



UNATTENDED DATA COLLECTION

Manual XALOC Beamline

- **Login to MXCube** using the credentials of your proposal (u202xxxxxxx)
- In ISPYB proposal>**GROUP** (below the login) set AUTO to differentiate the Automated Data Collection (ADC) datasets from the manual ones.
- Select **Automatic X-Ray** centring in Sample Tree>Centring.
- **Synchronize your samples with ISPyB** (Sample Tree>ISPyB). If the samples are not defined in ISPyB, add the puck positions in the comment field, below the data collection tabs (For example, “pos 1: CPS 3412, pos 2: CPS 3421” etc).
- In the **sample tree select those samples** you are interested to launch with similar parameters. To do that press CTR in your keyboard and click with your mouse (left click) the samples. Note that selecting the puck will select all samples. In case you select samples and pucks at the same time will lead to double data collections being programmed! Probably not desirable.
- In the **Standard data collection** tab choose the adequate **parameters** of your data collection. The standard parameters are 1800 images, 0.1° rotation, 0.01sec exposure and 30% transmission (choose according to susceptibility of the samples to X-rays). Modify it if needed. Select the minimum resolution you need, MXCube only will collect a dataset when the resolution detected is better than that (2.5 Å recommended).
- Once selected the samples of interest click the **Add to Queue** button. You can include several sets of samples with different data collection parameters to different queues so repeat previous steps for each class of samples.
- The last step is to click the **Collect Queue** button to start data collection. Verify first that the parameters and samples in the pop-up window are correct and if so click **Continue**.
- Done!