FEDERAL UNIVERSITY OF CEARÁ
Provost Office of Research and Graduate Studies

COURSE PROGRAM

1. IDENTIFICATION OF THE COURSE:	
1.1 Course	Graduate Program in Chemistry
1.2 Code:	CEP9444

2. MODALITY:	
Master (X)	PhD (X)

3. PERIOD	
Day (X)	Night ( )

4. IDENTIFICATION OF THE DISCIPLINE:	
Name:	CHEMOMETRICS
Code:	CEP9444
Study load:	64 hours
Credit:	04
Optional:	Yes (X) No ( )
Mandatory:	Yes ( ) No (X)
Specific Area:	Analytical Chemistry

5. RESPONSIBLE PROFESSOR:
Prof. Dr. Gisele Simone Lopes

6. SUBJECT:
The discipline of Chemometrics addresses aspects of experimental design and multivariate data analysis. Therefore, the student should be able, at the end of the course, to plan an experiment using all the variables, as well as be able to perform a multivariate data analysis.

7. PROGRAM UNIT:

1. Introduction to Chemometrics
2. Experimental Design
      2.1 Screening of variables
      2.2 Factorial Design
      2.3 Construction of models. Response Surface Methodology.
3. Multivariate data analysis

3.1 Problem definition. Data organization.
3.2 Pre-processing of original data.
3.3 Exploratory data analysis. Pattern Recognition.
3.4 Construction of Calibration Models. Classification.
3.5 Validation of the model.
3.6 Using the Model for Prevision.

8. EVALUATION:

Tests, frequency and oral presentation.

9. BIBLIOGRAPHY:

Basic
1. Neto, B.B., Scarminio, I.S., Bruns, R.E. "Como fazer experimentos", Editora Unicamp, 4ª ed., **2010**;
2. Beebe, K.R., Pell, R.J., Seasholtz, M.B. "Chemometrics A Pratical Guide", John Wiley & Sons, **1998**.
3. Brereton, R.G. "Applied Chemometrics for Scientists", Wiley & Sons, **2007**.

Complementary
1. Ferreira, M.M.C. "Quimiometria – Conceitos, Métodos e Aplicações", Editora da Unicamp, **2015**.

2. Box, G.E.P., Hunter, W.G., Hunter, S.S. "Statistics for Experimenters-An Introduction to Design, Data Analysis and Model Building", John Wiley & Sons, **1978.**

3. Teófilo, R.F., Ferreira, M.M.C. "Quimiometria II: Planilhas eletrônicas para cálculos de planejamentos experimentais, um tutorial". Química Nova, vol. 29, n.2, p.338-350, **2006**.

4. Correia, P.R.M., Ferreira, M.M.C. "Reconhecimento de padrões por métodos não supervisionados: explorando procedimentos quimiométricos para tratamento de dados analíticos". Química Nova, vol.30, n.2, p.481-487, **2007**.

5. Ferreira, M.M.C, Antunes, A.M., Melgo, M.S., Volpe, P.L.O. "Quimiometria I: calibração multivariada, um tutorial". Queimica Nova, vol.22, n.5, p., **1999**.