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

Institute of Pharmacy and Biotechnology
educational division (faculty/institute/academy) as higher education programme developer

COURSE SYLLABUS

COMPUTER TECHNOLOGIES IN SCIENTIFIC RESEARCH
course title

Recommended by the Didactic Council for the Education Field of:

28.04.01 NANOTECHNOLOGY AND MICROSYSTEM ENGINEERING
field of studies / speciality code and title

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

INNOVATIVE TECHNOLOGIES AND NANOTECHNOLOGIES IN MEDICINE, PHARMACY AND BIOTECHNOLOGY
higher education programme profile/specialisation title

2026

1. COURSE GOAL(s)

The course Computer Technologies in Scientific Research is part of the Master's programme «Innovative Technologies and Nanotechnologies in Medicine, Pharmacy and Biotechnology» (field of study 28.04.01 Nanotechnology and Microsystem Engineering), taught in Semester 2 of Year 1. The course is delivered by the Department of Pharmacy and Biotechnology. The course consists of 7 modules and 26 topics covering the fundamentals and practical aspects of applying computer technologies in modern scientific research.

The goal of this course is to equip students with professional competences in the use of modern computer technologies for effective collection, processing, analysis, visualisation and presentation of scientific data, as well as for improving the quality and efficiency of research activities.

2. REQUIREMENTS FOR LEARNING OUTCOMES

Mastering the course Computer Technologies in Scientific Research is aimed at the development of the following competences (competences in part):

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	Able to search for relevant information and data, perceive, analyse, memorise and communicate information using digital means, and apply algorithms when working with data from various sources for effective use in problem-solving; evaluate information for authenticity and reliability; draw logical conclusions from incoming information and data	GC-7.1. Able to search for relevant information and data, perceive, analyse, memorise and communicate information using digital means, and apply algorithms when working with data from various sources for effective use in problem-solving;
		GC-7.2. Evaluates information for authenticity and reliability; draws logical conclusions from incoming information and data;
		GC-7.3. Presents the outcomes of their work on corporate information platforms.

3.COURSE IN HIGHER EDUCATION PROGRAMME STRUCTURE

The course refers to the variable component of Block 1 (Disciplines/Modules) of the higher education programme curriculum.

Within the higher education programme students also master other disciplines (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	Able to search for relevant information and data, perceive, analyse, memorise and	Fundamentals of Statistics and Programming; Information Databases	Pre-graduation internship

Competence code	Competence descriptor	Previous courses/modules*	Subsequent courses/modules*
	communicate information using digital means, and apply algorithms when working with data from various sources; evaluate information for authenticity and reliability; draw logical conclusions from incoming information and data		

* 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 Computer Technologies in Scientific Research is 3 credits (108 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	Semesters/training modules			
			1	2	3	4
Contact academic hours		*36*	–	36	–	–
including:						
Lectures (LC)		18	–	18	–	–
Lab work (LW)		0	–	0	–	–
Seminars (workshops/tutorials) (S)		18	–	18	–	–
Self-studies		*54*	–	54	–	–
Evaluation and assessment (exam/passing/failing grade)		*18*	–	18	–	–
Course workload	academic hours_	**108**	–	–	–	
	credits	**3**	–	–	–	

*Table 4.2. Types of academic activities during the periods of higher education programme mastering (**part-time training**)**

Type of academic activities	Total academic hours	Semesters/training modules			
		1	2	3	4
Contact academic hours	*36*	–	36		
Lectures (LC)	18	–	18		
Lab work (LW)	0	–	0		
Seminars (workshops/tutorials) (S)	18	–	18		
Self-studies	*54*	–	54		

Type of academic activities		Total academic hours	Semesters/training modules			
			1	2	3	4
Evaluation and assessment (exam/ passing/failing grade)		*18*	–	18		
Course workload	academic hours_	**108**	–	108		
	credits	**3**	–	3		

* To be filled in regarding the higher education programme part-time training mode.

5. COURSE CONTENTS

Table 5.1. Course contents and academic activities types

Course module title	Course module contents (topics)	Academic activities types
Module 1: Fundamentals of Computer Technologies in Scientific Research	**Topic 1.1. The Role of Computer Technologies in Modern Scientific Research** History and stages of computer technology adoption in science. Classification of software tools by field of application. The impact of digitalisation on the speed and quality of research. Examples of breakthrough discoveries enabled by computational methods.	LC, S
	Topic 1.2. Types of Digital Data in Biochemical, Nanotechnology and Pharmaceutical Research Structured, unstructured and semi-structured data. Primary and secondary data in biochemistry, nanotechnology and pharmaceutics. Genomic, proteomic and metabolomic data. Data quality requirements and verification methods.	LC, S
	Topic 1.3. File Formats and Principles of Scientific Data Organisation Main scientific data storage formats: CSV, JSON, XML, HDF5, FASTA, PDB, etc. File naming conventions and directory structure principles. Metadata and its role in experiment documentation. Open data formats and FAIR standards (Findable, Accessible, Interoperable, Reusable).	LC, S
	Topic 1.4. Overview of Software Packages for Scientific Research General-purpose packages: Microsoft Office, LibreOffice, LaTeX. Specialised software for biochemistry and nanotechnology: OriginPro, GraphPad Prism, Avogadro, VESTA. Open-source tools: R, Python, ImageJ. Criteria for selecting software for a specific scientific task.	LC, S
Module 2: Software for Scientific Information Management	**Topic 2.1. Bibliographic Reference Management Systems** Purpose and functions of reference managers. Overview of popular systems: Zotero, Mendeley, EndNote, JabRef. Importing references from PubMed, Scopus, Web of Science. Generating bibliographies in various citation styles (APA, Vancouver, GOST 7.0.5). Collaborative literature work in a group.	LC, S

	Topic 2.2. Software for Experimental Data Organisation Structuring experimental data in Excel and Google Sheets. Using databases (Access, SQLite) for storing experimental results. Principles of data versioning and change control. Backup and cloud storage tools: OneDrive, Google Drive, Nextcloud.	LC, S
	Topic 2.3. Electronic Laboratory Notebooks and Laboratory Information Management Systems The concept of an electronic laboratory notebook (ELN) and its advantages over paper records. Overview of ELN systems: LabArchives, Benchling, RSpace, eLabFTW. Laboratory Information Management Systems (LIMS): structure, functions and equipment integration. Documentation requirements under GLP/GMP standards.	LC, S
Module 3: Analysis and Processing of Scientific Data	**Topic 3.1. Fundamentals of Statistical Data Analysis in Scientific Research** Descriptive statistics: mean, median, variance, standard deviation. Normality tests: Shapiro–Wilk, Kolmogorov–Smirnov. Parametric and non-parametric group comparison methods (t-test, Mann–Whitney U test). Correlation analysis. Type I and Type II errors, significance level, statistical power.	LC, S
	Topic 3.2. Statistical Software Packages for Data Processing Statistica: data entry, basic statistical tests, graphical output. R environment: stats, ggplot2, dplyr packages for analysis and visualisation. Python: Pandas, SciPy, Statsmodels libraries. SPSS for social and biomedical research. Comparative analysis of package capabilities.	LC, S
	Topic 3.3. Experimental Data Processing Technologies in Specialised Fields Processing spectroscopic data (IR, UV, NMR, mass spectrometry). Analysis of dynamic light scattering (DLS) and electron microscopy (TEM, SEM) data in nanotechnology. Processing chromatographic data (HPLC, GC). Specialised software: SpectraGryph, ImageJ, MestReNova.	LC, S

	Topic 3.4. Big Data Analysis Methods The concept of Big Data in scientific research. Dimensionality reduction methods: PCA, t-SNE, UMAP. Cluster analysis: hierarchical clustering, k-means. Bioinformatics pipelines for genomic data processing (RNA-seq, ChIP-seq). Parallel computing and cloud platforms: Galaxy, Google Colab.	LC, S
Module 4: Scientific Data Visualisation	**Topic 4.1. Principles of Effective Scientific Data Visualisation** Core principles of visual perception (Gestalt laws, data-ink ratio). Choosing the right chart type based on data nature. Common errors in graph construction: axis manipulation, chart junk. Requirements for figures in scientific journals: resolution, colour models, fonts.	LC, S
	Topic 4.2. Types of Charts and Diagrams for Presenting Scientific Results Scatter plots, line graphs, histograms, box plots, violin plots. Heatmaps and dendrograms for multivariate data. Scatter plots with regression curves. Specialised diagrams: volcano plots, MA-plots, Manhattan plots in bioinformatics.	LC, S
	Topic 4.3. Software Tools for Scientific Graphics Graph construction in OriginPro and GraphPad Prism. Vector graphics in Adobe Illustrator and Inkscape. ggplot2 (R) and Matplotlib/Seaborn (Python) for programmatic visualisation. Molecular graphics tools: PyMOL, ChimeraX, VESTA. Format requirements: SVG, EPS, TIFF for publications.	LC, S
	Topic 4.4. Creating Complex Visualisations for Scientific Publications Designing multi-panel figures with annotations. Composing graphical abstracts. Coordinating colour schemes and styles within a single article. Tools for diagrams and schematics: BioRender, ChemDraw, Draw.io. Preparing illustrations for presentations and posters.	LC, S
Module 5: Specialised Databases and Information Resources	**Topic 5.1. Overview of Specialised Databases in the Field of Study** Chemistry and biochemistry databases: PubChem, ChemSpider, ChEMBL, BRENDA. Nanotechnology databases: eNanoMapper, NanoHUB. Pharmaceutical databases: DrugBank, PharmGKB. Protein structure databases: PDB. Genomic and transcriptomic databases: NCBI, Ensembl, UniProt.	LC, S

	Topic 5.2. Strategies for Effective Scientific Information Retrieval Boolean operators and truncation in search queries. Using filters in PubMed, Scopus and Web of Science: date, document type, impact factor. MeSH terms as a tool for medical literature classification. Alert systems and RSS subscriptions for monitoring new publications. Evaluating source quality: impact factor, journal quartile, citation indices.	LC, S
	Topic 5.3. Using Online Resources for Research in Specialised Fields Open access to scientific data: PubMed Central, arXiv, SSRN, Zenodo. Data repositories: Figshare, Dryad, PANGAEA. Online tools for molecular modelling and docking: SwissDock, AutoDock Vina Online. Reproducible research platforms: GitHub, OSF (Open Science Framework).	LC, S
Module 6: Computer Technologies for Presenting Research Results	**Topic 6.1. Technologies for Preparing Scientific Publications** Scientific article structure (IMRAD) and manuscript formatting requirements. Working in Microsoft Word and LaTeX (Overleaf) with scientific content. Formatting equations, tables and figures according to journal requirements. Plagiarism checking: iThenticate, Antiplagiat. The peer review process and responding to reviewer comments.	LC, S
	Topic 6.2. Creating Effective Scientific Presentations Slide design principles: one-idea rule, minimalism, readability. Microsoft PowerPoint and Google Slides for academic presentations. Creating conference posters: structure and tools (PowerPoint, Canva, Inkscape). Oral presentation skills: talk structure, time management, Q&A handling.	LC, S
	Topic 6.3. Preparing Scientific and Technical Documentation Types of scientific and technical documentation: reports, technical specifications, method passports, patent applications. GOST requirements for technical reports. Patent documentation formatting: claims, description, drawings. Writing grant proposals: structure and requirements of funding bodies.	LC, S

	Topic 6.4. Collaborative Work Technologies and Scientific Data Sharing Collaborative document editing tools: Google Workspace, Microsoft 365 Online. Version control systems for code and data: Git, GitHub, GitLab. Collaborative research platforms: ResearchGate, Overleaf, OSF. Data exchange within a laboratory: cloud storage, VPN, corporate portals. Ethics of data sharing and authorship.	LC, S
Module 7: Artificial Intelligence Applications in Scientific Research	**Topic 7.1. Fundamentals of Artificial Intelligence and Machine Learning in Science** Concepts and classification of AI methods: machine learning, deep learning, neural networks. Types of AI tasks: classification, regression, clustering, generation. Key algorithms: random forests, gradient boosting, convolutional and recurrent networks. Frameworks: TensorFlow, PyTorch, scikit-learn. AI applications in biochemistry, nanotechnology and pharmaceutics.	LC, S
	Topic 7.2. Generative Language Models as a Tool for Scientific Work How large language models (LLMs) work: transformer architecture, pre-training and fine-tuning. Practical use of ChatGPT, Claude, Gemini and equivalents: literature summarisation, hypothesis formulation, writing and editing. Specialised scientific AI tools: Elicit, Consensus, ResearchRabbit, Semantic Scholar. Critical evaluation of LLM outputs: hallucinations, source verification. Ethics of AI use in scientific publications (COPE guidelines).	LC, S
	Topic 7.3. AI for Data Analysis and Predictive Modelling Neural networks for image analysis: microscopy, spectroscopy, electron microscopy of nanomaterials. Protein structure prediction with AlphaFold2 and ESMFold: principles and result interpretation. Machine learning-enhanced molecular docking: AutoDock-GPU, Gnina. AI in drug and nanomaterial development: generative molecular design, toxicity prediction. Automating experimental data processing with Python scripts and AI assistants.	LC, S

	Topic 7.4. Practical Workshop: AI Tools in Scientific Research Hands-on work with language models: crafting prompts for literature search and manuscript section generation. Working with AlphaFold2 via ColabFold: protein structure prediction and visualisation. Applying machine learning tools to analyse research data from the student's own field. Evaluating AI-generated content quality and verifying scientific accuracy. Designing a research workflow integrating AI tools.	LC, S

* - 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.	Everycom multimedia projector. Lenovo ThinkPad L530 laptop: Intel Core i3-2370M / 2.4 GHz / DDR3 4 GB. Internet access provided.
Seminar	A classroom for conducting seminars, group and individual consultations, current and mid-term assessment; equipped with a set of specialised furniture and technical means for multimedia presentations.	Everycom multimedia projector. Lenovo ThinkPad L530 laptop: Intel Core i3-2370M / 2.4 GHz / DDR3 4 GB. Internet access provided.
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.	Everycom multimedia projector. Lenovo ThinkPad L530 laptop: Intel Core i3-2370M / 2.4 GHz / DDR3 4 GB. Internet access provided.

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

7. RESOURCES RECOMMENDED FOR COURSE STUDY

Main readings:

1. Alekseev, D. S. Data Mining Technologies / D. S. Alekseev, O. V. Shchekochikhin. — 2nd ed. — St. Petersburg : Lan, 2024. — 176 p. — ISBN 978-5-507-48763-9. — Electronic text // Lan ELS. — URL: https://e.lanbook.com/book/362915

2. Mathematical Methods in Biology: Analysis of Biological Data in Statistica / S. N. Gashev et al. — 2nd ed. — Moscow : Yurayt, 2024. — 181 p. — ISBN 978-5-534-18668-0. — URL: https://urait.ru/bcode/545309

Additional readings:

1. Kruchinin, V. V. Computer Technologies in Scientific Research : study guide / V. V. Kruchinin. — Moscow : TUSUR, 2012. — 56 p. — Electronic text // Lan ELS. — URL: https://e.lanbook.com/book/11269

2. Computer Technologies in Scientific Research : study guide / E. N. Kosova et al. — Stavropol : NCFU, 2015. — 241 p. — Electronic text // Lan ELS. — URL: https://e.lanbook.com/book/155228

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 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 «Computer Technologies in Scientific Research».

* 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	**Kezimana Parfait**
position, department	name and surname

HEAD OF EDUCATIONAL DEPARTMENT:

Director	**Romashchenko Victoria Alexandrovna**
name of department	name and surname

HEAD
OF HIGHER EDUCATION PROGRAMME:

position, department	name and surname