Federal State Autonomous Educational Institution of Higher Education

PEOPLES' FRIENDSHIP UNIVERSITY OF RUSSIA named after P. Lumumba (RUDN University)

Faculty of Science

COURSE SYLLABUS

FUNDAMENTALS OF CONTEMPORARY MASS SPECTROMETRY

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:

«Pharmaceutical analysis in the production and drug quality control»

higher education programme profile/specialisation title

2025 г.

1. INTERNSHIP 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 the internship

Competence code	**Competence descriptor**	**Competence formation indicators** (within this course)
PC-1	To be able to plan work and choose adequate methods for solving research problems in the chosen field of chemistry, chemical technology or sciences related to chemistry	PC-1.1. To draw up a general plan of research and detailed plans for individual stages.
		PC-1.2. To select experimental and computational-theoretical methods for solving the problem based on the available material and time resources.
PC-2	To be able to perform patent information research in the chosen field of chemistry and/or related sciences	PK-2.1. To search for specialized information in patent information databases.
		PK-2.2. To analyze and summarize the results of a patent search on the subject of the project in the selected field of chemistry (chemical technology).

3. INTERNSHIP IN HIGHER EDUCATION PROGRAMME STRUCTURE

The discipline "FUNDAMENTALS OF CONTEMPORARY MASS SPECTROMETRY" refers to *the Elective Disciplines Module* of block B1 of the EP HE.

As part of the EP HE, students also master other disciplines and / or practices that contribute to the achievement of the planned results of mastering the discipline FUNDAMENTALS OF CONTEMPORARY MASS SPECTROMETRY".

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, internships***	**Subsequent courses/modules, internships***
PC-1	To be able to plan work and choose adequate	Actual problems of modern chemistry	Undergraduate practice

Competence code	Competence descriptor	Previous courses/modules, internships*	Subsequent courses/modules, internships*
	methods for solving research problems in the chosen field of chemistry, chemical technology or sciences related to chemistry	Chemistry of natural compounds Chemical methods of drug quality control in world pharmacopoeias pharmaceutical chemistry Modern information technologies in pharmacy Database Methodology Elemental analysis methods in drug quality control Physical and chemical bases of drug quality control Optical methods in pharmaceutical analysis Experimental research methods in pharmaceutical analysis Research work Experimental research methods in the chemistry of organic chemistry	
PC-2	To be able to perform patent information research in the chosen field of chemistry and/or related sciences	Actual problems of modern chemistry Chemistry of natural compounds Chemical methods of drug quality control in world pharmacopoeias pharmaceutical chemistry Modern information technologies in pharmacy Database Methodology Elemental analysis methods in drug quality control Physical and chemical bases of drug quality control Optical methods in pharmaceutical analysis Experimental research methods in pharmaceutical analysis Research work Experimental research	Undergraduate practice

Competence code	Competence descriptor	Previous courses/modules, internships*	Subsequent courses/modules, internships*
		methods in the chemistry of organic chemistry	

4. INTERNSHIP WORKLOAD

Course workload of the discipline «FUNDAMENTALS OF CONTEMPORARY MASS SPECTROMETRY» is 2 credits.

*Table 4.1. Types of educational work by periods of mastering EP VO for **FULL-TIME EDUCATION***

Types of academic activities		Total ac.h,	Semesters			
			1	2	3	4
Contact work ac.h.		*36*			36	
including:						
Lectures (**LC**)		18			18	
Lab Works (**LW**)		18			18	
Seminars (**PC**)						
Self-study, *ac.h.*		*18*			18	
Evaluation and assessment (exam or pass/fail grading), ac.h.		*18*			18	
Total labor intensity	**ac.h.**	**72**			**72**	
	ac.h.	**2**			**2**	

5. INTERNSHIP CONTENTS

*Table 5.1. Internship contents**

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

Modules	Contents (topics, types of practical activities)	Workload, academic hours
Section 4. Protocol for structure determination of unknowns by EI mass spectrometry.	Theme 4.1. The main fragmentation pathways and diagnostic ions for acyclic compounds with up to one functional group.	LK, LW
	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

* The contents of internship through modules and types of practical activities shall be FULLY reflected in the student's internship report.

6. INTERNSHIP EQUIPMENT AND TECHNOLOGY SUPPORT EQUIREMENTS

Table 6.1. Classroom Equipment and Technology Support Requirements

Classroom for Academic Activity Type	Audience equipment	Specialized educational / laboratory equipment, software and materials for mastering the discipline (if necessary)
Lecture Room	An auditorium for lecture-type classes, equipped with a set of specialized furniture; board (screen) and technical means of multimedia presentations.	
Laboratory room	Educational chemical laboratory for group laboratory-type classes, individual consultations, monitoring, intermediate certification, independent work	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
Room for independent work	An auditorium for independent work of students (can be used for seminars and	Room is equipped with a set of specialized furniture

Classroom for Academic Activity Type	Audience equipment	Specialized educational / laboratory equipment, software and materials for mastering the discipline (if necessary)
of students	consultations), equipped with a set of specialized furniture and computers with access to the EIOS.	there is wi-fi

* - the audience for independent work of students is indicated **MANDATORY**!

7. RECOMMENDED SOURCES FOR COURSE STUDIES

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.

Electronic libraries with access for RUDN by P. Lumumba students:

1. RUDN by P. Lumumba ELS and third-party ELS, to which university students have access on the basis of concluded agreements:

- RUDN by P. Lumumba Electronic Library System - RUDN EBS by P. Lumumba http://lib.rudn.ru/MegaPro/Web
- ELS "Университетская библиотека онлайн" http://www.biblioclub.ru
- EBS Юрайт http://www.biblio-online.ru
- ELS "Консультант студента" www.studentlibrary.ru - EBS "Lan" http://e.lanbook.com/
- EBS "Троицкий мост"

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/

* - all educational and methodological materials for independent work of students are placed in accordance with the current procedure on the page of the discipline in TUIS!

DEVELOPERS:

Assistant professor, Organic Chemistry Department		**R.S.Borisov**
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HEAD OF DEPARTMENT:

Organic Chemistry Department		**L. G. Voskressensky**
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