University of Zagreb

1. GENERAL INFORMATION				
1.1 Course teacher	Assoc. Prof. Tatjana Gazivoda Kraljević, PhD Assoc. Prof. Šime Ukić, PhD		1.6 Year of the study	1st (1st semester)
1.2 Name of the course	Process Analytical Technology		1.7. ECTS credits	5
1.3 Associate teachers	Matija Cvetnić, PhD Ivana Sokol, mag. appl. chem.		1.8. Type of instruction (number of hours L + E + S + e-learning)	TOTAL 60 (L: 30, E: 15, S: 15)
1.4. Study programme (undergraduate, graduate, integrated)	graduate		1.9. Expected enrolment in the course	20
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 (10% online)

2. COUSE DESCRIPTION	
2.1. Course objectives	Students will become familiar with sampling systems as well as the sensors/instruments applied in process analyzers and the physico-chemical principles on which these instruments are based. Students will learn how to access chemical analysis, eliminate possible interferences from the matrix, choose the correct analytical technique and extract the useful information from the resulting signal. Students will be able to apply spectroscopic methods (ultraviolet and visible spectroscopy (UV / VID), infrared spectroscopy (FTIR, NIR and Raman), single- and two-dimensional nuclear magnetic resonance (1D and 2D 1H and 13C NMR) and mass spectrometry in structure determination of known and newly synthesized compounds in solving chemical engineering problems.
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	• Compile and apply advanced knowledge of natural and technical sciences, particularly chemical engineering and environmental engineering in solving scientific, professional and general social problems. • Solve engineering problems using the scientific method combining expert knowledge from chemistry, environmental, and chemical engineering as well as material science and engineering. • Correlate expert knowledge from chemistry, chemical engineering and material engineering with awareness of influence on society, economy and environment. • Plan and independently perform experiments in order to confirm a hypothesis to estimate economic and ecological efficiency of processes. • Utilise advanced laboratory procedures and instruments for synthesis of new products, create sustainable processes, and solve problems of water, air and soil pollution.

	• 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. • Plan, document and monitor developmental activities of complex sustainable technological systems and processes. • Identify and analyse complex problems in technological processes of chemical and related industries. • 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. • Identify and discuss advantages, disadvantages and limitations of certain methods for preparation, synthesis, analysis and processing of samples in accordance with sustainable development and life cycle of products and processes. • Independently organise and plan timelines, apply a general methodology for project planning and management in a business environment • Evaluate technological processes and products from the perspective of high functionality in different conditions and environmental effects. • Create a critical analysis, evaluation and interpretation of personal results, and compare them with existing data in scientific and expert literature • Investigate and analyse implementation of innovative and incoming chemical technologies in multidisciplinary environment • Demonstrate independence and reliability in independent work, as well as effectiveness, reliability and adaptability in team work • Outline results of independent and teamwork in a written and oral form to non-experts and experts in a clear and coherent way. • Communicate with the scientific and professional community, as well as society in general in local and international surroundings • Develop work ethic, personal responsibility and tendency for further skill and knowledge acquisition, according to standards of engineering practice
2.4Expected learning outcomes at the level of the course (3 to 10 learning outcomes)	1. To define the fundamental principles of techniques applicable in process analyzers. 2. To explain the approach to analysis of an observed processes. 3. To apply different chemometric tools in data processing. 4. To interpret observations and measurement’s results. 5. To develop the ability to percept and solve complex problems those occur in analyzed process. 6. To analyze, interpret and present spectra obtained by spectroscopic methods UV/VIS, FTIR, 1D and 2D 1H and 13C NMR and mass spectrometry of known organic compounds. 7. To explain factors affecting spectral parameters in the analysis of UV/VIS, FTIR and 1H and 13C NMR spectra 8. To determine and confirm the structures of novel compounds based on complementary data obtained by various spectroscopic methods and mass spectrometry

2.5 Course content (syllabus)	**Lectures and seminars:** **WEEK 1.** Analytical system and analytical information. Quantitative and qualitative information. Influence of the matrix. Measurement error. Data quality. **WEEK 2.** Introduction to process analytics. Defining process analytics. Difference between laboratory analysis and process analysis. **WEEK 3.** Sampling in process analysis. Sampling errors. System heterogeneity problem: composition and distribution. **WEEK 4.** Chemometrics in process analytical technology. Experimental design. Signal processing. Data analysis. Regression analysis. Principal component analysis. **WEEK 5.** Chemometrics in process analytical technology. Validation and measurement uncertainty. Optimization and process management. Artificial Intelligence. **WEEK 6.** Monitoring of industrial-production processes. **WEEK 7.** Partial exam. **WEEK 8.** Ultraviolet-visible spectroscopy (UV/VIS): electronic transitions, basic photophysical processes, light absorption (Lambert-Beer's law), chromophore, examples of UV/VID spectra. **WEEK 9.** Infrared spectroscopy (FTIR, NIR and Raman): vibration of covalent bonds in molecules (stretching and bending), area of functional groups and fingerprint area, examples of spectra. **WEEK 10.** Nuclear Magnetic Resonance (^{1}H and ^{13}C NMR): physical principles, spectral parameters NMR (chemical shift δ, spin-spin coupling constant, J, relative signal intensity, bandwidth); Nuclear Overhauser Effect (NOE). **WEEK 11.** ^{1}H NMR spectroscopy: spin-spin coupling (1H-1 H), multiplet (rule n + 1), cleavage scheme. Interpretation of spin couplings and multiplets in 1H spectra of selected molecules. **WEEK 12.** ^{13}C NMR spectroscopy: decoupling techniques; COM and OFR spectra, APT, DEPT **WEEK 13.** Two-dimensional (2D) NMR spectroscopy: homonuclear 1H-1H (COSY, NOESY) and heteronuclear 1H-13C (HSQC, HMQC) correlation methods. **WEEK 14.** Mass spectrometry (MS): ionization methods, high resolution mass spectrometers, basic fragmentation of organic compounds. Gas chromatography and mass spectrometry (GC / MS) coupling, liquid chromatography and mass spectrometry (LC / MS). **WEEK 15.** Partial exam. **Laboratory practice:** **PRACTICE 1.** Making experimental design. **PRACTICE 2.** Determination of iron in unknown sample: data generation. **PRACTICE 3.** Determination of validation parameters. **PRACTICE 4.** Calculation of measurement uncertainty. **PRACTICE 5.** Obtaining and interpretation of qualitative and quantitative absorption spectra of selected molecules. **PRACTICE 6.** Obtaining and interpretation of IR spectra of selected molecules.

	PRACTICE 7. Analysis and interpretation of ^{1}H and ^{13}C NMR spectra of selected molecules in confirming their structures. **PRACTICE 8. - 9**. Analysis and standalone interpretation of ^{1}H NMR spectra in confirming the structures of the selected molecules. **PRACTICE 10. - 11.** Analysis and standalone independent interpretation of ^{13}C NMR spectra in confirming the structures of the selected molecules. **PRACTICE 12.** Interpretation of two-dimensional NMR spectra **PRACTICE 13. - 14.** Recording and analysis of MS spectra of the selected molecules based on fragments. Interpretation and presentation of analysed mass spectra for the selected molecules.

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)	2.7Comments:
2.8 Student responsibilities	Students are obligated to attend a minimum of 70 % of all lectures, seminars and laboratory practice.		

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

2.10. Required literature (available in the library and/or via other media)	**Title**	**Number of copies in the library**	**Availability via other media**
	F. W. Fifield, P. J. Haines. Environmental analytical chemistry, Blackwell Science, 2000.		YES
	R. M. Silverstein, F. X. Webster, D. J. Kiemle. Spectroscopic identification of organic compounds, Willey, 2005.	2	YES
	H. Friebolin. Basic One- and Two-Dimensional NMR Spectroscopy (3rd ed.), Wiley-VCH, Verlag, Weinheim, 1998.	2	NO
	K. A. Bakeev. Process Analytical Technology (2nd ed.) Wiley, 2010.		YES
	D. A. Skoog. D. M. West, F. J. Holler, S. R. Crouch, Fundamentals of Analytical Chemistry (9th ed.), Cengage Learning, 2013.		YES
2.11. Optional literature	R. Bruckner. Advanced organic chemistry, Elsevier, 2002.		

University of Zagreb

	B. D. Smith, B. Boggess, J. Zajicek. Organic Structure Elucidation, University of Colorado, 1998. E. Pretzsch, P. Bühlmann, C. Affolter, Structure Determination of Organic Compounds, Springer, 2000.
2.12. Other (as the proposer wishes to add)	