COURSE DESCRIPTION

Structure - Biological Activity Relationship

Academic year 2026-2027

1. Programme-related data

1.1. Higher Education Institution	Babeş-Bolyai University, Cluj-Napoca
1.2. Faculty	Faculty of Chemistry and Chemical Engineering
1.3. Department	Chemistry
1.4. Field	Chemistry
1.5. Level of study	Master's degree
1.6. Degree programme / Qualification	Advanced Chemistry (AC) / Chemist
1.7. Form of education	Full-time

2. Course-related data

2.1. Course title	**Structure - Biological Activity Relationship**			Course code	**CMR7222**
2.2. Course coordinator	Prof. Dr. Niculina Hădade				
2.3. Seminar coordinator	Prof. Dr. Niculina Hădade				
2.4. Year of study	II	2.5. Semester	2	2.6. Type of assessment	Exam
2.7. Course status	Optional			2.8. Course type	Specialisation subject

3. Total estimated time (hours per semester of teaching activities)

3.1. Number of hours per week	**4**	of which: 3.2. course	**2**	3.3. seminar/ laboratory/ project	**2**
3.4. Total of hours in the curriculum	56	of which: 3.5. course	28	3.6. seminar/ laboratory	**28**
Time allocation for individual study (IS) and self-taught activities (ST)					**hours**
Learning from textbooks, course materials, bibliography, and notes (IS)					33
Additional research in the library, on subject-specific electronic platforms, and on-site					14
Preparing seminars/ laboratories/ projects, assignments, reports, portfolios, and essays					14
Tutoring (professional guidance)					4
Examinations					2
Other activities					2
3.7. Total hours of individual study (IS) and self-taught activities (ST)				**69**	
3.8. Total hours per semester				**125**	
3.9. Number of credits				**5**	

4. Prerequisites (where applicable)

4.1. curriculum-related	Not applicable
4.2 skills-related	Not applicable

5. Specific conditions (where applicable)

5.1. course-related	Students will consult the course materials made available to them before each class. Materials and information will be provided on e-learning platforms. Interactive participation will be encouraged.
5.2. seminar/laboratory-related	Attendance at seminar and laboratory activities is mandatory under the conditions established by the regulations. Strict observance of occupational safety rules. Completion of the experiment sheet regarding risk factors and protective measures. Laboratory equipment is mandatory.

	The tasks that students must complete during each laboratory session are clearly defined and discussed with students at the beginning of the activity. Students are required to prepare the laboratory work and to know the working procedure, having available the necessary bibliographic material and the laboratory handout.

6.1. Competencies resulting from the completion of the degree programme *(as referred to in the curriculum)*[1]

Professional competencies	
Competency code	**Competency**
PC1	Demonstrate disciplinary expertise
PC4	Manage chemical testing procedures
PC5	Interact professionally in research and professional environments
Transversal competencies	
Competency code	**Competency**
TC2	Work in teams
TC3	Think critically

6.2. Learning outcomes relevant to the degree programme (as referred to in the curriculum)[2]

Learning outcomes targeted by the subject		
Competency code	**Knowledge and comprehension**	**Specific academic skills**
CP5, CT2	The graduate understands norms, roles and working practices specific to academic and professional research environments, including communication and collaboration standards.	The graduate interacts professionally in research and professional environments, gives and uses feedback, and argues scientific decisions within teams.
CP3, CT3	The graduate understands quality criteria and standards of scientific argumentation (coherence, validity, reproducibility, relevance) used to evaluate conclusions.	The graduate critically evaluates results and interpretations and communicates well-argued conclusions and recommendations in academic/professional contexts, adapting the message to audiences and purpose.

7. Subject-specific learning outcomes

Knowledge and comprehension
1. Explains the general principles of the structure-activity relationship and the main stages of rational drug design
2. Describes the sources of biologically active compounds, the concept of the lead compound, and the main screening techniques used for its identification.
3. Explains structural optimisation strategies for lead compounds, correlating structural changes with biological activity, selectivity, toxicity, and pharmacokinetic properties.
4. Describes the main types of drug-biological target interactions, the role of stereochemistry, and the mechanisms of action involved in the interaction of active compounds with receptors, enzymes, and nucleic acids.
Specific academic skills

[1] The professional and/or transversal skills targeted by the subject for which the course description is prepared will be copied from the curriculum of the degree programme. For each competency, the complete entry, including the competency code, will be copied with the exact wording that appears in the curriculum, without any changes. If no competency is copied from either of the two categories, the row corresponding to that category is deleted from the table.

[2] The learning outcomes relevant for the degree programme and targeted by the subject for which the course description is prepared will be listed. The entries, copied without any changes from the Curriculum by subject type (Core Subject/Specialisation Subject/Complementary Subject), are listed under the corresponding competency.

1. Critically analyses the relationship between chemical structure and biological activity for representative classes of bioactive compounds and drugs.
2. Evaluates and compares lead-compound identification and optimisation strategies using data from the scientific literature, experimental examples, and relevant validation criteria.
3. Communicates and supports, orally and in writing, conclusions regarding the selection, modification, and evaluation of biologically active compounds, integrating feedback and collaboration in seminar and laboratory activities.

8. Contents

8.1. Course	**Teaching and learning methods**	**Remarks[3]**
8.1.1. Structure-activity relationship: purpose and definitions. General overview of methods for identifying new drugs. Rational drug design.	Lecture, discussion, discovery learning, problem solving	2 hours
8.1.2. Identification of the lead compound. Sources of biologically active compounds.	Lecture, discussion, discovery learning, problem solving	2 hours
8.1.3. Identification of the lead compound. Screening techniques.	Lecture, discussion, discovery learning, problem solving	2 hours
8.1.4. Modification of the lead compound in order to improve its properties (activity, toxicity, absorption, metabolism, elimination). Homologous series, branching, bioisosteres.	Lecture, discussion, discovery learning, problem solving	2 hours
8.1.5. Modification of the lead compound in order to improve its properties (activity, toxicity, absorption, metabolism, elimination). Ring-chain transformation. Biologically active conformation.	Lecture, discussion, discovery learning, problem solving	2 hours
8.1.6. Modification of the lead compound in order to improve its properties. Peptidomimetics.	Lecture, discussion, discovery learning, problem solving	2 hours
8.1.7. Drug-biological target interaction. Types of interactions involved in drug-biological target complexes. Molecular recognition.	Lecture, discussion, discovery learning, problem solving	2 hours
8.1.8. Drug-biological target interaction. Determination of drug-receptor interactions. Receptor agonists and antagonists.	Lecture, discussion, discovery learning, problem solving	2 hours
8.1.9. Drug-biological target interaction. Mechanisms. Stereochemical considerations.	Lecture, discussion, discovery learning, problem solving	2 hours
8.1.10. Irreversible enzyme inhibitors.	Lecture, discussion, discovery learning, problem solving	2 hours
8.1.11. Reversible enzyme inhibitors.	Lecture, discussion, discovery learning, problem solving	2 hours
8.1.12. Drugs interacting with nucleic acids.	Lecture, discussion, discovery learning, problem solving	2 hours
8.1.13. Prodrugs of the drug-carrier type.	Lecture, discussion, discovery learning, problem solving	2 hours
8.1.14. Macromolecular drug delivery systems	Lecture, discussion, discovery learning, problem solving	2 hours
Bibliography		
1. Course materials in PDF format provided by the course coordinator. 2. Richard B. Silverman, Mark W. Holladay, The Organic Chemistry of Drug Design and Drug Action, 3rd edition, San Diego, CA: Academic Press, 2014. 3. D. Livingstone; Andrew M. Davis, Drug Design Strategies: Quantitative Approaches, Royal Society of Chemistry, Cambridge: RSC Publishing, 2012.		

[3] For example, organisational aspects, recommendations for students, specific aspects relating to the course/seminar, such as inviting experts in the field, etc.

4. M. V. Diudea, M. S. Florescu, and P. V. Khadikar, Molecular Topology and Its Applications, EFICON, Bucharest, 2006. 5. Reviews and articles from recent scientific literature (Wiley, ACS, RSC, Elsevier).		
8.2. Seminar/ laboratory	**Teaching and learning methods**	**Remarks**
8.2.1. Safety training. Presentation of the laboratory topics.	Experimentation, discussion, discovery learning, problem solving	4 hours
8.2.2. Four-step synthesis of benzocaine starting from p-toluidine: Preparation of N-acetyl-p-toluidine.	Experimentation, discussion, discovery learning, problem solving	4 hours
8.2.3. Four-step synthesis of benzocaine starting from p-toluidine: Preparation of N-acetyl-p-aminobenzoic acid.	Experimentation, discussion, discovery learning, problem solving	4 hours
8.2.4. Four-step synthesis of benzocaine starting from p-toluidine: Preparation of p-aminobenzoic acid.	Experimentation, discussion, discovery learning, problem solving	4 hours
8.2.5. Four-step synthesis of benzocaine starting from p-toluidine: Preparation and purification of benzocaine.	Discussion, discovery learning, problem solving	2 hours
8.2.6. Sources of prototype compounds. Screening methods and techniques. Aspirin, penicillins.	Experimentation, discussion, discovery learning, problem solving	2 hours
8.2.7. Identification of fragment-based prototype compounds. Study of complexes by mass spectrometry.	Discussion, discovery learning, problem solving	2 hours
8.2.8. Effect of structural modifications on efficacy and pharmacokinetic properties. Taxol.	Discussion, discovery learning, problem solving	2 hours
8.2.9. Optimisation of efficacy, selectivity, lipophilicity, and toxicity. Calculation of log P.	Discussion, discovery learning, problem solving	2 hours
8.2.10. Computational methods in lead-compound modification.	Experimentation, discussion, discovery learning, problem solving	4 hours
Bibliography: 1. Richard B. Silverman, Mark W. Holladay, The Organic Chemistry of Drug Design and Drug Action, 3rd edition, San Diego, CA: Academic Press, 2014. 2. K. C. Nicolaou and T. Montagnon, Molecules That Changed the World, Wiley-VCH, 2008. 3. Scientific articles corresponding to the course and laboratory topics (Wiley, ACS, Elsevier, RSC collections). 4. Laboratory handouts made available to students by the course coordinator. 5. Cercasov, F. Dumitrașcu, C.-V. Popa, C. Drăghici, Natural and Synthetic Compounds with Therapeutic Action, University of Bucharest Publishing House, 2004.		

9. Evaluation

Type of activity	9.1 Evaluation criteria[4]	9.2 Evaluation methods[5]	9.3 Percentage in the final grade
9.4. Course	Degree of understanding of the topics covered in the course and understanding of the notions illustrated through correct answers. Way of thinking, correctness, and argumentation of the solutions to problems and exercises	Oral examination. Exam fraud is punished by expulsion according to the UBB ECTS regulations.	60%
9.5. Seminar/ laboratory	Correctness of answers to exercises and problems, demonstrating understanding and acquisition of the topics.	Continuous assessment.	40%

[4] The evaluation criteria must directly reflect the learning outcomes targeted at the level of the degree programme respectively at the level of the subject. More specifically, the learning outcomes set out in the expected learning outcomes are assessed.

[5] Both final evaluation methods and ongoing evaluation strategies should be established.

	Presentation of a marketed drug, identification of the prototype, structural modifications, testing stages.	Continuous assessment.	
9.6 Minimum standard for passing			
Obtaining grade 5 (five) in the examination according to the grading scale, with access to the exam being conditional on passing the seminar assessment with at least grade 5 (five). Sources of biologically active compounds, screening methods, methods for structural validation, determination of ligand efficiency and therapeutic index. Identification of the pharmacophore, auxophoric groups, and drug-biological target interactions. Minimum grade 5 for each laboratory. Minimum grade 5 for each laboratory report.			

10. SDG labels (Sustainable Development Goals)[6]

	○	Sustainable Development Generic Label						
1 FĂRĂ SĂRĂCIE	2 FOAMETE „ZERO”	3 SĂNĂTATE ȘI BUNĂSTARE	4 EDUCAȚIE DE CALITATE	5 EGALITATE DE GEN	6 APĂ CURATĂ ȘI SANITAȚIE	7 ENERGIE CURATĂ ȘI LA PREȚURI ACCESIBILE	8 MUNCĂ DECENTĂ ȘI CREȘTERE ECONOMICĂ	9 INDUSTRIE, INOVAȚIE ȘI INFRASTRUCTURĂ
○	○	○	X	○	○	○	○	○
10 INEGALITĂȚI REDUSE	11 ORAȘE ȘI COMUNITĂȚI DURABILE	12 CONSUM ȘI PRODUCȚIE RESPONSABILE	13 ACȚIUNE CLIMATICĂ	14 VIAȚA ACVATICĂ	15 VIAȚA TERESTRĂ	16 PACE, JUSTIȚIE ȘI INSTITUȚII EFICIENTE	17 PARTENERIATE PENTRU REALIZAREA OBIECTIVELOR	No label applies
○	○	○	○	○	○	○	○	○

Date of entry:
17.04.2026

Signature of course coordinator

Prof. Dr. Niculina Hădade

Signature of seminar coordinator

Prof. Dr. Niculina Hădade

Date of approval in the department:
24.04.2026

Signature of the head of department

Prof. Dr. Monica Toșa

[6] Select a single label which, according to the *Implementation of SDG labels in the academic process*, best matches the subject. If the subject addresses sustainable development in a generic manner (i.e. by presenting/introducing the general framework of sustainable development, etc.), then the Sustainable Development generic label may be applied. If none of the labels describe the subject, select the last option: *"No label applies."*