SYLLABUS

1. Information regarding the programme

1.1 Higher education institution	**Babeș-Bolyai University**
1.2 Faculty	**Chemistry and Chemical Engineering**
1.3 Department	**Chemical Engineering**
1.4 Field of study	**Chemistry/Chemical Engineering**
1.5 Study cycle	**Master**
1.6 Study programme / Qualification	**Advanced Process Chemical Engineering**

2. Information regarding the discipline

2.1 Name of the discipline			**Artificial Intelligence in Chemistry and Biochemistry – CME7235**				
2.2 Course coordinator			Prof. dr. eng. Cristea Vasile Mircea				
2.3 Seminar coordinator			Vacant position.				
2.4. Year of study	**I**	2.5 Semester	**2**	2.6. Type of evaluation	**E**	2.7 Type of discipline	DS/Opt

3. Total estimated time (hours/semester of didactic activities)

3.1 Hours per week	**4**	Of which: 3.2 course	**2**	3.3 seminar/laboratory	**2**
3.4 Total hours in the curriculum	**56**	Of which: 3.5 course	**28**	3.6 seminar/laboratory	**28**
Time allotment:					hours
Learning using manual, course support, bibliography, course notes					**25**
Additional documentation (in libraries, on electronic platforms, field documentation)					**18**
Preparation for seminars/labs, homework, papers, portfolios and essays					**20**
Tutorship					**3**
Evaluations					**3**
Other activities:					**-**

3.7 Total individual study hours	**69**
3.8 Total hours per semester	**125**
3.9 Number of ECTS credits	**5**

4. Prerequisites (if necessary)

4.1. curriculum	• Basics of Chemistry
4.2. competencies	• Basic computer-using skills

5. Conditions (if necessary)

5.1. for the course	• Mobile phones should be switched off • No late arrival
5.2. for the seminar/lab activities	• Mobile phones should be switched off • Hand-held scientific calculator is required • No late arrival

6. Specific competencies acquired

Professional competencies	• The study of the relationship between the structure and the properties in designing, preparation and characterisation of materials for various applications. • Explanation and interpretation of concepts, properties, fundamental notions of the molecular recognition of the chemical compounds. • Application of the fundamental concepts to solve problems associated with the molecular recognition of the chemical compounds. • Critical analysis of the existing theories and models regarding the recognition of chemical compounds. • The ability to understand and interpret 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.
Transversal competencies	• Fulfilling the tasks according to the requirements within the deadlines, respecting the ethical and moral standards, and following the established working plan. • Fulfilling the tasks in agreement with the general objectives by integrating into a working group and distributing the tasks. • Communicating and arguing one's own ideas and points of view, clearly and concisely, using communication methods based on conventional and non-conventional IT • Getting information in English by using modern approaches.

7. Objectives of the discipline (outcome of the acquired competencies)

7.1 General objective of the discipline	• Achievement of knowledge regarding the preparation, characterization and usage of materials with ionic and molecular recognition properties. • Learning the fundamental concepts of artificial intelligence and demonstrating their use in applications in chemistry and chemical engineering
7.2 Specific objective of the discipline	• Developing the ability to select and use adequate methods in order to investigate properties by using compounds with ionic and molecular recognition properties.

8. Content

8.1 Course	Teaching methods	Remarks
8.1.1-2. 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	Lecture Explanation	Time allocated 2 hours

methods; Model evaluation and validation; Recurrent Artificial Neural Networks for dynamic modeling	Conversation Demonstration	
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
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 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 2 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 2 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 Autoregressive with Exogeneous Inputs Artificial Neural Networks (NARX)	Explanation Conversation Questioning Exercise	Time allocated 2 hours
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 2 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 2 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 2 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	Explanation Conversation Questioning Exercise	Time allocated 2 hours

presentations by students, followed by discussions and feedback		

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. Corroborating the content of the discipline with the expectations of the epistemic community, professional associations and representative employers within the field of the program

- By assimilating the theoretical and methodological concepts and by approaching the practical aspects included in the *Artificial Intelligence in Chemistry and Biochemistry* discipline, the students acquire consistent knowledge in accordance with the competences of the Diploma Supplement and qualifications in the ANC.

10. Evaluation

Type of activity	10.1 Evaluation criteria	10.2 Evaluation methods	10.3 Share in the grade (%)
10.4 Course	The rightness of the answers – achievement and understanding of the issues covered in the course	Oral exam.	80%
	The ability to apply the acquired knowledge		
10.5 Seminar/lab activities	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		
10.6 Minimum performance standards			
• Knowledge of molecular recognition basic concepts and principles of AI classification/prediction tools • Grade 5 (five) as weighted average of the grades obtained at 10.4 and 10.5			

Date	Signature of course coordinator	Signature of seminar coordinator
14.04.2024	Prof dr. eng. Cristea Vasile Mircea	

Signature of the head of department

Date of approval
22.04.2024

Prof. dr. eng. Graziella Liana Turdean
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