| ESRF | **Experiment title:** Crystal Structure of a putative esterase: a functional genomics approach | **Experiment number:** LS1657 |
|---|---|---|
| **Beamline:** ID14-2 | **Date of experiment:** from: 3-3-00 to: 4-3-00 | **Date of report:** Aug00 |
| **Shifts:** 3 | **Local contact(s):** Sigrid STURRMAN | *Received at ESRF:* |

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## Report:

We have cloned and expressed a gene controlled by the xylanolytic transcription factor XlnR from the filamentous fungus *Aspergilllus niger*, which is involved in the degradation of the polysaccharides xylan and cellulose. This gene encodes an extracellular protein having a significant homology to lipases/esterases of the $\alpha/\beta$ hydrolase family. It contains amino acids that could belong to functional catalytic triad. However, our first attempts to detect an esterase activity were unsuccessful. The protein is largely over-expressed as a soluble form and we thought it was a good example as functional genomics where a three-dimensional structure could lead to the finding of a substrate specificity. Crystals diffracted up to 2.1 Å resolution (Table 1). The structure was solved by molecular replacement with the AMoRe package using an original approach involving a chimeric template in which two thirds were taken from the Geotrichum candidum lipase (PDB code 1THG) and the remaining one third from mouse acetylcholinesterase (PDB code 1MAA). Indeed, attempts to solve the structure using either of the two models separately were unsuccessful. The chimeric model has a correlation coefficient and an R-factor value of respectively 19% and 49.7% in the 15 Å to 4 Å resolution range for two molecules in the asymmetric unit. The sequence identity between this protein and our chimeric model is low, but significant, and the current electron density maps are promising. Refinement process is underway.

**Table 1. Data collection and refine ment statistics**

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|---|---|
| Resolution (Å) | 2.1 |
| No. observations | 1 686 510 |
| No. unique | 104 768 |
| $R_{sym}$ (%) | 7.7 (42) |
| I/σ(I) | 7.2 (1.7) |
| Redundancy | 5.0 |
| Completeness (%) | 100 (100) |
| Resolution (Å) | 20- 2.1 |
| R-factor - R free (%) | 46 - 51 |