

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

CALENDAR AND THEMATIC PLAN
of lectures 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	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	13.09
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 <i>in silico</i> methods. Molecular descriptors, software for their calculation, QSAR-analysis. Lead- and hit-compounds, ways of their optimization.	2	27.09