

Program: Chemistry (15025012071P6)

Course: MULTIVARIATE ANALYSIS AND CALIBRATION

Code: PPGQU0056

Workload: 60 hours

Credits: 04

Syllabus:

Introduction: Definitions and terminologies; Exploratory analysis: Principal Component Analysis and Hierarchical Cluster Analysis; Classification: K-Nearest Neighbors and SIMCA; Multivariate Calibration: Multiple Linear Regression, Principal Component Regression, and Partial Least Squares Regression; Applications, state-of-the-art, and trends.

Bibliography:

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BRERETON, R. G. Chemometrics: Data Analysis for the Laboratory and Chemical Plant, John Wiley & Sons, Chichester-UK, 2003.

MASSART, D. L.; VANDEGINSTE, B. G. M.; DEMING, S. N.; MICHOTTE, Y.; KAUFMAN, L. Chemometrics: A Textbook, Elsevier Science B. V., Amsterdam, 2003.

BEEBE, K. R.; PELL, R. J.; SEASHOLTZ, M. B. Chemometrics – A Practical Guide, John Wiley & Sons: New York, 1998.

MARTENS, H.; NAES, T. Multivariate Calibration, John Wiley & Sons, New York, 1992.

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CAMO, A. S. The Unscrambler User's Guide, Trondheim, 2002.

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