



SUBJECT DATASHEET

Semester:	2009/10/1
Subject:	Chemometrics
Code:	VEMKKAB212K
Responsible department:	Department of Analytical Chemistry
Responsible department code:	MKKA
Responsible lecturer:	dr. Tamás Pap

Educational objectives:

Understanding of the fundamentals of chemometrics.

Detailed content of the subject:

1. Statistical evaluation of measured data. Theoretical basis. Distribution functions. Statistical moments. 2. Random and systematic errors. Functions of error propagation 3. Test of outliers, t-test, F-test. 4.. Analysis of variance. Techniques for one-way analysis of variance. Two-way analysis of variance. 5. Correlation analysis. Regression analysis. Linear and non-linear regression. 6. Principles of calibration. Modes of calibration. Test for linearity. 7. Experimental design. 2n type factorial design. Simplex method. Latin square design 8. Classification of samples by statistical method. Pattern recognition. Clusteranalysis. Nearest neighbour and k-th nearest neighbour method. 9. Definition of analog and digital signals. Classification of analog signals. The quality of the signal. The signal-to noise ratio. 10. Deterministic and periodic signals. Stationer and random signals. The type of noise and the source of noise. improvement of the quality of analog signal: filtering, modulation. 11. The digitization of the analog signals. Theory of Shannon. Transformation of analog-to-digital (A/D). 12. Examination of the signal-time functions in frequency domain. The Fourier Transform of the continous and discrete signals. 13. Improvement of the digital signal. Smoothing. Method of Savitzky-Golay. 14. Addition of spectra. Smoothing using Fourier-transformation.

Requirements:

The topics of the lectures.

Required and suggested references:

Dr. Inczédy János: Folyamatos és automatikus analízis. Műszaki Könyvkiadó, Budapest, 1984.