

COURSE DESCRIPTION

Academic year: 2026/2027	
University: Comenius University Bratislava	
Faculty: Faculty of Pharmacy	
Course ID: FaF.KFCh/06-Mgr-A/26	Course title: Pharmaceutical Chemistry (2)
Educational activities: Type of activities: lecture / laboratory practicals Number of hours: per week: 2 / 5 per level/semester: 28 / 70 Form of the course: on-site learning	
Number of credits: 8	
Recommended semester: 6.	
Educational level: I.II.	
Prerequisites:	
Recommended prerequisites: Recommendation. The KCHTL/04-Mgr-A/00 Organic Chemistry (1), KCHTL/05-Mgr-A/00 Organic Chemistry (2), KBMBL/03-Mgr-A/00 Biochemistry and KFCH/05-Mgr-A/00 Pharmaceutical Chemistry (1) courses are very strongly recommended to be successfully passed (with the final evaluation A-E) for the Pharmaceutical Chemistry (2) course.	
Course requirements: a) The Attendance at All Required Forms of Education Attendance at Lectures - active participation is strongly required (Lectures are the mandatory form of education!); Attendance at Laboratory Practicals - Student is obliged to complete all Laboratory Practicals following the schedule published at an official dashboard/web site of the Department of Pharmaceutical Chemistry FPharm CU (100% attendance at the Laboratory Practicals). b) Successful Course Completion Based On Successful Passing of All Semestral Preliminary Evaluations with Achievement of Adequate (Percentage) Success Students' knowledge will be verified in a written form at 3rd and 5th Laboratory Practical, respectively (two preliminary tests have to be passed); the content of preliminary tests, their evaluation as well as granting of preliminary evaluation will be the competence of particular teachers responsible for the teaching (supervising) of the Practicals. To pass successfully all scheduled Laboratory Practicals and semestral preliminary evaluations (2 preliminary tests), 60% or higher rate of the maximum evaluation score must be achieved from each test (in other words, 60% and more). The attendance of a student at a final evaluation (exam) from the Pharmaceutical Chemistry (2) course is based on successful passing of the requirements listed in both a) and b) sections. c) Successful Passing of the Final Evaluation (Exam) from the Pharmaceutical Chemistry (2) Course The exam from the Pharmaceutical Chemistry (2) course will be in a written form, i.e., a student will complete the test consisting of 25 questions. Each question will be evaluated by 2 points (the maximum number of points from the exam: 50 pts.).	

The set of questions will be based on the content of all pharmacodynamic groups listed in Syllabus of Lectures as well as Syllabus of Laboratory Practicals. Thus, the questions will cover i) definitions, chemical classifications of particular pharmacodynamic classes (with a very precise division of particular compounds – drugs), ii) chemical structures of selected compounds – drugs, iii) structure–(biological) activity, structure–pharmacokinetics as well as structure–toxicity relationships in detail (including comprehensible general chemical structure of the compounds from a relevant pharmacodynamic group as well as chemical structure one relevant compound at least) using the knowledge from general Pharmaceutical Chemistry as well as iv) knowledge regarding general biotransformation pathways applied for particular compounds – drugs.

The final written exam from Pharmaceutical Chemistry (2) course will last 120 minutes; particular terms, times and rooms for the exam will be listed in AIS-2.

Evaluation of the exam from the Pharmaceutical Chemistry (2) course will be as follows: 50–46 points (evaluation level „A“), 45–42 points („B“), 41–38 points („C“), 37–34 points („D“), 33–30 points („E“), less than 30 points („FX“; not passed).

Thus, minimal requirements for the Pharmaceutical Chemistry (2) course to be successfully passed are as follows: 60% (60% and more of the maximum point score).

Scale of assessment (preliminary/final): 0 / 100.a) Laboratory Practicals from the Pharmaceutical Chemistry (2) course. Successful completion of Laboratory Practicals, thus, the opportunity to participate in the final evaluation (exam) from the Pharmaceutical Chemistry (2) course, is based on successful completion of two preliminary evaluations. There is a requirement to obtain at least 60% or more of the maximum point score from each preliminary evaluation.

The obtained (point) evaluation from the preliminary ones is not explicitly taken into account in the final evaluation (exam).b) Exam from the Pharmaceutical Chemistry (2) course - weight in the final evaluation: 100%. The evaluation of the exam from the Pharmaceutical Chemistry (2) course and the assignment of relevant classification grades is provided in the „Conditions for Successful Completion of Lectures and Laboratory Practicals from the Pharmaceutical Chemistry (2) Course“ section. The exact score from the Laboratory Practicals will be not taken into consideration in the final evaluation (exam) from the Pharmaceutical Chemistry (2) course.

Learning outcomes:

Pharmaceutical/Medicinal Chemistry (the Pharmaceutical Chemistry (2) course) is a science unto itself, a central science positioned to provide a molecular bridge between basic science of biology and clinical science of medicine (analogous to chemistry being the (central) science between traditional disciplines of biology and physics). From a very broad perspective, a drug design may be divided into two phases fundamental concepts about: a) drugs, receptors, and drug–receptor interactions; b) drug–receptor interactions applied to human disease.

Pharmaceutical/Medicinal Chemistry is interdisciplinary, drawing very suitably on theoretical chemistry, organic chemistry, analytical chemistry, molecular biology, pharmacology, and biochemistry. Despite these complexities, Pharmaceutical/Medicinal Chemistry has its own clear line – the design and discovery of drug molecules with a comprehensive and precise definition and characterization of their properties, taking into account i) structural integrity of the drug molecules (in pharmaceutical, pharmacokinetic and pharmacodynamic phase, respectively), ii) their structural fragments (pharmacophore, toxicophore, metabophore, biophore, etc.; interchangeable bioisosteres), iii) structural properties, iv) physicochemical features (solubility, surface activity, acid-base and lipohydrophilic properties), v) shape properties (geometric, conformational, topological, steric), vi) stereochemical properties (optical isomers, enantiomers, geometric isomers), vii) electronic properties. Following that knowledge, structure–biological activity relationships, structure–pharmacokinetics relationships as well as structure–toxicity relationships are comprehensively investigated (SAR, QSAR).

Thorough and deep knowledge, understanding and correct interpretation of all relationships that are explained via this course is extremely important for (almost) all fields of pharmaceutical study.

Class syllabus:

Syllabus of Lectures

1ST WEEK: Drugs Influencing a Cardiovascular System. Cardiotonics, Cardiotonic Agents. Vasodilating Agents (Definitions, drugs - systematic chemical division, chemical structures of some compounds, mechanisms of action, structure–activity relationships, biotransformation pathways).

2ND WEEK: Antihypertensives. Drugs Influencing Veins (Definitions, drugs - systematic chemical division, chemical structures of some compounds, mechanisms of action, structure–activity relationships, biotransformation pathways).

3RD WEEK: Drugs Regulating Blood Coagulation Processes. Blood Substitutes. Lipid-Lowering Drugs – Treatment of Hypercholesterolemia. Treatment of Hypertriglyceridemia (Definitions, drugs - systematic chemical division, chemical structures of some compounds, mechanisms of action, structure–activity relationships, biotransformation pathways).

4TH WEEK: Hepatoprotective Agents. Diuretics, Anti-Diuresis Drugs. Ligands of Vasopressin Receptors (Definitions, drugs - systematic chemical division, chemical structures of some compounds, mechanisms of action, structure–activity relationships, biotransformation pathways).

5TH WEEK: Anthelmintics. Isecticidal Agents (Definitions, drugs - systematic chemical division, chemical structures of some compounds, mechanisms of action, structure–activity relationships, biotransformation pathways).

Discussion connected with the topics lectured previously

6TH WEEK: Cystic Fibrosis. Emerging Cystic Fibrosis Transmembrane Conductance Regulator Modulators as New Drugs for Cystic Fibrosis (Definitions, drugs - systematic chemical division, chemical structures of some compounds, mechanisms of action, structure–activity relationships, biotransformation pathways).

7TH WEEK: Antifungal Drugs. Anti-Protozoal Agents (Definitions, drugs - systematic chemical division, chemical structures of some compounds, mechanisms of action, structure–activity relationships, biotransformation pathways).

8TH WEEK: Antimalarial Drugs. Anti-Tuberculosis Drugs. Anti-Leprosy Drugs (Definitions, drugs - systematic chemical division, chemical structures of some compounds, mechanisms of action, structure–activity relationships, biotransformation pathways).

9TH WEEK: Antibacterial Chemotherapeutics/Antibiotics, part 1. beta-Lactam Antibiotics, beta-Lactamase Inhibitors (Definitions, drugs - systematic chemical division, chemical structures of some compounds, mechanisms of action, structure–activity relationships, biotransformation pathways).

10TH WEEK: Antibacterial Chemotherapeutics/Antibiotics, part 2. Diaminopyrimidines. Quinolones (Gyrase Inhibitors). Nitrofurans (Definitions, drugs - systematic chemical division, chemical structures of some compounds, mechanisms of action, structure–activity relationships, biotransformation pathways).

Discussion connected with the topics lectured previously.

11TH WEEK: Antiviral Agents (Definitions, drugs - systematic division, chemical structures of some compounds, mechanisms of action, structure–activity relationships, biotransformation pathways).

12th WEEK: Antitumor drugs, part 1. Alkylating compounds. Compounds forming complexes with DNA. Compounds generating reactive entities. Antimetabolites. Protein synthesis inhibitors. Antimitotic drugs (Definitions, drugs – systematic division, chemical structures of selected drugs, mechanisms of action, evaluation of structure–activity relationships, biotransformation).

13th–14th WEEK: Antitumor drugs, part 2. Angiogenesis inhibitors. PROTAC technology, PROTAC molecules. Molecular adhesives. Inhibitors of histone deacetylases and other proteins.

Inhibitors of histone methyltransferases. Inhibitors of the MAPK signaling pathway. Proteasome inhibitors (Definitions, drugs – systematic division, chemical structures of selected drugs, mechanisms of action, evaluation of structure–activity relationships, biotransformation).

Syllabus of Laboratory Practicals

1ST-12TH WEEK – PART A

At the Laboratory Practicals, students will calculate theoretical yields of particular reactions steps from convenient syntheses of biologically active compounds – drugs.

Selected drugs to be synthesized: Acetylsalicylic Acid, Paracetamol, Phenacetine, Methyl Salicylate, Parabens (Methyl Paraben, Ethyl Paraben, Propyl Paraben, Isopropyl Paraben, Butyl Paraben etc.), Benzocaine, Lidocaine (Lignocaine), Trimecaine, Sulfanilamide, Phthalylsulfathiazole, Succinylsulfathiazole, Disulfiram, Isoniazid.

Knowledge about the methods, which can be used to purify synthesized compounds (crystallization, adsorption thin-layer chromatography, distillation), purity verification (TLC), methods to determine their melting points; practical using of the knowledge.

Principles of spectral methods to confirm structural identity of compounds (Nuclear Magnetic Resonance (^1H NMR, ^{13}C NMR), Infrared Spectrometry, Ultraviolet/Visible Spectrophotometry, etc.), and chromatographic methods (High-Performance Liquid Chromatography; HPLC); spectral identification of synthesized compounds.

Knowledge about the determinations of some physicochemical properties and/or physicochemical constants related to reaction intermediates and final compounds – drugs, i.e., solubility in various solvents, melting point values, surface properties – surface tension γ (Traube stalagmometric method), electronic properties – $\log \epsilon$ values (UV/Visible Spectrophotometry), electronic properties – acid-base dissociation constants pK_a (titration methods), lipohydrophilic properties – retention factor $\log k$ (Reversed-Phase High-Performance Liquid Chromatography), partition coefficient $\log P_{\text{exp}}$ (shake-flask method), stability properties in acidic, alkaline and oxidizing media as well as kinetics studies; estimation of relevant parameters.

1ST-12TH WEEK – PART B

Extended knowledge regarding pharmacodynamic classes / particular drugs (introduced by a teacher; structure of the presentation: definitions, division of a pharmacodynamic class from a chemical point of view, chemical structures of particular compounds, brief but precise mechanisms of action, structure–activity relationships, structure–pharmacokinetics or structure–toxicity relationships eventually, biotransformation pathways of particular compounds) as follows:

- a) Analgesics–Antipyretics,
- b) Disulfiram,
- c) Drugs Supporting Acidosis. Antacids and Anti-Ulcer Drugs,
- d) Disinfectants and Antiseptics,
- e) Sulfonamides.

Recommended literature:

The Lectures from the Pharmaceutical Chemistry (2) Course

Abraham, D.J., & Rotella, D.P. (2010). Burger's Medicinal Chemistry and Drug Discovery, 8 Volume Set. 7th Ed. Wiley, Hoboken, NY, United States of America, 6416 pp.

Avendaño, C., & Menéndez, J.C. (2015). Medicinal Chemistry of Anticancer Drugs. 2nd Ed. Elsevier, Amsterdam, the Netherlands; Elsevier, Kidlington, Oxford, United Kingdom; Elsevier, Waltham, MA, United States of America, 744 pp.

Beale, J.M., & Block, J.H. (2011). Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry. 12th Ed. Wolters Kluwer Health (Lippincott Williams & Wilkins), Philadelphia, United States of America, 1022 pp.

Chackalamannil, S., Rotella, D., & Ward, S. (2017). Comprehensive Medicinal Chemistry III, 3rd Ed. Elsevier, Amsterdam, Netherlands, 4536 pp.

Desai, M.C., Meanwell, N.A., Thurston, D.E., Ganellin, R., Fox, D., Guccione, S., Martinez, A., Rotella, D., Belema, M., Sperandio, D., Shi, P.-Y., Jordan, R., Halcomb, R., Roberts, Ch., Johns, B.A., Griffin, S., Beaulieu, P.L., McCauley, J.A., Sofia, M., Xu, L., Guyer, B., & Peel, M.R. (2013). Successful Strategies for the Discovery of Antiviral Drugs: RSC (Drug Discovery). Drug Discovery Series No. 32, Royal Society of Chemistry, Cambridge, United Kingdom, 533 pp.

Firestine, S.M., Lister, T., Abel-Santos, E., Hedstrom, L., Melander, Ch., Fisher, S., Khursigara, C., Lazarides, L., Garneau-Tsodikova, S., & Balibar, C.J. (2017). Antibiotic Drug Discovery: New Targets and Molecular Entities. 1st Ed., Kindle Ed. Drug Discovery Series No. 58, Royal Society of Chemistry, Cambridge, United Kingdom, 285 pp.

Chackalamannil, S., Rotella, D., & Ward, S. (2017). Comprehensive Medicinal Chemistry III, 3rd. Ed. Elsevier, Amsterdam, Netherlands, 4536 pp.

Kos, J., & Garaj, V. (2020). Laboratory Practices from Pharmaceutical Chemistry. 1st Ed. Faculty of Pharmacy, Comenius University in Bratislava, 184 pp.

Patrick, G.L. (2017). An Introduction to Medicinal Chemistry. 6th Ed. Oxford University Press, New York, USA, 832 pp.

Roche, V.F., Zito, S.V., Lemke, T.L., & Williams, D.A. (2019). Foye's Principles of Medicinal Chemistry. 8th Ed. Wolters Kluwer Health Adis (ESP), Baltimore, USA, 1168 pp.

Silverman, R.B., & Holladay, M.W. (2015). The Organic Chemistry of Drug Design and Drug Action. 3rd. Ed. Elsevier, Waltham, USA, 521 pp.

Silverstein, R.M., Webster, F.X., Kiemle, D., & Bryce, D.L. (2014). Spectrometric Identification of Organic Compounds. 8th Ed. John Wiley & Sons, Hoboken, United States of America, 464 pp.

Wermuth, C., Aldous, D., Raboisson, P., & Rognan, D. (2015). The Practice of Medicinal Chemistry. 4th Ed. Academic Press (Elsevier), San Diego, CA, USA; Kidlington, Oxford, Great Britain, 903 pp.

Languages necessary to complete the course:

English language

Notes:

Past grade distribution

Total number of evaluated students: 0

A	ABS	B	C	D	E	FX
0,0	0,0	0,0	0,0	0,0	0,0	0,0

Lecturers: doc. PharmDr. Ivan Malík, PhD., Mgr. Róbert Šandrik, PhD., PharmDr. Lenka Stopková, PhD.

Last change: 11.06.2026

Approved by: doc. PharmDr. Ivan Malík, PhD.