Federal State Autonomous Educational Institution of Higher Education
PEOPLES' FRIENDSHIP UNIVERSITY OF RUSSIA
RUDN University

Faculty of Science

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

COURSE SYLLABUS

Artificial intelligence and additive technologies in chemistry

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

2026

1. COURSE GOAL

The goal of the course "Artificial intelligence and additive technologies in chemistry" is education of students with advanced methods and technologies at the intersection of chemistry, artificial Intelligence (AI) and additive manufacturing. The course aims to explore the principles of artificial intelligence and its applications to problems in chemistry, including modeling chemical processes, optimizing reaction conditions and the development of new materials. The course covers aspects of additive technologies, including 3D printing to create chemical reactors, devices for synthesis and analysis, as well as the development new materials with unique properties.

2. REQUIREMENTS FOR LEARNING OUTCOMES

Mastering the course “Artificial intelligence and additive technologies in chemistry” 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)
GC-7	Ability to look for the necessary sources of information and data, perceive, analyse, memorize and transmit information using digital means, as well as using algorithms when working with data obtained from various sources in order to effectively use the information received to solve problems; evaluate information, its reliability, build logical conclusions based on incoming information and data.	GC-7.1. Ability to use digital technologies and methods of searching, processing, analysing, storing and presenting information in the field of chemistry.
		GC-7.2. Ability to develop the conception of digital technologies and methods of searching, processing, analysing, storing and presenting information within the framework of the designated problem: to be able to formulate the purpose, objectives, justify the relevance, significance, expected results and possible areas of their application in the digital economy and modern corporate information culture.
		GC-7.3. Ability to monitor the use of digital technologies and methods of search, processing, analysis, storage and presentation of information in the field of chemistry, corrects deviations, makes additional changes to the plan for the use of digital technologies.
GPC-3	Ability to use computational methods and adapt existing software products to solve problems of professional activity.	GPC-3.1. Ability to use modern IT-technologies in the collection, analysis, and presentation of chemical profile information;
		GPC-3.2. Ability to use standard and original software products, if necessary, adapting them to solve the problems of professional activity;
		GPC-3.3. Ability to use modern computational

Competence code	Competence descriptor	Competence formation indicators (within this course)
		methods for processing chemical experiment data, modeling the properties of substances (materials) and processes with their participation
PC-2	Ability, based on a critical analysis of the results of research and development, to evaluate the prospects for their practical application and continuation of work in the chosen field of chemistry, chemical technology or sciences related to chemistry.	PC-2.2. Ability 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 "Artificial intelligence and additive technologies in chemistry" 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 code	Competence descriptor	Previous courses/modules*	Subsequent courses/modules*
GC-7	Ability to look for the necessary sources of information and data, perceive, analyse, memorize and transmit information using digital means, as well as using algorithms when working with data obtained from various sources in order to effectively use the information received to solve problems; evaluate information, its reliability, build logical conclusions based on incoming information and data.		The methods of working with databases Student Scientific-Research work Pre-graduation practical training
GPC-3	Ability to use computational	Bioenergy Bioproducts and	Experimental lab 3: Advanced Organic Synthesis

Competence code	Competence descriptor	Previous courses/modules*	Subsequent courses/modules*
	methods and adapt existing software products to solve problems of professional activity.	Biorefineries	Student Scientific-Research work Pre-graduation practical training
PC-2	Ability, based on a critical analysis of the results of research and development, to evaluate the prospects for their practical application and continuation of work in the chosen field of chemistry, chemical technology or sciences related to chemistry.	Bioproducts and Biorefineries	Experimental lab 3: Advanced Organic Synthesis Student Scientific-Research work Pre-graduation practical training

* 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 "Artificial intelligence and additive technologies in chemistry" is 2 credits (72 academic hours).

*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	Training modules			
			1	2	3	4
Contact academic hours		18			*18*	
Lectures (LC)		9			9	
Lab work (LW)		9			9	
Seminars (workshops/tutorials) (S)						
Self-studies		*54*			*54*	
Evaluation and assessment (exam/passing/failing grade)						
Course workload	academic hours	**72**			**72**	
	credits	**2**			**2**	

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. Artificial Intelligence in Chemical Research	Topic 1.1 Introduction to artificial intelligence for chemists The concept of artificial intelligence (AI), the history of its development and its main applications in science and technology. Overview of the use of AI in chemistry to solve scientific and practical problems. Basic principles and approaches of AI, the difference between machine learning and deep learning.	LC
	Topic 1.2 Fundamentals of machine learning and neural networks Key aspects of machine learning and neural networks. Types of learning (with teacher, without teacher, with reinforcement), algorithms and models, and their application in chemical research. Fundamentals of building, training and validating AI models.	LC
	Topic 1.3 Applications of AI in organic synthesis An overview of advanced developments in the use of AI in organic synthesis. Innovative application of machine learning for reactivity prediction, optimization of reaction conditions and development of new reaction pathways. Practical examples from current research.	LC
	Topic 1.4 Tools and databases for working with AI in chemistry Key tools, software and databases that are used to work with AI in chemistry. Issues of data availability, data preprocessing, and the importance of quality of data collection for successful AI applications. Examples of popular platforms and tools.	LC
Module 2. Fundamentals of additive technologies for chemical research	Topic 2.1 Introduction to additive technologies for chemists An overview of additive technologies, their history and development, and basic principles and capabilities for chemical research. Advantages of additive technologies over traditional manufacturing methods, including their ability to rapidly iterate designs, customize, and create complex structures.	LC
	Topic 2.2 Types of additive technologies and 3D printing	LC

Course module title	Course module contents (topics)	Academic activities types
	Various additive manufacturing techniques and technologies such as stereolithography (SLA), selective laser sintering (SLS), layer-by-layer deposition method (FDM) and others. Their main characteristics, advantages and limitations for use in chemical research.	
	Topic 2.3 Materials for additive manufacturing in chemistry Overview of materials used in additive manufacturing including plastics, metals, ceramics and composites. Suitability of materials for use in chemical research including chemical compatibility, heat resistance and mechanical properties.	LC, LW
	Topic 2.4 Applications of additive technologies in organic synthesis Specific applications of additive technologies in organic synthesis, including the fabrication of reactors, purification systems, and other laboratory devices. 3D printing applications that promote innovation in synthesis methodology, experiment optimization, and cost reduction.	LC, LW
	Topic 2.5 Development and integration of additive technologies into laboratory practice The process of developing and integrating additive technologies, device design, and tools for laboratory practice. Stages of design, material selection, printing and testing. Safety and cost effectiveness issues. Recommendations for getting started with additive technologies in the laboratory, including equipment selection.	LC, LW
Module 3. Artificial intelligence and additive technologies in modern organic synthesis and biomass valorization processes	Topic 3.1 Fundamentals of integrating AI and additive technologies in chemistry An overview of the opportunities offered by the combined use of AI and additive technologies in chemical synthesis. Basic principles and strategies	LC, LW

Course module title	Course module contents (topics)	Academic activities types
	for integrating these approaches to develop new chemical processes and devices. Examples of successful applications that demonstrate the potential of the combined approach.	
	Topic 3.2 Development of customizable catalysts using AI and 3D printing Development of customizable catalysts using the analytical capabilities of AI to predict catalytic activity and selectivity, and the application of additive technologies to their physical creation. The benefits of creating catalysts specifically tailored to specific reactions and opportunities for innovation in synthetic chemistry. Process design of biomass valorization.	LC, LW
	Topic 3.3 Automation of organic synthesis using AI and additive technologies Using AI to automate organic synthesis processes, including reaction planning and control of reactors produced by additive manufacturing methods. Strategies for integrating these approaches to create flexible, highly efficient and autonomous chemical production systems.	LC, LW
	Topic 3.4 The future of synthesis: AI and additive technologies as drivers of innovation and sustainability A look at the future prospects for the use of AI and additive technologies in organic synthesis. Potential directions for the development of these technologies, including the creation of smart materials, new approaches in process and device design, and the impact on sustainability and green chemistry. Challenges and opportunities for researchers and engineers in synthetic chemistry, biomass conversion and sustainability.	LC

* - 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	Projector, motorized screen

Type of academic activities	Classroom equipment	Specialised educational / laboratory equipment, software, and materials for course study (if necessary)
	with a set of specialised furniture; board (screen) and a set of devices for multimedia presentations.	for projectors, Wi-Fi
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 equipment of the chemical laboratory: fume hood SHVP-4, fume hood SHVP-2, rotary evaporator Hei-value digital G3B, rotary evaporator IKA, digital devices for determining the 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

Type of academic activities	Classroom equipment	Specialised educational / laboratory equipment, software, and materials for course study (if necessary)
		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

* The premises for students' self-studies are subject to **MANDATORY** mention

7. RECOMMENDED RESOURCES FOR COURSE STUDY

Main sources:

1. Gordeev E.G., Ananikov V.P., "Widely accessible 3D printing technologies in chemistry, biochemistry and pharmaceutics: applications, materials and prospects", *Russ. Chem. Rev.*, **2020**, 89, 1507-1561. http://dx.doi.org/10.1070/RCR4980
2. Erokhin K.S., Naumov S.A., Ananikov V.P., "Analysis, classification and remediation of defects in material extrusion 3D printing", *Russ. Chem. Rev.*, **2023**, 92, 11, RCR5103. https://www.uspkhim.ru/RCR5103
3. Meuwly, M. Machine Learning for Chemical Reactions. *Chem. Rev.* **2021**, *121* (16), 10218–10239. https://doi.org/10.1021/acs.chemrev.1c00033
4. Baum, Z. J.; Yu, X.; Ayala, P. Y.; Zhao, Y.; Watkins, S. P.; Zhou, Q. Artificial Intelligence in Chemistry: Current Trends and Future Directions. *J. Chem. Inf. Model.* **2021**, *61* (7), 3197–3212. https://doi.org/10.1021/acs.jcim.1c00619

Additional sources:

1. American Chemical Society ACS Publications: https://pubs.acs.org/
2. Royal Society of Chemistry RSC Publications: https://pubs.rsc.org/
3. Wiley on-line library http://onlinelibrary.wiley.com/
4. Electronic database SciFinder https://scifinder-n.cas.org/

Internet sources

1. Electronic libraries with access for RUDN students:
- 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"

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/
- www.scholar.google.ru

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

1. A set of lectures on "Artificial intelligence and additive technologies in chemistry"
2. The laboratory workshop on "Artificial intelligence and additive technologies in chemistry"

* 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		**Valentine Ananikov**
position, department	signature	name and surname

HEAD OF EDUCATIONAL DEPARTMENT:

Organic Chemistry Department		**Voskressensky L.G**
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HEAD OF HIGHER EDUCATION PROGRAMME:

Dean of Faculty of Science, Head of Organic Chemistry Department		**Voskressensky L.G**
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