



PROGRAMS AND BIBLIOGRAPHY

Subject	
Code	Name
QA854	Chemometrics

Vector
OF:S-5 T:002 P:000 L:000 O:000 D:000 HS:002 SL:002 C:002 AV:N EX:S FM:75%

Pre requirement
QA584

Summary
Importance of multivariate statistics in chemistry. Considerations on factorial design and optimization in chemistry. Application of multivariate analysis for the treatment of chemical data.

Program
Factorial design. Fractional factorial designs. Surface response methodology. Modeling of mixtures. Pattern recognition and classification. Principal component analysis. Multivariate calibration. Multivariate curve resolution. Analysis of higher order data. Use of software related to course topics for the treatment of chemical data.

Bibliography
<ol style="list-style-type: none">1. R., E. Bruns, I., S. Scarminio, B. de Barros Neto, Como fazer experimentos: aplicações na ciência e na indústria, 4ª ed., Bookman, SP, 2010.2. G. E. P. Box, J. S. Hunter, W. G. Hunter, Statistics for Experimenters, John Wiley and Sons, New Jersey, 2005.3. D. L. Massart, B. G. M. Vandeginste, L. M. C. Buydens, S. de Jong, P. J. Lewi, J. Smeyers-Verbeke, Handbook of Chemometrics and Qualimetrics: Part B, Elsevier, Amsterdam, 1998.4. R. G. Brereton, Chemometrics – Data Analysis for the Laboratory and Chemical Plant, Wiley, Chichester, 2003.5. M. Otto, Chemometrics - Statistics and Computer Application in Analytical Chemistry, Wiley-VCH, Weinheim, 1999.6. H. Martens e T. Naes, "Multivariate Calibration", Wiley, New York, 1991.7. M. M. C Ferreira, Quimiometria: Conceitos, métodos e Aplicações Ed. UNICAMP, 2015

Evaluation criteria
For grading policy, see: Regimento Geral de Graduação, Seção I – Normas Gerais, Capítulo V – Da Avaliação do Aluno na Disciplina. Students are required to attend 75 % of the lectures. For further details, see: Regimento Geral de Graduação, capítulo VI, seção X, artigo 72.