Schedule 2017

November

	Mon	Tue	Wed	Thu	Fri
W47	20th November M1 13-15	21st November M2 13-15	22nd November M3 13-15	23rd November M4 13-15	24th November M5 13-15
W48	27th November M6 13-15	28th November M7 13-15	29th November M8 13-15	30th November M9 13-15	1st December M10 13-15

M1	Introduction to Scientific Python, run scripts, create and manipulate Vectors, simple plotting
M2	Loops, switches and exceptions. String manipulation, Read and write files
M3	Clean data, create various plots for visual inspection (1D,2D, histograms, Distribution plots…). Handle the details.
M4	Create functions, advanced data formats and introduction in parameter optimisation
M5	Model building, parameter optimization and error evaluation
M6	SVD, PCA and global analysis
M7	Introduction to Anova, data mining, hypothesis testing and statistical methods
M8	
M9	Instrument control, introduction to more modules
M10	Exam

Course Preparation:

The course will be given in a computer room at the Chemistry Center (announced later).
There are 12 computer and 24 places available. The usage of Laptops is possible and highly recommended. As preparation please ensure that a version of Python 2.7 (not 3.x !!!) is installed. Python is based on a large number of modules that significantly enhance its capabilities. To effectively work with data a few of those packages are very useful. Please find below some instruction how to create the necessary environment on your computer.
This course runs this year for the first time this year and adjustments to the schedule might become necessary. At the end of each day there will be a small task that will help to connect the different modules of the course and has to be completed and submitted for evaluation on the next day. Participants should estimate up to an additional 1h for this task to be completed. Successful completion of each of these tasks is a necessary requirement for the credits. At the end of the course a number of analysis tasks will be given that have to be successfully completed and form the exam.

One key idea in this course is to achieve sufficient knowledge to work with data from your field of work. Please try to prepare a small dataset in the ASCII (plain text) format that represents a typical problem in your field. e.g. one matrix with time-spectrum, one dataset with many samples taken under a variety of parameter, a scan from any device/beamline... In order to accommodate such a wide spectrum of possibilities it will be necessary to have plain text (structured data that can be viewed with a program like Notepad on windows).

We will provide all necessary material during the course. There is an endless number of books to which we have access in the university. Each has a different approach and the choice is very individual. This literature is just a selection for further reading and specific questions. (all are digitally available at the moment)

- Data reduction and error analysis for the physical sciences / Philip R. Bevington, D. Keith Robinson
  http://ludwig.lub.lu.se/login?url=http://search.ebscohost.com/login.aspx?direct=true&db=cat01310a&AN=lovisa.001816207&site=eds-live&scope=site
- Chemometrics: Statistics and Computer Application in Analytical Chemistry
  http://onlinelibrary.wiley.com/book/10.1002/9783527699377
- Chemometrics in Food Chemistry
  http://ludwig.lub.lu.se/login?url=http://search.ebscohost.com/login.aspx?direct=true&db=cat01310a&AN=lovisa.004275337&site=eds-live&scope=site
- Pandas tutorial:
  https://pandas.pydata.org/pandas-docs/stable/tutorials.html
- An Introduction to Statistics with Python With Applications in the Life Sciences / by Thomas Haslwanter.
  http://ludwig.lub.lu.se/login?url=http://search.ebscohost.com/login.aspx?direct=true&db=cat01310a&AN=lovisa.004904188&site=eds-live&scope=site
- A Primer on Scientific Programming with Python [Elektronisk resurs] / by Hans Petter Langtangen.
  http://ludwig.lub.lu.se/login?url=http://search.ebscohost.com/login.aspx?direct=true&db=cat01310a&AN=lovisa.004197259&site=eds-live&scope=site
- Learning scientific programming with Python / Christian Hill, University College London and Somerville College, University of Oxford.
  http://ludwig.lub.lu.se/login?url=http://search.ebscohost.com/login.aspx?direct=true&db=cat01310a&AN=lovisa.004865586&site=eds-live&scope=site

Python Installation:
Windows user: (all versions)
To avoid installing all the packages step by step I would recommend to use one of the freely available pre-packaged distributions which contains all the necessary modules of this course. e.g.
https://www.anaconda.com/download/ or http://python-xy.github.io/
In addition I highly recommend to use either an advanced text editor or a specialized IDE (integrated development Environment). We will look on Spyder and Jupyter which are installed in these packages. But is good to have a better editor available then the normal notepad.
For Windows I would recommend notepad++ https://notepad-plus-plus.org/download/

Linux and Mac user: Depending on your distribution you have either a package handler or the “port” function (for mac). Please make sure that you have the following packages installed:
ipython, sys, os, pandas, scipy, numpy, matplotlib, scikit-learn, seaborn
(spyder, jupyter, lmfit we will touch but are optional)