Department of general and clinical pharmacology and pharmacognosy

ЗАТВЕРДЖУЮ

Проректор з науково-педагогічної роботи

_____ Едуард БУРЯЧКІВСЬКИЙ

01 вересня 2023 року

WORKING PROGRAM IN THE DISCIPLINE
«COMPUTER MODELING IN PHARMACY»
(full-time education)

Level of higher education: second (master's degree)

Field of knowledge: 22 «Health care»

Specialty: 226 «Pharmacy, industrial pharmacy»

Educational and professional program: Pharmacy, industrial pharmacy

2023

The program was compiled on the basis of the educational and professional program "Pharmacy, industrial pharmacy", training of specialists of the second (master's) level of higher education in the specialty 226 "Pharmacy, industrial pharmacy" field of knowledge 22 "Health care", approved by the Scientific Council of ONMedU (from 29.06 .2023, protocol No. 8).

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The work program was approved at the meeting of the department of pharmacology and pharmacognosy
Protocol No. 1 dated August 28, 2023

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Revised and approved at the meeting of the department of Pharmacology and Pharmacognosy
Protocol No. __ dated __/__/20__.

Head of the department _____ Yaroslav ROZHKOVSKY

Revised and approved at the meeting of the department of Pharmacology and Pharmacognosy
Protocol No. __ dated __/__/20__.

Head of the department _____ Yaroslav ROZHKOVSKY

1. Description of the discipline:

Name of indicators	Field of knowledge, specialty, specialization, level of higher education	Characteristics of the discipline	
Total number: Credits of ECTS: 3 Hours: 90 Content topics - 9	Field of knowledge 22 «Health care» Specialty 226 « Pharmacy, industrial pharmacy » Level of higher education second (master's degree)	*Full-time (day) education* *Selective discipline*	
		Course: III	*3*
		Semester:	*VI*
		Lectures	*0 hours*
		Seminars	*30 hours*
		Practical classes	*0 hours*
		Laboratories	
		Independent work	*60 hours*
		including individual tasks	*0 hours*
		Form of final control	*Credit*

2. Goals and objectives of the discipline

The purpose of teaching the discipline is: mastering the theoretical foundations and elements of the use of computer technologies in pharmacy, understanding the whole picture "from idea to product", acquaintance with modern approaches to the creation of innovative medicines

Gols:

- familiarization and practical skills of using the INTERNET network or electronic databases for professional activities;

- assimilation of available packages of computer programs for future professional activities.

- familiarization and development of innovative approaches to the creation of medicines (virtual screening, molecular modeling, docking, PASS analysis, optimization of the structure of leading compounds, combinatorial chemistry, highly efficient screening, etc.) and software for their implementation;

- study of modern medicines created using innovative technologies;

The process of studying the discipline is aimed at forming the elements of the following competencies:

IC - the ability to solve complex tasks and problems in a certain area of professional activity or in the learning process, involves research and / or innovation and is characterized by the complexity and uncertainty of conditions and requirements

General (GC):

GC 01. Ability to act in a socially responsible and conscious manner.

GC 0 2. Ability to apply knowledge in practical situations.

GC 03. Commitment to preserving the environment.

GC 04. Ability to think abstractly, analyze and synthesize, learn and be modernly trained.

GC 06. Knowledge and understanding of the subject area and understanding of professional activities.

GC 07. Ability to adapt and act in a new situation.

GC 08. Ability to communicate in a professional foreign language (mainly in English) at a level that ensures effective professional activity.

GC 09. Skills in the use of information and communication technologies.

GC 11. Ability to evaluate and ensure the quality of work performed.

Specialists (SC):

SC01. Ability to carry out health education work among the population.

SC02. Ability to advise on non-prescription and prescription drugs, medical devices and other pharmacy products; pharmaceutical care in the selection and sale of an over-the-counter medicinal product.

SC03. Ability to provide pre-medical care to patients and victims in extreme situations and in emergency conditions.

SC04. Ability to ensure the rational use of non-prescription and prescription drugs, medical devices and other goods in the pharmacy range.

SC07. Ability to ensure proper storage of medicines and pharmaceutical goods.

SC09. The ability to analyze and predict the main economic indicators of the activities of pharmacies, to calculate the main taxes and fees, to form prices for medicines and medical products in accordance with the current legislation of Ukraine.

SC11. Ability to analyze socio-economic processes in pharmacy

SC14. Ability to organize and carry out production activities of pharmacies for the manufacture of medicines in various dosage forms according to prescriptions of doctors and orders of medical institutions, including justification of technology and selection of auxiliary materials in accordance with the rules of good pharmacy practice.

SC16. The ability to organize and carry out the procurement of medicinal plant materials, choose ways to solve the problem of preserving and protecting thickets of wild medicinal plants, in accordance with current legislation.

SC17. The ability to carry out marketing management of the assortment, price, sales and communication policies of the subjects of the pharmaceutical market.

Program learning outcomes for the discipline: (PLO):

PLO01. To carry out professional activities in social interaction based on humanistic and ethical principles; to identify future professional activity as socially significant for human health.

PLO02. Apply knowledge of general and professional disciplines in professional activities.

PLO03. To comply with the norms of the sanitary and hygienic regime and the requirements of safety equipment when carrying out professional activities.

PLO04. Demonstrate the ability to independently search, analyze and synthesize information from various sources and use these results to solve typical and complex specialized tasks of professional activity.

PLO05. To position one's professional activity and personal qualities on the pharmaceutical labor market; formulate the goals of one's own activity taking into account public and industrial interests.

PLO06. Argue information for decision-making, bear responsibility for them in standard and non-standard professional situations; adhere to the principles of deontology and ethics in professional activity.

PLO11. Use methods of evaluating indicators of the quality of activity; identify reserves for increasing labor efficiency.

PLO20. To carry out a complex of organizational and management measures to provide the population and health care institutions with medicines and other products of the pharmacy assortment. Carry out all types of accounting in pharmacies, administrative records, product analysis processes.

PLO21. Calculate the main economic indicators of pharmacy establishments, as well as taxes and fees. Form all types of prices (wholesale, purchase and retail) for medicinal products and other products of the pharmacy assortment.

PLO22. Manage pharmaceutical organizations and determine its effectiveness using management functions. Make management decisions on the basis of the developed leadership and communication skills of pharmaceutical personnel regarding the strategic planning of enterprise activities.

PLO23. To take into account data on socio-economic processes in society for the pharmaceutical supply of the population, to determine the effectiveness and availability of pharmaceutical care in terms of medical insurance and reimbursement of the cost of drugs.

PLO24. Plan and implement professional activities on the basis of normative legal acts of Ukraine and recommendations of proper pharmaceutical practices.

PLO29. To ensure competitive positions and effective development of pharmaceutical organizations on the basis of the conducted research work on all elements of the marketing complex.

PLO30. Ensure quality control of medicines and document its results. To carry out quality risk management at all stages of the life cycle of medicinal products.

As a result of studying the discipline, the student has to
know:

• scope of tasks and basic principles of the application of mathematical methods and applied statistics in pharmacy and drug research;

• the scope and limits of the use of computer technologies in the tasks of drug research;

• rules for the statistical description of quantitative and qualitative data of clinical and pharmaceutical experiments, standards for providing statistically valid conclusions on drug research;

• methods of data analysis and computer technology tools used in drug research;

be able to:

• determine the stages of research of medicinal products requiring analysis by means of computer technology;

• conduct reconnaissance analysis of data from experiments on drug research using computer technology;

• choose an appropriate statistical analysis method depending on the study design and the properties of the source data;

• receive, read and understand the output of computer programs for the implementation of methods of statistical analysis and / or mathematical models in drug research;

• correctly formulate conclusions in the report on the research of medicinal products based on calculations obtained by means of computer technology;

own:

• professional and general competencies.

3. The content of the educational discipline

Topic 1. «Basic concepts of pharmaceutical informatics. Creation and maintenance of pharmaceutical and medical documentation by means of a word processor»

Topic 2. «Information technology tools. Special software for the professional activities of the pharmacist. Creation of chemical structures of biologically active substances using application software»

Topic 3. «Fundamentals of building information technologies for solving pharmaceutical problems. Information systems in a table processor environment. MS Excel spreadsheet processor, its purpose; basic technology work in its environment»

Topic 4. «Types of modern information technology. Decision support systems in a table processor environment. Modeling of elementary pharmaceutical calculations»

Topic 5. «Support of databases in ET. Data analysis in Excel. Graphic design of Excel documents»

Topic 6. «The principles of the structure of the Internet network and the Internet. Solution of information retrieval problems in the Internet»

Topic 7. «The basic services of the global network. Pharmaceutical resources and Ukrainian pharmacy on the Internet. Methods of effective information retrieval in the professional activity of a pharmacist. Practical search on the Internet for information about medicines and medicinal plants»

Topic 8. «Systems for processing multimedia information. MS Power Point program, its purpose and functionality. Creating presentations using MS Power Point. Plan content, develop scripts and create presentations using MS Power Point»

Topic 9. «The ability to demonstrate presentations using MS Power Point. Protection of coursework»

4. The structure of the discipline

Topic	Number of hours				
	That's all	Including			
		lectures	practical	seminars	IWS
Topic 1. «Basic concepts of pharmaceutical informatics. Creation and maintenance of pharmaceutical and medical documentation by means of a word processor»	10	0	4	0	6
Topic 2. «Information technology tools. Special software for the professional activities of the pharmacist. Creation of chemical structures of biologically active substances using application software»	2	0	2	0	0
Topic 3. «Fundamentals of building information technologies for solving pharmaceutical problems. Information systems in a table processor environment. MS Excel spreadsheet processor, its purpose; basic technology work in its environment»	2	0	2	0	0
Topic 4. «Types of modern information technology. Decision support systems in a table processor environment. Modeling of elementary pharmaceutical calculations»	10	0	4	0	6
Topic 5. «Support of databases in ET. Data analysis in Excel. Graphic design of Excel documents»	8	0	8	0	0
Topic 6. «The principles of the structure of the Internet network and the Internet. Solution of information retrieval problems in the Internet»	8	0	2	0	6
Topic 7. «The basic services of the global network. Pharmaceutical resources and Ukrainian pharmacy on the Internet. Methods of effective information retrieval in the professional activity of a pharmacist. Practical search on the Internet for information about medicines and medicinal plants»	14	0	2	0	12
Topic 8. «Systems for processing multimedia information. MS Power Point program, its purpose and functionality. Creating presentations using MS Power Point. Plan content, develop scripts and create presentations using MS Power Point»	16	0	4	0	12
Topic 9. «The ability to demonstrate presentations using MS Power Point. Protection of coursework»	20	0	2	0	18
Total	90	0	30	0	60

5. Topics of lectures / seminars / practical / laboratory classes

5.1 Thematic plan of lectures
Lectures classes are not provided

5.2. Topics of practical classes

№ п/п	Topic	Hours.
1	2	4
1.	Basic concepts of pharmaceutical informatics. Creation and maintenance of pharmaceutical and medical documentation using a word processor	2
2.	Electronic document flow in pharmacy. Protection of information.	2
3.	Toolkit of information technology. Special software for the pharmacist's professional activity. Creation of chemical structures of biologically active substances using application software.	2
4.	Automation of management processes in pharmacy. Automated control systems. Decision support systems. Expert systems. Pharmacy software.	4
5.	Basics of building information technologies for solving pharmaceutical problems. Information systems in a spreadsheet environment. MS Excel spreadsheet processor, its purpose; basic technologies of work in its environment.	2
6.	Concept of database. Principles of building modern databases. Chemical databases and their application in pharmacy.	2
7.	Types of modern information technologies. Decision support systems in a spreadsheet environment. Modeling of elementary pharmaceutical calculations.	2
8.	Database support in ET. Data analysis in Excel. Graphic design of Excel documents.	2
9.	Anti-virus programs. Classification of viruses. Protection methods.	2
10.	Pharmacy in the worldwide Internet. Principles of intranet and Internet network structure. Solving information and search tasks on the Internet. Practical search on the Internet for information about medicinal products and medicinal plants.	2
11.	Basic services of the global network. Pharmaceutical resources and Ukrainian pharmacy on the Internet. Methods of effective search for information in the professional activity of a pharmacist.	2
12.	Multimedia information processing systems. The MS Power Point program, its purpose and functionality. Creating presentations using MS Power Point. Content planning, script development and presentation creation using MS Power Point.	4
13	Modern medicines are created using innovative technologies.	2
	In total:	**30**

5.3. Topics of seminars classes
Seminars classes are not provided

5.4. Topics of laboratory classes
Laboratory classes are not provided

6. Independent work

№ п/п	Тема	Hours.
1	2	3

1.	MS Word text editor. Work with texts and tables	6
2.	MS Excel spreadsheet processor, its purpose and functionality. Construction, editing and formatting of diagrams in MS Excel.	6
3.	Practical search for information on the Internet on specific groups of medicinal products.	6
4.	Practical search for information on the Internet on specific groups of medicinal plants.	6
5.	Pharmacy computer networks. Automated workplace of a pharmacist.	6
6.	MS Power Point program, its purpose and functionality. Creating presentations using MS Power Point.	6
7.	Using a PC in preparing course work and creating a presentation	6
8.	Modern approaches to the study of the structure-activity relationship. The latest methods of finding medicines. Virtual screening. QSAR.	6
9.	Practical use of software packages ISIS (ISIS Base, ISIS Draw), CHEMOFFICE in pharmacy as a fully functional chemical and pharmaceutical database management system.	6
10.	Electronic communication. E-mail. Principles of correspondence. POP3, IMAP and SMTP protocols. Network etiquette. The chat system as a means of communication in real time. News distribution systems.	6
	Всього :	**60**

Practical exercises: conversation, solving situational problems, preparation and presentations, performing tasks on a computer.

Independent work: independent work with the textbook, independent work with the computer.

8. Control methods and criteria for evaluating learning outcomes

Current control: oral survey, testing, assessment of the performance of theoretical skills, solving situational tasks, assessment of class activity.

Final control: credit.

Evaluation of the current educational activity in a practical session:

1. Evaluation of theoretical knowledge on the subject of the lesson:

- methods: survey, solving a situational problem

- maximum score – 5, minimum score – 3, unsatisfactory score – 2.

2. Evaluation of practical skills and manipulations on the subject of the lesson:

- methods: assessment of the correctness of the performance of practical skills

- maximum score – 5, minimum score – 3, unsatisfactory score – 2.

3. Evaluation of work with a PC on the subject of the lesson:

- methods: assessment of the correctness of the performance of practical skills

- maximum score – 5, minimum score – 3, unsatisfactory score – 2.

The grade for one practical session is the arithmetic average of all components and can only have a whole value (5, 4, 3, 2), which is rounded according to the statistical method.

Current evaluation criteria in practical training

Rating	Evaluation criteria
"5"	The applicant is fluent in the material, takes an active part in discussing and solving the situational problem, confidently demonstrates practical skills when working with Microsoft Office software packages, databases, the ISIS program (ISIS Base, ISIS Draw), CHEMOFFICE, expresses his opinion on the subject of the lesson, demonstrates an individual approach to setting and solving algorithm

	problems.
"4"	The applicant has a good command of the material, participates in the discussion and solution of the situational problem, demonstrates practical skills when working with Microsoft Office software packages, databases, ISIS (ISIS Base, ISIS Draw), CHEMOFFICE, expresses his opinion on the topic of the lesson, demonstrates an individual approach to setting and solving the algorithm of problems
"3"	The applicant does not have sufficient knowledge of the material, is unsure of participating in the discussion and solving the situational problem, demonstrates practical skills when working with Microsoft Office software packages, databases, ISIS (ISIS Base, ISIS Draw), CHEMOFFICE, expresses his opinion on the subject of the lesson, demonstrates an individual an approach to setting up and solving an algorithm for problems with significant errors.
"2"	The applicant does not possess the material, does not participate in the discussion and solution of the situational problem, does not demonstrate practical skills when working with Microsoft Office packages, databases, ISIS (ISIS Base, ISIS Draw), CHEMOFFICE.

9. Distribution of points received by students of higher education

The grade for the discipline consists of 100.0% of the grade for the current academic performance.

The average score for the discipline is translated into a national score and converted into points on a multi-point scale.

The conversion of a traditional grade for a discipline into a 200-point grade is carried out by the information and computing center of the university using the "Contingent" program.

Table of conversion of a traditional assessment into a multi-point assessment:

national assessment	points
Excellent ("5")	185-200
Good ("4")	151-184
Satisfactory ("3")	120-150

Points from the discipline are independently converted to both the ECTS scale and the four-point scale. Points from the ECTS scale are not converted into a four-point scale and vice versa. Further calculations are carried out by the information and computing center of the university.

Conversion of traditional discipline grade and ECTS scores

ECTS assessment	Statistical indicator
«A»	Top 10% of students
«B»	The next 25% of students
«C»	The next 30% of students
«D»	The next 25% of students
«E»	The last 10% of students

An assessment on the ECTS scale is given by the educational unit of ONMedU or the dean's office after ranking the grades in the discipline among students who study in the same course and in one specialty. The ranking of students - citizens of foreign countries is recommended by the decision of the Academic Council to be carried out in one array

10. Methodological support of the discipline:
Working program of the academic discipline

- Syllabus
- Multimedia presentations
- Methodical developments for practical classes
- Methodical recommendations for independent work of higher education applicants

List of didactic methodological teaching aids

№№ п.п.	Equipment name used.	The numbers of topics in which the equipment is used	Notes (edit)
1.	Terminal station	All topics	30 units
2.	Internet resources of the department	All topics	30 units
3.	Software	All topics	
4.	Overhead	No. 1-2	1 unit
5.	Presentations of lectures (on electronic media)	No. 1-2	
6.	Multimedia projector	No. 1-2	1 unit
7	Ask for the ticket program	All topics	

11. List of questions for offset:

1. Expand the essence of the concept of electronic document and paperless technology.
2. Explain what hypertext-based electronic documents are.
3. What are the challenges facing the transition to paperless technology?
4. What measures are taken to ensure the confidentiality of information in electronic form?
5. List the devices for digitizing images.
6. Name and describe the types of scanners. Expand the essence of the computer text recognition process.
7. Determine the advantages of email over courier.
8. Give the classification of computer networks.
9. What relates to the communication equipment of computer networks.
10. Describe the communication software of computer networks.
11. What is meant by information security?
12. Highlight the main stages of development of information technology by the advantages of computer technology.
13. Name the main components of information technology expert systems.
14. What are the criteria for choosing options for the introduction of information technology at a pharmaceutical company.
15. Describe the technology for sorting the data table by one (two, three) keys in a table processor environment.
16. Give the classification of the database.
17. Give a definition of the concept of "logical operations".
18. Justify the need to predict the development of medico-pharmaceutical processes.
19. List the types of table processor diagrams.
20. Determine the charting technology.
21. Describe the technology for editing diagrams
22. Computer tools for automating the work of pharmacies.
23. Hardware and software for document flow automation in pharmacy
24. Protection of information in information systems in pharmacy.
25. Decision support systems in pharmacy and medicine.
26. Computer tools for economic analysis and management in pharmacy.
27. Components of modern electronic computers (computers) and their functional purpose.
28. Types, functions and capabilities of modern operating systems.
29. Chemical software package CHEMOFFICE, ISIS, ACDLabs and Java molecular editor
30. Computer tools for automating the work of pharmacies.
31. Operating system WINDOWS, its characteristics and capabilities.
32. Modern drugs and leading structures that are designed using CT.
33. Prediction of the activity of substance structures by the QSAR method.

34. Computer methods used in drug design.
35. Computer system for predicting the spectrum of biological activity PASS C & T.

List of required practical skills to be mastered.

_ Use the Windows operating system
_ Use the most common office programs (MS Word, etc.)
_ Use the most common spreadsheets (MS Excel, etc.)
_ Master the basic techniques of creating logical and mathematical functions
_ Work with books and sheets, in general
_ Create and edit spreadsheets
_ Operate with absolute and relative premises
_ Use when calculating formulas and functions
_ Master the construction, editing and formatting of diagrams.
_ Use database technology to process and analyze pharmaceutical information.
_ Search the existing drug databases and the Medline database
- Demonstrate the ability to perform functional data approximation and the construction of simple forecasts using spreadsheets.
- to use database technologies for processing and analyzing pharmaceutical information.
- demonstrate the ability to formalize and algorithmize medical tasks.
- demonstrate the ability to design, create, edit electronic forms and forms of medical records using a word processor.
- be able to carry out content planning, script development and creation of presentations using MS Power Point.
- to master the systems for processing multimedia information, the MS Power Point program, its purpose and functionality.
- to analyze the role of information, communication and computer technologies in pharmacy and medicine;
- to master the basic techniques of effective information retrieval in the professional activity of a pharmacist, the language of queries of an information retrieval system, to demonstrate the ability to solve information retrieval problems on the Internet.
- get acquainted with the existing pharmaceutical resources and resources of Ukrainian Pharmacy on the Internet, databases of pharmaceutical and medical information and the principles of searching for them, demonstrate the ability to practically search the Internet for information about medicines and medicinal plants.
- to demonstrate the ability to use special-purpose programs: Creation of structural chemical formulas and equations of chemical reactions by means of programs using the ISIS, CHEMOFFICE, ACDLabs programs, etc

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