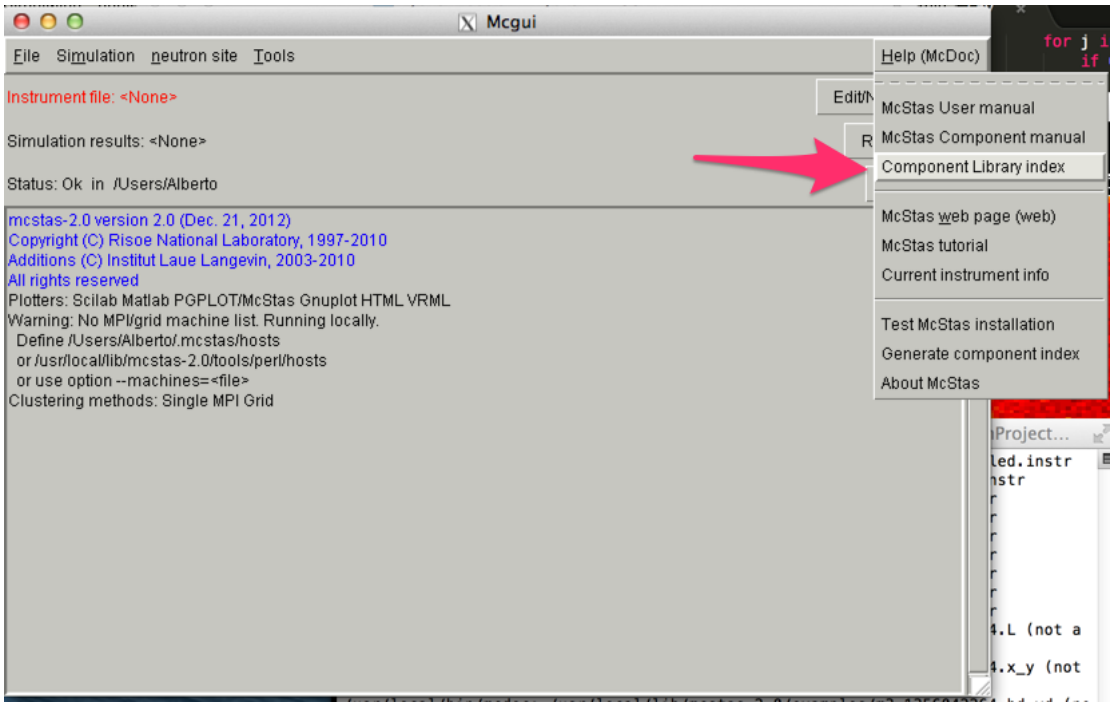
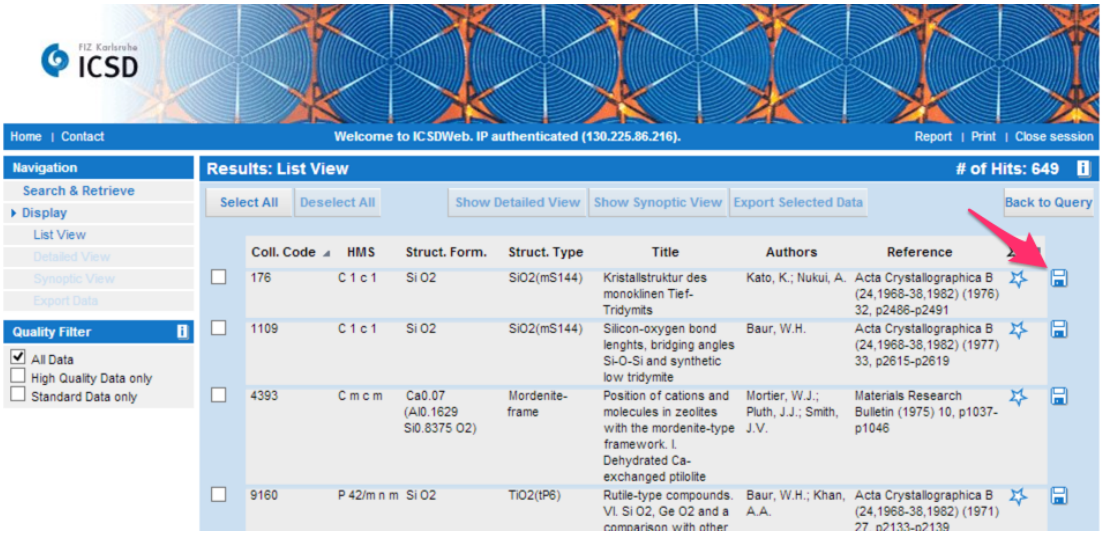
How to make a new .lau file for use with Single_crystal.comp, PowderN or Isotropic_Sqw – *by Alberto Cereser & Peter Willendrup, DTU Fysik*

1) Check that the .lau file is not already available in McStas. To do so, open a mcgui window, and select Help → Component Library index. Then check in the Data section.



2) Install Crystallographica (http://www.oxcryo.com/cg/crystallographica/). Crystallographica is for Windows only, so in case you are working with Linux or OSX you should first install a virtual machine running Windows, or use Wine (http://www.winehq.org/download);

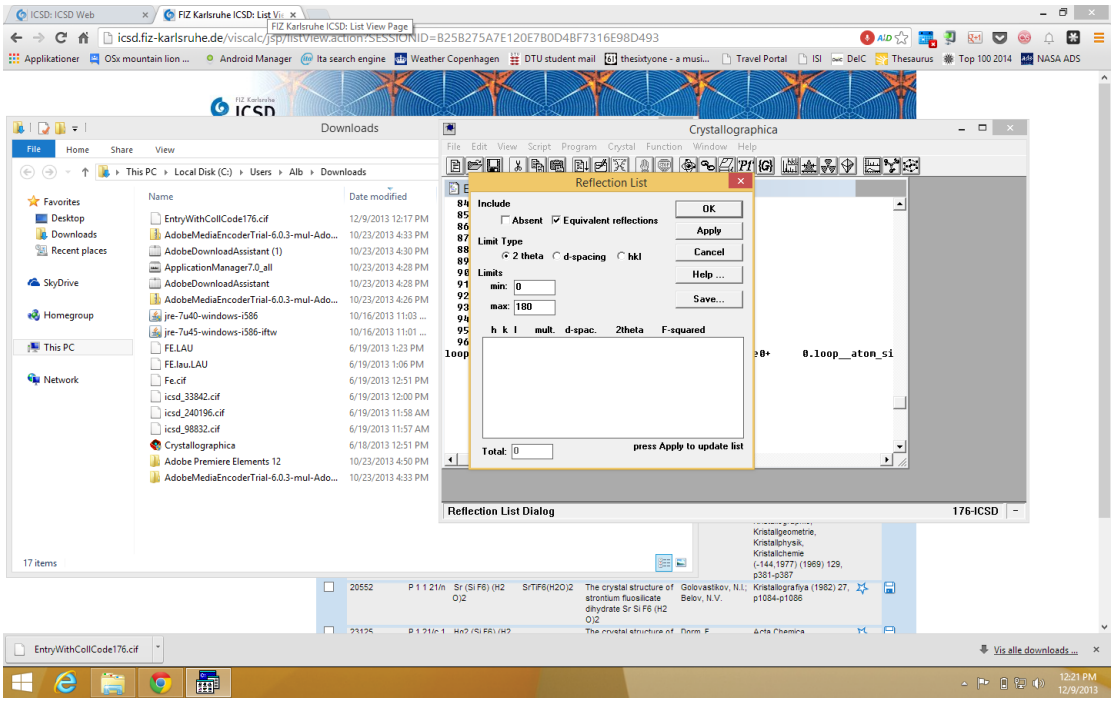
3) In the ICSD database (http://www.fiz-karlsruhe.com/icsd.html), look for the crystalline structure you want to study and download the .cif file.



4) Import the file in Crystallographica (File → Import CIF)

5) Select Crystal → Radiation → Neutron, and put the lower considered wavelength (this is required to indicate the resolution)

6) Select Crystal → Reflections. We suggest to select “Equivalent reflections”. This is however only needed if you intend to use the .lau file with Single_crystal.comp



7) Save the obtained file as .dat.

8) Open a mcgui window, and select Help → Component Library index. This will return a list of .lau files. Select one, and copy the header on the top of your .dat file. Correct the variables for the material you are using, and save the resulting file as .lau

9) Save a copy of your .lau file in the same folder of the .instr file you are working with.