



# Course Chemometrics in Excel



October 15-17, 2012, Sofia, [Sofia University](http://www.sofiauni.bg)

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:** Students, specialists, scientists. A basic knowledge of chemometric concepts and methods, e.g., PCA and PLS is desirable

**Language:** English

**Instructors:** DSc [Alexey Pomerantsev](http://www.chph.ras.ru) (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 Oct 7, 2012.

**Course Outline:**

*Day 1, Introduction, Explorative Analysis:*

- Matrix calculations in Excel ([Excel.xls](#))
- Chemometrics Add-In software ([Projection.xls](#))
- Computer exercises: PCA ([People.xls](#))

*Day 2 Calibration*

- Calibration: Problem
- Computer exercises: MLR, PCR, PLS, PLS2 ([Calibration.xls](#))

*Day 3 Classification*

- Classification: Overview of the problem
- Computer exercises: LDA, PLS-DA, SIMCA ([Iris.xls](#))

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.

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	A	B	C	D	E	F	G
1		<b>Window Factor Analysis</b>					
2		<b>Component A</b>					
3		Rows omitted from top					15
4			$P_a$		$t_z$		
5		220	=LoadingsPCA(OFFSET(Xdata,\$F\$3,0,-\$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		

