Затверджено
на засіданні кафедри
протокол № 1
від "31" серпня 2021 р

CALENDAR AND THEMATIC PLAN
of laboratory works of "**Computer modelling in pharmacy"**
for the 3^{d} Year students of the Faculty of Pharmacy
(autumn (V) semester of 2021/2022 educational year)

№	Theme	Hours	Date
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	01.09
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	08.09
3	Practical use of the Internet and digital databases for the information search about drugs	2	15.09
4	Search for the information on the drugs on the stages of pre-clinical/clinical study, their registration, usage.	2	22.09
5	Computational chemical programs and their functional possibilities (Accelrys, CHEMOffice, ACDLabs). Performing situational problems using different chemical editors (Accelrys Draw, ChemWin, ACDLabs Sketch).	2	29.09
6	Accelrys (ISIS) (Base, Draw) package's capabilities as the system for chemical databases operating. Processing of the chemical compounds' databases.	2	06.10
7	Operation of the chemical compounds' libraries. Using chemical editors to search for information in specialized databases.	2	13.10
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	20.10
9	Modern approaches to the design of new biologically active compounds. The concept of ligand-, target-based, "fragment-based" design, "structure-based" design.	2	27.10
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	03.11
11	Modern methods of structure-activity relationship study. Working out the QSAR-analysis methodology; software programs for its implementation	2	10.11
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	17.11
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	24.11

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	01.12
15	Lead-compounds structure optimization	2	08.12
16	Other algorithms and approaches of virtual screening and drug design	2	08.12
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	15.12
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	2	15.12
Total		36	