National Technical University of Ukraine
"Igor Sikorsky Kyiv Polytechnic Institute"

Department of Translational Medical Bioengineering

Fundamentals of Medicinal Chemistry and Biopharmaceutics

Working program of elective discipline (Course Syllabus)

Course Details	
PLevel of higher education	***First (Bachelor's) level***
Field of study	*16 Chemical and Bioengineering*
Speciality	*163 Biomedical Engineering*
Educational programme	*Medical Engineering*
Course status	*Elective course*
Mode of study	*Full-time (daytime)*
Year of study / semester	*3rd year, spring semester*
Course workload	*4 ECTS credits (120 hours)*
Forms of assessment	*Pass/fail test, modular assessment test, individual written assignment (essay)*
Course schedule	*26 hours – lectures; 28 hours – practical classe;: 66 hours – independent study* *According to the official timetable published at: https://schedule.kpi.ua/*
Language of instruction	*Ukrainian*
Course Instructor(s)	**Lecturer / Practical classes:** Associate Professor, PhD (Pharmaceutical Sciences) Olena I. Holembiovska Tel.: +380 67 234 22 48; E-mail: golembiovska-fbmi@lll.kpi.ua
Instructor profile	*https://bi.fbmi.kpi.ua/uk/holembiovska-ua/*
Course Delivery Platform	The course materials are available via the Moodle learning management system: https://do.ipo.kpi.ua/course/view.php?id=2738

Course Programme

1. Course Description, Aim, Subject Matter and Learning Outcomes

What will be studied

The course covers the scientific and methodological foundations for the application of chemical and physico-chemical laws and mechanisms of action of medicinal products, medical devices and related products at the molecular level, depending on their physical properties, dosage form and manufacturing technology, as well as their development (design) and synthesis.

Why this course is important

Knowledge of the fundamentals of medicinal chemistry enables future specialists to acquire skills in qualitative and quantitative prediction of biochemical processes involving medicinal products and medical devices in the human body.
Skills related to the assessment of the risk–benefit ratio, compatibility, indications and contraindications, based on data regarding the physiological state of the organism and taking into account biopharmaceutical, pharmacokinetic, pharmacodynamic and physico-chemical properties of medicinal products, are essential for informed decision-making in pharmaceutical and biomedical contexts.

Familiarity with regulatory documents and Good Pharmaceutical Practice (GxP) guidelines, as well as with the principles of development and testing of medicinal products and other parapharmaceutical products, contributes to the formation of pharmaceutical and engineering thinking and the ability to solve both typical and complex specialised professional problems.

What students will learn

Knowledge

- *fundamental concepts and laws of chemistry and methods of their application for solving applied problems in medicine and biopharmaceutical engineering;*
- *concepts of pharmacodynamics, pharmacokinetics and metabolism of biologically active molecules, and how these processes affect the activity of medicinal products, medical devices, etc., in the human body;*
- *principles of interaction of biologically active molecules with targets, the chemical nature and biochemical behaviour of general classes of drug targets;*
- *basic reactions and synthetic approaches in medicinal chemistry;*
- *key regulatory and legal acts governing pharmaceutical and biopharmaceutical activities in Ukraine and abroad;*
- *basic patterns of the influence of various factors on the therapeutic activity of biologically active molecules;*
- *fundamentals of general pharmacology.*

Skills

- *apply regulatory and legal acts governing pharmaceutical activities in Ukraine and abroad;*
- *apply chemical and physico-chemical methods of quantitative and qualitative analysis and draw conclusions regarding the possibility of their use in biomedical research; record and analyse laboratory experimental data;*
- *interpret the degree of activity of enzymes and receptors and use structure–activity databases;*
- *describe data on the structure and activity of medicinal products and medical devices;*
- *predict molecular metabolism and solubility depending on structural changes; apply various approaches, including combinatorial chemistry, to optimise molecular structure into a safe and effective medicinal product.*

*The main aim of the course **"Fundamentals of Medicinal Chemistry and Biopharmaceutics"** is to provide higher education students with **systematic theoretical knowledge and practice-oriented skills in medicinal chemistry and biopharmaceutics**, necessary for understanding the chemical nature, physico-chemical properties and mechanisms of action of biologically active substances and medicinal products, analysing structure–activity relationships, evaluating pharmacokinetic and pharmacodynamic characteristics, as well as applying experimental and computational methods in biomedical engineering in compliance with quality, safety and regulatory requirements.*
Students independently study additional core terminology and basic concepts of medicinal chemistry and biopharmaceutics, classification of medicinal products according to pharmacological groups, examples of medicinal substances belonging to different chemical classes and their physico-chemical properties, principles of classification of dosage forms and the role of excipients. They also familiarise themselves with pharmacopoeial monographs for medicinal substances and dosage forms, prepare for practical classes, and study the recommended educational and reference literature.

*Required **skills** for studying the course:*

1) *knowledge of a foreign language;*

2) *basic skills in working with educational and reference literature;*
3) *the ability to perceive and analyse educational information in chemistry, biochemistry and related disciplines;*
4) *skills in working with formulae, equations and graphical representations of chemical structures;*
5) *the ability to perform simple calculations and interpret numerical data;*
6) *skills of logical thinking and summarising educational material;*
7) *the ability to independently organise learning activities and prepare for classes;*
8) *basic computer skills and the ability to use electronic educational resources;*
9) *compliance with safety rules when working with chemical information and educational materials.*

Application of acquired knowledge and skills

The knowledge and skills acquired constitute an important tool for conducting research as well as organisational and production-related activities in the fields of biopharmaceutics, biotechnology and biomedical engineering.

Programme competencies *(in accordance with the educational programme "Medical Engineering"):*

GC-01 *Ability to apply knowledge in practical situations*
GC -02 *Knowledge and understanding of the subject area and understanding of professional activities*
GC -05 *Ability to conduct research at an appropriate level*
GC -06 *Ability to search, process, and analyze information from various sources*
GC -08 *Ability to make informed decisions*
GC -11 *Ability to assess and ensure the quality of work performed*

Professional competencies *(in accordance with the educational programme "Medical Engineering"):*

PC-03 *Ability to study and apply new methods and tools for analysis, modeling, design, and optimization of medical devices and systems*
PC-04 *Ability to ensure the technical and functional characteristics of systems and tools used in medicine and biology (for prevention, diagnosis, treatment, and rehabilitation)*
PC-05 *Ability to apply physical, chemical, biological, and mathematical methods in the analysis and modeling of the functioning of living organisms and biotechnical systems*
PC-06 *Ability to effectively use tools and methods for analysis, design, calculation, and testing in the development of biomedical products and services*
PC-08 *Ability to conduct research and observation on the interaction of biological, natural, and artificial systems (prostheses, artificial organs, etc.)*
PC-09 *Ability to identify, formulate, and solve engineering problems related to the interaction between living and non-living systems*
PC-11 *Ability to develop, plan, and conduct experiments using specified technical and biomedical techniques, applying mathematical methods in the analysis and modeling of the functioning of living organisms, systems, and processes in biology and medicine, computer processing, analysis, and synthesis of the obtained results*

Programme learning outcomes *(in accordance with the educational programme "Medical Engineering"):*

PLO -01 *The ability to apply knowledge of the fundamentals of mathematics, physics and biophysics, bioengineering, chemistry, engineering graphics, mechanics, materials resistance and strength, properties of gases and liquids, electronics, computer science, signal and image acquisition and analysis, automatic control, system analysis, and decision-making methods at a level necessary for solving biomedical engineering tasks*

PLO -02 *Formulate logical conclusions and reasoned recommendations regarding the assessment, operation, and implementation of biotechnical, medical-technical, and bioengineering tools and methods*

PLO -04 *Apply the provisions of regulatory and technical documents governing the procedure for product certification, production certification*

PLO -05 *Be able to use databases, mathematical and software tools for data processing and computer modeling of biotechnical systems*

PLO -11 *Conduct quality control and operational monitoring of medical equipment and materials for medical purposes, artificial organs, and prostheses*

PLO -18 *Understanding of fundamental-applied, medical-physical, and physico-chemical principles governing the functioning of biological objects, as well as bioengineering fundamentals of technologies and equipment for researching human body processes*

PLO -20 *Knowledge and application of research methods in biomedical engineering, methods and tools for organizing and processing experimental data, statistical methods for modeling and simulating processes and systems of physical and biological nature, modern programming technologies and supporting tools, methods for designing digital and microprocessor-based medical systems*

Integral competence: *The ability to solve complex, specialized problems and practical problems in biomedical engineering and in the process, which provides the use of specific theories and methods of chemical, biological and medical engineering, and is characterized by the complexity and non-strict terms.*

2. Prerequisites and Postrequisites of the Course *(place within the structural and logical framework of the educational programme)*

Prior to studying this course, students are expected to have completed the courses "Biochemistry" and "Human Anatomy and Physiology".
The course belongs to the cycle of elective courses; therefore, no mandatory (regulatory) links with other courses within the structural and logical framework of the educational programme are envisaged.

3. Course Content

Lecture Topics:

1. Medicinal chemistry and biopharmaceutics as the foundation of biomedical engineering: chemical and physico-chemical principles of biologically active molecules.
2. Properties of medicinal substances in solutions: solubility, ionisation, chemical equilibrium and their impact on bioavailability.
3. Physico-chemical factors of pharmacological activity: lipophilicity, polarity and intermolecular interactions.
4. Ligand–receptor interaction: pharmacodynamic mechanisms and analysis of structure–activity relationships.
5. Pharmacokinetics of medicinal products: absorption, distribution, metabolism and elimination, and their chemical determinants.
6. Modern approaches to drug development: rational design and optimisation of molecular structure.
7. Experimental and computational (in silico) methods in medicinal chemistry: modelling, databases and prediction of bioactivity.
8. Chemical reactions and synthetic approaches in medicinal chemistry: functional group modification and bioisosterism.

9. Pharmaceutical substances and excipients: chemical nature and their impact on pharmaco-technological properties.
10. Dosage forms and therapeutic systems: modified and controlled release of active substances.
11. Biopharmaceutical evaluation of medicinal products: bioavailability, bioequivalence and dissolution profiles.
12. Quality control of medicinal products: pharmacopoeial methods, stability and sterility.
13. Special pharmacology: quantitative dose–effect relationships, therapeutic index and safety fundamentals.

Practical Class Topics:

1. Analysis of physico-chemical properties of bioactive molecules as the basis of pharmacological activity.
2. Investigation of solubility and ionisation properties of bioactive molecules. Assessment of the effect of pH on bioavailability.
3. Construction of a chemical molecular structure using a graphical editor. Analysis of compliance with Lipinski's rule and basic ADME criteria.
4. Establishing the relationship between structure and biological activity and identification of pharmacophoric groups in the structure of bioactive molecules; investigation of their role in the formation of pharmacological activity.
5. Pharmacokinetic curve of a medicinal product: main phases and parameters (Cmax, Tmax, AUC, t½). Evaluation of pharmacokinetic parameters and their interpretation from the perspective of efficacy and safety of medicinal products. ADMET profiling of model compounds.
6. Stages of drug development: search for hit compounds and selection of a lead compound.
7. Introduction to experimental and computational modelling methods of medicinal products in medicinal chemistry. Computational prediction of biological activity of medicinal substances. Performance of docking prediction.
8. Fundamentals of chemical synthesis of medicinal substances. Influence of functional groups on the biological activity of a molecule. Bioisosteric replacement of functional groups as a method for optimising the properties of medicinal products.
9. Study of the influence of excipients on the pharmaco-technological properties of dosage forms and medical devices.
10. Analysis of dosage forms with modified and controlled release of active substances. Construction and comparison of release profiles.
11. Evaluation of bioavailability and bioequivalence of generic medicinal products and biosimilars. Construction of dissolution profiles of solid dosage forms.
12. Pharmacopoeial methods for quality control of medicinal products and stability analysis.
13. Quantitative analysis of the dose–effect relationship and evaluation of the therapeutic index of medicinal products.

4. Learning Materials and Resources

Core literature:

1. *Biopharmaceutics: textbook for higher education students / O. I. Tykhonov et al.; edited by O. I. Tykhonov. – 2nd revised and expanded edition. – Kharkiv: National University of Pharmacy, Zoloti Storinky, 2019. – 224 p.*
2. *Biopharmaceutics. Textbook for pharmaceutical higher education institutions and faculties. 2nd edition. Edited by V. V. Hladyshev / V. V. Hladyshev, L. L. Davtian, I. A. Biriuk et al. – Lviv: Publisher Marchenko T. V., 2023. – 176 p*
3. *Validation of analytical methods and tests (5.3.N.2) // State Pharmacopoeia of Ukraine: in 3 volumes / Ukrainian Scientific Pharmacopoeial Centre for Quality of Medicines. – 2nd edition. – Kharkiv, 2015. – Vol. 1. – pp. 910–929.*

4. State Pharmacopoeia of Ukraine: in 3 volumes / Ukrainian Scientific Pharmacopoeial Centre for Quality of Medicines. – 2nd edition. – Kharkiv, 2014. – Vol. 2. – 724 p.
5. State Pharmacopoeia of Ukraine: in 3 volumes / Ukrainian Scientific Pharmacopoeial Centre for Quality of Medicines. – 2nd edition. – Kharkiv, 2014. – Vol. 3. – 732 p.
6. State Pharmacopoeia of Ukraine: in 3 volumes / Ukrainian Scientific Pharmacopoeial Centre for Quality of Medicines. – 2nd edition. – Kharkiv, 2015. – Vol. 1. – 1135 p.
7. State Register of Medicinal Products of Ukraine. – [Electronic resource]. Available at: http://www.drlz.com.ua/
8. Law of Ukraine "On Medicinal Products" dated 04 April 1996 No. 123/96-VR.
9. Compendium: Medicinal Products. – [Electronic resource]. Available at: http://compendium.com.ua/
10. Krasnopolskyi Yu. M., Pylypenko D. M. Pharmaceutical Biotechnology: Biotechnologies for the Production of Finished Dosage Forms. Study guide. – Kharkiv: Madrid, 2020. – 279 p.
11. Medicinal Products. Stability Testing of Biotechnological/Biological Products (ICH Q5C): Guideline ST-N MoH of Ukraine 42-8.2:2013. – Kyiv: Ministry of Health of Ukraine, 2013. – 22 p. (MoH Standard).
12. Medicinal Products. Stability Testing: Guideline ST-N MoH of Ukraine 42-3.3:2004. – Kyiv: Ministry of Health of Ukraine, 2004. – 60 p. (MoH Standard).
13. Medicinal Products. Non-clinical Safety Studies as a Basis for Human Clinical Trials and Marketing Authorisation (ICH M3(R2)): Guideline ST-N MoH of Ukraine 42-6.0:2014. – Kyiv: Ministry of Health of Ukraine, 2014. – 45 p. (MoH Standard).
14. Medicinal Products. Bioequivalence Studies: Guideline ST-N MoH of Ukraine 42-7.1:2014. – Kyiv: Ministry of Health of Ukraine, 2014. – 62 p. (MoH Standard).
15. Medicinal Products. Manufacturing Site Dossier: Guideline ST-N MoH of Ukraine 42-4.1:2011. – Kyiv: Ministry of Health of Ukraine, 2011. – 8 p. (MoH Standard).
16. Medicinal Products. International Harmonised Requirements for Batch Certification: Guideline ST-N MoH of Ukraine 42-4.4:2011. – Kyiv: Ministry of Health of Ukraine, 2011. – 10 p. (MoH Standard)
17. Medicinal Products. Good Manufacturing Practice: Guideline ST-N MoH of Ukraine 42-4.0:2016. – Kyiv: Ministry of Health of Ukraine, 2016. – 335 p. (MoH Standard).
18. Medicinal Products. Good Clinical Practice: Guideline ST-N MoH of Ukraine 42-7.0:2008. – Kyiv: Ministry of Health of Ukraine, 2009. – 67 p. (MoH Standard).
19. Medicinal Products. Good Laboratory Practice: Guideline ST-N MoH of Ukraine 42-6.0:2008. – Kyiv: Ministry of Health of Ukraine, 2009. – 27 p. (MoH Standard).
20. Medicinal Products. Good Distribution Practice: Guideline ST-N MoH of Ukraine 42-5.0:2014. – Kyiv: Ministry of Health of Ukraine, 2014. – 67 p. (MoH Standard).
21. Medicinal Products. Good Storage Practice: Guideline ST-N MoH of Ukraine 42-5.1:2011. – Kyiv: Ministry of Health of Ukraine, 2011. – 19 p. (MoH Standard).
22. Medicinal Products. Good Agricultural and Collection Practice for Herbal Starting Materials: Guideline ST-N MoH of Ukraine 42-4.5:2012. – Kyiv: Ministry of Health of Ukraine, 2012. – 13 p. (MoH Standard).
23. Medicinal Products. Good Regulatory Practice: Guideline ST-N MoH of Ukraine 42-1.1:2013. – Kyiv: Ministry of Health of Ukraine, 2013. – 24 p. (MoH Standard).
24. Medicinal Products. Good Pharmacovigilance Practices: Guideline ST-N MoH of Ukraine 42-8.5:2015. – Kyiv: Ministry of Health of Ukraine, 2015. – 105 p. (MoH Standard).
25. Medicinal Products. Specifications: Test Procedures and Acceptance Criteria: Guideline ST-N MoH of Ukraine 42-3.2:2004. – Kyiv: Ministry of Health of Ukraine, 2004. – 33 p. (MoH Standard).
26. Medicinal Products. Specifications: Test Procedures and Acceptance Criteria for Biotechnological/Biological Products (ICH Q6B): Guideline ST-N MoH of Ukraine 42-8.3:2013. – Kyiv: Ministry of Health of Ukraine, 2013. – 34 p. (MoH Standard).
27. Medicinal Products. Quality Risk Management (ICH Q9): Guideline ST-N MoH of Ukraine 42-4.2:2011. – Kyiv: Ministry of Health of Ukraine, 2011. – 26 p. (MoH Standard).

28. Medicinal Products. Pharmaceutical Development (ICH Q8): Guideline ST-N MoH of Ukraine 42-3.0:2011. – Kyiv: Ministry of Health of Ukraine, 2011. – 13 p. (MoH Standard).
29. Medicinal Products. Pharmaceutical Development of Biotechnological and Biological Products: Guideline ST-N MoH of Ukraine 42-8.1:2013. – Kyiv: Ministry of Health of Ukraine, 2013. – 13 p. (MoH Standard).
30. Medicinal Products. Pharmaceutical Quality System (ICH Q10): Guideline ST-N MoH of Ukraine 42-4.3:2011. – Kyiv: Ministry of Health of Ukraine, 2011. – 22 p. (MoH Standard).
31. Licensing Conditions for Economic Activities in the Manufacture of Medicinal Products, Wholesale and Retail Trade in Medicinal Products, and Import of Medicinal Products (except APIs), approved by Resolution of the Cabinet of Ministers of Ukraine dated 30 November 2016 No. 929.
32. Order of the Ministry of Health of Ukraine dated 21 January 2013 No. 39 "On Approval of the Forms of Documents Used in State Quality Control of Medicinal Products Imported into Ukraine".
33. Quality Guidelines. Medicinal Products. Pharmaceutical Development: Guideline ST-N MoH of Ukraine 42-3.1:2004. – Kyiv: Ministry of Health of Ukraine, 2004. – 14 p. (MoH Standard).
34. Statistical Analysis of Chemical Experiment Results (5.3.N.1) // State Pharmacopoeia of Ukraine: in 3 volumes. Supplement 2. – 2nd edition. – Kharkiv, 2018. – pp. 77–112.
35. Tykhonov O. I., Yarnykh T. H. Pharmacy Technology of Medicines. – Vinnytsia: Nova Knyha, 2016. – 536 p.
36. Pharmaceutical Chemistry: textbook for students of higher pharmaceutical education institutions and faculties of higher medical education institutions (III–IV accreditation levels) / P. O. Bezuhlyi, I. S. Hrytsenko, I. V. Ukrainets et al. – Vinnytsia: Nova Knyha, 2011. – 560 p.
37. Fedorovska M. I. Biopharmaceutics: methodological guidelines for laboratory classes. – "Zoria-Plus" Publishing House, 2022. – 30 p.
38. Basic Organic Chemistry for the Life Sciences / Hrvoj Vančik. - Springer International Publishing, 2014. – 179 p.
39. Biochemistry and Molecular Biology: How Life Works / Kevin Ahern. - The Great Courses, 2019. – 408 p.
40. Davis A, Ward SimonE. The Handbook of Medicinal Chemistry: Principles and Practice. Royal Society of Chemistry; 2014.— ISBN 789 p. 978-1-84973-625-1
41. European Pharmacopoeia. – 11th ed. – Strasbourg: Council of Europe, 20123. – 6111 p.
42. In Silico Drug Discovery and Design: Theory, Methods, Challenges, and Applications / Claudio N. Cavasotto. - CRC Press, 2017. – 228 p.
43. Japanese Pharmacopoeia. – 18th ed. [Internet]. Pharmaceuticals and Medical Devices Agency. Available from: https://www.pmda.go.jp/english/rs-sb-std/standards-development/jp/0029.html
44. Li JJ. Medicinal chemistry for practitioners. John Wiley & Sons; 2020. 402 p.—ISBN 9781119607311
45. Nogrady T, Weaver DF. Medicinal chemistry: A Molecular and Biochemical Approach. Oxford University Press; 2005. 665 p.—ISBN 0-19-510455-2.
46. Pharmaceutical Dosage Forms and Drug Delivery / Ram I. Mahato, Ajit S. Narang. - CRC Press, 2017. – 728 p.
47. Small Molecule Medicinal Chemistry: Strategies and Technologies. Edited by Werngard Czechtizky and Peter Hamley. Wiley, Hoboken 2015. 528 pp.—ISBN 978-1-118-77160-0.
48. The British Pharmacopoeia. – 2025th ed. – London: HMSO, 2025. – 7248 p.
49. The Homoeopathic Pharmacopoeia of the United States. – Revision service. – official Compendium from July 1/1992.
50. The Practice of Medicinal Chemistry. 4th Edition / Camille Wermuth David Aldous Pierre Raboisson Didier Rognan. - Academic Press, 2015. – 902 p.
51. The United States Pharmacopoeia : The National Formulary. Available from: https://www.usp.org/

Additional literature:

1. Pertsev I. M., Piminov O. Kh., Slobodianiuk M. M. et al. Pharmaceutical and Biomedical Aspects of Medicinal Products. Study guide / edited by I. M. Pertsev. 2nd revised and expanded edition. – Vinnytsia: Nova Knyha, 2007. – 728 p.
2. Ruban O. A., Pertsev I. M., Kutseko S. A., Maslii Yu. S. Excipients in Medicinal Product Manufacturing: study guide for students of higher pharmaceutical education institutions / edited by I. M. Pertsev. – Kharkiv: Zoloti Storinky, 2016. – 720 p.
3. Hroshovyi T. A., Martseniuk V. P., Kucherenko L. I. et al. Mathematical Design of Experiments in Pharmaceutical Research. – Ternopil: TDMU Ukrmedknyha, 2008. – 367 p.

Навчальний контент

5. Methodology for Studying the Course (Educational Component)

Lectures are delivered following a classical format: the lecturer presents the relevant topic in a structured and visual manner. During the lecture and after its completion, students have the opportunity to ask questions. For certain topics within the lecture course, a discussion between the lecturer and students may be conducted in order to emphasise important, fundamental and problematic aspects. Students may take notes during lectures, and the lecture presentation and/or lecture notes or their selected parts are made available for download on the "Sikorsky" distance learning platform.

Practical classes are aimed at acquiring deeper knowledge and skills related to the topics covered in the lecture course and independently studied by students. The procedure for conducting a practical class includes the following stages: the instructor presents the basic (strategic) theses within the relevant topic; students deliver short presentations with pre-formulated problem questions related to the topic or complete practical tasks in accordance with the topic of the class; a discussion takes place between the presenter, other students and the instructor, aimed at clarifying all fundamental and applied aspects of the relevant topics in medicinal chemistry and biopharmaceutics.

Student presentations involve the preparation of an analytical note in the form of a short literature review in Ukrainian, as well as a visual presentation, which contributes to the development of written and oral academic Ukrainian language skills. When necessary, practical classes also include the study (familiarisation) of regulatory documents, methodological guidelines, etc., as well as the solution of situational problems. During the final practical class, students complete a module assessment test (MAT) in the form of a test. Materials useful for preparation for practical classes are made available for download on the "Sikorsky" distance learning platform.

Lectures and practical classes are conducted in accordance with the class schedule published at http://rozklad.kpi.ua/, following this sequence: lectures are conducted first, followed by practical classes upon their completion. Detailed information is communicated to students through appropriate communication channels, in particular via the "Sikorsky" and "Campus" platforms.

№	Topic	Programme Learning Outcomes	Основні завдання	
			Assessment Activity	Completion Time
1.	Medicinal chemistry and biopharmaceutics as the foundation of biomedical engineering: chemical and physico-chemical principles of bioactive molecules	PLO -01, PLO -18	Practical class 1	Week 1
2.	Properties of medicinal substances in solutions: solubility, ionisation, chemical equilibrium and their impact on bioavailability	PLO -01, PLO -18	Practical class 2	Week 2
3.	Physico-chemical factors of pharmacological activity: lipophilicity, polarity, intermolecular interactions	PLO -01, PLO-02	Practical class 3	Week 3
4.	Ligand–receptor interaction: pharmacodynamic mechanisms and analysis	PLO -01, PLO -02, PLO -18	Practical class 4	Week 4

№	Topic	Programme Learning Outcomes	Основні завдання	
			Assessment Activity	Completion Time
	of structure–activity relationships			
5.	Pharmacokinetics of medicinal products: absorption, distribution, metabolism, elimination and their chemical determinants	PLO -01, PLO -02	Practical class 5	Week 5
6.	Modern approaches to drug development: rational design and optimisation of molecular structure	PLO -02, PLO -05	Practical class 6	Week 6
7.	Experimental and computational (in silico) methods in medicinal chemistry: modelling, databases, prediction of bioactivity	PLO -05, PLO -20	Practical class 7	Week 7
8.	Chemical reactions and synthetic approaches in medicinal chemistry: functional group modification and bioisosterism	PLO -01, PLO -02	Practical class 8	Week 8
9.	Pharmaceutical substances and excipients: chemical nature and impact on pharmaco-technological properties	PLO -02, PLO -11	Practical class 9	Week 9
10.	Dosage forms and therapeutic systems: modified and controlled release of active substances	PLO -02, PLO -11	Practical class 10	Week 10
11.	Biopharmaceutical evaluation of medicinal products: bioavailability, bioequivalence, dissolution profiles	PLO -11, PLO -20	Practical class 11	Week 11
12.	Quality control of medicinal products: pharmacopoeial methods, stability, sterility	PLO -04, PLO -11, PLO -20	Practical class 12	Week 12
13.	Special pharmacology: dose–effect relationship, therapeutic index and safety of medicinal products	PLO -01, PLO -02, PLO -20	Practical class 13	Week 13-14
14.	Modular assessment test		Practical class 14	
15.	Essay	PLO- 02 PLO-05 PLO-18	Preparation and submission of the assignment	Week 14

6. Independent Student Work

The total volume of independent student work within the course amounts to 66 hours, including:

No.	Topics and questions assigned for self-study (with references to recommended literature)	Self-study hours
1	***Topic 1. Medicinal chemistry and biopharmacy as a foundation of biomedical engineering*** ***Questions for self-study:*** *"structure–property–effect" concept; minimum dataset needed to justify a hypothesis on activity/bioavailability; trade-offs potency ↔ solubility ↔ permeability ↔ safety; examples of different activity of the same molecule in different media;* ***additionally:*** *drug–device/combination products as an interface between medicinal chemistry and engineering.* ***References:*** *[40; 45; 50].*	5
2	***Topic 2. Properties in solutions: solubility, ionization, chemical equilibrium*** ***Questions for self-study:*** *pKa and degree of ionization; pH–solubility profile; salt formation (benefits/risks); effects of buffers, ionic strength, co-solvents and surfactants; typical errors when extrapolating in vitro → in vivo;* ***additionally:*** *supersaturation and precipitation after dissolution.* ***References:*** *[46; 45; 1; 2].*	6
3	***Topic 3. Physicochemical determinants of activity: lipophilicity, polarity, intermolecular interactions*** ***Questions for self-study:*** *LogP vs LogD; PSA, HBD/HBA; nonspecific binding to proteins/lipids;*	5

	intermolecular interactions (ionic, H-bond, π–π, hydrophobic) and their role in target binding; ***additionally:*** *structural "red flags" (excessive lipophilicity, reactive fragments).* ***References:*** *[45; 50; 44].*	
4	***Topic 4. Ligand–receptor interaction: pharmacodynamics and SAR ("structure–activity relationship")*** ***Questions for self-study:*** *pharmacophore and key interactions; selectivity vs off-target; role of stereochemistry; how to make SAR conclusions from small compound sets;* ***additionally:*** *mechanisms of false positives in bioassays (PAINS/aggregation — conceptually).* ***References:*** *[50; 40; 45].*	*5*
5	***Topic 5. Pharmacokinetics: ADME and chemical determinants*** ***Questions for self-study:*** *interpretation of Cmax/Tmax/AUC/t½; distribution and binding factors; metabolism (Phase I/II) as a function of structure; clearance and the role of lipophilicity/polarity;* ***additionally:*** *how PK profile affects dosing regimen and toxicity risk.* ***References:*** *[46; 50; 2].*	*6*
6	***Topic 6. Rational drug design and structure optimization*** ***Questions for self-study:*** *hit → lead → candidate; lead selection criteria; optimization of potency/selectivity/ADMET; compromise solutions;* ***additionally (term paper–oriented):*** *a critical review of lead selection criteria in modern medicinal chemistry (based on one case).* ***References:*** *[40; 44; 50].*	*6*
7	***Topic 7. In silico and experimental methods: modeling, databases, bioactivity prediction*** \n***Questions for self-study:*** *data sources and reliability; docking—problem formulation, target/ligand preparation; scoring interpretation;* ***additionally (term paper–oriented):*** *high-throughput screening vs in silico approaches—comparison, typical pitfalls, and the role of hypothesis validation.* ***References:*** *[42; 50; 44].*	*6*
8	***Topic 8. Chemical reactions and synthetic approaches: functional group modification and bioisosterism*** \n***Questions for self-study:*** *goals of structural modifications (solubility/metabolic stability/selectivity); bioisosteric replacements (typical examples); impact of functional groups on pKa/LogD;* ***additionally:*** *"metabolic hot spots" and conceptual strategies to block them.* ***References:*** *[40; 47; 45].*	*5*
9	***Topic 9. Drug substances and excipients: chemical nature and impact on pharmaco-technological properties*** ***Questions for self-study:*** *role of excipients; API–excipient compatibility; hygroscopicity/oxidation/hydrolysis; sorption to packaging materials;* ***additionally:*** *an engineering-style stability risk list (basic risk checklist).* ***References:*** *[35; 1; 2].*	*4*
10	***Topic 10. Dosage forms and therapeutic systems: MR/CR and controlled release*** ***Questions for self-study:*** *release mechanisms (diffusion/erosion/osmosis); factors affecting the profile; typical experimental artefacts;* ***additionally:*** *how to "read" a dissolution/release profile and what constitutes a meaningful difference between profiles.* ***References:*** *[46; 35; 1].*	*5*
11	***Topic 11. Biopharmaceutical evaluation: bioavailability, bioequivalence, dissolution profiles*** ***Questions for self-study:*** *BE rationale; dissolution profiles as a comparison tool; similarity criteria (conceptually);* ***additionally:*** *biosimilars—what "critical attributes" are and why they are harder to compare than small molecules.* ***References:*** *[14; 11; 2].*	*5*
12	***Topic 12. Quality control: pharmacopoeial methods, stability, sterility*** ***Questions for self-study:*** *specifications and acceptance criteria; structure of a pharmacopoeial method; basic validation/verification parameters; stability as a source of quality changes; sterility/microbiological risks (logic, without detailed methods);* ***additionally:*** *statistical interpretation of results (repeatability/dispersion).* ***References:*** *[3; 4; 5; 6; 34; 41; 51].*	*6*
13	***Topic 13. Special pharmacology: dose–response, therapeutic index, drug safety*** ***Questions for self-study:*** *typical dose–response curves; therapeutic index; factors shifting the "safety window"; basic causes of toxicity (off-target effects, reactive metabolites—conceptually);* ***additionally (term paper–oriented):*** *false positives and errors in bioassays and their consequences for safety assessment.* ***References:*** *[50; 45; 39].*	*8*
	Total	***66***

One of the main forms of semester assessment during the study of the course "Fundamentals of Medicinal Chemistry and Biopharmaceutics" is the preparation and defence of an essay. The essay is

prepared in accordance with established methodological requirements and within the timeframe specified by the instructor.

The main purpose of the essay is the in-depth study of a selected topic of the course through the analysis of scientific and technical sources, generalisation of theoretical material, as well as the development of skills in analysing and systematising information in the field of microprocessor technology. In the process of completing the essay, the student demonstrates the level of mastery of lecture material, the ability to work independently with literature sources, and the ability to present technical information accurately.

The student is entitled to prepare the essay only on a topic previously approved by the instructor, which ensures the relevance of the work to the content of the course and its educational objectives.

The calculation and graphical assignment is not checked for plagiarism; however, it must comply with the requirements of academic integrity. In the event of a violation of academic integrity, the work is annulled and not assessed.

Approximate List of Essay Topics:

1. *Review and critical analysis of criteria for lead compound selection in modern medicinal chemistry.*
2. *Structural approaches to the design of antibacterial compounds and overcoming drug resistance.*
3. *Molecular targets of anticancer therapy and modern principles of small-molecule design.*
4. *Microtubule inhibitors as anticancer agents: structural evolution, mechanism of action and selectivity issues.*
5. *Structural design of viral protease and polymerase inhibitors using HIV and SARS-CoV-2 as examples.*
6. *Opioid receptor ligands: modern approaches to the development of analgesics with improved safety profiles.*
7. *Structural optimisation of selective modulators of nuclear hormone receptors.*
8. *Small molecules interacting with DNA: modern principles of the design of intercalators and covalent ligands and their biological activity.*
9. *RNA as a target for small molecules in modern medicinal chemistry.*
10. *Molecular docking as a tool for the discovery and optimisation of medicinal substances: capabilities, limitations and errors in result interpretation.*
11. *High-throughput screening and in silico methods in drug development.*
12. *Pharmacophore modelling as a tool for rational drug design.*
13. *Caco-2 cell models for predicting the bioavailability of medicinal products.*
14. *Biopharmaceutical approaches to improving the oral bioavailability of medicinal products.*
15. *Strategies for enhancing drug penetration across the blood–brain barrier.*
16. *QSAR and 3D-QSAR methods for analysing structure–biological activity relationships: practical cases and limitations.*
17. *False-positive results and errors in biotesting of medicinal substances.*
18. *Biopharmaceutical evaluation of drug candidates at early stages of development.*
19. *COVID-19 as an example of rapid drug development: molecular targets and challenges.*
20. *Integration of medicinal chemistry and medical engineering in the development of medicinal products and medical devices.*

Programme learning outcomes, assessment activities and deadlines are announced to students during the first class.

Policy and Control

7. Course Policy (Educational Component)

Deadlines and incentive point

Students may be awarded incentive points. The total number of incentive points may not exceed 10 points.

Incentive points are awarded for the following activities: creation of unique infographics or other means of graphical interpretation of information for one of the course topics (5 points); participation in international or national scientific conferences, congresses, etc. (within the scope of the course subject), provided that conference abstracts are published (5 points); preparation of a manuscript of a review or experimental article or participation in competitions (provided a prize-winning place is obtained) related to the course subject (10 points).

Class attendance

No penalty points are assigned for absence from lectures. However, students are encouraged to attend lectures, as theoretical material is presented and practical skills necessary for the thorough development of relevant competencies are formed.

Attendance at practical classes is desirable, as these classes include short control tests / test tasks, explanations of subsequent practical assignments, and submission of completed practical work.

The assessment system is oriented towards awarding points for student activity as well as for completing tasks aimed at developing practical skills and abilities.

Missed assessment activities

Assessment activities scheduled to be completed during class sessions are conducted on a pre-determined date announced to students during the first week of the educational process. Completion of such assessment activities on another date is permitted only in the case of valid and/or force majeure circumstances.

If a student is absent from a practical class where a presentation is required, the presentation is either rescheduled for another practical class or replaced with the preparation of an analytical report on the relevant topic with a length of 5–10 pages (in the case of exceptional force majeure circumstances).

Missed assessment activities (defence of practical work) must be completed during subsequent classes, provided that the task scheduled for the current class is completed, or during consultation hours.

Missed short control tests are not retaken.

The result of the modular assessment test for a student who did not attend the assessment activity is zero. In such a case, the student may complete the modular assessment test at another time upon agreement with the instructor. Rescheduling of the modular assessment test is permitted only for valid reasons (force majeure circumstances).

An essay submitted after the established deadline is assessed with a reduction in weighted points.

Retesting within the modular assessment test is not provided.

Ensuring objectivity of student assessment

Objectivity of student assessment at all stages of mastering the course is ensured through the following mechanisms.
First, the use of test-based forms of knowledge assessment. Second, detailed guidelines regarding the rating-based system for assessing learning outcomes (Section 8 of the Syllabus). Third, the use by students and instructors of all available communication tools that ensure preservation of communication history (e-mail, social networks, messengers, etc.). Fourth, in the assessment of written student work, in case of disagreement with assessment results, another instructor with appropriate professional competence appointed by the department for the current academic year may be involved. In the absence of a consensus between instructors regarding the assessment of a student's work, the issue is considered at a department meeting, and resolution is carried out in accordance with the "Regulations on Appeals at Igor Sikorsky Kyiv Polytechnic Institute" (http://osvita.kpi.ua/node/182).

Procedure for appealing assessment results

After receiving comments from the instructor with justification of the assessment, the student has the right to individually ask any questions regarding the results of assessment activities. If the student disagrees with the assessment, they must provide arguments supporting their position and contact the dean of the faculty for further resolution of the issue (for details see the "Regulations on Appeals at Igor Sikorsky Kyiv Polytechnic Institute": http://osvita.kpi.ua/node/182).

Academic integrity

When using copyrighted content, results of analytical studies and/or other information, students must indicate the source. When using language models such as ChatGPT and others for completing written practical tasks or essays, such use must be explicitly indicated. The use of artificial intelligence is strictly prohibited for completing modular assessment tests, tests and other forms of knowledge assessment.

The policy and principles of academic integrity are defined in Section 3 of the Code of Honour of the National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute" (https://kpi.ua/code). If it is necessary to check academic texts prepared by students for textual borrowings, the student may contact the instructor directly or the department representative responsible for checking academic texts.

Ethical conduct

The norms of ethical conduct for students and staff are defined in Section 2 of the Code of Honour of the National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute" (https://kpi.ua/code).

Distance learning

Distance learning is conducted via the "Sikorsky" Distance Learning Platform.

Participation in online courses is provided in the case of force majeure circumstances (including quarantine measures) and for inclusive education of students with special needs, or upon agreement with students. If a small number of students wish to complete an online course on a specific topic, studying the material through such courses is permitted; however, students must complete all tasks предусмотрені by the course.

The student provides a document confirming completion of the distance course (in the case of completing the full course) or submits completed practical tasks from the distance course and, subject to passing an oral interview with the instructor on the covered topics, may receive grades for the assessment activities provided for the studied topics (short control tests / test tasks, practical work).

Inclusive education

The course is designed for study by students with special educational needs; however, the significant visual load should be taken into account. Depending on students' specific needs, the use of distance learning is possible.

8. Types of Assessment and Rating System for Learning Outcomes (RSLO)

Continuous assessment

Work during practical classes involves completion of practical assignments (13 assignments per student). Each assignment is assessed at 4 points (52 points in total).

Work during lectures and practical classes also includes short control tests in the form of a test consisting of 8 questions, with 0.5 points awarded for each correct answer. A total of 4 tests, 4 points each, are provided (16 points).

The modular assessment test (MAT) is assessed at 16 points. The essay is assessed at 16 points.

№	Assessment activity	%	Weight (points)	Quantity	Total
1.	Short control tests / test tasks	16	4	4	16
2.	Completion and defence of practical assignments	52	4	13	52
3.	Modular assessment test	16	16	1	16

№	Assessment activity	%	Weight (points)	Quantity	Total
4.	Essay	16	16	1	16
Total					100

Calendar assessment

Calendar assessment is conducted twice per semester as monitoring of the current level of fulfilment of syllabus requirements.

The first calendar assessment requires completion of at least practical assignments No. 1–2. The second calendar assessment requires completion of at least practical assignments No. 3–5 and the essay.

Criterion			First calendar assessment	Second calendar assessment
Timing of calendar assessments			Week 8	Week 14
Condition for obtaining a positive result	Current rating		≥ 8 points	≥ 20 points
	Completion of practical assignments	Practical assignments № 1-2	+	+
		Practical assignments № 3-5	-	+
	Modular assessment test	Assessed MAT	-	+
	Essay	Assessed essay	-	+

In the event of a violation of academic integrity during the course, the assessment activity is not credited.

Semester rating

The maximum semester rating of a student is 100 points. The sum of weighted points of assessment activities during the semester is:

RS = 40 + 20 + 20 + 20 = 100 points

Semester assessment: *The form of semester assessment is a pass (credit).*

Conditions for admission to semester assessment: *completion of all practical assignments; submission of the essay; completion of the modular assessment test with a score of at least 10 points; total semester rating of at least 60 points.*

If the semester rating is 60 points or higher, the student may receive the pass automatically. In case of disagreement, the student completes the pass assessment in the form of a test.

Assessment results are announced to each student individually in the presence of the student at the assessment activity or remotely (by e-mail). Results are also recorded in the "Electronic Campus" system.

Optional conditions for admission to the examination

1. *Activity during practical classes.*
2. *Positive results of the first and second attestations.*
3. *Attendance of lectures.*

Correspondence table of rating points and grades according to the university scale

Number of points	Grade (university scale)
100–95	Excellent
94–85	Very good
84–75	Good
74–65	Satisfactory
64–60	Sufficient
Less than 60	Unsatisfactory
Admission conditions not fulfilled	Not admitted

9. Additional Course Information (Educational Component)

The questions included in the semester assessment correspond to the topics of lectures and practical classes.

Recognition of learning outcomes acquired through non-formal / informal education is carried out in accordance with the "Temporary Regulations on the Procedure for Recognition of Learning Outcomes Acquired by Students of Igor Sikorsky Kyiv Polytechnic Institute through Non-formal / Informal Education" (https://osvita.kpi.ua/node/119).

Description of material, technical and information support of the course

The syllabus, lecture presentations and guidelines for practical classes are available in the Electronic Campus system and the Sikorsky online learning platform.

Laboratory equipment. General analytical equipment, including extractors, vacuum filtration unit, rotary evaporator, analytical balances, equipment for potentiometric measurements, pH meters, UV–visible spectrophotometer, electrophoresis equipment, thin-layer chromatography (TLC) developing chamber, etc.

Multimedia equipment. In the case of distance learning, Zoom and Google Meet videoconferencing services are used.

Course syllabus:

Prepared by: *O. I. Holembiovska*

Approved *by the Department of TMBE (Minutes No. 1 dated 28 August 2023)*

Approved *by the Faculty / Educational and Scientific Institute Methodological Committee (Minutes No. 1 dated 1 September 2023)*