



Chemometrics in Excel – Interactive Educational Programme

Monday, 25 June 2012, Budapest, Conference CAC-2012



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

Language: English

Instructors: DSc. [Oxana Rodionova](#) (ICP RAS, Moscow)
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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 May 1, 2012.

Course Outline:

Part 1, Introduction 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 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 [CAC-2012 conference site](#)

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	A	B	C	D	E	F	G
1		Window Factor Analysis					
2		Component A					
3		Rows omitted from top					15
4			P_a		t_z		
5		220	=LoadingsPCA(OFFSET(Xdata,\$F\$3,0,1-\$F\$3))				
6		225	0.223	2	0.091		
7		230	0.170	3	0.522		
8		235	0.149	4	1.000		
9		240	0.182	5	1.131		
10		245	0.213	6	1.018		