

Introduction to Three-Dimensional Electron Diffraction / MicroED (NTU)

All software listed below are freely available to academic user.

RED processing (REDp)

Installation and Tutorial: <https://www.mmk.su.se/zou/electron-crystallography-software/rotation-electron-diffraction-red>

Note: REDp is for Windows only. Mac users can run REDp in a virtual windows machine.

XDS

Installation: https://xds.mr.mpg.de/html_doc/downloading.html

For installation in Win 10/11, please see attached instructions.

XDS WIKI: <https://strucbio.biologie.uni-konstanz.de/xdswiki/index.php/Xds>

XDS and XDSGUI tutorial: <https://www.youtube.com/watch?v=3WU9NrILECo>

Small Molecules:

Shelx package:

Installation: <http://shelx.uni-goettingen.de/>

Please add the path of Shelx in the Windows environment variables, so that shelx can be called in all folders.

Shelxle (GUI):

Installation: <https://www.shelxle.org/shelx/eingabe.php>

VESTA:

Installation: <https://jp-minerals.org/vesta/en/download.html>

Macromolecules:

PHENIX:

Installation: <https://phenix-online.org/download/>

Tutorials: https://phenix-online.org/documentation/reference/tutorial_channel.html

COOT and WinCOOT:

COOT Installation: <https://www2.mrc-lmb.cam.ac.uk/personal/pemsley/coot/>

WinCOOT Installation: <https://bernhardcl.github.io/coot/wincoot-download.html>

Tutorial: <https://www2.mrc-lmb.cam.ac.uk/personal/pemsley/coot/web/tutorial/>

Videos: <https://www.youtube.com/c/PaulEmsley/videos>

Other useful software:

DIALS:

Installation: <https://dials.github.io/installation.html>

Tutorial (MyD88^{TIR} Protein, Small Wedge):

<https://dials.github.io/documentation/tutorials/3DED/MyD88.html>

PETS 2.0:

Installation: <http://pets.fzu.cz/>

Tutorial: http://pets.fzu.cz/download/pets2_manual.pdf

Contacts: <https://www.fzu.cz/en/research/research-topics/methodology-structural-electron-crystallography>

JANA:

Installation and information: <http://jana.fzu.cz/>

Yearly workshop: <http://jana.fzu.cz/#workshops1>

Manual (Cookbook): <http://jana.fzu.cz/workshops/Jana2006%20Cookbook.pdf>

SIR2019:

Installation: <http://www.ba.ic.cnr.it/softwareic/sir/sir2014-download-2/>

Information: <http://www.ba.ic.cnr.it/softwareic/sir/>

Manual: <http://www.ba.ic.cnr.it/softwareic/sir/wp-content/uploads/sites/3/kalins-pdf/Sir2019.pdf>

Olex2:

Installation: <https://www.olexsys.org/olex2/>

CCP4:

Installation: www.ccp4.ac.uk/download

Tutorials: https://www.ccp4.ac.uk/?page_id=1072

Phaser: [https://www.phaser.cimr.cam.ac.uk/index.php/Phaser Crystallographic Software](https://www.phaser.cimr.cam.ac.uk/index.php/Phaser_Crystallographic_Software)

MrBump: <https://www.ccp4.ac.uk/schools/APS-2011/tutorials/mrbump/mrbump-aps2011.pdf>

Refmac Manual: <https://www.ccp4.ac.uk/html/refmac5/keywords/xray-principal.html>

CCP4Cloud:

Installation: www.ccp4.ac.uk/download

Registration for an account: cloud.ccp4.ac.uk

MyD88 Tutorial on CCP4Cloud: "My Projects" -> "Demo Projects" -> "Select demo project" -> "upper directory" -> "tutorial-data" -> "iUCR-25" -> "MyD88"

UCSF:

Installation: <https://www.rbvi.ucsf.edu/chimerax/download.html>

Tutorials: <https://www.rbvi.ucsf.edu/chimerax/tutorials.html> and <https://www.rbvi.ucsf.edu/chimerax/docs/videos/>

Information: <https://www.rbvi.ucsf.edu/chimerax/index.html>

ISOLDE:

Installation: <https://isolde.cimr.cam.ac.uk/download/>

Tutorial: <https://isolde.cimr.cam.ac.uk/documentation/>

Information: <https://isolde.cimr.cam.ac.uk/>

ImageJ:

Installation: <https://imagej.nih.gov/ij/download.html>

Notepad++:

Installation: <https://notepad-plus-plus.org/downloads/>

DigitalMicrograph (Gatan microscopy Suite):

Installation: <https://www.gatan.com/products/tem-analysis/gatan-microscopy-suite-software>