Code: QA854

Name: Quimiometria

Name in English: Chemometrics

Name in Spanish: Quimiometria

Subject type: Weekly

Approval Type: Grade and frequency

Characteristic: Regular

Frequency: 75%

Period Type / Offering period: Semi-annual / Every period

Requires Final Exam: Yes

Vectors

T	L	P	O	PE	OE	SL	WEEKS	CREDITS
2	**0**	**0**	**0**	**0**	**0**	**2**	**15**	**2**

Occurrence on curriculum:

Pre requirement: QA584 ou QA585

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.

Basic Bibliography

1) BRUNS, R.E.; SCARMINIO, I.S.; NETO, B.B. **Como fazer experimentos: aplicações na ciência e na indústria**. 4. Ed. Porto Alegre: Bookman, 2011. E-book.
2) BOX, G.E.P.; HUNTER, J.S.; HUNTER, W.G. **Statistics for Experimenters**. Hoboken: John Wiley & Sons, 2005. 639 p.
3) MASSART, D.L.; VANDEGINSTE, B.G.M.; BUYDENS, L.M.C.; JONG, S.; LEWI, P.J.; SMEYERS-VERBEKE, J. **Handbook of Chemometrics and Qualimetrics: Part B**. Amsterdam: Elsevier, 1998. 713 p.

Supplementary Bibliography

1) BRERETON, R.G. **Chemometrics – Data Analysis for the Laboratory and Chemical Plant**. Hoboken: Wiley, 2003. 489 p. E-book.
2) OTTO, M. **Chemometrics - Statistics and Computer Application in Analytical Chemistry**. Weinheim: Wiley-VCH, 1999. 314 p.
3) MARTENS, H.; NAES, T. **Multivariate Calibration**. New York: John Wiley & Sons, 1989. 419 p.
4) FERREIRA, M.M.C. **Quimiometria: Conceitos, métodos e Aplicações**. Campinas: UNICAMP, 2015. 493 p.
5) HARRIS, D.C. **Análise Química Quantitativa**. 9. Ed. Rio de Janeiro: LTC, 2017. 774 p.