XChem lab checklist

- ☐ Have your Diamond FedID and password in hand
- ☐ Check if there is enough pucks/pins for your experiment and recycle if needed
- ☐ Image your plate at the Research Complex
- ☐ Set xchempath in your linux bashrc if you are new on the platform
- ☐ Run: preparevisit to create the XChem visit directories
- ☐ Open SoakDB: /dls/labxchem/data/PROPOSAL/VISIT/processing/lab36/
- ☐ Input your protein acronym (this must match what is in your ERA)
- ☐ Rank your crystals using TexRank (remember to set to Formulatrix and 1 drop) and export the target list CSV file
- ☐ Watch out for X/Y coordinates > +/-1400 in the exported CSV file
- ☐ If using plate ≠ SwissCi-3drop, change the plate type in SoakDB
- ☐ Export Echo soaking CSV files from SoakDB
- ☐ Open compound plate under argon gas
- ☐ Transfer compounds for soaking to your crystal drops using the Echo
- ☐ Flush compound plate with argon gas before sealing it
- ☐ Update the transfer status to "Done" in SoakDB
- ☐ Export the harvesting CSV file for the shifter
- ☐ Scan the required pucks out at the scan in/out workstation
- ☐ Scan your pucks on the Shifter software in the same order you are going to use them and select the first row of the puck list
- ☐ Mount your crystals
- ☐ Scan your open pucks/pins on the puck scanner station
- ☐ Seal your pucks and store in the dewars and write down the cane tape number
- ☐ If using plate ≠ SwissCi-3drop, before you import the harvesting CSV file back, be sure you still have the right plate type selected in SoakDB
- ☐ Import your harvesting CSV shifter file back into SoakDB
- ☐ Click on "update status" in the SoakDB ISpyB section
- ☐ Add beamline visit, unit cell dimensions and data collection parameters for UDC in SoakDB as necessary
- ☐ Click on "Export to ISpyB" in the SoakDB ISpyB section
- ☐ Open Putty and connect to **ssh.diamond.ac.uk** (click on "yes" if a pop-up window asking to add the RSA key appears)
- ☐ Login with your FedID and password and go to your visit ispyb directory: /dls/labxchem/data/**PROPOSAL**/**VISIT**/processing/lab36/ispyb/
- ☐ Run the script: csv2ispyb **your-exported-ispyb-csv-file.csv**
- ☐ Log onto ISpyB and check that a new shipment with your pucks has been created
- ☐ Go to SoakDB "Pucks" tab, click on "Update/Save changes" then on "Yes". Update the puck table with: the puck location, the data collection parameters, the beamline visit number, your name, your target name and your local contact
- ☐ Copy the new/relevant lines into the XChem-Queue Google spreadsheet
- ☐ Close your SoakDB
- ☐ Scan your unused pucks back in the scan in/out workstation

XChem team