| ESRF | Experiment title: BAG Marseille | Experiment number: LS-1363 Date of report: 22.2.99 |
|-----------|---|---|
| Beamline: | Date of experiment: from: 16 Feb 1999 7am to: 17 Feb 1999 7am | |
| Shifts: | Local contact(s): Sean Mc Sweeney | Received at ESRF: |

Names and affiliations of applicants (* indicates experimentalists):

Yves Bourne*, Alain Roussel*, Silvia Spinelli*, Kieron Brown*, Mariella Tegoni*, Christian Cambillau

Report: 15 shifts have been attributed to the BAG, 3 on ID14, 3 on BM14 and 9 on ID2.

We report here the 3 shifts on ID14-EH4, which took place one week ago. Despite problems on the line (shutter, etc) leading to the lost of one shift (start at 1 pm), 18 data sets have been collected, 2 of which have been integrated to date, the others being still underway. Most crystals have been transported frozen in liquid N2. A few frames have been evaluated on the line for each data set, however. All of them showed improved quality of the diffraction pattern. These 3 shifts have produced a tremendous amount of valuable data with huge improvements in the diffraction quality.

Table 1: List of the data sets:

- Enzyme GlmU with effectors 3 data sets at 2.2 Å (ca 3Å at home)
- Acetyl choline esterase with inhibitors. 3 data sets.
- Lipase HGL with inhibitors. 3 data sets at 3.2-2.8 Å (between 6 Å at home.
- Nitrate reductase. Intermediates along the d heme reduction (after microspectrophotometric characterization at ESRF: 2 data sets at 2.8 Å.

- Odorant Binding Proteins (native) at very high resolution: porcine at 1.4Å resolution, Bovine at 1.2 Å resolution (with natural ligand bound inside).
- Aphrodisin Se-Met. A data set has been collected at 2.1 Å resolution at the Se absorption edge. Test data set for ulterior MAD experiment.
- Hyperthermophilic Threonine Dehydrogenase 3 data sets of native and derivatives.
- Hyperthermophilic enzyme AARE: 1 data set.

Table 2:

| Project: | GlmU-Glc-Nac | HGL (cubic: I23) |
|--------------|--------------|------------------|
| Resolution | 30-2.2 | 30-3.2 |
| Overall I/oI | 6.0 | 5.5 |
| Overall Rsym | 6.7 | 9.8 |
| Multiplicity | 3.5 | 7.5 |
| Completeness | 98 | 99.9 |