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| **Study program:** Chemistry (PhD) | | |
| **Course title: Advanced Chemometrics Course (H334C)** | | |
| **Name of lecturer/lecturers: Violeta D. MItić** | | |
| **Type of course: elective** | | |
| **Number of ECTS allocated 10** | | |
| **Course objectives**  **Acquaintance of students with basic concepts and techniques of advanced data processing and making statistical conclusions.** | | |
| **Course outcomes**  **After completing the course, the student should be able to:**  **- select and apply appropriate chemometric methods in data analysis in different areas fundamental research, especially in the field of quality control;**  **- understands the importance of optimization and experimental design;**  **- use computer programs for statistical processing of data both for parametric methods and for**  **non-parametric statistical methods**  **- choose and apply optimal methods of multivariate analysis, classification and modeling of data;**  **- by choosing the representative variables responsible for the variations in the data set by performing the reduction data**  **- optimizes the process monitoring and control system by reducing the number of measured parameters and their frequency measurements by classifying and grouping data** | | |
| **SYLLABUS**  *Introduction to chemometric data analysis, concept and application. Methods for statistical data processing. Preparation of the data matrix. Selection of appropriate chemometric techniques, preliminary statistical analysis. Examining the distribution type. Measurement uncertainty. Removal of external values of points. Parametric and non-parametric statistics. Elements of statistical inference: statistical evaluation, hypothesis testing. Statistical tests (one-way and two-way tests, parametric and non-parametric tests, one-way analysis of variance ANOVA). Calibration methods, correlation and regression. Optimization and experimental design (randomization, types of experimental design, optimization methods). Exploratory analysis and pattern recognition. Methods of multivariate analysis (parametric and non-parametric), principles, advantages and disadvantages, choice and application: Analysis of the main components (PCA), factor analysis (FA), cluster analysis (grouping analysis), hierarchical andnon-hierarchical (CA). Application of factor analysis methods in chemistry. Models that provide a quantitative relationship between the structure of molecules and their biological activity – QSAR modeling. Basic principles of setting up a mathematical QSAR model. Molecular descriptors. Interaction of parameters, evaluation of the success of the experiment. Application and interpretation of statistical results analysis* | | |
| **References**  1. James N. Miller and Jane C. Miller Statistics and Chemometrics for Anllytical Chemistry, Ellis Horwood imprint 1995  2. А. Перић-Грујић, Основи хемометрије, ТМФ, Београд, 2012 | | |
| **Active teaching classes** | **Lectures 105** | **Laboratory work** |
| **Teaching mode** | | |
| **ASSESSMENT METHODS AND CRITERIA (Max 100 points)** | | |
| **Activity during lectures 10; teaching colloquia 45; written examination 35 points;** | | |