Syllabus "Computer modelling in Pharmacy"

1. General information	
Faculty	Pharmaceutical
Educational Program	22 Healthcare, 226 Pharmacy, industrial pharmacy the second (master's) level, full-time
Academic year	2021-2022
Subject	Computer modelling in Pharmacy, OK 21
Department	Department of Pharmaceutical, Organic and Bioorganic chemistry Pekarska 69, Lviv, Tel. +38(032)275-59-66, 275-59-77, 278-64-34 Kaf_pharmchemistry@meduniv.lviv.ua
Head of the Department	Roman Lesyk, Doctor of Science, Professor roman.lesyk@gmail.com
Year of study	3^{d} year
Semester	5
Type of course / module	Compulsory
Lecturers	Anna Kryshchyshyn-Dylevych, PhD, DSc, associate professor, kryshchyshyn.a@gmail.com ; Andriy Lozynskyy PhD, ssociate professor, lozynskyiandrii@gmail.com ; Sergiy Golota PhD, associate professor, golota_serg@yahoo.com
Erasmus yes/no	No
The person responsible for the syllabus	Anna Kryshchyshyn- Dylevych, PhD, DSc, assoc. prof. kryshchyshyn.a@gmail.com; A. Lozynskyy, PhD, assoc. prof.; lozynskyiandrii@gmail.com
Number of credits ECTS	**14**
Number of hours	90 (lectures – 4 hours, Practical classes – 36 hours, Out-of-class Work – 50 hours)
Language of study	English
Information about consultations	Each Thursday at 13^{05}-15^{20}
Address, telephone and regulations of the clinical base, office ... (if	

necessary)	

2. Short annotation to the course

The discipline "Computer modelling in pharmacy" belongs to the obligatory 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 novel drug development.

3. The purpose and objectives of the course

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.

The main tasks are:

1. acquire skills for searching medical and biological information on the INTERNET or electronic databases for professional activities;
2. astering the available software packages for future professional activities;
3. 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;
4. study of modern drugs created with the usage of innovative technologies.

Competences and learning outcomes, the formation of which provides the study of the Discipline

ЗК – General competencies; ФК – Special responsibility

ЗК 2. The ability to apply knowledge in practical situations;

ЗК 6. Knowledge and understanding of the subject area and comprehension of the profession.;

ЗК 11. Ability to assess and ensure the quality of performed work.;

ЗК 12. Ability to perform research at the appropriate level.

ФК 12 Ability to use knowledge of regulations, legislation of Ukraine, and recommendations of good pharmaceutical practices in professional activities

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 medicines;

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.

4. Prerequisites of the course

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

5. Program learning outcomes

List of the learning outcomes

Learning outcome code	The content of the learning outcome	Reference to the code of the competence matrix
Зн – Knowledges Ум – skills		ПРН – program learning

AB – independence and responsibility K – competence		outcomes
Зн-1	to know the methods of knowledge implementation in solving practical issues	*ПР 1, ПР2, ПР3* *ПР5, ПР7,* *ПР12, ПР15, ПР16, ПР17, ПР18, ПР19, ПР20*
Зн-2	structure and features of professional activity;	
Зн-3	methods of searching for pharmaceutical information in the global network	
Зн-4	components of the health care system, planning and evaluation of scientific research	
Зн-5	basics of the law system and pharmaceutical legislation; basic mechanisms of state regulation of pharmaceutical activity	
Зн-6	state regulation of the quality of medicines	
Зн-7	algorithms for drug development	
Ум-1	use professional knowledge to solve practical situations	
Ум-2	carry out professional activities that require updating and integration of knowledge	
Ум-3	to ensure quality performance of professional work	
Ум-4	search for scientific sources of information; to choose the appropriate method for carrying out the scientific research; use methods of mathematical analysis and modeling, theoretical and experimental research in pharmacy	
Ум-5	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	
К-1	To establish connections with business entities	
К-2	To form a communication strategy in professional activity	
К-3	Establish connections to ensure performance of the quality work	
К-4	To use the information data from scientific sources	
К-5	To form conclusions and professionally apply laws and regulations	

K-6	To carry out quality control of medicines and their certification	
K-7	To develop methods of quality control of pharmaceutical products	
AB-1	To be responsible for timeliness of the decisions made	
AB-2	To be responsible for professional development with a high level of autonomy	
AB-3	To be responsible for the high quality work performance	
AB-3	To be responsible for the development and implementation of planned projects	
AB-4	To be responsible for the qualified and timeliness use of the regulations in professional activities	
AB-5	To be responsible for certifying and preventing the spread of counterfeit medicines	
AB-6	Be responsible for the validity of the developed quality control methods	

6. Format and scope of the course

Format of the course	Full-time course, distance-learning course	
Type of classes	Number of hours	Number of groups
Lectures	**52**	16
Practical classes	**216**	16
Seminars	**-**	
Out of class work	**152**	16

7. Topics and content of the course

Class type code	Topic	Content of the training	Code of the training result	Lecturer
Л – lecture, П – practical class, СРС – out-of-class work				
Л-1 *(lecture-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,	To acquaint the students with the basic techniques and principles of searching for specialized information, its evaluation and analysis	*Зн 1-4,6,8,9 Ум 1,5,7-9,10,11*	Anna Kryshchyshyn-Dylevych, PhD, DSc, assoc. prof.

	patents; main publishers of scientific information. Software used in pharmacy (R&D, industrial, drugstore).			
Л-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.	To acquaint students with the innovative technologies in pharmacy, drug-design methodologies (virtual screening, combinatorial chemistry, high throughput screening, molecular-modelling)	*Зн 1-4,6,8,9 Ум 1,5,7-9,10,11*	Anna Kryshchyshyn-Dylevych, PhD, DSc, assoc. prof.
П-1 *(практичне заняття 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	To acquaint students with office software packages, software licensing in Ukraine	*Зн 1-4,6,8,9 Ум 1,5,7-9,10,11*	R. Lesyk, PhD, DSc, prof.; A. Kryshchyshyn-Dylevych, PhD, DSc, assoc. prof.; A. Lozynskyy, PhD, assoc. prof.; I. Yushyn, assist. prof.

П-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.	Introduce the students to pharmaceutical resources on the Internet	*Зн 1-4,6,8,9 Ум 1,5,7-9,10,11*	R. Lesyk, PhD, DSc, prof.; A. Kryshchyshyn-Dylevych, PhD, DSc, assoc. prof.; A. Lozynskyy, PhD, assoc. prof.; I. Yushyn, assist. prof.
П-3	Practical use of the Internet and digital databases for the information search about drugs	To acquaint the students with the practical use of the Internet and electronic databases on drugs	*Зн 1-4,6,8,9 Ум 1,5,7-9,10,11*	R. Lesyk, PhD, DSc, prof.; A. Kryshchyshyn-Dylevych, PhD, DSc, assoc. prof.; A. Lozynskyy, PhD, assoc. prof.; I. Yushyn, assist. prof.
П-4	Search for the information on the drugs on the stages of pre-clinical/clinical study, their registration, usage	To acquaint students with the algorithm of searching for information about drugs and/or biologically active compounds at the stage of preclinical/clinical research	*Зн 1-4,6,8,9 Ум 1,5,7-9,10,11*	R. Lesyk, PhD, DSc, prof.; A. Kryshchyshyn-Dylevych, PhD, DSc, assoc. prof.; A. Lozynskyy, PhD, assoc. prof.; I. Yushyn, assist. prof.
П-5	Computational chemical programs and their functional possibilities (Accelrys, CHEMOffice, ACDLabs). Performing situational problems using different chemical editors (Accelrys Draw, ChemWin, ACDLabs Sketch).	To acquaint students with different chemical software (Accelrys, CHEMOffice, ACDLabs)	*Зн 1-4,6,8,9 Ум 1,5,7-9,10,11*	R. Lesyk, PhD, DSc, prof.; A. Kryshchyshyn-Dylevych, PhD, DSc, assoc. prof.; A. Lozynskyy, PhD, assoc. prof.; I. Yushyn, assist. prof.

П-6	Accelrys (ISIS) (Base, Draw) package's capabilities as the system for chemical databases operating. Processing of the chemical compounds' databases.	To acquaint students with the usage of Accelrys (ISIS) (Base, Draw) package y as the system for chemical and pharmaceutical databases operating	*Зн 1-4,6,8,9 Ум 1,5,7-9,10,11*	R. Lesyk, PhD, DSc, prof.; A. Kryshchyshyn-Dylevych, PhD, DSc, assoc. prof.; A. Lozynskyy, PhD, assoc. prof.; I. Yushyn, assist. prof.
П-7	Operation of the chemical compounds' libraries. Using chemical editors to search for information in specialized databases.	Introduce students to libraries of chemical compounds. Using chemical editors to search for information in specialized databases	*Зн 5, 9, 10 Ум 2,3,4,6*	R. Lesyk, PhD, DSc, prof.; A. Kryshchyshyn-Dylevych, PhD, DSc, assoc. prof.; A. Lozynskyy, PhD, assoc. prof.; I. Yushyn, assist. prof.
П-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	To acquaint students with modern approaches to the drug development	*Зн 1-4,6,8,9 Ум 1,5,7-9,10,11*	R. Lesyk, PhD, DSc, prof.; A. Kryshchyshyn-Dylevych, PhD, DSc, assoc. prof.; A. Lozynskyy, PhD, assoc. prof.; I. Yushyn, assist. prof.
П-9	Modern approaches to the design of new biologically active compounds. The concept of ligand-, target-based, "fragment-based" design, "structure-based" design.	To acquaint students with modern approaches to the design of new biologically active compounds	*Зн 1-4,6,8,9 Ум 1,5,7-9,10,11*	R. Lesyk, PhD, DSc, prof.; A. Kryshchyshyn-Dylevych, PhD, DSc, assoc. prof.; A. Lozynskyy, PhD, assoc. prof.; I. Yushyn, assist. prof.
П-10	Calculation of a series of structure's molecular descriptors. Lipinski's rule of five.	To acquaint students with the calculation of molecular descriptors of the structure	*Зн 1-4,6,8,9 Ум 1,5,7-*	R. Lesyk, PhD, DSc, prof.; A. Kryshchyshyn-

	Computational presentation of molecular structure and information on biological/pharmacological effects of real or virtual compounds	(Lipinsky's rules).	*9,10,11*	Dylevych, PhD, DSc, assoc. prof.; A. Lozynskyy, PhD, assoc. prof.; I. Yushyn, assist. prof.
П-11	Modern methods of structure-activity relationship study. Working out the QSAR-analysis methodology; software programs for its implementation	To acquaint students with modern approaches to the study of the structure-activity relationship and the development of the methodology of QSAR-analysis	*Зн 1-4,6,8,9 Ум 1,5,7-9,10,11*	R. Lesyk, PhD, DSc, prof.; A. Kryshchyshyn-Dylevych, PhD, DSc, assoc. prof.; A. Lozynskyy, PhD, assoc. prof.; I. Yushyn, assist. prof.
П-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.	To acquaint students with the usage of 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).	*Зн 1-4,6,8,9 Ум 1,5,7-9,10,11*	R. Lesyk, PhD, DSc, prof.; A. Kryshchyshyn-Dylevych, PhD, DSc, assoc. prof.; A. Lozynskyy, PhD, assoc. prof.; I. Yushyn, assist. prof.
П-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	To acquaint students with practical use of molecular modelling methods (molecular mechanics methods and semiempirical quantum chemical methods) for the molecules' 3D structure modelling in the drug design process	*Зн 1-4,6,8,9 Ум 1,5,7-9,10,11*	R. Lesyk, PhD, DSc, prof.; A. Kryshchyshyn-Dylevych, PhD, DSc, assoc. prof.; A. Lozynskyy, PhD, assoc. prof.; I. Yushyn, assist. prof.
П-14	Molecular docking as one of the prediction methods of binding affinity between ligands and	To acquaint students with the use of docking research as a method of predicting the evaluation of the	*Зн 1-4,6,8,9 Ум 1,5,7-9,10,11*	R. Lesyk, PhD, DSc, prof.; A. Kryshchyshyn-Dylevych, PhD,

	biomacromolecules – potential targets for the drugs. Correlation of the scoring functions with the experimental data	binding of ligands to biomacromolecules		DSc, assoc. prof.; A. Lozynskyy, PhD, assoc. prof.; I. Yushyn, assist. prof.
П-15	Lead-compounds structure optimization	To acquaint students with the methods of lead-compounds optimization	*Зн 1-4,6,8,9 Ум 1,2,5,7-9,10,11*	R. Lesyk, PhD, DSc, prof.; A. Kryshchyshyn-Dylevych, PhD, DSc, assoc. prof.; A. Lozynskyy, PhD, assoc. prof.; I. Yushyn, assist. prof.
П-16	Other algorithms and approaches of virtual screening and drug design	To acquaint students with other algorithms and approaches of virtual screening and drug design	*Зн 1-4,6,8,9 Ум 1,2,5,7-9,10,11*	R. Lesyk, PhD, DSc, prof.; A. Kryshchyshyn-Dylevych, PhD, DSc, assoc. prof.; A. Lozynskyy, PhD, assoc. prof.; I. Yushyn, assist. prof.
П-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.	Introduce students to the use of computer technologies in automation of the working places in the pharmacies	*Зн 1-4,5,6,8,9 Ум 1,5,7-9,10,11*	R. Lesyk, PhD, DSc, prof.; A. Kryshchyshyn-Dylevych, PhD, DSc, assoc. prof.; A. Lozynskyy, PhD, assoc. prof.; I. Yushyn, assist. prof.
П-18	Organization of communication and integration of manufacturers, distributors (wholesale and retail) and specialists in the field of pharmacy. Functional possibilities of the “Morion”	To acquaint students with the automated marketing analysis of the offer of wholesale firms.	*Зн 1-4,6,8,9 Ум 1,5,7-9,10,11*	R. Lesyk, PhD, DSc, prof.; A. Kryshchyshyn-Dylevych, PhD, DSc, assoc. prof.; A. Lozynskyy, PhD, assoc. prof.;

	company. Online pharmacy, opportunities and realities			I. Yushyn, assist. prof.
CPC-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.	To acquaint students with modern office software packages (Microsoft Office, OpenOffice, StarOffice, etc.), their advantages and disadvantages, the conditions of their licensing	*Зн 1-4,6,8,9 Ум 1,5,7-9,10,11*	R. Lesyk, PhD, DSc, prof.; A. Kryshchyshyn-Dylevych, PhD, DSc, assoc. prof.; A. Lozynskyy, PhD, assoc. prof.; I. Yushyn, assist. prof.
CPC-2	Search for information about drug of a certain pharmacological group on the INTERNET according to the lecturer's instructions.	To teach students to search for information about drugs of a certain pharmacological group on the INTERNET	*Зн 1-4,6,8,9 Ум 1,5,7-9,10,11*	R. Lesyk, PhD, DSc, prof.; A. Kryshchyshyn-Dylevych, PhD, DSc, assoc. prof.; A. Lozynskyy, PhD, assoc. prof.; I. Yushyn, assist. prof.
CPC-3	Search and systematization of information from the MEDLINE database on the topic given by the teacher.	Introduce students to the MEDLINE database	*Зн 1-4,6,8,9 Ум 1,5,7-9,10,11*	R. Lesyk, PhD, DSc, prof.; A. Kryshchyshyn-Dylevych, PhD, DSc, assoc. prof.; A. Lozynskyy, PhD, assoc. prof.; I. Yushyn, assist. prof.
CPC-4	Computer approaches in predicting the toxicity and pharmacokinetic parameters of potential drug-like molecules.	Introduce students to computer approaches for predicting the toxicity and pharmacokinetic parameters of potential drugs	*Зн 1-4,6,8,9 Ум 1,5,7-9,10,11*	R. Lesyk, PhD, DSc, prof.; A. Kryshchyshyn-Dylevych, PhD, DSc, assoc. prof.; A. Lozynskyy, PhD, assoc. prof.; I. Yushyn,

				assist. prof.
CPC-5	Combinatorial chemistry and high throughput screening as *in silico* modern approaches to drug search.	To acquaint students with the concept of combinatorial chemistry and high throughput screening	*Зн 1-4,6,8,9 Ум 1,5,7-9,10,11*	R. Lesyk, PhD, DSc, prof.; A. Kryshchyshyn-Dylevych, PhD, DSc, assoc. prof.; A. Lozynskyy, PhD, assoc. prof.; I. Yushyn, assist. prof.
CPC-6	Concepts, classification and types of molecular descriptors and their use in modeling the structure-activity relationship	To acquaint students with the concept, classification and types of molecular descriptors and their use in modeling the structure-activity relationship	*Зн 1-4,6,8,9 Ум 1,5,7-9,10,11*	R. Lesyk, PhD, DSc, prof.; A. Kryshchyshyn-Dylevych, PhD, DSc, assoc. prof.; A. Lozynskyy, PhD, assoc. prof.; I. Yushyn, assist. prof.
CPC-7	Comparative characteristics of algorithms and existing docking software	To acquaint students with the methods of molecular docking	*Зн 1-4,6,8,9 Ум 1,5,7-9,10,11*	R. Lesyk, PhD, DSc, prof.; A. Kryshchyshyn-Dylevych, PhD, DSc, assoc. prof.; A. Lozynskyy, PhD, assoc. prof.; I. Yushyn, assist. prof.
CPC-8	Software packages used to implement the practical activities of the pharmacist abroad	To acquaint students with the software packages used to implement the practical activities of a pharmacist abroad	*Зн 1-4,6,8,9 Ум 1,5,7-9,10,11*	R. Lesyk, PhD, DSc, prof.; A. Kryshchyshyn-Dylevych, PhD, DSc, assoc. prof.; A. Lozynskyy, PhD, assoc. prof.; I. Yushyn, assist. prof.
CPC-9	Model of a comprehensive software product to meet the needs of	To acquaint students with methods of automation of the working place at	*Зн 1-4,6,8,9 Ум 1,5,7-*	R. Lesyk, PhD, DSc, prof.; A. Kryshchyshyn-

	automation of the working place at pharmacies.	pharmacies	*9,10,11*	Dylevych, PhD, DSc, assoc. prof.; A. Lozynskyy, PhD, assoc. prof.; I. Yushyn, assist. prof.

8. Verification of the learning outcomes

Current control is carried out during training sessions and aims to check the mastering of students' the learning material (it is necessary to describe the forms of current control during training sessions). Forms of assessment of current educational activities should be standardized and include control of theoretical and practical training. The final grade for the current educational activity is set on a 4-point (national) scale.

Learning outcome code	Code of the type of classes	Method of verification of learning outcomes	Enrollment criteria
Зн 1-10 *Ум 1-11* *К 1-9* *АВ 1-8*	*Л-1-26* *П-1-72* *СРС1-71*	**Types of educational activities of students are:** a) lectures b) practical classes c) out of class work. Thematic plans of lectures, practical classes, out of class work ensure the implementation in the educational process of all topics included in the content of the program. **The lecture course** consists of 2 lectures. The topics of the lecture course reveal the problematic issues of the relevant sections of computer technologies in pharmacy. During lectures, students develop theoretical basic knowledge; a motivational component and a general-indicative stage of mastering scientific knowledge during out of class work are formed. The lecture course makes maximum use of various didactic tools - multimedia presentations, educational films, slides. **Practical classes** are aimed at control of the mastering the theoretical material, formation of practical skills and abilities, as well as the ability to analyze and apply the acquired knowledge to solve practical	**A grade of "5" (excellent) -** the student 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) -** 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. Each lesson begins with a test to assess the initial level of knowledge and determine the degree of students' readiness for classes. The lecturer determines the purpose of the lesson and creates a positive cognitive motivation; answers questions that had arisen while preparing to the classes. One of the stages of the lesson is to carry out the practical task according to the instructions of the teacher. At the final stage of the lesson in order to assess the student's mastery of the topic he is asked to solve the situational tasks The teacher summarizes the lesson, gives students tasks for independent work, points out the main issues of the next topic and offers a list of recommended reading. The duration of the practical lesson is two academic hours.	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) -** 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) -** 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.
Current educational activity			
Current control is carried out during practical classes and includes: a) MCQ with one correct answer, with the definition of the correct sequence of actions, with the definition of conformity, with the definition of a certain area in the photo or diagram ("recognition"); The control is carried out using the Misa training platform.			

b) individual oral examination, interview;
c) solving typical situational problems;
e) control of practical skills.
When assessing the mastery of each topic for current learning activities the student is graded on a 4-point (traditional) scale. This takes into account all types of work provided by the discipline's program.
Scores on the traditional scale are converted into points.
The student's out of class work is assessed in practical classes and is part of the final assessment of the student.

Final control		
Type of final control	Credit	Enrollment criteria
Enrollment criteria of credit		
Credit	Credit is a form of final control of mastering by the student of theoretical and practical material on academic discipline. The final control is carried out in writing, using the Misa training platform, according to the schedule. Lasts 2 academic hours.	The maximum number of points – *200*

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:

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

For convenience, the table of recalculation on a 200-point scale is given:

The grade for the discipline, which ends with a credit, is defined as the sum of points. 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.

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).

9. Course policy

The policy of the course is determined by the system of requirements for the student in the study of the discipline
"Computer modeling in pharmacy" is based on the principles of academic integrity. Students are explained the value of acquiring new knowledge, the need for independent performance of all types of work, tasks provided by the work program of this discipline. Lack of references to used sources, fabrication of sources, writing off, interference in the work of other students are examples of possible academic dishonesty. Detection of signs of academic dishonesty in the student's work is the basis for its non-enrollment by the teacher, regardless of the extent of plagiarism or deception. Literary sources may be provided by the teacher exclusively for educational purposes without the right to transfer to third parties. Students are encouraged to use other literature sources not provided by the recommended list.

10. Literature

Main literature sources:

1. Kryshchyshyn, A. P., Kaminskyy, D. V., Atamanyuk, D. V., & Lesyk, R. B. (2015). Computer technologies in pharmacy-Filling in the gaps in Ukrainian PharmD curriculum. Currents in Pharmacy Teaching and Learning, 7(4), 556-559.
2. Mohs, R. C., & Greig, N. H. (2017). Drug discovery and development: Role of basic biological research. Alzheimer's & Dementia: Translational Research & Clinical Interventions, 3(4), 651-657.
3. Perkins, R., Fang, H., Tong, W., & Welsh, W. J. (2003). Quantitative structure-activity relationship methods: Perspectives on drug discovery and toxicology. Environmental Toxicology and Chemistry: An International Journal, 22(8), 1666-1679. D.L.Banville Mining chemical structural information from the drug literature // DDT. – 2006. – Vol.11, N 1/2. – P. 36-42.
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11. Equipment, logistics and software of the discipline

Methodical support:

- Working curriculum of the discipline;
- Multimedia support of lectures,
- Abstracts of lectures on the discipline;
- Methodical recommendations and developments for the lecturer;
- Misa learning platform;
- Methodical instructions for practical classes for students;
- Methodical materials that provide independent work of students;
- Tests and control tasks for practical classes;
- Questions and tasks for the final control.

12. Additional information

The department has a permanent student research group. Meetings take place in the auditorium №1,2.

Practical classes are held in the classrooms of the department at st. Pekarska, 69. Building of pharmaceutical chemistry.
Web site of the department - e-mail Kaf_pharmchemistry@meduniv.lviv.ua

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