Chemometrics in Excel – Interactive Educational Programme

Sunday, 11 September 2011, Belgrade, Conference EUROanalysis 2011

Chemometrics is a very practicable discipline. Therefore, in teaching chemometrics it is important not to explain the methods only, but to provide a student with a full access and ability to perform all relevant calculations as well. Not all universities have easy access to the special chemometric software packages. For this case a special Excel Chemometrics Add In has been designed. This software provides:

(1) a lecturer with the possibility to present the teaching material in an interactive mode;

(2) a student with the full access and ability to perform all relevant calculations for the data analysis.

The course consists of two blocks: Part 1 – Introduction, and Part 2 - Advanced

Audience: The persons involved in teaching of chemometrics. A basic knowledge of chemometric concepts and methods is desirable

Language: English

Instructor: DSc. Oxana Rodionova (ICP RAS, Moscow)

Course materials:

- Matrix calculations in Excel (web tutorial)

- Projection methods in Excel (web tutorial)

- Useful Formulae for Chemometrics Add-In (web tutorial)

Additional materials will be available for the participants on July 21, 2011.

Course Outline:

Part 1, Introduction 9h00 - 12h00 deals with:

- Teaching of chemometrics in an interactive web-based mode

- Main features of Chemometrics Add-In software (Projection.xls)

- Special technique for matrix calculations in Excel (Excel.xls)

- Computer exercises: basic Excel matrix calculations (Task.xls)

Part 2 Advanced 13h00 - 17h00 deals with:

- Overview of interactive materials: (Iris.xls, MCR.xls)

- Computer exercises: Calibration problem (Calibration.xls)

- Computer exercise: real-world problems

Chemometrics Add-In is specially designed software for Microsoft Excel. The package consists of two files Chemometrics.dll and Chemometrics.xla. The main projection functions can be applied as ordinary user-defined functions in Excel

The core functions for the PCA/PLS decompositions are designed to ensure very fast calculations even for the rather large data sets (200 samples by 4500 variables). They are programmed in C++ language and linked to Excel via DLL.

Full individual license for Chemometrics Add-In software will be provided for all registered attendees.

Participants are encouraged to use their **own laptops** with Excel 2007 and Chemometrics Add-In installed.

Registration via conference site

Additional information: rcs@chph.ras.ru to Oxana Rodionova.