University of Zagreb

1. GENERAL INFORMATION				
1.1 Course teacher	Prof. Tomislav Bolanča, PhD Assoc. Prof. Šime Ukić, PhD		1.6 Year of the study	2 (3rd semester)
1.2 Name of the course	Chemometrics		1.7 ECTS credits	5
1.3 Associate teachers	Matija Cvetnić, PhD		1.8 Type of instruction (number of hours L + E + S + e-learning)	Total: 60 (L 30 ,E 0,S 30)
1.4 Study programme (undergraduate, graduate, integrated)	graduate		1.9 Expected enrolment in the course	10
1.5. Status of the course	☐ mandatory	☒ elective	1.10 Level of application of e-learning (level 1, 2, 3), percentage of online instruction (max. 20%)	3

2. COUSE DESCRIPTION	
2.1. Course objectives	To introduce students to the importance of the use of mathematical and statistical methods to process real experimental data, to conduct multi-variant analysis and apply experimental design strategies. To insure their interaction with computer using standard software environment (MS Excel, MatLab, Statistica).
2.2. Enrolment requirements and/or entry competences required for the course	-
2.3. Learning outcomes at the level of the programme to which the course contributes	• Solve engineering problems using the scientific method combining expert knowledge from chemistry, environmental, and chemical engineering as well as material science and engineering. • Plan and independently perform experiments in order to confirm a hypothesis to estimate economic and ecological efficiency of processes. • Apply different analytical techniques, analytical and numerical methods, as well as software tools in creative problem solving of engineering challenges, proposing sustainable technological solutions. • Optimise complete and sustainable technological processes using analysis and modelling aimed at waste minimization utilising the strategy of the closed cycle manufacturing. • Apply tools, methods and standards for monitoring and assessing the quality of processes and products, as well as their environmental impact, and to predict potential risks in working with technological processes and developing products. • Create a critical analysis, evaluation and interpretation of personal results, and compare them with existing data in scientific and expert literature • Demonstrate independence and reliability in independent work, as well as effectiveness, reliability and adaptability in team work

	• Develop work ethic, personal responsibility and tendency for further skill and knowledge acquisition, according to standards of engineering practice		
2.4. Expected learning outcomes at the level of the course (3 to 10 learning outcomes)	1. To define data distributions. 2. To apply statistical hypothesis tests in chemistry. 3. To use methods of exploration of data in real chemical systems. 4. To apply methods of modelling and optimization 5. To extract useful information. 6. To calibrate analytical system, to process measured signal in order to obtain useful information.		
2.5. Course content (syllabus)	Lectures: **WEEK 1.** Introduction to chemometrics. Types of experimental data. The relationship between experimental data, information and knowledge. **WEEK 2.** Basic Statistics in chemometrics. Probability. The distribution of the data. Types and sources of errors. **WEEK 3.** Application of the t-test and F - test. Analysis of variance. Heteroscedascity. Cohran's test. **WEEK 4.** Outlier tests. Dixon test. Grubbs test. **WEEK 5.** Experimental design. Random blocks. Latin squares. **WEEK 6.** Factor design. The use of blocking. Multi-factor analysis of variance. **WEEK 7.** Introduction to modelling and optimization. Linear regression. Weighting factors. Multi-linear regression. Nonlinear regression. Response surface modelling. **WEEK 8.** Partial exam **WEEK 9.** Signal processing. Signal detection, limits of detection and decision. Filtering. Smoothing. Signal modulation. Fourier transformation. Deconvolution. **WEEK 10.** Calibration. Linear range. Sensitivity. Measurement uncertainty. **WEEK 11.** Exploratory data analysis. Complex sample data. Patten recognition. Pre-treatment of data. Filling. Scaling. Rotation. **WEEK 12.** Hierarchical cluster analysis. Distance and similarity. Single, full and centroid connection. Dendrograms. **WEEK 13.** Principal component analysis. Covariance matrix. Eigenvectors. Eigenvalues. **WEEK 14.** Artificial neural networks. The types and topologies of artificial neural networks. Basics of algorithms for learning. Validation. Generalization. Classification. Linear and nonlinear model. K - nearest neighbour methodology. Independent modelling by class analogy **WEEK 15.** Partial exam.		
2.6. Format of instruction:	☒ lectures ☐ seminars and workshops ☒ exercises ☐ online in entirety ☒ partial e-learning ☐ field work	☒ independent assignments ☐ multimedia and the internet ☐ laboratory ☐ work with mentor ☐ (other)	2.7. Comments:
2.8. Student responsibilities	Students are obligated to attend a minimum of 70% of all lectures and seminars		

2.9. Monitoring student work	Class attendance	YES		Research		NO	Oral exam		NO
	Experimental work	YES		Report		NO	(other)		NO
	Essay		NO	Seminar paper	YES		(other)		NO
	Preliminary exam	YES		Practical work	YES		(other)		NO
	Project		NO	Written exam	YES		ECTS credits (total)	5	

	Title	Number of copies in the library	Availability via other media
2.10. Required literature (available in the library and/or via other media)	1. P. Gemeprline. Practical Guide to Chemometrics, 2nd ed., CRC Press, Boca Raton, 2006.	1	YES
	2. R. G. Brereton. Chemometrics Data Analysis for the Laboratory and Chemical Plant, Wiley, West Sussex, 2003.	1	YES
	3. P. C. Meier, R. E. Zund, Statistical Methods in Analytical Chemistry, 2nd ed., Wiley, New York, 2000.	1	YES
2.11. Optional literature	J. Zupan, J. Gasteiger, Neural Networks in Chemistry and Drug Design, Wiley-VCH, Weinheim, 1999. J. W. Einax, H. W. Zwanziger, S. Geiß, Chemometrics in Environmental Analysis, Wiley-VHC, Weinheim, 1997.		
2.12. Other (as the proposer wishes to add)			