Course: Chemometrics		
Language: English		
Lecturer: Tomislav Bolanča		
TEACHING	**WEEKLY**	**SEMESTER**
Lectures	**2**	**30**
Laboratory	**2**	**30**
Seminar	**0**	**0**
		Overall: 60
		ECTS: 5

PURPOSE:

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).

THE CONTENTS OF THE COURSE:

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 modeling and optimization. Linear regression. Weighting factors. A multi-linear regression. Nonlinear regression. Response surface modeling.
Week 8: Signal processing. Signal detection, limits of detection and decision. Filtering. Smoothing.
Week 9: Signal modulation. Fourier transformation. Deconvolution.
Week 10: Calibration. Linear range. Sensitivity. Measurement uncertainty.
Week 11: Exploratory data analysis. Complex sample data. Patten recognition. Pretreatment 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.
Week 15: Classification. Linear and nonlinear model. K - nearest neighbor

methodology. Independent modeling of class analogy methodology**.**

GENERAL AND SPECIFIC COMPETENCE:

Educating students about the modern approach of creating experimental work and processing experimental data with the aim of extracting useful information and the formation of new knowledge.

KNOWLEDGE TESTING AND EVALUATION:

Attendance to the lectures, seminar work, colloquia, 2 tests, exercises.

MONITORING OF THE COURSE QUALITY AND SUCCESSFULNESS:

Student Survey.

LITERATURE:

- Paul GemeprlineEd.Practical Guide to Chemometrics, 2nd Ed. CRC Press, Taylor & FrancisG roup, 2006, Boca Raton, USA, 2006.
- Richard G. Brereton: Chemometrics Data Analysis for the Laboratory and Chemical Plant, John Wiley & Sons Ltd, West Sussex, UK, 2003.
- Peter C. Meier,Richard E. Zund, Statistical Methods in Analytical Chemistry, 2nd Ed. John Wiley & Sons Ltd, New York, USA, 2000.
- Ivan Šošić, Primijenjena statistika, Školska knjiga, Zagreb, Hrvatska, 2004.
- J. Zupan, J. Gasteiger, Neural Networks in Chemistry and Drug Design, Wiley-VCH, Weinheim, Germany, 1999.