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

NMR of organic compounds

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

2024

1. COURSE GOAL(s)

The goal of the course "NMR of organic compounds" is to develop students' skills in establishing the structures of complex organic compounds by deciphering nuclear magnetic resonance spectra (hereinafter referred to as NMR) in the Trial program, allowing editing feeds. These skills are of great practical importance, since every synthetic chemist is faced with the task of establishing and proving the structure of the data obtained during the experiment. The greatest attention is paid to ^{1}H и ^{13}C NMR spectroscopy of organic compounds.

2. REQUIREMENTS FOR LEARNING OUTCOMES

Mastering the discipline "NMR 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-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-1.2. Selects experimental and computational-theoretical methods for solving the problem based on the available material and time resources
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 "NMR of organic compounds" refers to the *Electives* of block B1 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-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	Methods of Organic Chemistry Fundamentals of biotechnology Research work Experimental methods in the chemistry	Chemistry of natural compounds Fundamentals of drug design Chemistry of heterocyclic compounds Stereochemistry Reseacrh work Undergraduate practice
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	Experimental methods in the chemistry Theoretical organic chemistry	Mass spectrometry of organic compounds Stereochemistry Reseacrh work Undergraduate practice

4. COURSE WORKLOAD AND ACADEMIC ACTIVITIES

The total workload of the course is "NMR of organic compounds" 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	Semesters			
			1	2	3	4
Contact academic hours		*54*		*54*		
including:						
Lectures (**LC**)		36		36		
Lab Work (**LW**)		18		18		
Seminars (workshops/tutorials) (S)						
Self-studies		*36*		*36*		
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

Modules	Themes	Types of academic activities
Section 1. Introduction and theoretical foundations of the NMR method	Theme 1.1. NMR spectroscopy and its place among physical methods for studying the processes and products of organic chemistry. Elements of the theory of the NMR phenomenon.	LC, LW
	Theme 1.2. The history of the development of the method (I. Rabi, F. Bloch, E. Purcell). Spin numbers and magnetic moment of atoms, Zeeman effect, Larmor frequencies.	LC, LW
	Theme 1.3. Magnetic resonance conditions. Decay of free induction. Times of longitudinal and transverse relaxation.	LC, LW
Section 2. The structure of the NMR spectrometer	Theme 2.1. Types of NMR spectrometers. Schematic diagram of the apparatus. Opportunities.	LC, LW
	Theme 2.2. Description of the method of analysis, the output data obtained after the removal of the spectrum.	LC, LW
Section 3. Parameters of 1H and 13C NMR spectra	Theme 3.1. Solvents used, internal and external standards. Parameters of NMR spectra, their informative value. Width and intensity of the NMR line.	LC, LW
	Theme 3.2. Integration. Chemical shift. Chemical shifts of 1H and 13C nuclei of organic molecules.	LC, LW
	Theme 3.3. The concept of the fine structure of the 1H and 13C NMR spectra, SSCC. Spin-spin interaction.	LC, LW
Section 4. NMR features of various classes of organic compound	Theme 4.1. Characteristic signals in proton and carbon spectra of alkenes, alkynes, arenes, carboxylic acids and carbonyl compounds. Their use to establish structure.	LC, LW
Section 5. Trial Program	Theme 5.1. Acquaintance and basic methods of working in Trial programs: Fourier transform of spectra, adjustment of phases of the 1st and 2nd orders, integration, correlation of signals, editing of spectra, etc.	LC, LW
Section 6. Decoding of 1H spectra of unknown compound	Theme 6.1. Transformation of 1H NMR fids for further work with the spectrum: determination of the spatial structure of organic compounds from the data	LC, LW
Section 7. Decoding of 13C spectra of unknown compounds	Theme 7.1. Transformation of 1H NMR fids for further work with the spectrum: determination of the spatial structure of organic compounds from 13C NMR data.	LC, LW
Section 8. Decoding the spectra of unknown compounds from the totality of NMR data.	Theme 8.1. Transformation of 1H NMR fids for further work with the spectrum: determination of the spatial structure of organic compounds from the totality of 1H and 13C NMR data, taking into account the SSCC values.	LC, LW

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.	A set of specialized furniture; specialized chemical laboratory equipment: IR Fourier spectrometer BRUKER "MPA", gas chromatography-mass spectrometer FOCUS-DSQ with a turbomolecular pump 250 l / s, gas cylinder (helium), fume hood, air conditioning, computer, wi-fi available In NMR spectroscopy, the instruments of the Scientific and Educational Center for Collective Use of RUDN University are used: http://www.rudn.ru/index.php?pagec=5972, http://ccp.rudn.ru/?pagec=940 Laboratory work is carried out in the building of the Center for Collective Use of RUDN University under the guidance of the staff of the center, who are equipped with Jeol "JNM-ECA 600" and Jeol "JNM-ECA 400" NMR spectrometers.
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.	

7. RESOURCES RECOMMENDED FOR COURSE STUDY

Main reading:

1. Slikter Ch. Fundamentals of the theory of magnetic resonance.

Additional reading:

1. Zaitsev B.E. Fundamentals of NMR spectroscopy: Lecture notes / B.E. Zaitsev. - M.: Publishing House of RUDN University, 2009.

2. Ernst R., Bodenhausen J., Vokaun A. NMR in one and two dimensions: TRANS. from English. ed. K. M. Salikhova, M.: Mir, 1990.

3. Sergeev N. M. NMR spectroscopy (for organic chemists): M.: Publishing house of Moscow State University, 1981.

4. Deroum E. Modern NMR methods for chemical research. M.: Mir, 1992.

5. Günter H. Introduction to the course of NMR spectroscopy: TRANS. from English. M.: Mir, 1984.

Resources of the information and telecommunications network "Internet":

1. RUDN Electronic Library System (ELS) and third-party ELS, to which university students have access on the basis of concluded agreements:

- RUDN Electronic Library System - RUDN EBS
  http://lib.rudn.ru/MegaPro/Web
  http://lib.rudn.ru:8080/MegaPro/Web
- Databases Scopus
  https://www.scopus.com/
- Databases Web of Science
  http://apps.webofknowledge.com/WOS_GeneralSearch_input.do?product=WOS&search_mode=GeneralSearch&SID=N1cZ3JYEClUJdm14VTK&preferencesSaved=
- Organic Chemistry Portal
  http://www.organic-chemistry.org/
- Databases Reaxys
  https://www.reaxys.com/reaxys/secured/search.do

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. A course of lectures on the discipline "NMR of organic compounds".
2. Laboratory workshop on the discipline "NMR 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.

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 the Department of Organic Chemistry		**F. I. Zubkov**

Position, Department	Signature	name and surname

HEAD OF EDUCATIONAL DEPARTMENT:

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

HEAD
OF HIGHER EDUCATION PROGRAMME:

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