



Chemometrics in Excel

June 20, 2010, Budapest, Hungary, SCAC-2010 preconference course

The aim of the course is to provide the participants with simple and powerful tool for basic multivariate analysis. The core functions for projection methods are presented as worksheet functions in Excel, a most widely spread data handling environment. All calculations are carried out in Excel books, and all regular Excel capacities can be applied for additional calculations: charts, data export and import, templates, etc. During the course, attendees will have a wide opportunity for the hands-on data analysis.

Audience: (postgraduate) students, specialists, scientists with a basic knowledge in chemometrics and Excel

Language: English

Instructors: DSc. [Alexey Pomerantsev](#) (ICP RAS, Moscow)
DSc. [Oxana Rodionova](#) (ICP RAS, Moscow)

Course materials:

- Matrix calculations in Excel ([web tutorial](#))
- Projection methods in Excel ([web tutorial](#))
- Supplementary xls-files
- Chemometrics Add-In software

will be provided for the participants on May 20, 2010. To refresh the Excel skills it is highly recommended to read the tutorials and to carry out exercises.

Course Outline:

Introduction (Brief reminders)

Matrix calculations in Excel

Basic projection methods PCA, PLS

Main features of *Chemometrics.Add-In*

Computer exercises

Basic Excel calculation

Explorative (one-block) data analysis: PCA and classification

Multivariate calibration

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.

The course is part of SCAC-2010 and **free of charge for the conference participants**. 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 by email: rcs@chph.ras.ru to Oxana Rodionova.

	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		