

<b>Course title: Introduction to chemometrics</b>					
	<b>Specialty</b>	<b>Semester</b>	<b>Number of ECTS</b>	<b>Number of hours in the class</b>	<b>Form</b>
	<b>Foreign students</b>	<b>summer</b>	<b>1</b>	<b>15</b>	<b>Lecture</b>
<b>Name of lecturer: Dr. hab. Tomasz Puzyn</b>					
<b>Objective of the course (expected learning outcomes and competences to be acquired)</b>					
Presenting students with the scope for application of chemometric methods in chemistry.					
<ul style="list-style-type: none"> <li>• Gaining the students skills in the use of the most important chemometric methods (analyses and results interpretation)</li> <li>• Introducing students to accessible software implementing chemometric methods</li> </ul>					
<b>Prerequisites:</b> Completed courses of Mathematics, Statistical methods in chemistry and Analytical chemistry.					
<b>Teaching methods:</b> Lecture with multimedia presentation;					
<b>Course contents</b>					
A. Lecture: 1. Introduction to chemometric methods; specification of multidimensional data sets, differences between chemical statistics and chemometrics, fields of interest in chemometrics, type of chemometric methods, review of computational software utilizing chemometric methods, (R, MATLAB, Statistica, Origin, SPSS)					
2. Methods of preliminary control and verification of chemometric data sets, problem of lacking data, transformations of variables, normalization of data set, correlation and covariation.					
3. Methods revealing the internal structure of the chemical data: similarity between objects in the multidimensional space of variables, hierarchical cluster analysis (HCA) as an example of technique to analyze similarities; principal component analysis (PCA) as an example of technique to make projections. Examples of application of these methods in different fields of chemistry.					
4. Developing models describing relationships in chemical processes with application of regression or classification methodology: linear regression of one or multiple variables (LR and MLR), principal component regression (PCR) and partial least squares regression (PLS); linear discriminant analysis (LDA), nonlinear k-nearest neighbors classifier (kNN); application of artificial neural networks (ANN), methods to select the optimal combination of variables in the model (genetic algorithms); validation of developed models. Examples of application of these methods in different fields of chemistry.					
<b>Recommended reading:</b>					
A. Primary literature:					
S. D. Brown, R. Tauler, B. Walczak (red): Comprehensive chemometrics. Chemical and biochemical data analysis. Amsterdam: Elsevier, 2009					
R. Kramer: Chemometric techniques for quantitative analysis. New York: Marcel Dekker, Inc, 2005					
<b>Assessment methods:</b>					
Written exam with open questions					
Written test exam					
Oral exam					
<b>Language of instruction:</b> English					