ESRF	Experiment title: **Cellulases.** *BAG: Uppsala (II)*	**Experiment number:** LS-1520 g
Beamline: ID14-EH4	**Date of experiment:** from: 10 Dec 1999 to: 12 Dec 1999	**Date of report:** 29 Aug 2000
Shifts: 2	**Local contact(s):** Sean McSweeney	*Received at ESRF:*

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Report:

During this visit to ID14-4 more than 60 crystals were tested and 5 datasets were collected. The time was used for Ribokinase (Experiment report LS-1520 e), Allose-binding protein (Experiment report LS-1520 f) and Cellulases, reported here.

Three datasets were collected of ligand complexes with Cellobiohydrolase 58 (synonyms: CBH 58, CBH 1-4, Cel7D) from the white-rot fungus *Phanerochaete chrysosporium:* Two of them, both at 1.5 A, were from crystals of CBH 58 co-crystallised with the *(R)*-enantiomer of an adrenergic beta-receptor antagonist, *(R)*-propranolol. CBH 58 can be immobilised on silica and used as a chiral selector molecule in chromatographic enantio-separation of adrenergic beta-blockers and some other compounds. We have earlier obtained a structure with the preferred *(S)*-enantiomer of propranolol bound in the active site, and have made several attempts to obtain a structure with the other enantiomer, *(R)*-propranolol. Our hope with the current experiments was that with altered conditions for co-

crystallisation together with the higher resolution obtained at the synchrotron, we should be able to distinguish the electron density for the ligand, even if the occupancy was way below 1. Weak electron density is evident at the expected binding site, but the interpretation is not straightforward. One data-set at 1.6 A, was collected of CBH 58 co-crystallised with high concentration of glucose, 0.2 M. Structure refinement is pending.

Very small crystals (less than 50 um) were tested of the cellulases EG 2 and EG 5 from *Trichoderma reesei*. They showed protein diffraction to 1.8 and 1.7 A resolution, respectively, but were too disordered to be useful for data collection.

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