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Информация о владельце:  
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Должность: Ректор  
Дата подписания: 06.05.2026 15:20:55  
Уникальный программный ключ:  
ca953a0120d891083f939673078ef1a989dae18a

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

**Institute of Pharmacy and Biotechnology**

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

**COURSE SYLLABUS**

**COMPUTER TECHNOLOGIES IN SCIENTIFIC RESEARCH**

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course title

**Recommended by the Didactic Council for the Education Field of:**

**33.04.01 INDUSTRIAL PHARMACY**

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field of studies / speciality code and title

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

**BIOPHARMACEUTICAL TECHNOLOGIES AND PHARMACEUTICAL  
PRODUCTION MANAGEMENT**

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higher education programme profile/specialisation title

## 1. COURSE GOAL(s)

The course "Computer Technologies in Scientific Research" is part of the Master's programme "Biopharmaceutical Technologies and Pharmaceutical Production Management" in the field of study 33.04.01 "Industrial Pharmacy" and is taught in Semester 2 of Year 1. The course is delivered by the Department of Agrobiotechnology. The course consists of 7 modules and 26 topics and is aimed at studying the fundamental principles and practical aspects of using computer technologies in pharmaceutical and biopharmaceutical scientific research.

The goal of the course is to develop students' professional competencies in using modern computer technologies for effective collection, processing, analysis, visualisation, and presentation of scientific data in the areas of drug development, quality control, and pharmaceutical production management, as well as to improve the quality and productivity 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)
PC-5	Ability to apply statistical quality management methods, statistical methods used in evaluating the results of testing technological processes and validation	PC-5.1. Knows statistical data processing methods, statistical quality management methods, and economic analysis methods;
		PC-5.2. Uses modern methods for searching and analysing information on biological data and medicinal chemistry.

## 3. COURSE IN HIGHER EDUCATION PROGRAMME STRUCTURE

The course "Computer Technologies in Scientific Research" is part of the variable component of Block 1 "Disciplines (Modules)" of the higher education programme curriculum.

Within the higher education programme, students also master other disciplines and/or internships that contribute to the achievement of the expected learning outcomes of this course.

*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-5	Ability to apply statistical quality management methods, statistical methods used in evaluating the results of testing technological processes and validation	Bioanalytical Research in Drug Development, Registration and Quality Control; Intellectual Property Protection	—

\* 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
<i>Contact academic hours</i>		36	–	36	–	–
including:						
Lectures (LC)		18	–	18	–	–
Lab work (LW)		0	–	0	–	–
Seminars (workshops/tutorials) (S)		18	–	18	–	–
<i>Self-studies</i>		54	–	54	–	–
<i>Evaluation and assessment (exam/passing/failing grade)</i>		18	–	18	–	–
<b>Course workload</b>	academic hours	<b>108</b>	–	–	–	–
	credits	<b>3</b>	–	–	–	–

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

Type of academic activities		Total academic hours	Semesters/training modules			
			1	2	3	4
<i>Contact academic hours</i>		8	–	8		
Lectures (LC)		4	–	4		
Lab work (LW)		0	–	0		
Seminars (workshops/tutorials) (S)		4	–	4		
<i>Self-studies</i>		97	–	97		
<i>Evaluation and assessment (exam/passing/failing grade)</i>		18	–	18		
<b>Course workload</b>	academic hours	<b>108</b>	–	108		
	credits	<b>3</b>	–	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
<p align="center"><b>Module 1: Fundamentals of Computer Technologies in Scientific Research</b></p>	<p><b>Topic 1.1. The Role of Computer Technologies in Modern Scientific Research</b> 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.</p>	LC, S
	<p><b>Topic 1.2. Types of digital data in research on biochemical technologies, nanotechnologies, and pharmaceuticals</b> Structured, unstructured and semi-structured data. Primary and secondary data in biochemistry, nanotechnology and pharmaceuticals. Genomic, proteomic and metabolomic data. Data quality requirements and verification methods.</p>	LC, S
	<p><b>Topic 1.3. File Formats and Principles of Scientific Data Organisation</b> Main formats for storing pharmaceutical data: CSV, XML, JSON, SDF, MOL, CIF. ALCOA+ principles for data documentation (Attributable, Legible, Contemporaneous, Original, Accurate). Metadata and its role in the regulatory dossier. FAIR and CDISC standards for clinical data exchange.</p>	LC, S
	<p><b>Topic 1.4. Overview of Software Packages for Scientific Research</b> General-purpose scientific software: Microsoft Office, LaTeX, R, Python. Specialised packages for pharmaceuticals: Empower (Waters), Chromeleon, Analyst (Sciex), PharmaSoft. Drug formulation software: DissoCubes, GastroPlus, PK-Sim. Quality control and statistics: Minitab, JMP, SPC tools. Validation criteria for computerised systems per GAMP 5.</p>	LC, S
<p align="center"><b>Module 2: Software for Scientific Information Management</b></p>	<p><b>Topic 2.1. Reference management systems</b> Purpose and functions of reference managers in research. Overview of popular systems: Zotero, Mendeley, EndNote. Importing references from PubMed, Scopus, Web of Science. Creating bibliographic lists in APA, Vancouver, GOST 7.0.5 styles. Searching and tracking clinical guidelines and regulatory documents (ICH, EMA, FDA, GRSL).</p>	LC, S
	<p><b>Topic 2.2. Software for Experimental Data Organisation</b> 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.</p>	LC, S

	<p><b>Topic 2.3. Electronic Laboratory Notebooks and Laboratory Information Management Systems</b>  Concept of electronic laboratory notebook (ELN) and advantages over paper records in GLP/GMP context. Overview of ELN systems: LabArchives, Benchling, IDBS E-WorkBook. Laboratory information management systems (LIMS): structure, functions, integration with analytical equipment. Validation of computerised systems per GAMP 5. 21 CFR Part 11 requirements for electronic signatures and records.</p>	LC, S
<p><b>Module 3: Analysis and Processing of Scientific Data</b></p>	<p><b>Topic 3.1. Fundamentals of Statistical Data Analysis in Scientific Research</b>  Descriptive statistics: mean, median, variance, RSD. Normality tests: Shapiro–Wilk, Kolmogorov–Smirnov. Parametric and non-parametric comparison methods (t-test, ANOVA, Mann–Whitney). Correlation and regression analysis. ICH Q2(R1) statistical requirements for analytical method validation: accuracy, precision, linearity, detection/quantitation limits.</p>	LC, S
	<p><b>Topic 3.2. Software packages for statistical processing of pharmaceutical data</b>  Minitab: statistical process control (SPC), Shewhart charts, Gage R&amp;R reproducibility analysis. JMP for design of experiments (DoE) and development data analysis. R environment: stats, ggplot2, dplyr, mixOmics packages. Python environment: Pandas, SciPy, Statsmodels libraries. SPSS for clinical and biopharmaceutical research.</p>	LC, S
	<p><b>Topic 3.3. Design of experiments (DoE) and technological process optimisation</b>  Principles of experimental design: full and fractional factorial design, central composite design (CCD), Box–Behnken design. DoE application in drug formulation development: optimisation of composition and process parameters. Response surface methodology (RSM) and Design Space per ICH Q8(R2). Software tools: JMP, Design-Expert, Minitab</p>	LC, S
	<p><b>Topic 3.4. Big Data Analysis Methods</b>  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.</p>	LC, S
<p><b>Module 4: Scientific Data Visualisation</b></p>	<p><b>Topic 4.1. Principles of Effective Scientific Data Visualisation</b>  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.</p>	LC, S

	<p><b>Topic 4.2. Types of Charts and Diagrams for Presenting Scientific Results</b>  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.</p>	LC, S
	<p><b>Topic 4.3. Software Tools for Scientific Graphics</b>  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.</p>	LC, S
	<p><b>Topic 4.4. Creating comprehensive visualisations for scientific publications</b>  Developing multi-panel figures with annotations. Compiling graphical abstracts. Coordinating colour schemes and styles within a single article. Tools for creating diagrams and schemes: BioRender, ChemDraw, Draw.io. Preparing illustrations for presentations and posters..</p>	LC, S
<p><b>Module 5: Specialised Databases and Information Resources</b></p>	<p><b>Topic 5.1. Overview of specialised databases in industrial pharmacy and biopharmaceutics</b>  Pharmaceutical databases: DrugBank, PharmGKB, ChEMBL, PubChem. Drug formulation and technology databases: Drugs@FDA, EMA Product Database, GRLS. Pharmacokinetics and metabolism databases: ADME-Tox. Protein and biopharmaceutical target databases: UniProt, PDB. Pharmacopoeia databases: State Pharmacopoeia of the Russian Federation (online), EP, USP-NF.</p>	LC, S
	<p><b>Topic 5.2. Strategies for Effective Scientific Information Retrieval</b>  PubMed search using MeSH terms and Boolean operators. Scopus and Web of Science: filtering by document type, journal, citation. Navigating regulatory databases: ICH Guidelines, EMA Scientific Guidelines, FDA Guidance Documents, Ministry of Health of the Russian Federation. Regulatory framework monitoring: GMP, GLP, GCP — current editions and changes. Alert systems and RSS subscriptions for tracking new publications and regulatory updates..</p>	LC, S

	<p><b>Topic 5.3. Online resources for industrial pharmacy research</b>  Open repositories: PubMed Central, Zenodo, Figshare. Drug formulation resources: Pharma Excipients Database, Inactive Ingredient Database (FDA). Online calculators and predictive models: pkCSM, SwissADME (ADME/Tox prediction). Reproducible research platforms: OSF, GitHub. Standardisation resources: ISPE, PDA, ASTM in open access</p>	LC, S
<p><b>Module 6: Computer Technologies for Presenting Research Results</b></p>	<p><b>Topic 6.1. Technologies for Preparing Scientific Publications</b>  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.</p>	LC, S
	<p><b>Topic 6.2. Creating Effective Scientific Presentations</b>  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&amp;A handling.</p>	LC, S
	<p><b>Topic 6.3. Preparing regulatory and scientific-technical documentation</b>  Structure of regulatory dossier CTD (Common Technical Document): modules M1–M5. Preparing documents for section M2 (Summaries): QOS, NCS, CES using computer tools. Formatting technological regulations, SOPs, and validation protocols. GOST requirements for scientific and technical reports. Patent documentation in pharmaceuticals: claims, description, examples. Electronic document submission: eCTD, EAEU formats.</p>	LC, S
	<p><b>Topic 6.4. Collaborative Work Technologies and Scientific Data Sharing</b>  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.</p>	LC, S

<b>Module 7: Artificial Intelligence Applications in Scientific Research</b>	<p><b>Topic 7.1. Fundamentals of Artificial Intelligence and Machine Learning in Science</b>  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 pharmaceuticals.</p>	LC, S
	<p><b>Topic 7.2. Generative Language Models as a Tool for Scientific Work</b>  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).</p>	LC, S
	<p><b>Topic 7.3. AI for Data Analysis and Predictive Modelling</b>  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.</p>	LC, S
	<p><b>Topic 7.4. Practical Workshop: AI Tools in Scientific Research</b>  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.</p>	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](http://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.elsevier.com/locate/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**

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position, department

name and surname

### **HEAD OF EDUCATIONAL DEPARTMENT:**

**Director**

**Romashchenko Victoria**

**Alexandrovna**

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name of department

name and surname

### **HEAD OF HIGHER EDUCATION PROGRAMME:**

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position, department

name and surname