis of Ganciclovir (Cytovene®, Roche, Green Chemistry Award 2000).	LC
	Topic 2.3 Real examples of application of Green Chemistry principles II in pharma synthesis: Synthesis of Sertraline (Zoloft®, Pfizer, Green Chemistry Award 2002), Synthesis of Aprepitant (Emend®, Merck &Co., Green Chemistry Award 2005); Synthesis of Sitagliptin (Juvenia <sup>TM</sup> , Merck	LC, LW
	&Co. Green Chemistry Award 2006).  Topic 2.4 Flow approaches to sustainable pharmaceuticals synthesis	LC, LW

<sup>\* -</sup> 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 a set of devices for multimedia	1 -
Lab work	presentations.  A classroom for laboratory work, individual	1 0
Lao work	consultations, current and mid-term assessment; equipped with a set of specialised	1
	furniture and machinery.	laboratory: fume hood SHVP-4, fume hood SHVP-
		2, rotary evaporator Heivalue digital G3B, rotary
		evaporator IKA, digital devices for determining the

Type of academic activities	Classroom equipment	Specialised educational / laboratory equipment, software, and materials for course study (if necessary)
		melting point SMP10; electronic laboratory scales AND EK-610, MK-M flask heaters of different volumes, drying cabinet, magnetic stirrer MRHei-Mix S, magnetic stirrer with heating MRHei-Standart, refractometer, combined laboratory water bath, vacuum chemical station RS3001 VARIO-pro, circulation cooler Rotacool Mini, rotary plate pump vacuum RZ2.5, membrane vacuum chemical pump MZ2CNT, Steinel thermal air blower, Spectroline UV lamp, electronic vacuum controller with CVC3000 detect Vacuumbrand valve, stainless steel emergency cabin SHVV, chemical dishes, refrigerator; wi-fi
Self-studies	A classroom for self-studies (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.	Faculty of Science Reading Room Ordzhonikidze D.3. Coworking area Monday - Friday 10.00 - 22.00 Reading room of the main building of the RUDN Coworking area Monday - Saturday 9.00 - 23.00 Hall No. 2 Monday - Thursday 10.00 - 17.45 Friday 10.00 - 16.45 Hall No. 6 Monday - Thursday 10.00 - 17.45 Friday 10.00 - 16.45 Friday 10.00 - 16.45

<sup>\*</sup> The premises for students' self-studies are subject to **MANDATORY** mention

# 7. RECOMMENDED RESOURCES FOR COURSE STUDY

#### Main sources:

- 1. L. D. Field, S. Sternhell y J. R. Kalman, Organic Structures from Spectra, Wiley, 2002.
- 2. Green Chemistry in the synthesis of pharmaceuticals, S. Kar, H. Sanderson, K. Roy, E. Benfenati, J. Leszczynski, Chem. Rev. 2022, 122, 3637-3710.
- 3. Green Chemistry and Sustainability metrics in the pharmaceutical manufacturing sector, J. Becker, C. manske, S. Randl, Current Opinion in Green and Sustainable Chemistry 2022, 33, 100562

## Additional sources:

- 1. Website of the American Chemical Society ACS Publications: Chemistry journals, books, and references https://pubs.acs.org/
- 2. http://www.thieme.com/journals-main
- 3. http://onlinelibrary.wiley.com/
- 4. http://www.springer.com/gp/products/journals
- 5. Server with the ability to search for methods for synthesizing compounds http://www.orgsyn.org/

#### Internet sources

- 1. Electronic libraries with access for RUDN students:
- RUDN Electronic Library System (RUDN ELS) <a href="http://lib.rudn.ru/MegaPro/Web">http://lib.rudn.ru/MegaPro/Web</a>
- EL "University Library Online" <a href="http://www.biblioclub.ru">http://www.biblioclub.ru</a>
- EL "Yurayt" http://www.biblio-online.ru
- EL "Student Consultant" www.studentlibrary.ru
- EL "Lan" <a href="http://e.lanbook.com/">http://e.lanbook.com/</a>
- EL "Trinity Bridge"

## Databases and search engines:

- electronic foundation of legal and normative-technical documentation <a href="http://docs.cntd.ru/">http://docs.cntd.ru/</a>
  - Yandex search engine <a href="https://www.yandex.ru/">https://www.yandex.ru/</a>
  - Google search engine <a href="https://www.google.ru/">https://www.google.ru/</a>
  - Scopus abstract database <a href="http://www.elsevierscience.ru/products/scopus/">http://www.elsevierscience.ru/products/scopus/</a>
  - www.scholar.google.ru

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

- 1. A set of lectures on "Modern organic synthesis and pharmacology"
- 2. The laboratory workshop on "Modern organic synthesis and pharmacology"
- \* 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.

# **DEVELOPERS:**

Organic Chemistry Department		Luigi Vaccaro
position, department	signature	name and surname
Organic Chemistry Department		Rafael Luque
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name of department	signature	name and surname
HEAD OF HIGHER EDUCATION PROGRAMME: Dean of Faculty of Science,		
Head of Organic Chemistry		Voskressensky L.G
Head of Organic Chemistry  Department		Voskressensky L.G