NEW CALIBRATION STRATEGIES IN SPECTROCHEMICAL ANALYSIS
TWRF 9:00-11:00 AM, November 16 - 26, 2021

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When: November 16 - 26, 2021
Where: Centro de Energia Nuclear na Agricultura (CENA), University of São Paulo

Course objectives
➢ Explore the fundamental concepts associated with least-squares regression and the traditional external standard calibration, internal standardization and standard additions methods.
➢ Understand the advantages and limitations of each of the traditional calibration methods.
➢ Introduce new approaches to calibration such as the interference standard (IFS), standard dilution analysis (SDA), and multi-energy (MEC), multi-isotope (MICal), multispecies (MSC) and multi-flow (MFC) calibration methods.
➢ Discuss the theoretical basis of each new strategy, as well as their application in atomic absorption, atomic emission and mass spectrometry.
➢ Provide the basic knowledge in calibration methods to enable informed decisions on the most appropriate strategy to solve the analytical problem at hand.

Suggested literature


**Outline**

This is a two-week course held Tuesday through Friday (TWRF) between November 16th and 26th, 2021. There will be opportunity for hands-on data processing using MS Excel and ICP-OES, ICP-MS, MIP-OES and HR-CS FAAS experimental results. Thus, you will need a computer with MS Excel installed for class and homework exercises. We will also introduce and use the programming language and free software environment R (R Foundation for Statistical Computing, Vienna, Austria) for in-class and homework calculations. Instruction on how to install and use R will be given during the course.

Depending on availability of instrumentation, laboratory experiments applying the new calibration methods will also be performed. Below is a list of topics to be covered in the course.

1. Introduction
2. Fundamentals of least-squares regression
   2.1. Ordinary least-squares regression
   2.2. Weighted least-squares regression
3. Traditional calibration methods
   3.1. Fundamentals, advantages and limitations of external standard calibration (EC)
   3.2. Fundamentals, advantages and limitations of internal standardization (IS)
   3.3. Fundamentals, advantages and limitations of standard additions (SA)
4. New calibration methods for spectrochemical analysis
4.1. The interference standard method (IFS)
4.2. Standard dilution analysis (SDA)
4.3. Multi-energy calibration (MEC)
4.4. Multi-isotope calibration (MICal)
4.5. Multispecies calibration (MSC)
4.6. Multi-flow calibration (MFC)

5. Analyte estimation for calibration methods with both variables subject to error

Grading
The course will include directed study exercises that may involve calculation, literature searching, participation in class discussions, data processing exercises, and lab reports. Each activity will be graded in a scale between 1 and 10, and the final grade will be the average of all individual activities. The letter grade scale used to attribute to the final grade is shown below.

A ≥ 93%
90% < A- < 92%
87% < B+ < 89%
83% < B < 86%
80% < B- < 82%
77% < C+ < 79%
73% < C < 76%
70% < C- < 72%
67% < D+ < 69%
63% < D < 66%
60% < D- < 62%
F < 60%