COURSE DESCRIPTION

Artificial Intelligence in Chemistry and Biochemistry

Academic year 2026 - 2027

1. Programme-related data

1.1. Higher Education Institution	Babeș-Bolyai University of Cluj-Napoca
1.2. Faculty	Chemistry and Chemical Engineering
1.3. Department	Chemical Engineering
1.4. Field	Chemical Engineering
1.5. Level of study	Master
1.6. Degree programme / Qualification	Organic and Biochemical Processes Engineering
1.7. Form of education	Full time education

2. Course-related data

2.1. Course title	**Artificial Intelligence in Chemistry and Biochemistry**			Course code	**CME7234**
2.2. Course coordinator	Vacant position				
2.3. Seminar coordinator	Vacant position				
2.4. Year of study	II	2.5. Semester	4	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)	24
Additional research in the library, on subject-specific electronic platforms, and on-site	20
Preparing seminars/ laboratories/ projects, assignments, reports, portfolios, and essays	15
Tutoring (professional guidance)	4
Examinations	4
Other activities: consultations and discussions with the course/seminar coordinators and with the tutor	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	Basics of Chemical Engineering
4.2 skills-related	Basic computer-using skills

5. Specific conditions (where applicable)

5.1. course-related	Students should switch off the mobile phones during courses and seminars. Students attending the courses should be present at the courses without any time delay.
5.2. seminar/laboratory-related	The deadline for presenting the homework results will be agreed by the seminar teaching person and the students. No delay is accepted for the presentation of the homework results unless well-founded reasons (health care) are proven.

	In case of presenting the homework with delay, the grade will be penalized by 0.5 points/week of delay. Students should be present at the compulsory seminars/laboratories without any time delay.

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

Professional competencies	
Competency code	**Competency**
PC1	Description, analysis and use of fundamental concepts and theories in the field of organic chemistry, biochemistry, microbiology, genetics and molecular biology
PC2	Description, analysis and use of fundamental concepts and theories in the field of engineering sciences and biotechnologies
PC3	Description, analysis and use of methods of analysis, characterization and control specific to natural products and biosynthesis products
PC4	The operation of installations and processes in the field of organic and biochemical processes
PC5	Modelling biological systems/bioengineering structures and processes of fine organic synthesis
Transversal competencies	
Competency code	**Competency**
TC1	Independent execution of complex professional assignments and autonomous development of project-research activities by using computer-assisted techniques and by observing the norms of professional ethics and moral conduct
TC3	Self-assessment of professional performances and determining the continuous training needs, permanent information and documentation in the field of activity and related areas, according to the needs of the labour market

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**
PC1, PC2, PC4, PC5	1. The student/graduate knows effective ecological synthesis methods	1. The student/graduate proposes sustainable (bio)technologies for synthesis and implements them (partially) experimentally
PC1, PC2, PC4, PC5, TC1	2. The student/graduate knows the operations and equipment used in organic processes and bioprocesses involved in obtaining and developing useful products	2. The student/graduate develops operational schemes and tools for obtaining useful products (pharmaceuticals, food products, other synthetic compounds), performs equipment calculations and modelling/optimization
PC2, PC4, PC5, TC3	3. The student/graduate knows the basic principles of a (bio)process, the stages of technology development, and methods for separating useful products	3. The student/graduate proposes technologies for obtaining useful products, including their separation/purification steps.

7. Subject-specific learning outcomes

Knowledge and comprehension

[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. The student applies the study of the relationship between the structure and the properties in designing, preparation and characterisation of materials for various applications
2. The student knows to explain and interpret concepts, properties, fundamental notions of the molecular recognition of the chemical compounds
3. The student applies the fundamental concepts to solve problems associated with the molecular recognition of the chemical compounds
4. The student selects and uses adequate methods in order to investigate properties by using compounds with ionic and molecular recognition properties
5. The student understands and interprets the space-and-time evolution of a chemical system, to abstract and represent it in the form of a mathematical model using the methods of artificial intelligence
Specific academic skills
1. The student fulfils the tasks according to the requirements within the deadlines, respecting the ethical and moral standards, and following the established working plan
2. The student communicates and argues one's own ideas and points of view, clearly and concisely, using communication methods based on conventional and non-conventional IT tools

8. Contents

8.1. Course	**Teaching and learning methods**	**Remarks[3]**
8.1.1. Introduction / overview of Artificial Intelligence and Machine Learning; Brief history and evolution of applications in Chemistry and Biochemistry	Lecture Explanation Conversation Demonstration	Time allocated 2 hours
8.1.2. Basic concepts of chemistry and biochemistry that are within the scope of artificial intelligence applications	Lecture Explanation Conversation Demonstration	Time allocated 2 hours
8.1.3. Data Preprocessing: Data cleaning and preparation; Feature selection and engineering; Handling missing data	Lecture Explanation Conversation Demonstration	Time allocated 2 hours
8.1.4. Supervised Learning: Regression techniques in chemistry and biochemistry; Classification methods; Model evaluation and validation; Recurrent Artificial Neural Networks for dynamic modeling	Lecture Explanation Conversation Demonstration	Time allocated 2 hours
8.1.5. Unsupervised Learning: Clustering algorithms; Dimensionality reduction techniques; Applications in chemical and biochemical data analysis	Lecture Explanation Conversation Demonstration	Time allocated 2 hours
8.1.6. Deep Learning Fundamentals: Introduction to neural networks; Deep learning architectures; Convolutional Neural Networks (CNNs) for image analysis in biochemistry	Lecture Explanation Conversation Demonstration	Time allocated 2 hours
8.1.7. Applications of ML in Drug Discovery: Drug-target interactions prediction; QSAR (Quantitative Structure-Activity Relationship) modeling; Virtual screening and compound design	Lecture Explanation Conversation Demonstration	Time allocated 2 hours
8.1.8. Molecular Dynamics Simulation and AI: Introduction to Molecular Dynamics Simulation; Enhancing simulations with AI/ML; Protein folding prediction using deep learning	Lecture Explanation Conversation Demonstration	Time allocated 2 hours

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

8.1.9. Cheminformatics and Bioinformatics: Chemical databases and data mining; Sequence analysis in bioinformatics; Drug design using cheminformatics approaches	Lecture Explanation Conversation Demonstration	Time allocated 2 hours
8.1.10. AI in Systems Biology: Network biology and systems modeling; Metabolic pathway analysis using ML; Predicting gene regulatory networks	Lecture Explanation Conversation Demonstration	Time allocated 2 hours
8.1.11. AI in Protein Engineering: Protein structure prediction; Protein engineering and design using AI techniques; Directed evolution and machine learning	Lecture Explanation Conversation Demonstration	Time allocated 2 hours
8.1.12. AI in Analytical Chemistry; Analytical instrumentation and data analysis; Spectroscopy data analysis using ML; Chromatographic data analysis	Lecture Explanation Conversation Demonstration	Time allocated 2 hours
8.1.13. AI in Chemical Engineering: Chemical process modeling, control and optimization using AI tools	Lecture Explanation Conversation Demonstration	Time allocated 2 hours
8.1.14. Ethical and Social Implications: Bias and fairness in AI models; Privacy concerns in biomedical data; Responsible AI in chemistry and biochemistry research; Emerging directions	Lecture Explanation Conversation Demonstration	Time allocated 2 hours

Bibliography

1. LeCun, Y., Bengio, Y., & Hinton, G. (2015). Deep learning. Nature, 521(7553), 436-444.
2. Schneider, G., & Fechner, U. (2005). Computer-based de novo design of drug-like molecules. Nature Reviews Drug Discovery, 4(8), 649-663.
3. Min, S., Lee, B., Yoon, S. (2017). Deep learning in bioinformatics. Briefings in Bioinformatics, 18(5), 851–869.
4. Aliper, A., Plis, S., Artemov, A., Ulloa, A., Mamoshina, P., & Zhavoronkov, A. (2016). Deep Learning Applications for Predicting Pharmacological Properties of Drugs and Drug Repurposing Using Transcriptomic Data. Molecular Pharmaceutics, 13(7), 2524–2530.
5. Sliwoski, G., Kothiwale, S., Meiler, J., & Lowe, E. (2014). Computational Methods in Drug Discovery. Pharmacological Reviews, 66(1), 334–395.
6. Simon Haykin, (1994). Neural Networks A Comprehensive Foundation, Mcmillan Publishing Company, Englewood Cliffs, NJ 07632.

8.2. Seminar/ laboratory	**Teaching and learning methods**	**Remarks**
8.2.1-2. Introduction to Python, Matlab Deep Learning Toolbox and Data Handling; Setup Python environment and necessary libraries (NumPy, Pandas); Introduction to Jupyter Notebooks; Basic data handling exercises: loading datasets, data visualization, summary statistics	Explanation Conversation Questioning Exercise	Time allocated 4 hours
8.2.3-4. Data Preprocessing; Data cleaning: handling missing values, outlier detection; Feature selection and engineering: identifying relevant features, creating new features; Hands-on exercises with real chemical and biochemical datasets	Explanation Conversation Questioning Exercise	Time allocated 4 hours
8.2.5-6. Supervised Learning; Implementing regression models for chemical property prediction; Building classification models for protein function prediction; Model evaluation and validation techniques; Nonlinear	Explanation Conversation Questioning Exercise	Time allocated 4 hours

Autoregressive with Exogeneous Inputs Artificial Neural Networks (NARX)		
8.2.7-8. Unsupervised Learning; Clustering techniques for chemical compound grouping; Dimensionality reduction methods (PCA, t-SNE) for visualization; Practical applications in analyzing biochemical data sets	Explanation Conversation Questioning Exercise	Time allocated 4 hours
8.2.9-10. Deep Learning Fundamentals; Introduction to deep learning frameworks (TensorFlow, Keras); Implementing simple neural networks for chemical data analysis; Shallow Artificial Neural Networks; Hands-on exercise: image classification for protein structure prediction	Explanation Conversation Questioning Exercise	Time allocated 4 hours
8.2.11-12. Applications in Drug Discovery; Predicting drug-target interactions using machine learning models; Virtual screening of chemical compounds for drug discovery; Case studies and group discussions on recent research in drug discovery using AI/ML	Explanation Conversation Questioning Exercise	Time allocated 4 hours
8.2.13-14. Project Work and Presentation; Students work on a final project applying AI/ML techniques to a chemistry or biochemistry problem; Guidance and support from instructors on project development; Project presentations by students, followed by discussions and feedback	Explanation Conversation Questioning Exercise	Time allocated 4 hours
Bibliography 1. TensorFlow Documentation: https://www.tensorflow.org/ 2. Keras Documentation: https://keras.io/ 3. Scikit-learn Documentation: https://scikit-learn.org/stable/documentation.html 4. PyTorch Documentation: https://pytorch.org/docs/stable/index.html 5. Bioinformatics.org: https://www.bioinformatics.org/ 6. Matlab Deep Learning Toolbox: https://www.mathworks.com/help/deeplearning/		

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	The rightness of the answers – achievement and understanding of the issues covered in the course	Oral exam/Essay presentation	80%
	The rightness of the answers – achievement and understanding of the issues covered in the course		
9.5. Seminar/ laboratory	Active participation to the seminar, achievement and correct understanding of the issues covered in the seminar	Short presentation throughout the semester	20%
	The ability to apply the acquired knowledge		
9.6 Minimum standard for passing			

[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.

Knowledge of molecular recognition basic concepts and principles of AI classification/prediction tools Understanding the role, area of utilization and principles on which instruments of the artificial intelligence is based Obtaining the minimum grade of 5 for each of the following: examination, seminar work and solving the homework

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

	○	Eticheta generală pentru Dezvoltare durabilă

								
○	○	○	○	○	○	○	○	◉
								Nu se aplică nici o etichetă
○	○	○	○	○	○	○	○	○

Date of entry:
...

Signature of course coordinator

vacant

Signature of seminar coordinator

vacant

Date of approval in the department:
...

Signature of the head of department

Prof. habil. dr. ing. Graziella L. Turdean

[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."*