

# CHIMIOMÉTRIE 2016

**Séminaires précongrès - Dimanche 17 Janvier**

**Pre-conference courses - Sunday 17 January**

**Titre du séminaire / Course title**

**Chemometrics without Equations (or Hardly Any)**

**Enseignant / Trainer**

The course will be led by PLS\_Toolbox creator and Eigenvector Research President Dr. Barry M. Wise. Wise holds a doctorate in chemical engineering and has experience in a wide variety of applications spanning chemical process monitoring, modeling and analytical instrument development. He has extensive teaching experience, having presented over 100 chemometrics courses. Each spring Wise organizes and teaches at Eigenvector University, the most comprehensive offering of chemometrics classes in the world.

**Description / Course details**

Chemometrics without Equations (CWE) concentrates on two areas of chemometrics: 1) exploratory data analysis and pattern recognition, and 2) regression. Participants will learn to safely apply techniques such as Principal Components Analysis (PCA), Principal Components Regression (PCR), and Partial Least Squares (PLS) Regression. Examples will include problems drawn from process monitoring and quality control, predicting product properties, and others. The target audience includes those who collect and/or manage large amounts of data that is multivariate in nature. This includes bench chemists, process engineers, and managers who would like to extract the maximum information possible from their measurements.

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## **Course Outline**

### **1.0 Introduction**

**1.1 what is chemometrics?**

**1.2 resources**

### **2.0 Pattern Recognition Motivation**

**2.1 what is pattern recognition?**

**2.2 relevant measurements**

**2.3 some statistical definitions**

### **3.0 Principal Components Analysis**

**3.1 what is PCA?**

**3.2 scores and loadings**

**3.3 interpretation**

**3.4 supervised and unsupervised pattern recognition**

**3.5 examples**

### **4.0 Regression**

**4.1 what is regression?**

**4.2 classical least squares (CLS)**

**4.3 inverse least squares (ILS)**

**4.4 principal components regression (PCR)**

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**4.5 partial least squares regression (PLS)**

**4.6 examples**

**5.0 Summary**

## **Public / Expected public**

Chemometrics Without Equations (or Hardly Any) is designed for those who wish to explore the problem solving power of chemometric tools, but are discouraged by the high level of mathematics found in many software manuals and texts. Course emphasis is on proper application and interpretation of chemometric methods as applied to real-life problems. The objective is to teach in the simplest way possible so that participants will be better chemometrics practitioners and managers.

## **Prérequis / Specific needs**

No prior knowledge of chemometrics is required to take CWE. Students wishing to participate in hands on exercises should bring a laptop with either Solo 8.0 or PLS\_Toolbox 8.0 installed. (PLS\_Toolbox 8.0 requires MATLAB R2008a or newer.) Demo copies of Solo or PLS\_Toolbox will work fine for the course and are available via download at

<https://software.eigenvector.com/toolbox/download/>

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The software must be INSTALLED AND TESTED PRIOR TO THE COURSE as we will not have time to do software installs in class.