APPROVED
Vice Rector for Academic Affairs

A.A. Voronov

Work program of the course (training module)

course:	English Language. Drug discovery/Английский язык в фармаисследованиях
major:	Applied Mathematics and Physics
specialization:	General and Applied Physics/Общая и прикладная физика
	Landau Phystech-School of Physics & Research
	Foreign Languages Department
term:	1
qualification:	Master

Semesters, forms of interim assessment:

1 (fall) - Pass/fail exam

2 (spring) - Grading test

Academic hours: 120 AH in total, including:

lectures: 0 AH.

seminars: 120 AH.

laboratory practical: 0 AH.

Independent work: 60 AH.

In total: 180 AH, credits in total: 4

Number of course papers, tasks: 4

Authors of the program:

O.V. Gudkova, старший преподаватель

E.N. Vikhrova, candidate of philological sciences, associate professor

The program was discussed at the Foreign Languages Department 30.06.2023

Annotation

The program is aimed to form a holistic understanding of the main problems, types and forms of intercultural activity in the aspect of using new digital technologies at the present stage, to develop students' ability to perceive relevant information in English, analyze English-language materials in the specialty and discuss options for solving various interdisciplinary problems at the intersection AI and the real world, taking into account the social context, as well as improving communication skills in the professional field related to the use of AI; to form and develop practical skills in oral and written communication, correlating with the areas of activity of the future graduate; skills of conducting intercultural dialogue to solve communicative and social problems with representatives of other cultures in academic and professional activities. Successful mastery of the course will allow students to replenish their lexicon with vocabulary used in texts on the relevant topic, master the skills of using lexical and grammatical material included in the course program, and also develop communication skills (at level B2-C1 according to the Common European Classification).

1. Study objective

Purpose of the course

Basics of new drug development; methods used in the identification of target molecules; application of various technologies and methods in the development of new drugs; methods of modeling and optimization of new drugs; basics of drug quality control and compliance with safety and efficacy standards; developing an understanding of the main stages and processes involved in the development of new drugs; developing skills in analytical processing of a large array of information on the topic of specialization; mastering the practical skills necessary for the development of new drugs; developing the skills necessary for the development of new drugs.

Tasks of the course

Develop lexical skills to understand and use specific terminology in the field of drug development; study grammar structures for working with scientific literature and understanding the basic processes related to drug development; develop listening skills and understanding of speech by scientific specialists in the field of drug development; activate skills of active reading of scientific articles, drug development reports, and solving tasks related to drug development; familiarize oneself with specific tasks related to drug development and the requirements imposed on the drug development process; develop teamwork and project management skills in the field of drug development; apply information technologies and scientific resources for obtaining and processing data on drug development; familiarize oneself with the basic principles of drug development regulation in different countries and regions; develop the ability to solve communicative tasks in various situations of intercultural communication using language means; conduct interpersonal and professional communication in a foreign language taking into account cultural differences.

2. List of the planned results of the course (training module), correlated with the planned results of the mastering the educational program

Mastering the discipline is aimed at the formation of the following competencies:

Code and the name of the competence	Competency indicators
UC-1 Use a systematic approach to critically analyze a problem, and develop an action plan	UC-1.1 Systematically analyze the problem situation, identify its components and the relations between them
	UC-1.2 Search for solutions by using available sources
	UC-1.3 Develop a step-by-step strategy for achieving a goal, foresee the result of each step, evaluate the overall impact on the planned activity and its participants
UC-2 Able to manage the project through all stages of implementation	UC-2.1 Set an objective within a defined scientific problem; formulate the agenda, relevance, significance (scientific, practical, methodological, or other depending on the project type), forecast the expected results and possible areas of their application
	UC-2.2 Forecast the project outcomes, plan necessary steps to achieve the outcomes, chart the project schedule and monitoring plan
	UC-2.3 Organize and coordinate the work of project stakeholders, provide the team with necessary resources

	UC-2.4 Publicly present the project results (or results of its stages) via reports, articles, presentations at scientific conferences, seminars, and similar events
UC-3 Organize and manage a team, and develop the team strategy to achieve the objectives	UC-3.1 Organize and coordinate the work of the project stakeholders and help resolve disputes and conflicts
	UC-3.2 Consider the interests, specific behavior, and diversity of opinions of team members/colleagues/counterparties
	UC-3.3 Foresee the results (consequences) of both individual and collective actions
	UC-3.4 Plan teamwork, distribute tasks to team members, hold discussions of different ideas and opinions
UC-4 Use modern communication tools in the academic and professional fields, including those in a foreign language	UC-4.1 Exchange business information in oral and written forms in Russian and at least one foreign language
	UC-4.2 Use the acquired skills to write, translate, and edit various academic texts (abstracts, essays, reviews, articles, etc.)
	UC-4.3 Present the results of academic and professional activities at various academic events, including international conferences
	UC-4.4 Use modern ICT tools for academic and professional collaboration
UC-5.1 Analyze and consider cultural diversity in intercultural interactions	UC-5.1 Identify specific philosophical and scientific traditions in major world cultures
	UC-5.2 Define the theoretical and practical significance of cultural and linguistic factors within various interrelated philosophical and scientific traditions
UC-6 Determine priorities and ways to improve performance through self-assessment	UC-6.1 Achieve personal growth and professional development, determine priorities and ways to improve performance
	UC-6.2 Evaluate performance results in correlation with the set objectives and applied methods

3. List of the planned results of the course (training module)

As a result of studying the course the student should:

know:

-- The interconnection, influence, and interaction of language and culture.
- The role of language as an integral part of culture in a person's life, their behavior, and communication with speakers of other languages and different cultures, national identity.
- Understanding of the cultural-anthropological view of human beings, their lifestyle, ideas, views, customs, value systems, and perception of the world, both their own and that of others.
- The influence of culture through language on human behavior, their perception of the world and life in general.
- The history of the emergence, development stages, and methods of teaching intercultural communication.
- The concept of "culture," its role in the communication process, as well as its relation to such concepts as "socialization," "enculturation," "acculturation," "assimilation," "behavior," "language," "identity," and "global citizenship."
- The influence of various social transformations on the change of cultural identity.
- The peculiarities of perceiving other cultures, the reasons for prejudices and stereotypes in intercultural interaction.
- Mechanisms for forming intercultural tolerance and dialogue of cultures.
- Types, forms, models, and structural components of intercultural communication.
- Norms and styles of intercultural communication.
- Mental characteristics and national customs of representatives of different cultures, cultural standards on ethnic, political, and economic levels.
- The linguistic worldview of speakers of a foreign language and the features of their worldview.
- Ethical and moral norms of behavior in a cross-cultural environment.
- Language norms of oral communication culture, ethical and moral norms of behavior, accepted in the country of the studied language; stereotypes and ways to overcome them; etiquette norms of the countries of the studied language.
- Methods of systemic and critical analysis; methods of developing strategies for identifying and solving problem situations.
- The stages of the project life cycle; stages of project development and implementation; methods of project development and management.
- Methods of team formation; methods of effective team management; basic leadership theories and leadership styles.
- Rules and regularities of personal and business oral and written communication; modern communication technologies in Russian and foreign languages; existing professional communities for professional interaction.
- Regularities and features of socio-historical development of different cultures; peculiarities of intercultural diversity in society; rules and technologies of effective intercultural interaction.
- Methods of self-assessment, self-control, and self-development.

be able to:

-- Apply methods for studying cultural systems and intercultural situations.
- Perceive, analyze, interpret, and compare cultural facts.
- Determine the role of basic cultural concepts in intercultural communication.
- Find adequate solutions in different intercultural communication situations.
- Analyze the peculiarities of intercultural communication in a collective.
- Reflect on the orientation system of their own culture.
- Recognize and correctly interpret nonverbal signals during intercultural communication.
- Create a communicative portrait of a representative of another linguistic culture.
- Reveal the significance of concepts and actions in an intercultural situation.
- Analyze similarities and differences in communication behavior from the positions of interacting cultures.
- Adequately realize their communicative intention in communication with representatives of other lingual cultures.
- Adapt to different linguistic and non-linguistic norms of behavior when encountering another culture.
- Determine the reasons for communication failures and apply methods to overcome them.
- Take the position of a partner in intercultural communication and identify possible conflicts as being rooted in the values and norms of their culture.
- Successfully overcome barriers and conflicts in communication and achieve mutual understanding.
- Reveal the connection and influence of language and culture.
- Tolerantly relate to representatives of other cultures and languages.
- Analyze the main stages and regularities of the historical development of society to form a civil position.
- Respectfully and carefully treat historical heritage and cultural traditions.
- Use models of social situations, typical scripts of interaction of participants in intercultural communication.
- Be guided by the principles of cultural relativism and ethical norms, presupposing the rejection of ethnocentrism and respect for the uniqueness of the foreign language culture and value orientations of the foreign community.
- Overcome the influence of stereotypes and carry out intercultural dialogue in general and professional communication.
- Model possible communication situations among representatives of different cultures and societies.
- Apply methods of a systemic approach and critical analysis of problem situations; develop a strategy of actions, make specific decisions for its implementation.
- Develop a project considering analysis of alternative implementation options, determine target stages, main work directions; explain the goals and formulate tasks related to the preparation and implementation of the project; manage the project at all stages of its life cycle.
- Develop a plan of group and organizational communication for the preparation and implementation of the project; formulate tasks for team members to achieve the set goal; develop a team strategy; apply effective leadership styles to lead the team to achieve the set goal.
- Apply communicative technologies, methods, and ways of business communication for academic and professional interaction in practice.
- Determine the theoretical and practical significance of the cultural and linguistic factor during the interaction of various philosophical and scientific traditions.
- Understand and tolerantly perceive the intercultural diversity of society; analyze and consider the diversity of cultures in the process of intercultural interaction.
- Solve tasks of personal and professional development, determine and implement priorities for improving one's own activities; apply self-assessment and self-control methodologies.

master:

- - Norms of etiquette and behavior when communicating with representatives of a foreign culture.
- Principles of tolerance in resolving intercultural conflicts.
- Methods of communicative research, the ability to apply acquired knowledge in scientific research, oral and written communication.
- Communicative strategies and tactics characteristic of other cultures.
- Skills of correct intercultural communication, independent analysis of intercultural conflicts in communicating with representatives of other cultures and methods of their resolution.
- Ability to correctly interpret specific manifestations of verbal and non-verbal communicative behavior in different cultures.
- Communication skills in oral and written forms in Russian and foreign languages for solving tasks of interpersonal and intercultural interaction.
- Skills oriented towards ethical and moral norms of behavior accepted in the cross-cultural society.
- Necessary interactional and contextual knowledge that allows overcoming the influence of stereotypes and adapting to changing conditions when interacting with representatives of different cultures.
- Methodology of systemic and critical analysis of problem situations; methods of goal setting, determining ways to achieve it, and developing action strategies.
- Methods of project development and management; methods for evaluating the need for resources and project effectiveness.
- Ability to analyze, design, and organize interpersonal, group, and organizational communications within a team to achieve the set goal; methods of organization and team management.
- Methodology of interpersonal business communication in Russian and foreign languages, using professional language forms, means, and modern communication technologies.
- Methods and skills of effective intercultural interaction.
- Technologies and skills for managing one's cognitive activities and their improvement based on self-assessment, self-control, and lifelong learning principles.

4. Content of the course (training module), structured by topics (sections), indicating the number of allocated academic hours and types of training sessions

4.1. The sections of the course (training module) and the complexity of the types of training sessions

№	Topic (section) of the course	Types of training sessions, including independent work			
		Lectures	Seminars	Laboratory practical	Independent work
1	Topic 1. Deep Learning in Drug Discovery		20		10
2	Topic 2. Design and Synthesis		20		10
3	Topic 3. Design and Optimization		20		10
4	Topic 4. Biological Investigation		20		10
5	Topic 5. Bio-AI revolution		20		10
6	Topic 6. Trends in Drug Discovery		20		10
AH in total			120		60
Exam preparation	0 AH.				
Total complexity	180 AH., credits in total 4				

4.2. Content of the course (training module), structured by topics (sections)

Semester: 1 (Fall)

1. Topic 1. Deep Learning in Drug Discovery

Integration of deep learning methods into the process of drug discovery. Deep learning algorithms for processing large arrays of genetic and molecular data. Virtual screening. Predictive modeling. Efficiency and safety in drug development. Personalized medicine. Analyzing large sets of genomic and clinical data to identify patterns and relationships. Alternative in silico methods. Identification of novel specific inhibitors. New chemical class drugs for cancer therapy.

Communicative tasks: communicate orally and in writing: explain and discuss Drug Discovery in the context of scientific disciplines such as biology, chemistry, and pharmacology; hypothesize and form judgments based on a large body of scientific literature; discuss relationships and patterns; translate scientific texts with respect to cultural context and genre and style; transform scientific texts in oral and written communication; participate in a simulation of a scientific conference.

2. Topic 2. Design and Synthesis

Design and synthesis of promising innovative compounds as key components of Drug Discovery. Chemical structure of drug candidate. Study of factors such as solubility, stability and bioavailability. In vitro and in vivo experiments and human clinical trials. High-throughput screening. Computer modeling. Optimization of the synthesis process taking into account factors such as yield, purity and reproducibility. Drugs for the treatment of inflammation and inflammatory diseases. Combinations of creative thinking, scientific knowledge and technical expertise. Communicative tasks: communicate orally and in writing: explain the concept of resistance and its mechanisms; discuss technological advances and automation; discuss the development and synthesis of new drugs; analyze methods of testing a large number of compounds for their potential therapeutic effects; translate scientific texts in oral and written communication; predict the properties of new drug candidates before they are synthesized; translate scientific texts with respect to cultural context and genre and style; analyze and synthesize scientific literature.

3. Topic 3. Design and Optimization

Design and optimization in drug development: maximizing efficacy and minimizing side effects. Molecular targeting. Computational modeling and genomic analysis. Chemical structure. Pharmacokinetics. Toxicity. Optimization of toxicity by structural modifications. Clinical trials. Determination of efficacy, safety and optimal dosing regimen of the drug. Communicative tasks: communicate orally and in writing: describe the molecular target, chemical structure, pharmacokinetics, toxicity and clinical efficacy of drug candidates; discuss any potential safety issues; describe the development cycles of vaccines and antiviral agents; translate scientific texts taking into account cultural context and genre and style; transform scientific texts in oral and written communication.

Semester: 2 (Spring)

4. Topic 4. Biological Investigation

Biological mechanisms that contribute to the development of a particular disease or condition. Key proteins or enzymes involved in the disease process. High-throughput screening. Rational drug design. Preclinical trials. Clinical trials. Virtual screening. Coping with SARS-CoV-2 and the health problems that accompany COVID-19. Communicative tasks: communicate orally and in writing: describe sequential biological studies; describe types of screening; transform scientific texts in oral and written communication; translate scientific texts taking into account cultural context and genre and style.

5. Topic 5. Bio-AI revolution

Artificial Intelligence (AI) and Machine Learning (ML) technologies and their application in the field of biology to solve complex problems. Recent advances in biotechnology and how they are contributing to the development of AI systems that can be used in drug discovery, gene editing, and other areas of biology. The impact of these technologies on advancing research and discovery in medicine and health care, including precision medicine, personalized therapies, disease diagnosis and prevention. The ethical and social implications of the Bio-AI revolution, including issues related to privacy, data ownership, and the potential for misuse or unintended consequences. How to evaluate and interpret biological data, such as genomic and proteomic data, using AI and ML to make predictions and model biological systems. Communicative tasks: communicate orally and in writing: effectively communicate ideas, opinions, and conclusions using scientific language and terminology; conduct extensive research and extract information from scientific literature, scientific databases, and other sources to support their work; collaborative learning and interdisciplinary problem solving skills.

6. Topic 6. Trends in Drug Discovery

Recent advances in drug discovery, including high-throughput screening, computational drug design, and network pharmacology. Novel drug targets, including those based on genomics, epigenomics and proteomics, as well as recent advances in personalized medicine and precision medicine. Advanced drug delivery systems, including liposomal formulations, nanoparticle-based systems and drug-eluting implants. Advanced drug design and optimization techniques including combinatorial chemistry, fragment-based drug design and biomimetic drug design. Regulatory framework for pharmaceutical development, including intellectual property rights, FDA approval and clinical trials. Novel pharmaceutical and biotechnology research, including vaccines, biologics, and biosimilars. Communication Objectives: communicate orally and in writing: analyze and evaluate recent trends and advances in drug discovery and their impact on health care, society, and the environment; acquire the technical skills necessary to work with scientific and technical data, including data mining, statistical analysis, and data visualization; effectively communicate research results and solve critical problems using innovative technologies and methodologies.

5. Description of the material and technical facilities that are necessary for the implementation of the educational process of the course (training module)

A classroom for conducting training sessions provided for by the course (training module) program, equipped with training facilities and technical means of training: an interactive smartboard (screen), a multimedia projector, sound reproducing equipment, a computer for the teacher with the possibility to connect to the Internet and provide access to the MIPT electronic information and educational environment.

6. List of the main and additional literature, that is necessary for the course (training module) mastering

Main literature
1. Navigate A2 Elementary [Text], Coursebook with video and Oxford online skills /J. Hughes, K. Wood ; add. material by Paul, immett ; series adviser C. Walter. -United Kingdom, Oxford Unversity Press, 2015
2. Language Leader : PRE-Intermediate [Text] : Coursebook and CD-ROM / I. Lebeau, G. Rees ; Language Reference and Extra Practice by Diane Hall .— Harlow : Pearson Longman, 2008 .— 112 p. - ISBN 978-0-582-84778-1.
3. Language Leader : Elementary [Text] : Coursebook and CD-ROM / I. Lebeau, G. Rees ; Language Reference and Extra Practice by Diane Hall .— Harlow : Pearson Longman, 2008 .— 160 p. - ISBN 978-0-582-84768-2.

Additional literature
1. Иностранный язык в сфере профессиональной коммуникации : комплексные учебные задания, учебное пособие / И. В. Беляева, Е. Ю. Нестеренко, Т. И. Сорогина. — Москва, Флинта, 2017.— URL: https://e.lanbook.com/book/92749 (дата обращения: 04.02.2021). - Полный текст (Режим доступа : из сети МФТИ / Удаленный доступ)
2. Английский язык для медиков / под редакцией Н. П. Глинской. – Москва: Юрайт, 2022.

3. Cambridge English for Scientists [Text] /T. Armer ; Series Editor: J. Day. Edinburgh, Cambridge University Press, 2011

Рекомендуемые литературные источники для самостоятельного изучения

1. Cotton D., Falvey D., Kent S. (2012) Market Leader Elementary. Coursebook, 3 ed., Pearson Education.

2. Cotton D., Falvey D., Kent S. (2012) Market Leader Pre-intermediate. Coursebook, 3 ed., Pearson Education.

3. Глоссарий русскоязычных терминов в медицинской химии. О. Н. Зефирова, К. В. Балакин, М. Ю. Красавин, В. А. Палюлин, В. В. Поройков, Е. В. Радченко, Н. Ф. Салахутдинов, А. А. Спасов, В. П. Фисенко, С. О. Бачурин. Известия Академии наук. Серия химическая, 2019, № 12. С. 2381-2395.

4. Practice of Medicinal Chemistry, Ed. C. Wermuth, Academic Press, London, UK, 2003. https://www.google.ru/books/edition/The_Practice_of_Medicinal_Chemistry/dUNfJmllmqwC?hl=ru&gbpv=1

7. List of web resources that are necessary for the course (training module) mastering

1. http://uefap.com/reading/readfram.htm - дополнительные тексты для чтения
2. http://uefap.com/writing/writfram.htm - задания по развитию навыков письменной речи
3. https://owl.purdue.edu/owl_exercises/esl_exercises/paraphrase_and_summary_exercises/intermediate_paraphrase_exercises.html - упражнения по письменному реферированию на более высоком уровне
4. http://ted.com – сайт с видео-отрывками, которые магистранты смотрят в качестве домашнего задания
5. Grammarly – бесплатный онлайн-сервис на основе искусственного интеллекта для помощи в написании текстов на английском языке (https://www.grammarly.com/)
6. Reverso - веб-сайт, специализирующийся на автоматизированном переводе и помощи в изучении языка. Сайт предлагает онлайн-словари, перевод в контексте, проверку орфографии, поиск синонимов и средства грамматического спряжения (https://context.reverso.net)
7. Linguee — онлайн-словарь и система контекстуального поиска переводов, позволяющая найти, как слова и фразы переводились людьми в существующих билингвистических текстах (https://www.linguee.ru/)
8. Ludwig.guru - лингвистическая поисковая система, которая проверяет грамматику, синтаксис, стилистику и последовательность предложений на английском языке (https://ludwig.guru/)
9. Quizlet - сервис для быстрого создания тестов, которые помогут запомнить любой материал разными способами (на слух, написание и т.д.) (https://quizlet.com/ru)
10. Glossary maker – сервис для создания списка лексических единиц по уровню сложности, включая определения, синонимы, антонимы, производные слова и др. https://www.wordsmyth.net/

8. List of information technologies used for implementation of the educational process, including a list of software and information reference systems (if necessary)

Practical classes are held with the use of multimedia technologies: multimedia presentations, work on an interactive smartboard, Internet information resources.

Independent work of students is conducted using a virtual learning environment system based on LMS MIPT which helps students get access to various sources of multimedia information, makes it possible to organize communication of all participants in the educational process, provides for interactive control and self-control of tasks, and testing.

To form language skills, the platform of the virtual learning environment LMS contains a set of interactive exercises created on the basis of the test module built into the LMS MIPT.

9. Guidelines for students to master the course

Students who are mastering the discipline/module "English Language. Drug Discovery" should acquire intercultural communicative competence, including: linguistic competence (the ability to correctly construct grammatical forms and syntactic structures in accordance with the norms of the studied language), sociolinguistic competence (the ability to use and transform language forms in accordance with the situation of foreign language communication), sociocultural competence (the ability to consider verbal and non-verbal behavior accepted in the country of the studied language), social competence (the ability to interact with communication partners, mastery of appropriate strategies), discursive competence (the ability to understand and achieve coherence in individual statements in significant communicative models), strategic competence (the ability to use the most effective strategies when solving communicative tasks), subject competence (knowledge of subject-related information when organizing one's own speech or understanding the speech of others), pragmatic competence (the ability to communicate and implement any speech while taking into account the conditions under which the speech act is carried out (listening, writing), the status of the addressee, the subject of discussion, and so on) to develop personal and professional qualities, a sense of the social significance of their professional activities, respectful adherence to the principles of ethics, morality, and tolerance.

Assessment funds for course (training module)

major:	Applied Mathematics and Physics
specialization:	General and Applied Physics/Общая и прикладная физика
	Landau Phystech-School of Physics & Research
	Foreign Languages Department
term:	1
qualification:	Master

Semesters, forms of interim assessment:

1 (fall) - Pass/fail exam

2 (spring) - Grading test

Authors:

O.V. Gudkova, старший преподаватель

E.N. Vikhrova, candidate of philological sciences, associate professor

1. Competencies formed during the process of studying the course

Code and the name of the competence	Competency indicators
UC-1 Use a systematic approach to critically analyze a problem,and develop an action plan	UC-1.1 Systematically analyze the problem situation, identify its components and the relations between them
	UC-1.2 Search for solutions by using available sources
	UC-1.3 Develop a step-by-step strategy for achieving a goal, foresee the result of each step, evaluate the overall impact on the planned activity and its participants
UC-2 Able to manage the project through all stages of implementation	UC-2.1 Set an objective within a defined scientific problem; formulate the agenda, relevance, significance (scientific, practical, methodological, or other depending on the project type), forecast the expected results and possible areas of their application
	UC-2.2 Forecast the project outcomes, plan necessary steps to achieve the outcomes, chart the project schedule and monitoring plan
	UC-2.3 Organize and coordinate the work of project stakeholders, provide the team with necessary resources
	UC-2.4 Publicly present the project results (or results of its stages) via reports, articles, presentations at scientific conferences, seminars, and similar events
UC-3 Organize and manage a team, and develop the team strategy to achieve the objectives	UC-3.1 Organize and coordinate the work of the project stakeholders and help resolve disputes and conflicts
	UC-3.2 Consider the interests, specific behavior, and diversity of opinions of team members/colleagues/counterparties
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	UC-4.3 Present the results of academic and professional activities at various academic events, including international conferences
	UC-4.4 Use modern ICT tools for academic and professional collaboration
UC-5.1 Analyze and consider cultural diversity in intercultural interactions	UC-5.1 Identify specific philosophical and scientific traditions in major world cultures
	UC-5.2 Define the theoretical and practical significance of cultural and linguistic factors within various interrelated philosophical and scientific traditions
UC-6 Determine priorities and ways to improve performance through self-assessment	UC-6.1 Achieve personal growth and professional development, determine priorities and ways to improve performance
	UC-6.2 Evaluate performance results in correlation with the set objectives and applied methods

2. Competency assessment indicators

As a result of studying the course the student should:

know:

-- The interconnection, influence, and interaction of language and culture.
- The role of language as an integral part of culture in a person's life, their behavior, and communication with speakers of other languages and different cultures, national identity.
- Understanding of the cultural-anthropological view of human beings, their lifestyle, ideas, views, customs, value systems, and perception of the world, both their own and that of others.
- The influence of culture through language on human behavior, their perception of the world and life in general.
- The history of the emergence, development stages, and methods of teaching intercultural communication.
- The concept of "culture," its role in the communication process, as well as its relation to such concepts as "socialization," "enculturation," "acculturation," "assimilation," "behavior," "language," "identity," and "global citizenship."
- The influence of various social transformations on the change of cultural identity.
- The peculiarities of perceiving other cultures, the reasons for prejudices and stereotypes in intercultural interaction.
- Mechanisms for forming intercultural tolerance and dialogue of cultures.
- Types, forms, models, and structural components of intercultural communication.
- Norms and styles of intercultural communication.
- Mental characteristics and national customs of representatives of different cultures, cultural standards on ethnic, political, and economic levels.
- The linguistic worldview of speakers of a foreign language and the features of their worldview.
- Ethical and moral norms of behavior in a cross-cultural environment.
- Language norms of oral communication culture, ethical and moral norms of behavior, accepted in the country of the studied language; stereotypes and ways to overcome them; etiquette norms of the countries of the studied language.
- Methods of systemic and critical analysis; methods of developing strategies for identifying and solving problem situations.
- The stages of the project life cycle; stages of project development and implementation; methods of project development and management.
- Methods of team formation; methods of effective team management; basic leadership theories and leadership styles.
- Rules and regularities of personal and business oral and written communication; modern communication technologies in Russian and foreign languages; existing professional communities for professional interaction.
- Regularities and features of socio-historical development of different cultures; peculiarities of intercultural diversity in society; rules and technologies of effective intercultural interaction.
- Methods of self-assessment, self-control, and self-development.

be able to:

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- Perceive, analyze, interpret, and compare cultural facts.
- Determine the role of basic cultural concepts in intercultural communication.
- Find adequate solutions in different intercultural communication situations.
- Analyze the peculiarities of intercultural communication in a collective.
- Reflect on the orientation system of their own culture.
- Recognize and correctly interpret nonverbal signals during intercultural communication.
- Create a communicative portrait of a representative of another linguistic culture.
- Reveal the significance of concepts and actions in an intercultural situation.
- Analyze similarities and differences in communication behavior from the positions of interacting cultures.
- Adequately realize their communicative intention in communication with representatives of other lingual cultures.
- Adapt to different linguistic and non-linguistic norms of behavior when encountering another culture.
- Determine the reasons for communication failures and apply methods to overcome them.
- Take the position of a partner in intercultural communication and identify possible conflicts as being rooted in the values and norms of their culture.
- Successfully overcome barriers and conflicts in communication and achieve mutual understanding.
- Reveal the connection and influence of language and culture.
- Tolerantly relate to representatives of other cultures and languages.
- Analyze the main stages and regularities of the historical development of society to form a civil position.
- Respectfully and carefully treat historical heritage and cultural traditions.
- Use models of social situations, typical scripts of interaction of participants in intercultural communication.
- Be guided by the principles of cultural relativism and ethical norms, presupposing the rejection of ethnocentrism and respect for the uniqueness of the foreign language culture and value orientations of the foreign community.
- Overcome the influence of stereotypes and carry out intercultural dialogue in general and professional communication.
- Model possible communication situations among representatives of different cultures and societies.
- Apply methods of a systemic approach and critical analysis of problem situations; develop a strategy of actions, make specific decisions for its implementation.
- Develop a project considering analysis of alternative implementation options, determine target stages, main work directions; explain the goals and formulate tasks related to the preparation and implementation of the project; manage the project at all stages of its life cycle.
- Develop a plan of group and organizational communication for the preparation and implementation of the project; formulate tasks for team members to achieve the set goal; develop a team strategy; apply effective leadership styles to lead the team to achieve the set goal.
- Apply communicative technologies, methods, and ways of business communication for academic and professional interaction in practice.
- Determine the theoretical and practical significance of the cultural and linguistic factor during the interaction of various philosophical and scientific traditions.
- Understand and tolerantly perceive the intercultural diversity of society; analyze and consider the diversity of cultures in the process of intercultural interaction.
- Solve tasks of personal and professional development, determine and implement priorities for improving one's own activities; apply self-assessment and self-control methodologies.

master:

- - Norms of etiquette and behavior when communicating with representatives of a foreign culture.
- Principles of tolerance in resolving intercultural conflicts.
- Methods of communicative research, the ability to apply acquired knowledge in scientific research, oral and written communication.
- Communicative strategies and tactics characteristic of other cultures.
- Skills of correct intercultural communication, independent analysis of intercultural conflicts in communicating with representatives of other cultures and methods of their resolution.
- Ability to correctly interpret specific manifestations of verbal and non-verbal communicative behavior in different cultures.
- Communication skills in oral and written forms in Russian and foreign languages for solving tasks of interpersonal and intercultural interaction.
- Skills oriented towards ethical and moral norms of behavior accepted in the cross-cultural society.
- Necessary interactional and contextual knowledge that allows overcoming the influence of stereotypes and adapting to changing conditions when interacting with representatives of different cultures.
- Methodology of systemic and critical analysis of problem situations; methods of goal setting, determining ways to achieve it, and developing action strategies.
- Methods of project development and management; methods for evaluating the need for resources and project effectiveness.
- Ability to analyze, design, and organize interpersonal, group, and organizational communications within a team to achieve the set goal; methods of organization and team management.
- Methodology of interpersonal business communication in Russian and foreign languages, using professional language forms, means, and modern communication technologies.
- Methods and skills of effective intercultural interaction.
- Technologies and skills for managing one's cognitive activities and their improvement based on self-assessment, self-control, and lifelong learning principles.

3. List of typical control tasks used to evaluate knowledge and skills

Представлено в прикреплённом файле.

4. Evaluation criteria

Presented in the attached file

Assessment of knowledge, skills, abilities characterising the stages of competence formation in the discipline "English Language. Modern State of Artificial Intelligence", that is carried out in the form of current and intermediate control, carried out with the help of MIPT point-rating system (BRS).

Assessment of successful mastering of the material in the discipline is expressed in a 100-point scale and consists of the quality assessment of current work in the semester (80 points) and the rating assessment for the final credit work at the end of the semester (20 points).

5. Methodological materials defining the procedures for the assessment of knowledge, skills, abilities and/or experience

The grade for the current work in the semester is given as a weighted average score based on the results of three point-rating attestations during the semester.

Current progress control is conducted during the semester to monitor the assimilation of students' knowledge, skills and level of proficiency in a foreign language to solve communicative problems in socio-cultural, academic and professional-business spheres of activity, timely identification of difficulties in mastering the discipline (module) and their elimination, as well as the provision of timely advisory individual assistance to students.

The control of current academic achievement includes testing of knowledge, skills and competences:
in classes (surveys, interactive discussions, reports, presentations, role-playing games, control tasks for different types of speech activities and tests to check lexico-grammatical skills);
according to the results of individual independent work (preparation of oral reports, performance of online practice tests and tasks for control and self-control of listening, reading, writing and lexico-grammatical skills in LMS MIPT.

in the course of individual consultations with students who have academic arrears.

Intermediate certification (credit/differential credit) is held in oral and written form at the end of each semester to determine the compliance of the level of competence in the discipline (module) to the requirements of the educational standard of MIPT in the direction of training in the scope of the work programme. Assessment for credit/differential credit is 20% of the total grade for the semester.

Written work at intermediate certification is conducted in the form of a test. Assessment is made by adding the points received by students for all tasks, and calculating the ratio of points to the maximum possible number of points for written work.

The oral part of the credit/differential credit/exam is taken by a teacher who does not teach in the given group. The grade is awarded on the basis of the criteria for evaluating a monologic/dialogic statement. In the final grade for the oral and written part of the test, equal weight is given to the skills in all types of speech activity: listening, reading, speaking and writing.

Intermediate certification on completion of the discipline (module) is held in the 9th semester in the form of credit and in the 10th semester in the form of differentiated credit, each of them consists of 2 parts: oral form (reading/speaking/audition/translation) and written form: written work, testing to determine the level of language competence (English), to solve communicative problems in socio-cultural, academic and professional-business spheres of activity, as well as for the development of professional and personal qualities of the student.

The final rating for the semester by mastering a discipline (module) or course of study (elective course) is a maximum of 100 points and is formed as a sum of points consisting of the following components:

Current rating (points based on the results of the current control of academic performance in the semester) - a maximum of 80 points, including:

     5 % - class attendance (0 - 4 points);

     15 % - academic activity at classes (0 - 12 points);

     60 % - current control milestones (control points) (0 - 48 points);

     20 % - fulfilment of written work for the semester (0 - 16 points), including:

     10 % current practical assignment (0 -8 points);

     10 % final practical assignment (0 - 8 points).

Intermediate certification (credit, differentiated credit, examination) - 20 points, including:

     50 % - for the oral part (0 - 10 points);

     50% - for the written part (0 - 10 points).

The rating points, which constitute the current rating, are recorded by a pedagogical staff member of the JJD in the electronic journal. During the academic term for each discipline (module) the student must have accumulated a current rating of at least 48 rating points (60% of the maximum value of the current rating).

4. List of typical questions, tasks, topics used for end-of-term assessment

End-of-term assessment in the course (training module) "English Language. Drug Discovery" is held at the end of each semester.

Semester (Fall) – pass/fail exam:
Written part: a test on the material studied.
Oral part: project.

Examples of typical tasks to the written and oral parts of the pass/fail exam.

Written part – a test

Ex.1 Complete the following table with the synonyms from the box below:

decrease, keep, assist, begin, preserve consume, release, appear, enquire, end, climb, show, reside, cease

Verbs

Formal	Informal
(1)	seem
ascend	(2)
(3)	help
(4)	stop
commence	(5)
(6)	use
(7)	shorten
demonstrate	(8)
(9)	ask
(10)	keep
(11)	free
(12)	live
retain	(13)

Adjectives

responsible, incorrect, energetic, lucky, whole, sufficient, amiable, vacant, inexpensive, enough, worse

Formal	Informal
(14)	friendly
complete	(15)
(16)	lively
fortunate	(17)
(18)	wrong
inferior	(19)
(20)	cheap
(21)	empty
	(22) enough

Describe the company you work for or know well. Use the Worksheet below.

Company Name - The official name of your company registered in the state where you do business.

Company Structure - Examples include sole proprietorship, LLC, partnership, or corporation.

Management and ownership -Names of the main people behind the ownership and management of the company.

Company location - Where is the company's headquarters located?

Company History - When was your company founded, what prompted you to start it, and what needs does your company fulfill?

Mission Statement - A mission statement is a concise statement expressing the purpose of your company. Keep your mission statement to one or two sentences.

Products/Services and Target Market - A brief statement of what you intend to sell and to whom.

Goals - A brief statement of what you want to accomplish in the near future, based on the information contained in the rest of the business plan as well as your long-term growth goals.

Vision - A vision statement is a statement of how you see the future of the company.

Company Description Worksheet

Business Name	
Company Mission Statement	
Company Philosophy/ Values	
Company Vision	
Goals & Milestones	
Target Market	
Industry/ Competitors	
Legal Structure/ Ownership	

Oral part – project

Project structure

Stage	Aims	Students Activity
Initiation	clarification of the goal, proposition, and the starting point	do market research; formulate the concept; evaluate the prospects
Planning	Proposition analysis; data collection; goal setting; assessment criteria; team formation (if necessary); detailed staffing; procurement; project controls plans	set the aim and objective; gather the relevant data; specify the successful result
Research	data research; brainstorming; working strategy; action plan approval	synthetise and analise all the data gathered; start the project
Performance	project fulfilment	accomplish the work of the project
Feedback	project analysis; success and failure evaluation	give and get a detailed feedback on the project; correct the items of the project (if necessary)
Defence	project presentation	explain the choice; talk through the results; prove its feasibility and actuality

Criteria for evaluating end-of-term assessment tasks

Assessment criteria

Stages	Assessment criterion	Self-reflection	Instructor	Colleagues
Defence	Presentation (20 points)			
	QA session (10 points)			
Project	Creativity (5 points)			
	Novelty (5 points)			
	Impact (5 points)			
	Relevance (5 points)			

Project presentation assessment criteria

Criterion	Criterion details	1 point	2 points
Content	The accuracy, relevance, and depth of the information presented		
Organization	The logical flow and structure of the presentation, including clear introduction, main points, and conclusion		
Delivery	The effectiveness of the presenter's communication skills, including clarity, volume, and pace of speech, as well as eye contact and body language		
Visual aids	The quality and appropriateness of any supporting visual aids such as PowerPoint slides, handouts, or props		
Engagement and audience interaction	The ability to engage and maintain the interest of the audience through active participation, questions, or other interactive methods		
Time management	The ability to effectively manage the allocated presentation time and stay within the given time limits		
Confidence and enthusiasm	The level of confidence, enthusiasm, and passion displayed by the presenter during the delivery		
Clarity of message	The ability to clearly convey the main message or objective of the presentation		
Use of supporting evidence	The appropriate use of credible sources and evidence to support arguments or claims made in the presentation		

3. List of typical questions, tasks, topics used for in-progress assessment

Topic 1. Machine learning vs Deep learning

Classroom work: checking understanding of the content of the read text, viewed or listened to video fragment about the history of the science of artificial intelligence, followed by a conversation on the content; discussion in the form of hypotheses about what is happening in what is read or seen; problematic discussion.

Independent work on the development of communication skills, working with information resources, studying the material of practical classes, reading the main and recommended literature on the topic.

Sample task for speaking

Difference between Machine Learning and Deep Learning

Machine learning and deep learning both are subsets of artificial intelligence but there are many similarities and differences between them.

Task 1 Distribute the descriptive criteria into the proper column:

1. Requires the larger volume of dataset compared to machine learning
2. A model is created by relevant features which are manually extracted from images to detect an object in the image
3. Relevant features are automatically extracted from images. It is an end-to-end learning process
4. It requires a high-performance computer with GPU
5. Apply statistical algorithms to learn the hidden patterns and relationships in the dataset
6. Better for the low-label task
7. Better for complex task like image processing, natural language processing, etc.
8. More complex, it works like the black box interpretations of the result are not easy
9. Can work on the smaller amount of dataset
10. Takes less time to train the model
11. Uses artificial neural network architecture to learn the hidden patterns and relationships in the dataset
12. Less complex and easy to interpret the result
13. Takes more time to train the model
14. It can work on the CPU or requires less computing power as compared to deep learning

Machine Learning	Deep Learning
1.	
2.	
3.	
4.	
5.	
6.	

7.	

Task 2 Challenges in Deep Learning
Deep learning has made significant advancements in various fields, but there are still some challenges that need to be addressed. Discuss some of the main challenges, their impact, and ways to reduce it in deep learning:

1. Data availability
2. Computational Resources
3. Time-consuming
4. Interpretability
5. Overfitting

Topic 2. Chemoinformatics

Classroom work: checking the understanding of the content of the read text, viewed or listened to video clip about approaches and models to the construction of artificial intelligence, followed by a conversation on the content; discussion of problematic issues.
Independent work with information resources, studying the material of practical classes, reading the main and recommended literature on the topic, preparing a report on the topic.

Sample task for vocabulary work

Chemoinformatics, also known as cheminformatics, is an advanced interdisciplinary field that blends principles from chemistry, computer science, and information science. It revolves around the use of computational methods and tools to analyze and interpret chemical data, enabling researchers and scientists to draw meaningful insights, make predictions, and facilitate drug discovery and development.

specialized vocabulary and terminology:

1. QSAR	a. Unique binary or hashed representations of molecular structures for database searching and clustering.
2. molecular docking	b. The process of simulating the binding of a small molecule (ligand) to a macromolecule (protein) to predict their interactions.
3. chemical descriptor	c. A structured vocabulary that defines and categorizes chemical entities and concepts, enhancing data integration and semantic searching.
4. chemoinformatics software	d. A multi-dimensional space where each dimension represents a chemical property, used to map and explore compound diversity.
5. chemical fingerprints	e. The sequence of steps and processes involved in chemoinformatics analysis, from data retrieval to model generation.
6. machine learning algorithms	f. A method used to correlate the chemical structure of compounds with their biological activity or other properties quantitatively.

7. chemical informatics workflow	g.	Software applications and libraries tailored for chemoinformatics tasks, such as Cheminformatics toolkits (e.g., RDKit, ChemAxon).
8. chemometric analysis	h.	The fusion of chemical and biological data to gain a comprehensive understanding of drug-target interactions.
9. pharmacophore	i.	Advanced computer programs designed for tasks like molecular modeling, virtual screening, and chemometric analysis.
10. chemical space	j.	A method used to rapidly test large compound libraries for biological activity.
11. cheminformatics databases	k.	A numerical or binary value that characterizes a specific chemical property, often used for quantitative analysis.
12. cheminformatics tools	l.	Statistical and mathematical methods used to extract information from chemical data, such as principal component analysis (PCA) and clustering.
13. molecular dynamics simulation	m.	Specialized repositories of chemical data, including chemical structures, properties, and biological activities.
14. chemical ontology	n.	Computational techniques used to train models that can predict chemical properties or classify compounds based on input data.
15. toxicophore	o.	The integration of genomics and chemoinformatics to identify connections between chemical compounds and specific genes or proteins.
16. chemogenomics	p.	Refers to processes or experiments conducted in a computer simulation rather than in a physical laboratory.
17. chemical information extraction	q.	A molecular framework that represents the essential features required for a molecule to interact with a specific biological target.
18. HTS	r.	Computational technique for studying the physical movements of atoms and molecules over time.
19. biological data integration	s.	The process of automatically extracting relevant chemical information from unstructured text, such as research papers or patents.
20. in silico	t.	A molecular substructure or pattern that is associated with toxicity, used for predictive toxicology.

Key applications of chemoinformatics. Discuss the usage and significance:
1. Drug Discovery and Development
2. Virtual Screening
3. Toxicology Prediction
4. Chemical Property Prediction
5. Materials Science
6. Environmental Chemistry

7. Food Chemistry
8. Chemical Patent Analysis
9. Chemical Database Management
10. Personalized Medicine
11. Chemical Education
12. Chemical Informatics in Agriculture
13. Cosmetic and Fragrance Design
14. Predictive Modeling
15. Quality Control

Topic 3. Design and Optimization

Classroom work: discussion of problematic issues and exchange of opinions (understanding of arguments and their evaluation); checking of understanding of what was heard/viewed, expressing hypotheses, writing a story about events preceding or following them;

Independent work with information resources, studying the material of practical classes, reading the main and recommended literature on the topic; creative individual /group task: compilation of associograms on concepts and events from the point of view of their own and foreign language culture, presentation in presentation format; analysis of cases of situations of intercultural communication.

Sample task for reading

Task 1 Try to guess the content of the article titled "Development, validation, and evaluation of a deep learning model to screen cyclin-dependent kinase 12 inhibitors in cancers" with the help of the questions below:

1. What is the primary objective of the article, and what problem does it aim to address in the field of cancer research?

2. Can you provide an overview of the deep learning model developed in the article for screening cyclin-dependent kinase 12 (CDK12) inhibitors?

3. How was the deep learning model validated and evaluated in the study, and what were the key performance metrics used?

4. Were there any unique challenges or considerations in developing a model for CDK12 inhibitors, especially given their similarity to CDK13?

5. What role does virtual screening play in the methodology, and how does it complement the deep learning approach?

6. Can you summarize the results of the study regarding the identification of potential CDK12 inhibitors, including any novel findings?

7. Did the study involve experimental validation of the predicted CDK12 inhibitors, and if so, what were the outcomes?

8. Were there specific datasets or compound libraries used for testing the deep learning model, and how large were these datasets?

9. How does the article discuss the potential implications of the findings for cancer treatment and drug discovery?

10. Are there any insights into the efficiency and effectiveness of the deep learning model in comparison to traditional drug discovery methods?

Abstract _ Introduction

Task 2 Acronyms

Explain the acronyms from the provided text:

1. CDK12 - Cyclin-dependent kinase 12:

2. CDK13 - Cyclin-dependent kinase 13:

3. DTI - Drug-Target Interaction:

4. IC50 - Half-maximal inhibitory concentration:

5. HER2 - Human Epidermal Growth Factor Receptor 2:

6. GNN - Graph Neural Network:

7. GCN - Graph Convolutional Neural Network:

8. QSAR - Quantitative Structure-Activity Relation:

9. CADD - Computer-Aided Drug Discovery:

10. VS - Virtual Screening:

11. MPG - Molecular Pre-training Graph-based:

12. BERT - Bidirectional Encoder Representations from Transformers:

13. GPT-3 - Generative Pre-trained Transformer 3:

14. HTS - High-Throughput Screening:

Task 3 Answer the questions concerning the core vocabulary:

1. **Deep Learning**:

   - What is the fundamental concept behind deep learning in machine learning?

   - How is deep learning different from traditional machine learning?

2. **In Silico**:

   - What does the term "in silico" mean in the context of scientific research?

   - How is in silico research different from in vitro or in vivo research?

3. **Drug Discovery**:

   - What is the primary goal of the drug discovery process?

   - What are the key stages involved in drug discovery?

4. **Cyclin-dependent kinase 12 (CDK12)**:

   - What is the role of CDK12 in cellular processes?

   - Why is CDK12 significant in cancer research?

5. **Transcription-related**:

   - How does CDK12 relate to transcription processes in cells?

   - What are the implications of CDK12 being transcription-related?

6. **Biomarker**:

   - What is a biomarker, and why are they important in medicine and research?

   - How can CDK12 function as a biomarker in cancer?

7. **Therapeutic Target**:

   - What is meant by the term "therapeutic target" in drug development?

   - Why is CDK12 considered a potential therapeutic target in cancer treatment?

8. **CDK12 Inhibitor**:

   - What is the purpose of a CDK12 inhibitor in cancer treatment?

   - Why is the development of selective CDK12 inhibitors challenging?

9. **CDK13**:

   - How does CDK13 relate to CDK12, and why is their similarity important?

   - Are there any specific functions or roles associated with CDK13?

10. **Virtual Screening**:

    - What is virtual screening in the context of drug discovery?

    - How does virtual screening complement experimental High-Throughput Screening (HTS)?

11. **Workflow**:

    - What does a typical virtual screening workflow entail?

    - How does a well-designed workflow contribute to the efficiency of drug discovery?

12. **Transformer Architecture**:

    - What is the significance of the term "Transformer architecture" in deep learning?

    - How is it used in the context of Drug-Target Interaction (DTI) modeling?

13. **Drug-Target Interaction (DTI) Model**:

    - What is the purpose of a DTI model in drug discovery?

    - How does it assist in predicting interactions between drugs and target proteins?

14. **Self-supervised Pre-trained Molecular Graph Models**:

    - What is the role of self-supervised learning in molecular graph modeling?

    - How are these models pre-trained, and why is it important?

15. **Protein Sequence Models**:

    - How are protein sequence models used in the context of drug discovery?

    - What information can be extracted from protein sequences?

16. **Predictive Model**:

    - What is the main objective of a predictive model in deep learning?

- How do predictive models contribute to the identification of potential drug candidates?

17. **Compound Library**:

    - What is a compound library, and why is it important in drug discovery?

    - How large is the compound library mentioned in the text?

18. **Molecular Docking**:

    - How does molecular docking work in the context of virtual screening?

    - What information is derived from molecular docking simulations?

19. **Kinase Assay**:

    - What is the purpose of a kinase assay in drug development?

    - How is the effectiveness of CDK12 inhibitors assessed through kinase assays?

20. **THZ531**:

    - What role does THZ531 play in the context of CDK12 inhibition?

    - How does its effectiveness compare to other compounds mentioned in the text?

21. **CICAMPA-01, CICAMPA-02, CICAMPA-03, CICAMPA-04, CICAMPA-05, CICAMPA-06, CICAMPA-09**:

    - What are these compounds, and how are they related to CDK12 inhibition?

    - How do their inhibitory effects compare to each other?

22. **In Vitro**:

    - What does "in vitro" mean, and how does it relate to laboratory experiments?

    - Why was the BT-474 cell line used in the in vitro experiments?

23. **IC50**:

    - What does IC50 represent in the context of drug development?

    - Why is it significant to have an IC50 value less than 3 μM?

24. **HER2**:

    - What is the relevance of HER2 in breast cancer research?

    - How does CDK12 amplification relate to HER2-positive breast cancer?

25. **BT-474**:

    - What is the BT-474 cell line, and why is it used in the study?

    - What role does it play in testing CDK12 inhibitors?

26. **Computational Screening**:

    - How does computational screening differ from experimental screening methods?

    - What advantages does computational screening offer?

27. **Graph Neural Network (GNN)**:

- What is the purpose of a Graph Neural Network (GNN) in deep learning?

- How is it applied to problems in drug discovery?

28. **Graph Convolutional Neural Network (GCN)**:

- How does a Graph Convolutional Neural Network (GCN) extend the capabilities of a standard CNN?

- In what drug discovery tasks has GCN shown promise?

29. **Node-level, Edge-level, and Graph-level Tasks**:

- What are these different levels of tasks in graph-based deep learning?

- How are they relevant to molecular graph modeling?

30. **Multi-perceptron Predictor**:

- What is the function of a multi-perceptron predictor in graph-based deep learning?

- How does it contribute to the prediction of node properties?

31. **Graph Pooling**:

- What is graph pooling, and why is it performed in graph-based deep learning?

- What information is retained or aggregated during graph pooling?

32. **Self-supervised Learning**:

- How does self-supervised learning work, and what is its main objective?

- What types of tasks are used as pretext tasks in self-supervised learning?

33. **Molecular Pre-training Graph-based Deep Learning Framework (MPG)**:

- What is the purpose of the MPG framework in molecular graph modeling?

- How has it advanced the field of molecular property prediction?

34. **Bidirectional Encoder Representations from Transformers (BERT)**:

- How is BERT applied in natural language processing, and what does it achieve?

- In what ways has BERT been adapted for tasks involving protein sequences?

35. **Generative Pre-trained Transformer 3 (GPT-3)**:

- What are the primary capabilities of GPT-3 in natural language understanding?

- How has GPT-3 been used in the context of protein structure and function prediction?

36. **High-Throughput Screening (HTS)**:

- What is High-Throughput Screening, and how does it differ from virtual screening?

- What are the advantages and limitations of HTS?

37. **Phosphorylation**:

- What is phosphorylation, and why is it relevant to CDK12 and cellular activities?

- How does phosphorylation affect protein functions?

Topic 4. Biological Investigation

Classroom work: heuristic conversation with the statement of hypotheses about the prospects of bio investigation; discussion of the text.

Independent work with information resources, studying the material of practical classes, reading the main and recommended literature on the topic; creative task for the communicative translation of academic text.

Sample task for reading

Read the text and prepare a short review about the described sphere of AI application:
READING 1

Task 1 Before reading the extract from an article "Deep learning in drug discovery: an integrative review and future challenges", work with the key vocabulary

> To gain favor _ Data acquisition _ Conventional _ Extensively _ Regression _ To escalate _
>
> Compilation _ Array _ To distribute _ Sampling layer _ Output layer _ To precede _ To subject to __ To flatten

1. The company used various techniques to _____ their customers and increase their sales.

2. _____ is the process of collecting and gathering information for analysis.

3. The _____ methods of manufacturing were replaced with more advanced technologies.

4. The researchers _____ studied the effects of the new drug on a large group of participants.

5. The _____ in the research showed a strong correlation between age and income.

1. Data acquisition refers to:

  a) The process of analyzing data

  b) The process of collecting data

  c) The process of distributing data

  d) The process of summarizing data

2. The output layer in deep learning models is responsible for:

  a) Gathering data

  b) Distributing data

  c) Analyzing data

  d) Providing final results

Fill in the gaps with the vocabulary from above. You may need to change the form of the words:

1. _____analysis is often used in statistical modeling to establish a relationship between variables and predict outcomes.
2. _____is the process of collecting and gathering information, which is further analyzed for insights and patterns.
3. _____methods of manufacturing were extensively replaced with advanced technologies to improve efficiency and productivity.
4. An _____is a data structure that stores a collection of elements of the same type in a sequential manner.
5. The _____of the research findings has been completed, and the report will be published soon.
6. The _____function in programming is used to convert a multidimensional array into a one-dimensional array.
7. The _____in deep learning models extracts relevant features from the input data for further processing.
8. The _____in deep learning models produces the final results or predictions based on the processed data.
9. The sampling process should _____the data analysis to ensure a representative sample is obtained.
10. To _____the workload evenly, the team assigned different tasks to each member according to their skills and expertise.
11. To _____with their customers, the company implemented various marketing strategies and offered attractive discounts.
12. To _____the conflict, both parties resorted to aggressive tactics and confrontational language.
13. To _____the hypothesis _____rigorous testing, the researchers designed a series of experiments and collected relevant data.

Task 2 Before reading the extract from an article "Deep learning in drug discovery: an integrative review and future challenges", discuss the following questions:

How has Machine Learning and Deep Learning revolutionized the world's perspective?

Explain the difference between linear and nonlinear functions.

What are Sigmoid Curve, Hyperbolic Tangent, and Rectified Linear Unit?

READING

Deep learning (DL) techniques

Detecting spam, recommending videos, classifying images, and retrieving multimedia ideas are just a few of the techniques used where machine learning (ML) has lately gained favor in research. Deep learning (DL) is one of the most extensively utilized ML methods in these applications. The ongoing appearance of new DL studies is due to the unpredictability of data acquisition and the incredible progress made in hardware technologies. DL is based on conventional neural networks but outperforms them significantly. Furthermore, DL uses

transformations and graph technology to build multi-layer learning models. With their groundbreaking invention, Machine Learning and Deep Learning have revolutionized the world's perspective. Deep learning approaches have revolutionized the way we tackle problems. Deep learning models come in various shapes and sizes, capable of effectively resolving problems that are too complex for standard approaches to tackle.

Classic neural networks

As shown in Fig. 2, Multi-layer perceptron are frequently employed to recognize Fully Connected Neural Networks. It involves converting the algorithm into simple two-digit data inputs (Mukhamediev et al. 2021). This paradigm allows for both linear and nonlinear functions to be included. The linear function is a single line with a constant multiplier that multiplies its inputs. Sigmoid Curve, Hyperbolic Tangent, and Rectified Linear Unit are three representations for nonlinear functions. This model is best for categorization and regression issues with real-valued data and a flexible model of any kind.
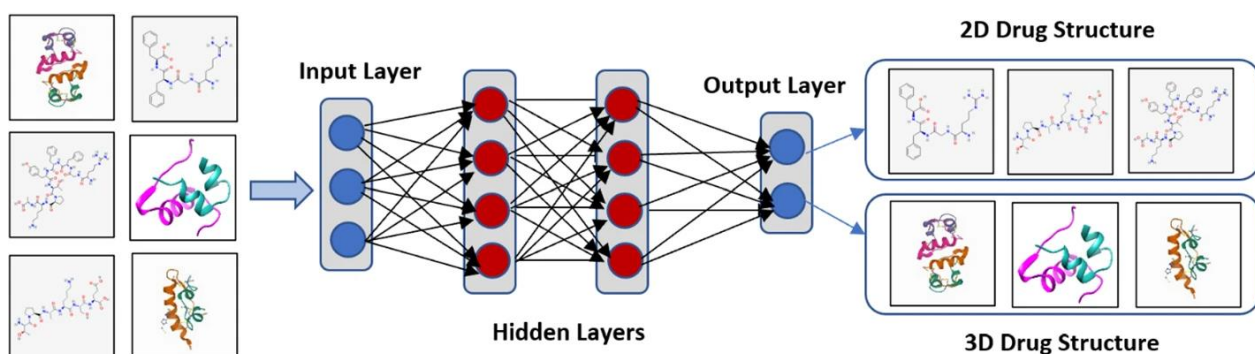
Convolutional neural networks (CNN)

As shown in Fig. 3, The classic convolutional neural network (CNN) model is an advanced and high-potential variant ANN, which was developed to manage escalating complexity levels, as well as data pretreatment and compilation. It is based on how an animal's visual cortex's neurons are arranged (Amashita et al. 2018). One of the most flexible algorithms for the processing of data with and without images is CNNs. CNN can be processed through 4 phases:

— For analyzing basic visual data, such as picture pixels, it includes one input layer that is often the case a 2D array of neurons.
— Some CNNs analyze images on their inputs using a single-dimensional output layer of neurons coupled to distributed convolutional layers.
— Layer number 3, called as the sampling layer, is included in CNNs and restricts the number of neurons which it took part in the relevant network levels.
— The sampling and output layers are joined by one or more connected layers in CNNs.
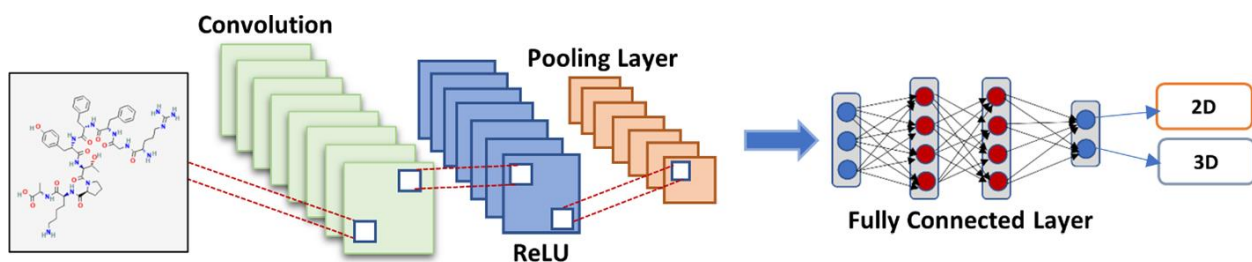
This network concept can potentially aid in extracting relevant visual data in pieces or smaller units. In the CNN, the neurons are responsible for the group of neurons from the preceding layer.

After the input data has been included into the convolutional model, the CNN is constructed in four steps:

— Convolution: The method produces feature maps based on supplied data., which are then subjected to a purpose.
— Max-Pooling: It aids CNN in detecting an image based on supplied changes.
— Flattening: The data is flattened in this stage so that a CNN can analyze it.
— Full Connection: It's sometimes referred to as a "hidden layer" which creates the loss function for a model.

Adapted from https://link.springer.com/article/10.1007/s10462-022-10306-1

Topic 5. Bio-AI revolution

Classroom work: oral survey, discussion of questions on the topic of the section; checking the understanding of the content of the read text about the use of artificial intelligence in various spheres of life with a discussion of examples from native and foreign cultures; watching videos discussing problematic issues; modeling communication situations.
Independent work with information resources, studying the material of practical classes, reading the main and recommended literature on the topic.

Sample task for listening

Watch the Video From idea to medicine | Drug development at Roche - YouTube
Ex. 1 Take notes on:
1.   Identifying a molecular drug target
2.   Identifying a first lead compound
3.   Lead optimisation
4.   Preclinical safety and efficacy trials
5.   Clinical trials in man
6.   Regulatory approval and launch

Ex. 2 Watch the video again. Fill in the gaps with the words and phrases as you hear them
1.   Identifying a molecular drug target Researchers   need   to   understand   the underlying mechanisms of the disease as fully as possible. Molecules on the pathways that influence the development or progression of the disease are potential drug (1)_____ .
2.   Identifying a first lead compound   … Basically, there are two options here. Researchers can look for a small chemical compound that will (2) _____. … Or they can look for a large biological molecule. Automated tests are used to (3) _____ first lead compounds. …

These tests (4) _____ thousands of compounds. … The search then consists of identifying and (5) _____ the antibody of the most favorable characteristics. It is sometimes also possible to isolate and produce a protein that occurs naturally in the body and (6)_____ with the body.

      3.   Lead optimisation   … Chemists start with a first lead compound and then generate, test, and (7) _____a succession of structurally related compounds until they come up with an optimal active structure. Wherever possible, they use computer aided molecular (8) _____ to better understand how active compounds and the target interact. The goal is to find a compound that has the desired effect, is well – (9)_____, and doesn't cause unacceptable side effects. The expression "multidimensional optimization" is commonly used because the aim is to optimize many other characteristics besides (10) _____ . … These include the rate at which a compound is absorbed into the blood stream, the average duration of its presence in the body. … In the case of large biological molecules, characterization, isolation and large-scale (11) _____ all are a challenge.

      4.   Preclinical safety and efficacy trials … Investigations at this stage focus primarily on safety, (12) _____, and efficacy. Then they can be performed in (13)_____ culture. … As far as possible Roche uses (14)_____ testing methods. …

      5.   Clinical trials in man Phase 1: A new drug is tested under close medical (15) _____ .

      Phase 2: … A new drug is tested on a small number of patients to determine its effectiveness. … These trials generate information on the optimal doze, dozing (16)_____, and route to the administration.

      Phase 3: It's often difficult to find patients to fill all the (17) _____ criteria. The aim is to demonstrate that the new drug is more effective. To ensure maximum objectivity these trials are usually double-(18) _____.

      6.   Regulatory approval and launch   Medicine cannot be sold in a country without approval. … The regulatory reveal process … may take months or years. If the outcome is positive the drug can be sold in a country concerned. In a sense, a package (19) _____ is a distillation of the (20) _____research and development process. The information it contains is important both for health professionals and for the patients.

Topic 6. Trends in Drug Discovery

Classroom work: checking the understanding of the content of the read text (viewed or listened to a video clip), followed by a conversation on the content.

Independent work with information resources, studying the material of practical classes, reading the main and recommended literature on the topic; writing an e-mail to a business partner, taking into account his cultural affiliation.

Sample task for speaking

What can you comment on the following questions:

1.   What are the current trends in the way patients, doctors, and healthcare providers are transforming their attitude to care delivery?

2.   What is the correct balance between preserving patient-centric information and ensuring the quality and accessibility of this data?

3.   What do you know about the standards for producing next-generation sequencing (NGS) data, handling bioinformatics, data deposition, and supporting medical decision-making?

Sample task for written task

Task 1: Select a Research Paper

Choose a research paper from your field of interest. It can be from a journal, academic database, or a preprint repository.

Task 2: Reading and Understanding

Read the research paper carefully, taking notes as you go along. Pay attention to the following aspects:

- Research question or hypothesis
- Methodology and data collection
- Results and findings
- Discussion and conclusion
- Strengths and weaknesses

Task 3: Summarize the Research Paper

Write a concise summary of the research paper. Include the following elements:

- Briefly state the research question or objectives.
- Summarize the methods used in the study.
- Highlight the key findings and results.
- Note any conclusions or implications drawn by the authors.

Task 4: Assess the Methodology

Evaluate the methodology used in the research paper. Answer the following questions:

- Was the research design appropriate for the research question?
- Were the data collection methods suitable and well-described?
- Were there any limitations in the methodology?

Task 5: Evaluate the Results

Assess the presentation and interpretation of results in the research paper. Consider these points:

- Are the results clearly presented, using tables, figures, or graphs when necessary?
- Do the authors provide sufficient context and explanation for the results?
- Are there any statistical or analytical issues to consider?

Task 6: Analyze the Discussion

Analyze the discussion section of the research paper. Answer the following questions:

- Do the authors effectively link their results to the research question?
- Are alternative interpretations considered and discussed?
- Do the authors acknowledge any limitations or potential biases in their findings?

Task 7: Consider the Contribution

Evaluate the contribution of the research paper to the field. Discuss:

- How does this research paper advance knowledge or understanding in the field?
- Does it address a significant research gap or problem?
- Are there practical implications or applications of the findings?

Task 8: Critique the Paper

Provide a critical assessment of the research paper. Discuss:

- What are the strengths of the paper? Be specific.
- What are the weaknesses or limitations of the study?
- Are there areas where the paper could be improved?

Task 9: Write the Review

Based on your assessment, write a review of the research paper. Follow a structured format, including:

- Introduction: Briefly introduce the paper and its topic.
- Summary: Summarize the key aspects of the paper.
- Evaluation: Provide a balanced evaluation of the paper, highlighting strengths and weaknesses.
- Conclusion: Offer a concluding statement about the paper's contribution and significance.

Task 10: Proofread and Edit

Carefully proofread and edit your review for clarity, grammar, and style. Ensure that your review is well-organized and free of errors.

Repeat these tasks with different research papers to practice and improve your skills in writing reviews of research articles.

Criteria for evaluating in-progress assessment tasks as regards to modules

Criteria for evaluating written speech are used when students write works of such genres as an email, argumentative text (paragraph, text of a project), summary.

Grades for tests assessing skills of using vocabulary and grammar in reading and listening are calculated as the ratio of the number of correct answers of the student to the maximum possible number of points for the test.

In-progress assessment of oral and written speech is based on evaluation criteria

Writing assessment criteria

Email evaluating criteria (Formal Letter)

Maximum number of points – 10

Criteria	Grade points
1. Statement of all the main ideas	2
2. Compliance with the email format	1
3. Considering the cultural affiliation of the addressee	2
4. Language correctness	1
5. Logical and coherent presentation	1
6. Official style of presentation	2
7. Length (120-150 words)	1
Total	**10**

Criteria for evaluating a prepared monologue statement on the studied topics
(report, description, story)

Maximum number of points – 10

Criteria	Description	Grade points
Grammar	Poor knowledge of simple grammatical forms / does not try to use more complex constructions	0
	Limited knowledge of simple grammatical forms / does not try to use more complex constructions	1
	Good use of simple grammatical forms / poorly tries to use more complex constructions	2
	Good use of simple grammatical forms / tries to use more complex constructions	3
Vocabulary	Uses individual words and phrases	0
	Uses a limited vocabulary to discuss familiar situations	1
	Mainly uses the appropriate vocabulary to discuss familiar topics	2
	Uses the appropriate vocabulary to discuss a number of familiar topics	3

Fluency	A significant number of hesitation pauses / frequent repetition of information	0
	Gives answers that go beyond a short phrase, with some pauses / sentences mostly correspond to the subject / there are some repetitions / uses only the basic techniques of logical communication	1
	Pronounces long fragments of speech with uncertainty / mainly correctly uses a number of linkers / there is a certain number of repetitions	2
	Pronounces long fragments of speech, making hesitation pauses/ uses linkers correctly / uses few repetitions	3
Pronunciation	Limited phonological skills; the statement is mostly understandable	0.5
	Shows good phonetic and phonological skills at the level of words/sentences	1
Total: maximum 20 points		