ESRF	Experiment title: The Structure of the Catalytic Module from *Pseudomonas cellulosa* Xyn10C	**Experiment number**: LS-1811
Beamline: ID14-4	**Date of experiment**: from: 11/11/00 to: 13/11/00	**Date of report**: 30/08/01
Shifts: 1	**Local contact(s)**: Sean McSweeney	*Received at ESRF:*

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Report:

The structure of the plant cell wall is composite in nature, comprising many, often complex, polysaccharides and the carbon cycle is absolutely dependent on the breakdown of such plant material. Many enzymes are involved in this essential process, including polysaccharide hydrolases, lyase and esterases. Xylan is the major constituent of hemicellulose, the second most abundant polysaccharide on Earth. This polymer is cleaved by xylanases, enzymes belonging to families 10 and 11 of the glycoside hydrolases (GH10 and GH11, respectively). The process of xylan degradation is complex and many organisms posses multiple xylanase genes. Although the three dimensional structures of numerous GH10 xylanases have been reported, in order to understand the multiplicity of enzymes involved in plant cell wall degradation, the structure of Xyn10C from *Pseudomonas cellulosa* was solved and compared to that of the homologous enzyme Xyn10A from the same organism.

Crystals of the catalytic module of Xyn10C were obtained from 100 mM Tris/HCl buffer, pH 7.5, containing 150 mM KSCN and 25 % (w/v) PEG4000. These crystals belong to space group $P2_12_12_1$ (a=44.14, b=78.75 Å, c=172.22 Å) and contain one molecule in the asymmetric unit. 500 images of 0.35 degrees were collected on beamline ID14-4 at the ESRF, Grenoble (Nov 2000). The structure of Xyn10C was solved by molecular replacement using the program AMoRe and one molecule of Xyn10A (PDB code 1CLX) as the search model. As expected, the substrate binding cleft of Xyn10C is very similar to that of Xyn10A. The only major difference in the –2 to +2 subsite region of the active site is at position 43. This residue is a glutamate in the majority of GH10 enzymes and interacts with the C2-OH group of a xylosyl residue occupying the –2 subsite. However, a subfamily of enzymes posses a glycine at this position. A complex of Xyn10C is currently being prepared to determine what functional role, if any, is played by Gly 43.