Federal State Autonomous Educational Institution of 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

MASS SPECTROMETRY OF ORGANIC COMPOUNDS

course title

Recommended by the Didactic Council for the Education Field:

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

2025

1. COURSE GOAL(s)

The goal of the course "Mass spectrometry of organic compounds" is to gain an understanding of the features of the fragmentation of various classes of organic compounds under electron ionization, the skills to obtain and analyze the totality of the spectral characteristics of organic compounds.

2. REQUIREMENTS FOR LEARNING OUTCOMES

Mastering the discipline "Mass spectrometry of organic compounds " is aimed at developing the following competencies (parts of competencies) among students:

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

Competence code	**Competence descriptor**	**Competence formation indicators** (within this course)
PC-2	To be able to base on a critical analysis of the results of research and development, to assess the prospects for their practical application and the continuation of work in the chosen field of chemistry, chemical technology or sciences related to chemistry	PC-2.2. To determine possible directions for the development of work and prospects for the practical application of the results obtained

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***
PC-2	To be able to base on a critical analysis of the results of research and development, to assess the prospects for their practical application and the continuation of work in the chosen field of chemistry, chemical technology or	Molecular spectral analysis NMR of organic compounds Research work Experimental methods in the chemistry	Undergraduate practice

Competence code	Competence descriptor	Previous courses/modules*	Subsequent courses/modules*
	sciences related to chemistry		

* 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 4 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	Semesters			
			1	2	3	4
Contact academic hours		*54*			54	
including:						
Lectures (**LC**)		36			36	
Lab Works (**LW**)		18			18	
Seminars (workshops/tutorials) (S)						
Self-studies		*72*			72	
Evaluation and assessment (exam/passing/failing grade)		*18*			18	
Course workload	academic hours_	**108**			**144**	
	credits	**3**			**4**	

5. COURSE CONTENTS

Table 5.1. Course contents and academic activities types

Course module title	Course module contents (topics)	Academic activities types*
Section 1. Principles of fragmentation of medicinal organic compounds under conditions of electron ionization (EI)	Theme 1.1. Basic methods of ionization and separation of ions in mass spectrometry.	LC
	Theme 1.2. The main mechanisms of bond breaking and splitting of organic compounds under the conditions of mass spectrometry with electron ionization, possible rearrangement processes. Basic mass spectral rules.	LC, LW
Section 2. Fragmentation of hydrocarbons under EI conditions	Theme 2.1 Characteristic features of the fragmentation of alkanes, alkenes, alkynes, cycloalkanes, aromatic hydrocarbons under the conditions of mass spectrometry with electron ionization.	LC, LW
Section 3. Fragmentation of heterocyclic compounds under EI conditions	Theme 3.1. Characteristic features of the fragmentation of nitrogen-, oxygen- and sulfur-containing aliphatic and aromatic heterocyclic compounds under the conditions of mass	LC, LW

Course module title	Course module contents (topics)	Academic activities types*
	spectrometry with electron ionization, ortho-effect.	
Section 4. Fragmentation of halogen derivatives under EI conditions	Theme 4.1. Characteristic features of the fragmentation of halogen derivatives under the conditions of mass spectrometry with electron ionization.	LC, LW
	Theme 4.2. Polyisotope elements and calculation of their content.	
Section 5. Fragmentation of compounds with an amino group under EI conditions	Theme 5.1. Characteristic features of the fragmentation of aliphatic and aromatic amines under the conditions of mass spectrometry with electron ionization. Using derivatization to study amines with GC/MS.	LC, LW
Section 6. Fragmentation of compounds with a hydroxyl group under EI conditions	Theme 6.1. Characteristic features of the fragmentation of aliphatic alcohols and phenols, dialkyl, alkyl aryl and diaryl ethers under conditions of mass spectrometry with electron ionization.	LC, LW
	Theme 6.2. Analogies between electron ionization and tandem mass spectrometry.	LC, LW
Section 7. Fragmentation of compounds with a carboxyl group under EI conditions	Theme 7.1. Characteristic features of the fragmentation of carboxylic acids, alkyl and aryl esters, phthalic acid derivatives under conditions of mass spectrometry with electron ionization.	LC, LW
Section 8. Fragmentation of compounds with several functional groups under EI conditions	Theme 8.1. Characteristic features of the fragmentation of amino acids and their derivatives under the conditions of mass spectrometry with electron ionization.	LC, LW
	Theme 8.2. Use of Husek's reagents for the analysis of amino acids and protozoan peptides by GC/MS. Analysis of hydroxy and oxo acids.	LC, LW

* - 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.	
Lab work	A classroom for laboratory work, individual consultations, current and mid-term assessment; equipped with a set of specialised	Room is equipped with a set of specialized furniture; specialized equipment of the

Type of academic activities	Classroom equipment	Specialised educational / laboratory equipment, software, and materials for course study (if necessary)
	furniture and machinery.	spectroscopy laboratory: manual press, scales, consumables for sample preparation, Thermo DSQ II mass spectrometer
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 reading:

1. McLafferty, Fred W., ed. Mass spectrometry of organic ions. Elsevier, 2012.
2. Scheinmann, Feodor, ed. An introduction to spectroscopic methods for the identification of organic compounds: Mass spectrometry, ultraviolet spectroscopy, electron spin resonance spectroscopy, nuclear magnetic resonance spectroscopy (recent developments), use of various spectral methods together, and documentation of molecular spectra. Elsevier, 2013.
3. Pretsch, Ernö, Philippe Bühlmann, Christian Affolter, Ernho Pretsch, P. Bhuhlmann, and C. Affolter. Structure determination of organic compounds. Vol. 13. Berlin: Springer, 2009.

Additional reading:

Watson, J. Throck, and O. David Sparkman. Introduction to mass spectrometry: instrumentation, applications, and strategies for data interpretation. John Wiley & Sons, 2007.

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"

2. Databases and search engines:

- electronic fund of legal and normative-technical documentation http://docs.cntd.ru/
- Yandex search engine https://www.yandex.ru/
- Google search engine https://www.google.ru/
- abstract database SCOPUS http://www.elsevierscience.ru/products/scopus/

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

1. The set of lectures on the course "Mass spectrometry of organic compounds".

2. The laboratory workshop on the course "Mass spectrometry of organic compounds"

* 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:

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Position, Department	Signature	name and surname

HEAD OF EDUCATIONAL DEPARTMENT:

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HEAD OF HIGHER EDUCATION PROGRAMME:

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