ESRF	Experiment title: **Cellobiose dehydrogenase.** *BAG: Uppsala (II)*	**Experiment number**: LS-2187
Beamline: ID14-EH4	**Date of experiment**: from: 4 May 2002 to: 6 May 2002	**Date of report**: 1 Sep 2002
Shifts: 0.2	**Local contact(s)**: Raimond Ravelli	*Received at ESRF:*

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Report:

The fungal flavocytochrome cellobiose dehydrogenase (CDH) participates in lignocellulose degradation with a proposed role in the early events of wood degradation. The 755-residue protein consists of a *b*-type cytochrome linked to a large FAD-binding domain which can be separated proteolytically to yield the individual proteins. CDH catalyzes the oxidation of cellobiose to yield cellobiono-1,5-lactone with the concomitant reduction of FAD. Reducing equivalents are then transferred, one by one, to the cytochrome domain and subsequently to an external electron acceptor. We are undertaking X-ray crystallographic studies on the structure-function relationship of CDH, and have recently reported the structures of the two domains of CDH from *Phanerochaete chrysosporium*.

The structure of the CDH cytochrome domain revealed a for cytochromes unusual fold: a fibronectin-like β-sandwich consisting of a five-stranded and six-stranded β-sheet with the protoheme bound relatively surface exposed at one face of the β-core. Moreover, unique features were found for the Met-His ligation of the *b*-type heme, i.e., a near-perpendicular arrangement of the Fe ligands. To investigate the heme-coordinating aspects of CDH further, a mutant was produced where the Met ligand was replaced by His, which is more prevalent in *b*-type cytochromes. Data was collected on a crystal (0.01 mm^3) of space group $P6_5$ to 1.9 Å resolution (R_{sym} 7.8%). The structure has now been determined and refined, and a manuscript describing the spectroscopic and structural analysis of the *bis*-His CDH cytochrome is currently in preparation.