Course Unit Descriptor

Study Programme: Food Engineering

Course Unit Title: Chemometrics

Course Unit Code: DKKI12

Name of Lecturer(s): Prof. Sanja Podunavac-Kuzmanović, PhD; Assoc. Prof. Lidija Jevrić, PhD

Type and Level of Studies: Master Academic Degree

Course Status (compulsory/elective): Elective

Semester (winter/summer): Summer

Language of instruction: English

Mode of course unit delivery (face-to-face/distance learning): Face-to-face

Number of ECTS Allocated: 7

Prerequisites: None

Course Aims:

The aim of the course is to provide the theoretical and practical knowledge to students in the field of chemometrics, including the application of suitable software for statistical processing and modeling of experimental data and the mathematical prediction of various factors (quality of food products, biological activity of compounds, chromatographic behavior of compounds, outcomes of laboratory experiments). Also, the objective of the course is to acquire the knowledge and skills in the planning and optimization of experiments.

Learning Outcomes:

After completing the course, the student will be able to practically apply chemometrics methods in laboratory analysis, food quality analysis and design of experiments. The student will be trained to apply various chemometric methods to predict different analytical factors and to classify analytical data, in order to save the time and reduce financial costs in everyday analytical and technological practice.

Syllabus:

Theory

General principles of chemometrics. Multivariate statistical methods. Interdependence methods. Molecular modeling. Principal component analysis. Factor analysis. Grouping analysis. QSPR and QSAR analysis. Correlation analysis. Regression analysis. Univariate linear regression. Multiple linear regression. Validation of chemometric models. Neural networks. Future trends in chemometrics. Chemometrics of real samples. Chemometrics in laboratory analysis and food quality control.

Practice

Chemometric processing of chemical data. Chemometric statistics. Formation of chemometric models. Validation of chemometric models. Application of software for chemometric data processing and optimization. Case studies.

Required Reading:

1. S. Luna (editor), Chemometrics: Methods, Applications and New Research. Novascience Publishers, New York (2017)
2. J. M. Miller, J. C. Miller, Statistics and Chemometrics for Analytical Chemistry, 6th Edition, Pearson Education Limited, Harlow (2010)
3. K. H. Esbensen, Multivariate Data Analysis - In Practice, 5th Edition, CAMO Software AS, Oslo, Norway (2009)
4. S. S. Ražić, Chemometrics in the Analysis of Real Samples – From Theory to Application, Univerzitet u Beogradu,

Farmaceutski fakultet, Beograd (2011)			
Weekly Contact Hours:	**Lectures:** 3	**Practical work:** 3	
Teaching Methods: Lectures and students group work			
Knowledge Assessment (maximum of 100 points):			
Pre-exam obligations	points	**Final exam**	points
Active class participation	5	written exam	35
Practical work	10	oral exam	-
Preliminary exam(s)	50		
Seminar(s)	-		
The methods of knowledge assessment may differ; the table presents only some of the options: written exam, oral exam, project presentation, seminars, etc.			