ESRF	**Experiment title:** BAG-LEBS-2003-2	**Experiment number:** 30-01-627
Beamline: BM-30 A	**Date of experiment:** from: 08/10/2003 at 8h00 to: 11/10/2003 at 8h00	**Date of report:** 11/12/2003
Shifts: 9	**Local contact(s):** Dr. Philippe Carpentier	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Solange Morera* (research assistant, CR1), Laurent Lariviere* (Ph.D. student), Marc Graille* (Post-Doc), LEBS, 1, Av. de la Terrasse, 91190 Gif-Sur-Yvette, France

and Lionel Tresaugues* (Ph.D. student Orsay), Institut de Biochimie et Biophysique Moléculaire et Cellulaire, Universite Paris-Sud, Orsay, France

Report:

Solange Morera, Laurent Lariviere: Structural studies of the Beta Glucosyl Transferase in complex with DNA (2 shifts):

We collected 4 data sets of BGT:
1-one in complex with a 13mer DNA fragment at 2.9 A resolution. We are now analysing the structure.
2-three of BGT crystals soaked with UDP-Gal and/or potential inhibitors/substrates. Unfortunately these structures do not show a ligand.

L. Tresaugues, M. Graille (4.5 shifts) : yeast *Saccharomyces cerevisiae* Structural Genomics project

The systematic names of the genes are used. More details on every orf can be found on http://genomics.eu.org:targets.html

1) YLR011w (target 131).
Spacegroup $P2_12_12$ a=58A; b=75A;c=153A.
Resolution 1.9A
Completion: 97 %.

This protein contains 191 residues and has unknown function. During this session, we have collected a 3 wavelengths MAD dataset but as phasing was not possible, we have collected a highly redundant SAD dataset from a second crystal (redundancy of 24). We have then been able to solve to 2.5A resolution. Resolutiuon was further improved by a 1.9A resolution dataset also collected during this beam time allocation. Searches for structural homologues revealed that this protein is close to many FAD bining protein and the best structural match was found to be *Bacillus subtilis* azobenzene reductase. In addition, FAD was found to be bound to the protein, hence alowing identification of the active site.

2)YHR049w (target 136).
Spacegroup I432 a=b=c=207A.
Resolution 1.7A
Completion 100 %

The structure of this protein has been solved in the presence of ATP during the last semester to 2.9A resolution. To investigate ligand specificity of this protein, we have undertaken co-crystallisation trials with other nucleotides. A crystal grown in the presence of GTP has diffracted to 1.7A resolution. The structure is currently under refinement (R_f=24.3%; R=22%) and the GTP is well bound to the protein. We have also collected a 2.3A resolution dataset from crystal grown in the presence of ATP (same space group and unit cell parameters), that is currently under refinement.

3) RRM.
Spacegroup $P4_132$
Resolution 3.3A.
Completion 100%.
Three datasets to 3.3A resolution (one native and 2 from crystals soaked in heavy atom solutions) have been collected. Analysis of the difference Patterson maps indicate that no derivative is well bound in the crystal.

4) Neocarzinostatin mutants.
Spacegroup: $P6_5$.
Resolution: 1.8A.
Completion: 100%
Neocarzinostatin (NCS) is an antitumour antibiotic protein isolated from the actinomycetes *Streptomyces carzinostaticus* whose structure has been previously solved to 1.5Å resolution. A directed evolution strategy was used to confer to this protein the ability to bind a human hormone. Three different crystal forms have been obtained from a NCS-steroid complex. We have collected one dataset from each crystal form (spacegroups $P2_12_12_1$, $P2_12_12$, $P6_5$). The structure has been refined against the best resolution dataset and the steroid is very well defined in the 2Fo-Fc electron density map, thus allowing a good understanding of the role of the mutation for steroid binding.