

COURSE SYLLABUS

1. Identification

Code and title: QUP 152 - Chemometrics

Professor: Marco Flôres Ferrão and Adriano de Araújo Gomes

Level: Master and Doctorate

Credit hours: 2

Revised: August_2021

2. Summary

Exploratory Analysis: PCA and HCA. Fundamentals and applications in environmental chemistry, food chemistry, pharmaceutical chemistry and in the field of fuels and biofuels. Pattern recognition techniques. Fundamentals and applications in food analysis, petrochemical and drug analysis. Multivariate regression. Fundamentals and applications in instrumental techniques, environmental chemistry, food chemistry, pharmaceutical chemistry and in the field of fuels and biofuels.

3. Objective

Understand and apply the basic techniques of multivariate data treatment seeking a more adequate solution in the evaluation of chemical data in the environmental, pharmaceutical, technology and food and fuel areas.

4. Contents

- Fundamentals of Principal Component Analysis (PCA);
- Hierarchical Cluster Analysis (HCA);
- Construction of classification models: SIMCA (Soft Independent Modeling of Class Analogy) and KNN Method;
- Principal Component Regression (PCR);
- Partial Least Squares Regression (PLS);
- Introduction to sample selection methods and variables

5. Assessment

The evaluation will take place through the analysis of scientific articles, seminars and a written evaluation. The student, who obtains a final grade of A, B or C, awarded as per the list below, will be considered approved:

A: grade equal to or above 9.0

B: grade equal to or above 7.5 and below 9.0

C: grade equal to or above 5.0 and below 7.5

D: grade below 5

FF: lack of frequency

6. Methodology

Lectures, exercises lists, seminars and examinations.

7. Bibliography

- 7.1 Ferreira, Márcia M. C. Quimiometria: Conceitos, Métodos e Aplicações. Campinas: Editora da Unicamp, 2015, 493p.
- 7.2 Brereton, Richard G. Chemometrics: applications of mathematics and statistics to laboratory systems. New York: Ellis Horwood, 1993. 307 p .
- 7.3 Massart, D. L. et al. Chemometrics: a textbook. Amsterdam: Elsevier, 1988. 488p.
- 7.4 Steven D. Brown (Editor), Romã Tauler (Editor), Beata Walczak (Editor). Comprehensive Chemometrics, Elsevier Science, 2009. 4 volumes.
- 7.5 Brown S. D., Tauler R. Walczak B. Comprehensive Chemometrics, Elsevier Science, 2009.