Federal State Autonomous Educational Institution of Higher Education

PEOPLES' FRIENDSHIP UNIVERSITY OF RUSSIA
RUDN University

Faculty of Science

COURSE SYLLABUS

FUNDAMENTALS OF CONTEMPORARY MASS SPECTROMETRY

course title

Recommended by the Didactic Council for the Education Field:

04.03.01 «Chemistry»

field of studies / speciality code and title

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

«Chemistry»

higher education programme profile/specialisation title

2026 г.

1. COURSE GOAL(s)

The purpose of mastering the discipline "FUNDAMENTALS OF CONTEMPORARY MASS SPECTROMETRY " 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 "FUNDAMENTALS OF CONTEMPORARY MASS SPECTROMETRY" is aimed at developing the following competencies (parts of competencies) among students:

Table 2.1. List of competences that students acquire during course study

Competence code	**Competence descriptor**	**Competence formation indicators** (within this course)
GC-1	To be able to search, critically analyze and synthesize information, apply a systematic approach to solve the tasks	GC-1.1. To analyze the task, highlighting its basic components;
		GC-1.2. To determine and rank the information required to solve the problem;
		GC-1.5. To analyze and contextually processes information to solve assigned tasks with the formation of their own opinions and judgments.
PC-1	To be able to use the acquired knowledge of the theoretical foundations of the fundamental sections of chemistry in solving professional problems	PC-1.1. To understand the basic principles, laws, methodology of the studied chemical disciplines, the theoretical foundations of physical and physico-chemical research methods;
		PC-1.2. To use fundamental chemical concepts in his professional activities;
		PC-1.3. To interpret the results obtained using the basic concepts of chemical disciplines.

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 that contribute to the achievement of the expected learning outcomes as the internship results.

Competence code	Competence descriptor	Previous courses/modules*	Subsequent courses/modules*
GC-1	To be able to search, critically analyze and synthesize information, apply a systematic approach to solve the tasks	Philosophy Mathematics Physics Computer science Inorganic chemistry Analytical chemistry Organic chemistry Physical chemistry Fundamentals of quantum chemistry Introduction to the specialty Advanced excel Basics of Python programming Infographics and presentation technology SQL beginner course Python for data analysis Digital business communications Introduction to the chemistry of coordination compounds Fundamentals of nanochemistry Chemistry of medicinal substances	Selected chapters of chemistry Experimental research methods in chemistry Undergraduate practice
PC-1	To be able to use the acquired knowledge of the theoretical foundations of the fundamental sections of chemistry in solving professional problems	Inorganic chemistry Analytical chemistry Physical chemistry Organic chemistry Fundamentals of quantum chemistry Chemical technology Introduction to the specialty Introduction to the chemistry of coordination compounds Fundamentals of nanochemistry Chemistry of medicinal substances Educational practice Structure of matter High-molecular compounds	Selected chapters of chemistry Experimental research methods in chemistry Research work Undergraduate practice

4. COURSE WORKLOAD AND ACADEMIC ACTIVITIES

Course workload of the discipline «FUNDAMENTALS OF CONTEMPORARY MASS SPECTROMETRY» is 4 credits.

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

Types of academic activities		**Total academic hours**	**Semesters**			
			7			
Contact academic hours		*72*	*72*			
including:						
Lectures (**LC**)		36	36			
Lab Works (**LW**)		36	36			
Seminars (workshops/tutorials) (**S**)						
Self-studies		*72*	*72*			
Evaluation and assessment (exam/passing/failing grade)						
Course workload	academic hours_	**144**	**144**			
	credits	**4**	**4**			

5. COURSE CONTENTS

*Table 5.1. Course contents and academic activities types**

Modules	**Contents (topics, types of practical activities)**	**Workload, academic hours**
Section 1. Basic principles of mass spectrometry	Theme 1.1. Principles of the mostly used methods for ions generation. Soft and hard ionization techniques.	LK
	Theme 1.2. Principles of the mostly used methods for ions separation and detection. Magnetic sector, quadrupole, quadrupole ion trap, linear ion trap, Orbitrap, ion cyclotron resonance and time-of-flight mass analyzers.	LK, LW
Section 2. Tandem mass spectrometry	Theme 2.1 Ion activation techniques: collision-induced dissociation, electron-transfer and electron-capture dissociation, photon-induced fragmentation. Multiply reaction monitoring	LK, LW
Section 3. Basic principles of mass spectral data interpretation.	Theme 3.1. The main fragmentation pathways of organic compounds. Bond scission and rearrangement mechanisms. Odd and even electron ions. The use of mass spectra databases, match and reverse match factors, head-to-tail and side-by-side comparison of mass spectra.	LK, LW
Section 4. Protocol for structure determination of	Theme 4.1. The main fragmentation pathways and diagnostic ions for acyclic compounds with up to one functional group.	LK, LW

Modules	Contents (topics, types of practical activities)	Workload, academic hours
unknowns by EI mass spectrometry.	Theme 4.2. The main fragmentation pathways and diagnostic ions for cyclic compounds with up to one functional group.	
	Theme 4.3. The main fragmentation pathways and diagnostic ions for aromatic compounds with up to one functional group	LK, LW
	Theme 4.4. The main fragmentation pathways and diagnostic ions for acyclic compounds with more than one functional group	LK, LW
	Theme 4.5. The main fragmentation pathways and diagnostic ions for cyclic compounds with more than one functional group	LK, LW
	Theme 4.6. The main fragmentation pathways and diagnostic ions for aromatic compounds with more than one functional group	LK, LW
Section 5 Quantitative analysis	Theme 5.1. Methods of quantitative analysis, calibration procedures for external and internal standards, isotope dilution technique.	LK, 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 furniture and machinery.	Room is equipped with a set of specialized furniture; specialized equipment of the 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.	Room is equipped with a set of specialized furniture there is wi-fi

* 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"

1. Databases and search engines:

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

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

1. The set of lectures on the course "FUNDAMENTALS OF CONTEMPORARY MASS SPECTROMETRY".

2. The laboratory workshop on the course "FUNDAMENTALS OF CONTEMPORARY MASS SPECTROMETRY".

* 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

Evaluation materials and a point-rating system* for assessing the level of formation of competencies (parts of competencies) based on the results of mastering the discipline "FUNDAMENTALS OF CONTEMPORARY MASS SPECTROMETRY" are presented in the Appendix to this Work Program of the discipline.

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:

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Position, Department	Signature	Full name

HEAD OF EDUCATIONAL DEPARTMENT:

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HEAD
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