Danylo Halytsky Lviv National Medical University

Department of Pharmaceutical, Organic and Bioorganic Chemistry

APPROVED
The first vice-rector for scientific and pedagogical work
prof. Mechyslav Gzhegotskyi
_____
“___”_____2021

WORKING PROGRAM OF THE DISCIPLINE

Computer modeling in pharmacy
training of specialists of the second (master's) level of higher education
field of knowledge 22 "Health"
specialty 226 "Pharmacy, industrial pharmacy"

Discussed and approved
at the methodical meeting of the department of pharmaceutical, organic and bioorganic chemistry
Protocol № 1
from "31" August 2021
Head of Department
prof. Lesyk R.

Approved
profile methodical commission in pharmaceutical disciplines
Protocol № 3
from "31" August 2021
Chairman of the profile methodical commission
assoc. prof. Bilous S.

Working curriculum of discipline Computer modeling in pharmacy for 3th year students of the Faculty of Pharmacy, studying in the specialty 226 "Pharmacy" compiled by prof. Lesyk R, assoc prof. Kaminskyy D., assoc prof. Kryshchyshyn-Dylevych A., assoc prof. Lozynskyi A., senior lect. Novikevych OT on the basis of the sample program of the elective discipline modern methods of research of biological systems, approved by the State Institution "Central Methodical Cabinet for Higher Medical Education of the Ministry of Health of Ukraine" and the curriculum approved by the profile methodical commission (protocol №3 from 31.08.2021)

Changes and additions to the curriculum for the academic discipline for 2021-2022 academic year

№	Contents of changes (additions)	Date and № protocol of the meeting	Notes
	None		

Head of Department
Prof. Lesyk Roman _____
(підпис)

Introduction

The syllabus for *«***Computer modelling in pharmacy***»*
in accordance with the Standard of Higher Education of *the second (master's) level*
Field: 22 *"Health"*
Specialty: 226 "Pharmacy"
Master's Degree Programme in Pharmacy

Description of the discipline (abstract)

The last decades of the XX century were characterized by a number of factors that became the objective reasons for the slowdown of the innovation process in pharmacy. These factors are natural (deterioration of the ecological situation, rapid mutation of microorganisms), political and social (deterioration of market conditions due to the influence of government agencies and public organizations), of economic, scientific and technical origin. These facts do not allow the pharmaceutical industry to adequately respond to the permanent changes in the environment and social transformations that determine the health of each individual. Therefore, the urgent task of the practical and research sectors of pharmacy has been the generation of fundamentally new approaches, including computer technologies. Today, it is difficult to imagine a qualified pharmacist without a deep knowledge of modern computer programs and the competent use of databases, including specialized, to perform their professional work. In the scientific field, the approach to the search for drugs has fundamentally changed, due to the use of advances in biotechnology, molecular biology, experimental pharmacology, improved methodology of pharmaceutical/organic synthesis. Recently, a number of new technologies have been introduced, which are generalized in the so-called "drug design" approach, which includes virtual and highly effective screening, molecular docking, QSAR analysis, combinatorial chemistry. This radically changed the initial stage of drug development. These technologies, which are based on the use of modern computer programs, are the methodological basis of modern pharmaceutical chemistry. Thus, knowledge of the theoretical foundations of computer technology in pharmacy and practical use in education and future work is a necessary prerequisite for training a highly qualified specialist with higher pharmaceutical education.

Annotation

The discipline "Computer Modeling in Pharmacy" belongs to the compulsory disciplines of the cycle of professionally-oriented training of specialists in the specialty "Pharmacy". The course is based on the general laws of chemical and medical-biological sciences and allows students to master the theoretical foundations and elements of computer technology in pharmacy, understanding the holistic picture "from idea to drug", acquaintance with modern approaches to creating innovative drugs.

The study of the discipline is carried out in the 3rd year, the study includes: 90 hours (lectures - 4 hours, practical classes - 36 hours, self-study - 50 hours).

The program is divided into three content blocks: 1) principles and approaches to the search for specialized information; 2) approaches to the drug development (drug design); 3) the use of computer programs in practical pharmacy. The program contains

the necessary list of knowledge, skills and abilities, taking into account the international requirements for the credit transfer system, international regulations and standards governing the professional activities and training of masters of pharmacy.

The structure of the discipline	**The number of credits, hours**				**Year of study, semester**	**Type of control**
	Total	**Auditorium**		**Self-study**		
		Lectures	**Pract. Class.**			
Module 1 Thematic modules 3	3 credits ECTS / 90 hours	4	36	50	3d year, V sem.	credit

The subject of study of the discipline is
Approaches and methods of information search, innovative drug development, software packages used in practical pharmacy.

Interdisciplinary links: bioorganic and pharmaceutical/medical chemistry, biophysics, biochemistry, normal and pathological physiology, pharmacology, toxicological chemistry.

Interdisciplinary links: bioorganic and pharmaceutical/medical chemistry, biophysics, biochemistry, normal and pathological physiology, pharmacology, toxicological chemistry.

1. Aim and purposes of the learning discipline

1.1. The purpose of teaching the discipline is: mastering the theoretical background and elements of the usage of computer technology in pharmacy, understanding the holistic picture "from idea to drug", acquaintance with modern approaches to the creation of innovative drugs.

1.2. The main tasks are:

- To acquire skills for searching medical and biological information on the INTERNET or electronic databases for professional activities;
- Mastering the available software packages for future professional activities;
- The acquaintance and mastering of innovative approaches to drug development (virtual screening, molecular modeling, docking, QSAR-analysis, optimization of structure of lead-compounds, combinatorial chemistry, highly effective screening, etc.) and software for their implementation;
- Study of modern drugs created with the usage of innovative technologies.

1.3. Competences and learning outcomes, the formation of which provides the study of the discipline

in accordance with the Standard of Higher Education the discipline provides acquiring by the students the next **competences**:

- *general:* ЗК2; ЗК6; ЗК11; ЗК12.
- *special:* ФК 12; ФК 19; ФК 20.

ЗК – General competencies; ФК – Special responsibility

Competence matrix

№	Competence	Knowledge	Skills	Communication	Autonomy and responsibility
1	**ЗК 2.** The ability to apply knowledge in practical situations	to know the methods of knowledge implementation in solving practical issues	use professional knowledge to solve practical situations	To establish connections with business entities	To be responsible for timeliness of the decisions made
2	**ЗК 6.** Knowledge and understanding of the subject area and comprehension of the profession.	To know the state regulation of the quality of medicines	carry out professional activities that require updating and integration of knowledge	To form a communication strategy in professional activity	To be responsible for professional development with a high level of autonomy
3	**ЗК 11.** Ability to assess and ensure the quality of performed work	To know the evaluation methods of performance indicators	To ensure quality performance of professional work	Establish connections to ensure performance of the quality work	To be responsible for the high quality work performance
4	**ЗК 12.** Ability to perform research	To know the components of the health care system,	To search for scientific sources of information; to	To use the information data	To be responsible for

	at the appropriate level	planning and evaluation of scientific research	choose the appropriate method for carrying out the scientific research; use methods of mathematical analysis and modeling, theoretical and experimental research in pharmacy.	from scientific sources	the development and implementation of planned projects
7	**ФК 12.** Ability to use knowledge of regulations, legislation of Ukraine, and recommendations of good pharmaceutical practices in professional activities	To know basics of the law system and pharmaceutical legislation; basic mechanisms of state regulation of pharmaceutical activity; The principles of pharmaceutical care organization, basic principles of the population pharmaceutical supply organization; legal and ethical norms of pharmaceutical activity	- to use normative-legal acts regulating pharmaceutical activity in Ukraine and abroad; to monitor and identify changes and additions to domestic pharmaceutical legislation; - compile information on the material and technical base of the pharmacy and drugstore, as well as organizational documents necessary for their activities; - to form relationships with patients and doctors in order to meet the ethical criteria of the WHO and the principles of good pharmacy practice to promote drugs on the market, minimize abuse and misuse of drugs	To form conclusions and professionally apply laws and regulations	To be responsible for the qualified and timeliness use of the regulations in professional activities
8	**ФК 19.** Ability to organize and control the quality of medicines in accordance with the requirements of the current State Pharmacopoeia of Ukraine and good practices in pharmacy, determine methods of sampling for control of medicines and standardize them in accordance with current requirements, prevent the spread of counterfeit	To know the state regulation of the quality of medicines; - chemical reactions kinetics and catalysis; - chemical reactions velocity and equilibrium; physical-chemical properties of medicines; - methods of qualitative and quantitative analysis of drugs; - analysis of dosage forms in the production process; - tests for the purity of drugs; - potentiometric analysis; - quality indicators of parenteral, solid, soft and aerosol dosage forms; - stability and shelf life of drugs; - analysis of purified water,	- to determine the presence of impurities in raw materials and drugs; - to determine basic characteristic of drugs using physical methods of analysis; - to determine basic characteristic of drugs by visual and instrumental methods (transparency, color, pH, refractive index, angle of rotation, density); - to perform analysis of purified water, highly purified water and water for injections by chemical instrumental methods – to determine alcohol concentration in the solutions; - to take samples of medicinal substances, plant raw material, auxiliary	Carry out quality control of drugs and their certification	Be responsible for certifying and preventing the spread of counterfeit drugs

	medicines	highly purified water and water for injections; - purification, processing and disposal of industrial waste.	materials for analysis; - to fill up the quality passport, to carry out serial control; - to determine stability of medicines under the storage during the established shelf life.		
9	**ФК 20**. Ability to develop methods for quality control of medicines, including active pharmaceutical ingredients, medicinal plant raw materials and excipients using physical, chemical, physicochemical, biological, microbiological, pharmacotechnological and pharmacoorganoleptic control methods	To know: - qualitative analysis of cations and anions; - drugs of inorganic nature; - elemental analysis and analysis by functional groups; - functional analysis of organic compounds by functional groups; - general methods of analysis of inorganic and organic drugs; - chemical titrimetric methods of analysis; - chromatographic methods of identification, study of purity and quantitative content of drugs; - optical activity and specific rotation; - gravimetric method of analysis; - functional analysis of organic compounds; - basic concepts of titrimetric analysis; - spectral methods of analysis	- to determine cations and anions of active substances of inorganic nature in raw materials, intermediates and finished products by chemical methods; - to determine the functional groups of active substances of organic nature in raw materials, semi-finished products, finished products; - to prepare titrated, working solutions and solutions of indicators from chemical reagents and to establish percentage concentration and molarity by titrimetric and physicochemical methods	Develop methods of quality control of pharmaceutical products	Be responsible for the validity of the developed quality control methods

Learning outcomes:

Integrative final program learning outcomes (ПРН – program learning outcomes), the formation of which is facilitated by the discipline:
ПРН 1 Carry out professional activities in social interaction based on humanistic and ethical principles; identify future professional activities as socially significant for human health.
ПРН 2 Apply knowledge of general and professional disciplines in professional activities.
ПРН 3 Adhere to the norms of sanitary and hygienic regime and safety requirements in carrying out professional activities.
ПРН 4 Demonstrating 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.
ПРН 6 Argue information for decision-making, be responsible for them in standard and non-standard professional situations; adhere to the principles of deontology and ethics in professional activities.
ПРН 7 Perform professional activities using creative methods and approaches.
ПРН 8 Carry out professional communication in the state language, use the skills of oral communication in a foreign language, analyzing texts of professional orientation and translate foreign language information sources.
ПРН 9 Carry out professional activities using information technologies, "Information Databases", navigation systems, Internet resources, software and other information and communication technologies.
ПРН 12 Analyze the information obtained as a result of scientific research, summarize, systematize and use it in professional activities.
ПРН 14 To determine the advantages and disadvantages of drugs of different pharmacological groups, taking into account their chemical, physicochemical, biopharmaceutical, pharmacokinetic and pharmacodynamic features. To recommend to consumers over-the-counter medicines and other products of the pharmacy range with the provision of counseling and pharmaceutical care.
ПРН 16 To determine the impact of factors influencing the processes of absorption, distribution, deposition, metabolism and excretion of the drug and due to the condition, features of the human body and physicochemical properties of drugs.
ПРН 19. Predict and determine the impact of environmental factors on the quality of medicines and consumer characteristics of other products of the pharmacy range during their storage.
ПРН 20 Implement a set of organizational and managerial measures to provide the population and health care facilities with medicines and other products of the pharmacy range. Carry out all types of accounting in pharmacies, administrative records, processes of commodity analysis.
ПРН 24 Plan and implement professional activities on the basis of regulations of Ukraine and recommendations of good pharmaceutical practices.
ПРН 30 Ensure quality control of medicines and document its results. Manage quality risks at all stages of the life cycle of medicines.
ПРН 31 Carry out all types of quality control of medicines; draw up quality certificates for the batch of the medicinal product and the certificate of analysis, taking into account

the requirements of current regulations, the State Pharmacopoeia of Ukraine and the results of quality control. Develop specifications and quality control methods in accordance with the requirements of the current State Pharmacopoeia.

According to the learning outcomes the student should:
- know the basic packages of modern computer programs used in pharmacy;
- learn to use databases, specialized (medical-biological and chemical-pharmaceutical) information available on the INTERNET or on electronic media;
- know the approaches and principles of information retrieval on the INTERNET;
- be able to search for specialized information;
- know the basic approaches and principles to the search and innovative drug development;
- to get acquainted with innovative technologies in pharmacy, and in particular pharmaceutical and medical chemistry, and their software;
- get acquainted with chemical software packages (used for molecular modeling, docking, study of structure-activity relationship;
- master the basic techniques of obtaining structural information, building databases, virtual screening based on available packages of computer programs;
- get acquainted with modern medicines and lead structures that have been designed using computer technologies;
- know the aspects of using modern software packages in the field of practical pharmacy (pharmacy, wholesale company).

2. Information volume of the academic discipline

3 Credits ECTS, 90 hours are allocated for the study of the discipline.

Structure of the discipline:

Content module 1. **Basic techniques and principles of searching for specialized information using computer technologies. Pharmacy on the Internet**

Contents of the program. Computer operating systems and their types, licensing conditions. Basic techniques and principles of searching for specialized information on the INTERNET. Pharmaceutical resources on the INTERNET. Electronic libraries. Databases of specialized information. Ukrainian pharmacy on the Internet.
Specific goals:
- study of approaches and principles of information retrieval on the INTERNET and their use to search for specialized information;
- study and practical use of basic databases of specialized medical-biological and chemical-pharmaceutical information;
- acquaintance with the presentation of pharmacy on the INTERNET.

Topic 1. Modern office software packages, software licensing in Ukraine. Main principles of the information search on the Internet. Search servers, HTTP-protocol,

hyperlink system. Information relevancy/reliability estimation, “information filter” systems

Topic 2. Pharmaceutical resources in the Internet. Search in the data bases containing pharmaceutical and biomedical information, bibliographic and full-text database of scientific journals, patent data bases (MEDLINE, RxLIST, State register of medicines of Ukraine). Patent databases. Information availability.

Topic 3. Practical use of the Internet and digital databases for the information search about drugs.

Topic 4. Search for the information on the drugs on the stages of pre-clinical/clinical study, their registration, usage.

Content module 2. Modern approaches and methodology for drug development (drug design)

Contents of the program. Basic chemical and pharmaceutical software packages and their use. A brief history of the development of approaches to the development of medicines. Successes and achievements of pharmaceutical/medical chemistry. Brief description of innovative technologies in pharmacy and drug-design methodology. Virtual screening (selection of REOS, 2D-similarity, generation of 3D-conformations and assessment of their similarity to pharmacologically active compounds). Molecular descriptors, QSAR analysis. Methodology of molecular flexible docking. Combinatorial chemistry and total highly effective screening. Quantum chemical and mathematical bases of molecular modeling methods. The concept of lead-structure and its optimization.

Specific goals:

- study of approaches and principles to search and creation of innovative medicines;
- study of the main methodological approaches to "drug design".
- mastering the skills of working with chemical software packages;
- mastering the skills of working with software packages used for molecular modeling, docking, structure-activity relationship study.

Topic 5. Computational chemical programs and their functional possibilities (Accelrys, CHEMOffice, ACDLabs). Performing situational problems using different chemical editors (Accelrys Draw, ChemWin, ACDLabs Sketch).

Topic 6. Accelrys (ISIS) (Base, Draw) package’s capabilities as the system for chemical databases operating. Processing of the chemical compounds’ databases.

Topic 7. Operation of the chemical compounds’ libraries. Using chemical editors to search for information in specialized databases.

Topic 8. Modern methods of drug discovery (main strategies). Virtual libraries, virtual screening, methods and algorithms, program packages for different stages of the virtual screening realization

Topic 9. Modern approaches to the design of new biologically active compounds. The concept of ligand-, target-based, "fragment-based" design, "structure-based" design.

Topic 10. Calculation of a series of structure's molecular descriptors. Lipinski's rule of five. Computational presentation of molecular structure and information on biological/pharmacological effects of real or virtual compounds.

Topic 11. Modern methods of structure-activity relationship study. Working out the QSAR-analysis methodology; software programs for its implementation.

Topic 12. Usage of the ACDLabs and PASS C&T software and packages available on the Internet for the virtual screening and prediction of the virtual compounds' biological activity (2D similarity). Estimation of the pharmacokinetic parameters and prediction of the biological active substances' metabolism.

Topic 13. Practical use of the molecular modelling (molecular mechanics methods and semiempirical quantum chemical methods) for the molecules' 3D structure modelling in the drug design process.

Topic 14. Molecular docking as one of the prediction methods of binding affinity between ligands and biomacromolecules – potential targets for the drugs. Correlation of the scoring functions with the experimental data.

Topic 15. Lead-compounds structure optimization.

Topic 16. Other algorithms and approaches of virtual screening and drug design.

Content module 3. **The use of computer technologies in practical pharmacy.**
Contents of the program. Use of the software packages in practical pharmacy ("warehouse" programs, consolidated e-price list, etc.). "Means of communication" and cooperation within the vertical of the pharmaceutical industry.
Specific goals:

- study of the aspects of modern software packages usage of in the field of practical pharmacy (pharmacy, wholesale company);
- know the approaches to the organization of "communication" within the vertical of the pharmaceutical industry.

Topic 17. Computer technologies application in automation of the working places in the pharmacies, wholesale pharmaceutical companies. Examples of the used software. Functional requirements to the needed software.

Topic 18. Organization of communication and integration of manufacturers, distributors (wholesale and retail) and specialists in the field of pharmacy. Functional possibilities of the "Morion" company. Online pharmacy, opportunities and realities.

3. Structure of the learning discipline

№	Topic	Lecturs	Practical classes	Out-of-class work	Individual work
Content module 1. ***Basic techniques and principles of searching for specialized information using computer technologies. Pharmacy on the Internet***					
1	Modern office software packages, software licensing in Ukraine. Main principles of the information search on the Internet. Search servers, HTTP-protocol, hyperlink system. Information relevancy/reliability estimation, "information filter" systems	**0,5**	**2**	**4**	Work with educational and methodical literature, Internet resources; work on solving individual situational tasks
2	Pharmaceutical resources in the Internet. Search in the data bases containing pharmaceutical and biomedical information, bibliographic and full-text database of scientific journals, patent data bases (MEDLINE, RxLIST, State register of medicines of Ukraine). Patent databases. Information availability	**1,0**	**2**		
3	Practical use of the Internet and digital databases for the information search about drugs		**2**	**4**	
4	Search for the information on the drugs on the stages of pre-clinical/clinical study, their registration, usage.		**2**	**4**	
Total according to the content module 1			**8**	**12**	
Content module 2. ***Modern approaches and methodology for drug development (drug design)***					
5	Computational chemical programs and their functional possibilities (Accelrys, CHEMOffice, ACDLabs). Performing situational problems using different chemical editors (Accelrys Draw, ChemWin, ACDLabs Sketch).		**2**		Work with educational and methodical literature, Internet resources; appropriate software packages and modules Work on solving individual situational tasks
6	Accelrys (ISIS) (Base, Draw) package's capabilities as the system for chemical databases operating. Processing of the chemical compounds' databases.		**2**		
7	Operation of the chemical compounds' libraries. Using chemical editors to search for information in specialized databases.		**2**		
8	Modern methods of drug discovery (main strategies). Virtual libraries, virtual screening, methods and algorithms, program packages for different stages of the virtual screening realization	**0,5**	**2**	**4**	
9	Modern approaches to the design of new biologically active compounds. The concept of ligand-, target-based, "fragment-based" design, "structure-based" design.	**0,5**	**2**	**4**	
10	Calculation of a series of structure's molecular descriptors. Lipinski's rule of five. Computational presentation of molecular structure and information on biological/pharmacological effects of real or virtual compounds	**0,5**	**2**	**4**	
11	Modern methods of structure-activity relationship	**0,5**	**2**	**4**	

	study. Working out the QSAR-analysis methodology; software programs for its implementation				
12	Usage of the ACDLabs and PASS C&T software and packages available on the Internet for the virtual screening and prediction of the virtual compounds' biological activity (2D similarity). Estimation of the pharmacokinetic parameters and prediction of the biological active substances' metabolism.		**2**	**4**	
13	Practical use of the molecular modelling (molecular mechanics methods and semiempirical quantum chemical methods) for the molecules' 3D structure modelling in the drug design process.		**2**	**4**	
14	Molecular docking as one of the prediction methods of binding affinity between ligands and biomacromolecules – potential targets for the drugs. Correlation of the scoring functions with the experimental data.		**2**	**4**	
15	Lead-compounds structure optimization		**2**		
16	Other algorithms and approaches of virtual screening and drug design.		**2**	**4**	
Total according to the content module 2			**24**	**32**	
Content module 3. ***The use of computer technologies in practical pharmacy.***					
17	Computer technologies application in automation of the working places in the pharmacies, wholesale pharmaceutical companies. Examples of the used software. Functional requirements to the needed software	**0,25**	**2**	**3**	Work with educational and methodical literature, Internet resources; appropriate software packages and modules Writing a CV
18	Organization of communication and integration of manufacturers, distributors (wholesale and retail) and specialists in the field of pharmacy. Functional possibilities of the "Morion" company. Online pharmacy, opportunities and realities	**0,25**	**2**	**3**	
Total according to the content module 3			**4**	**6**	
Total hours 90/3,0 credits ECTS		**4**	**36**	**50**	
Final control					**1cr., Credit**

Classroom load – 44,4%; out-of-class work – 55,6%.

4. Topics of the lectures

№	Topic of the lecture	Number of hours
Content module 1. **Basic techniques and principles of searching for specialized information using computer technologies. Pharmacy on the Internet.** ***Content module 3***. **The use of computer technologies in practical pharmacy**		
1	Basic principles and approaches to the information search. Pharmacy on INTERNET. Characteristic of the most important information databases. Characteristics of the most important databases of medical/pharmaceutical information (PubMed, Science-direct etc.), bibliographic and full text databases of scientific journals, patents; main publishers of scientific information. Software used in pharmacy (R&D, industrial, drugstore).	2
Content module 2. Modern approaches and methodology for drug development (drug design)		
2	Background for innovative technology. Short history of drug development process. Successes and achievements of pharmaceutical and medicinal chemistry. Innovative technologies – methodology of drug design (virtual screening, combinatorial chemistry, high throughput screening, molecular-modelling, molecular docking and the software for these approaches implementation). Basic strategies of drug development, stages from "molecule to drug", role and significance of *in silico* methods. Molecular descriptors, software for their calculation, QSAR-analysis. Lead- and hit-compounds, ways of their optimization.	2
TOTAL		**4**

5. Теми практичних занять

№	Topic of the practical class	Number of hours
Content module 1. **Basic techniques and principles of searching for specialized information using computer technologies. Pharmacy on the Internet**		
1	Modern office software packages, software licensing in Ukraine. Main principles of the information search on the Internet. Search servers, HTTP-protocol, hyperlink system. Information relevancy/reliability estimation, “information filter” systems	2
2	Pharmaceutical resources in the Internet. Search in the data bases containing pharmaceutical and biomedical information, bibliographic and full-text database of scientific journals, patent data bases (MEDLINE, RxLIST, State register of medicines of Ukraine). Patent databases. Information availability	2
3	Practical use of the Internet and digital databases for the information search about drugs	2
4	Search for the information on the drugs on the stages of pre-clinical/clinical study, their registration, usage.	2
Total		**8**
Content module 2. ***Modern approaches and methodology for drug development (drug design)***		
5	Computational chemical programs and their functional possibilities (Accelrys, CHEMOffice, ACDLabs). Performing situational problems using different chemical editors (Accelrys Draw, ChemWin, ACDLabs Sketch).	2
6	Accelrys (ISIS) (Base, Draw) package’s capabilities as the system for chemical databases operating. Processing of the chemical compounds’ databases.	2
7	Operation of the chemical compounds’ libraries. Using chemical editors to search for information in specialized databases.	2
8	Modern methods of drug discovery (main strategies). Virtual libraries, virtual screening, methods and algorithms, program packages for different stages of the virtual screening realization	2
9	Modern approaches to the design of new biologically active compounds. The concept of ligand-, target-based, "fragment-based" design, "structure-based" design.	2
10	Calculation of a series of structure’s molecular descriptors. Lipinski’s rule of five. Computational presentation of molecular structure and information on biological/pharmacological effects of real or virtual compounds	2
11	Modern methods of structure-activity relationship study. Working out the QSAR-analysis methodology; software programs for its implementation	2
12	Usage of the ACDLabs and PASS C&T software and packages available on the Internet for the virtual screening and prediction of the virtual compounds’ biological activity (2D similarity). Estimation of the pharmacokinetic parameters and prediction of the biological active substances’ metabolism.	2
13	Practical use of the molecular modelling (molecular mechanics methods and semiempirical quantum chemical methods) for the molecules’ 3D structure modelling in the drug design process.	2
14	Molecular docking as one of the prediction methods of binding affinity between ligands and biomacromolecules – potential targets for the drugs. Correlation of the scoring functions with the experimental data.	2
15	Lead-compounds structure optimization	2
16	Other algorithms and approaches of virtual screening and drug design.	2
Total		**24**
Content module 3. ***The use of computer technologies in practical pharmacy.***		
17	Computer technologies application in automation of the working places in the pharmacies, wholesale pharmaceutical companies. Examples of the used software. Functional requirements to the needed software	2
18	Organization of communication and integration of manufacturers, distributors (wholesale and retail) and specialists in the field of pharmacy. Functional possibilities of the “Morion”	2

	company. Online pharmacy, opportunities and realities	
Total		4
Number of hours of practical classes of the discipline		**36**

6. Topics of the out-of-class work

№	Topic	Number of hours	Type of control
Content module 1. **Basic techniques and principles of searching for specialized information using computer technologies. Pharmacy on the Internet.**			
1	Modern office software packages (Microsoft Office, OpenOffice, StarOffice, etc.), advantages and disadvantages, licensing conditions. Use of office programs (text editors, spreadsheets, presentation systems and database management systems) in pharmacy.	4	Current control on practical classes/e-reports
2	Search for information about drug of a certain pharmacological group on the INTERNET according to the lecturer's instructions.	4	
3	Search and systematization of information from the MEDLINE database on the topic given by the teacher..	4	
Total		**12**	
Content module 2. ***Modern approaches and methodology for drug development (drug design).***			
4	Computer approaches in predicting the toxicity and pharmacokinetic parameters of potential drug-like molecules	8	Current control on practical classes/e-reports
5	Combinatorial chemistry and high throughput screening as *in silico* modern approaches to drug search.	8	
6	Concepts, classification and types of molecular descriptors and their use in modeling the structure-activity relationship	8	
7	Comparative characteristics of algorithms and existing docking software	8	
Total		**32**	
Content module 3. ***The use of computer technologies in practical pharmacy.***			
8	Software packages used to implement the practical activities of the pharmacist abroad	3	Current control on practical classes/e-reports
9	Model of a comprehensive software product to meet the needs of automation of the working place at pharmacies.	3	
Total		**6**	
Number of hours of out-of-class work on the discipline		**50**	

7. Methods of studies

Explanatory-illustrative, problematic presentation, partially-exploratory.
Studying Computer modelling in pharmacy students use textbooks, lecture notes, methodological guidelines, chemical computer software, molecular models, laboratory devices and glassware necessary for performing experiments.

Methods for organization and accomplishment of studies are:
a) lectures
b) practical classes
c) students' independent study
d) control work.

The topics of the lecture course cover the problematic issues of the appropriate sections of Computer modelling in pharmacy

Practical classes according to the methods of their organizations are seminar and laboratory classes; provide laboratory studies of the quality of drugs. Students are recommended to draw up research protocols in laboratory classes.

The structure of the organization of practical classes includes:
- Discussion and explanation of the most difficult issues of the topic;
- Written survey;
- Execution of practical works.
- The result of the class.

8. Methods of control

Types of control: initial, current and final.

Form of final control according to the curriculum: credit (5 semester).

The initial control of theoretical training is carried out at the beginning of each class.

Current control is carried out at each class in accordance with specific objectives, as well as during the individual work of the teacher with the student for those topics that the student develops independently and they are not part of the structure of the practical lesson. A standardized form of control of theoretical and practical training of students is used. At each practical lesson the student answers test tasks, questions on the topic of practical lesson, knowledge of which is necessary to understand the current topic, lecture course and independent work related to the current lesson, demonstrates knowledge and skills of practical skills according to the theme of laboratory class.

The test is performed individually according to the tasks of the lecturer and is evaluated by the appropriate assessment before the session.

Students' independent work is assessed during the current control of the topic in the relevant lesson. Assimilation of topics that are submitted only for independent work is controlled during the final control. Assessment of practical training of students - as a result of the practical part - is made in the form of a protocol.

Criteria for evaluating current learning activities:

A grade of "5" (excellent) gets the student who perfectly mastered the theoretical material of the topic, demonstrates deep and comprehensive knowledge of the topic, the main provisions of scientific sources and recommended literature, logically thinks and builds the answer, freely uses the acquired theoretical knowledge in analyzing practical material, expresses his attitude to certain problems, demonstrates high level of practical skills acquisition.

Grade "4" (good) gets the student has well mastered theoretical material of the lesson, knows the main aspects of primary sources and recommended literature, expresses his views on certain problems, but assumes certain inaccuracies and errors in the logic of the presentation of theoretical content or in the implementation of practical skills.

Grade "3" (satisfactory) gets the student has mainly mastered the theoretical knowledge of the subject, is guided by primary sources and recommended literature, but unconvincingly answers, confuses concepts, additional questions cause the student uncertainty or lack of stable knowledge; answering questions of a practical nature, reveals inaccuracies in knowledge, is unable to assess facts and phenomena, relates them to future activities, makes mistakes in the implementation of practical skills.

Grade "unsatisfactory" (2) gets the student has not mastered the studied material of the topic, does not know the scientific facts, definitions, almost does not navigate in the original sources and recommended literature, there is no scientific thinking, practical skills are not formed.

Final control is carried out at the end of the semester.

9. Scheme of accrual and distribution of points received by students:

The grade in the discipline is based on the results of current educational activities and is expressed on a scale:

- "credited"

the student must receive for the current academic activity at least 3.0 (expressed as the arithmetic mean of points for classes included in the structure of the discipline - according to the Regulations on the working curriculum of the discipline and guidelines for its development (protocol of CMC Danylo Halytsky LNMU №2 from 23.04.2015);

- «not credited»

the student must receive for the current academic activity less than 3.0 (expressed as the arithmetic mean of points for classes included in the structure of the discipline - according to the Regulations on the working curriculum of the discipline and guidelines for its development (protocol of CMC Danylo Halytsky LNMU №2 from 23.04.2015).

The maximum number of points that a student can score for the current educational activity in the study of the discipline is 200 points.

The minimum number of points that a student must score for the current academic activity to enroll in the discipline is 120 points.

The calculation of the number of points is based on the grades received by the student on a 4-point (national) scale during the study of the discipline, by calculating the arithmetic mean (CA), rounded to two decimal places. The resulting value is converted into points on a multi-point scale as follows:

$$x = \frac{CA \times 200}{5}$$

Students' independent work is assessed during the current control of the topic in the relevant lesson.

Points from the discipline are independently converted into both the ECTS scale and the 4-point (national) scale. ECTS scale scores are not converted to a 4-point scale and vice versa. The scores of students studying in one specialty, taking into account the number of scores scored in the discipline are ranked on the ECTS scale as follows:

Point ECTS	Statistical indicator
A	The best 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

Ranking with assignments of grades "A", "B", "C", "D", "E" is carried out for students of this course who study in one specialty and have successfully completed the study of the discipline. Students who received FX, F ("2") ratings are not included in the list of ranked students. Students with an FX score after repassing the exam receive an "E" score automatically.

Discipline scores for students who have successfully completed the program are converted into a traditional 4-point scale according to the absolute criteria, which are given in the table below:

Points in the discipline	Score according to a 4-point scale
From 170 to 200 points	5
From 140 to 169 points	4
From 139 points to the minimum number of points that a student must score	3
Below the minimum number of points that a student must score	2

The ECTS score is not converted to the traditional scale, as the ECTS scale and the four-point scale are independent.

The objectivity of the assessment of students' learning activities is checked by statistical methods (correlation coefficient between ECTS assessment and assessment on a national scale).

10. Methodological support

Guidelines for preparation for practical classes and independent work:

- plan of lectures,
- plans of practical classes,
- tasks for laboratory work, out-of class work,
- questions, tasks and MCQ for current and final control of knowledge and skills of students, after attestation monitoring of acquired knowledge and skills in the discipline.

11.The list of questions submitted for the final (current) control

1. Operating systems and licensing conditions.
2. Types of electronic media and their capacity.
3. Advantages and disadvantages of operating systems used in Ukraine.
4. The main components of office software packages and their functional purpose.
5. Basic services of the INTERNET, principles of network construction.
6. Cyrillic and English search servers on the INTERNET.
7. Protocols of information exchange, their purpose.
8. Domain name system.
9. Degrees of reliability and reliability of information on the INTERNET.
10. Pharmaceutical resources on the INTERNET.
11. Pharmaceutical and medical databases. Bases of existing drugs.
12. Electronic libraries containing pharmaceutical periodical literature.
13. Higher pharmaceutical and medical institutions on the INTERNET.
14. International and regional reputable pharmaceutical and medical institutions on the INTERNET.
15. Sources of patent information on the INTERNET.
16. Basic modern strategies for drug development.
17. The main stages and paths "from the idea/molecule to the drug".
18. Methods for determining the biological activity of compounds.
19. Chemical editors.
20. Capabilities of databases of chemical information management.
21. Virtual library - definition, types, methods of construction, limits of use.
22. Virtual screening. Describe the concept, its stages.
23. Software for virtual screening.
24. Combinatorial chemistry, principles, possibilities of application.
25. High throughput screening.
26. Docking. Principles and approaches.
27. Basic methods of molecular modeling of 3D-structure of molecules.
28. QSAR analysis. Basic provisions and applied value.
29. Lipinsky's rules. The concept of "medicine".
30. Concepts and types of molecular descriptors. Methods of their calculation and establishment.
31. Features of optimization of lead-structures.
32. Modern drugs developed using computer technologies.
33. Stages of planning research in pharmaceutical chemistry.

34. Principles of construction and functional requirements for warehousing programs for use in practical pharmacy.
35. The concept of electronic pharmacy, advantages, disadvantages, realities of usage.
36. The concept of consolidated e-mail, problems of use and standardization of information (methods of overcoming).

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