Integrative Structural Biology School
5-12 June 2015
Software for X-ray Macromolecule Crystallography (MX) and Small Angle X-ray Scattering (SAXS)

Here is a list of recommended crystallography software to be installed on your computer before coming to the school. The table below summarizes the software to be installed.

	Linux	**Mac OS X**	**Windows**
XDS	X	X	
SHELX	X	X	X
CCP4	X	X	X
Coot			X
iMOSFLM			X
Pymol	(X)	(X)	(X)
ATSAS	X	X	X

X: to be installed. (X): optional (but recommended...).

Note for installation on Windows

PC 64-bit with Windows 7 or 8 is required (check that you have an “exploitation system 64-bit” by opening the “configuration panel” in your PC and checking the file “system”).

For software installation, you **MUST** follow this order of installation: CCP4, Coot, SHELX, iMOSFLM.

Coot and iMOSFLM has to be installed separately (see above), whereas it is part of the CCP4 installation for other Oss.

During installation of SHELX, you **MUST** change the path: Path proposed during installation: `c:\user\username\AppData\Local\shelx64` to be changed to `c:\CCP4\6.5\bin\`

List of software

Required for: MX Data reduction
Package name: XDS
To be installed on all OSs but Windows
Available for: Linux 32 bit, Linux 64 bit, Mac OS X
Can be downloaded from: http://xds.mpimf-heidelberg.mpg.de/html_doc/downloading.html
Installation: download the .tar.gz file, uncompress / untar and place binaries where appropriate
Special conditions: no restriction for academics (present license expires December 2015).

Required for: MX anomalous phasing
Package name: SHELX
To be installed on all OSs
Available for: Linux 32 bit, Linux 64 bit, Mac OS X, PC Windows 64 bit
Can be downloaded from: http://shelx.uni-ac.gwdg.de/SHELX/download.php
Installation: download the compressed files, uncompress and place binaries where appropriate.
Special conditions: SHELX binaries has to be installed prior to CCP4, in a location where CCP4 can see them when you run ccp4i. SHELX is free for academics, but a license and a pre-registration are required, with a valid email address. Upon pre-registration, the answer to the Xtal question (space group 19) is: P212121

Required for: almost everything in MX
Package name: CCP4 Program Suite v6.5
To be installed on all OSs
Available for: Linux 32 bit and 64 bit, Mac OS X, PC Windows 32 bit and 64 bit
Can be downloaded from: http://www.ccp4.ac.uk/download
Installation: download the package manager generated automatically and run it. Alternatively, download the CCP4 and Arp/Warp packages and install them the usual way (no need for the Balbes database).
Special conditions: no restriction for academics

Required for: graphics program for visualization of electron density maps
Package name: Coot
To be installed on Windows only (this is part of CCP4 package for other OSs)
Available for: Linux 32 bit and 64 bit, Mac OS X, PC Windows 32 bit and 64 bit
Can be downloaded from: http://www.ccp4.ac.uk/download/#os=windows
Installation: coot v0.8.1 (32 bit)
Special conditions: no restriction for academics

Required for: MX data reduction
Package name: iMOSFLM
To be installed on Windows only (this is part of CCP4 package for other OSs)
Can be downloaded from:
http://www.mrc-lmb.cam.ac.uk/harry/imosflm/ver713/introduction.html
Special conditions: none. Use the “Windows installer”

Required for: display structures, generate images and movies
Package name: Pymol
To be installed on all Oss (optional)
Available for: Linux 32 bit and 64 bit, Mac OS X 10.7 to 10.10, PC Windows 32 bit and 64 bit
Can be downloaded from: http://pymol.org/edu/?q=educational/
Installation: Just download the .tar.gz file, uncompress / untar and place binaries where appropriate
Special conditions: Educational-use-only PyMOL builds available at no cost to teachers and students. License and pre-registration are required, with a valid email address.

Required for: SAXS data processing
Package name: ATSAS
To be installed on all OSs
Available for: Linux 32 bit and 64 bit, Mac OS X, Windows XP 32 bit, Windows 7 64 bit
Can be downloaded from: http://www.embl-hamburg.de/biosaxs/download.html
Installation: Upon login on the web site, download the right package.
Special conditions: Free for academics, but a license and a pre-registration are required, with a

valid email address.

Assistance

If you need assistance, please contact:
For installation on Mac computers: Marie-Hélène LeDu (Marie-Helene.LEDU@cea.fr), Dominique Housset (dominique.housset@ibs.fr).
For installation on Windows: Patrice Gouet (patrice.gouet@ibcp.fr)
For installation on Linux systems: Jean-Luc Ferrer (jean-luc.ferrer@ibs.fr), Dominique Housset (dominique.housset@ibs.fr)

Some time will also be dedicated at the beginning of the school (Saturday 6, 01:30PM-03:30PM) to fix the last issues.