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| **Title and Code** of the subject: **Chemometry, MTBE743A** | **ECTS Credit Points: 3** |
| **Type** of the subject: optional | |
| **Ratio of theory and practice: 50/50** (credit%) | |
| **Type and number of classes per semester**: 14 hour(s) lecture and 14 hour(s) practice per **semester**  Number of teaching hours / week : eg.:1+1 (lecture and practice) | |
| **Type of exam**: practical course mark | |
| **Subject in the curriculum:** semester 3 | |

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| **Summary of content - theory**: The development and application of sensitive and selective analytical methods is required for the effective development and quality control in the food industry. One can recently witness a silent revolution either in the process automation and or in analytical technology. The food industry is a part of this evolution. Various companies offer PAT (process analytical technology) systems based on image and spectroscopic sensory (NIR, RAMAN) analysis. These technical solutions are  presented by dozens of spectacular booklets and more or less well trained service engineers. Less information is provided about how the actual qualitative and quantitative results are computed from the sensor signals. Although for a company it is crucial for the in-house development and maintenance of a PAT system customized for a product or production step using the existing expert team. This course offers a basic insight into the most widely used multivariate classification and calibration techniques with easily understandable practical examples. |
| Course objectives:….  1-2. Introduction to the spectroscopic methods, interaction of the material and the electromagnetic radiation, methods and sensors in the daily routine  3-4. Evolution and properties of spectra. Construction of data matrices, visual observation, basic descriptive statistical tools.  5-6. Classification methods (I): factor analysis, PCA (principal component analysis), LDA (linear  discriminant analysis)  7-8. Classification methods (II):), ANN (artificial neural networks), SIMCA (self-independent modelling of class analogies) , SVM (support vector machines), cluster analysis  9-10. Regression methods (I): linear and multilinear regression, PCR (principal component regression)  11-12. Regression methods (II): PLS, PLS-DA (partial least squares regression and discriminant analysis)  13-14. Internal and external validation |
| **Summary of content - practice**: |
| Skills to be learnt:…    1-4. Non-destructive determination of elemental composition of alloys and its use in classification models  5-8. RAMAN spectrum recording and classification of various cheese samples (PCA, LDA)  9-12. Determination of food dye concentration by image analysis and multivariate regression (PLS, PCR)  13-14. Application of NIR spectroscopy in the analysis of different skin types (LDA, SIMCA) |
| **Literature, handbooks in English** |
| Füstös László: A sokváltozós adatelemzés módszerei, Módszertani Füzetek, 2009/1.  S.N. Deming, Y. Michotte, D.L. Massart, L. Kaufman, B.G.M. Vandeginste: Chemometrics:  A Textbook, Elsevier, 1988 |

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| **Responsible lecturer: Dr János Elek, PhD** |

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| **Terms of course completion:** |
| 1. Completing assignments / exercises 2. Submitting essay 3. Giving presentation |
| **Form of examination:** |
| practice grade mark |
| **Requirement(s) to get signature:** |
| Addentance to seminars – maximum 3 absences are allowed per semester. |