Report of experiment MX608 at ID 23.2 (21-22 July 2007)

During the 3 shifts assigned to our bag we have been able to test 50 crystals thanks to the sample changer. We have also performed 8 data collections and 1 SAD experiment, until the beam dropped for vacuum problems.
The beamline is well equipped, but the experimental hutch is too humid, therefore we experienced the presence of ice in the sample changer, whose motor got stuck several times and needed to be reset almost at every basket change. Moreover not all the barcodes were read under the scan procedure, despite they were all coming from the same batch of Hampton cryo-vials.
Data Backup was straightforward, as well as indexing and processing. The presence of the package CRANK was very useful to obtain preliminary maps of the SAD experiment.
We collected 2 data sets of the Norcoclaurine synthase (Nausica) from *Thalictrum flavum* soaked with Osmium for two different time-spans. A native data set was already collected earlier this year. In both cases, the cell was isomorphous within error with the native one: space group $P3_121$, cell dimensions a=b=86.39Å, c=118.25Å. Despite a 50% attenuation of the beam and an exposure time of 1second, the first crystal suffered from radiation damage so the initial resolution of 2.8 dropped to 3.5Å, and the phasing power was not enough to solve the structure. The second crystal was less anisotropic and suffered less radiation damage keeping the resolution at 2.9Å all throughout.
After that we collected 1 native data set of a new construct of HbA in which the two alpha chains and the two beta chains are fused each one in one polypeptide chain. The crystals diffracted very anisotropically, nevertheless we collected 1 data set at 3Å resolution and we are trying to place the subunits by MR. The space group was C2 with cell dimensions a= 235.14, b= 53.06, c=135.73, beta=123.36. The asymmetric unit contains two tetramers, as judged from the Matthews coefficient.
We then collected 4 datasets of 2 crystal forms of SmTGR cocrystallised with either GSH or GSSG. Each crystal grew from a different drop condition, therefore we decided to collect them all. We are performing MR to solve the structure and verify the presence of the ligands. In both cases the space group is C2 with slightly different cell dimensions: a=142.18, b=104.33, c= 59.84, beta= 112.35 for the ones with GSH, and a=141.57, b=102.88, c=59.11, beta=112.62 for the ones with GSSG.
The SAD experiment was performed on the SeMet derivative of Laminarinase endo-ß-glucanase (LamA) from *Pyrococcus furiosus*. The best crystal diffracted well enough, at 2.7Å resolution, C2 space group and cell dimensions a=120.97, b= 72.91, c=92.05, beta=100.61. the preliminary maps look promising, and we are tracing the protein.
Finally we started collecting one crystal of SmGpx which was the highest diffracting one (1.5Å), but we managed to collect only 57° before the beam died. So the data collection was not complete since the space group is P212121 with dimensions a=41.57, b= 60.58, c=62.88.