



Experiment title:
Cellobiohydrolase 58 from *Phanerochaete chrysosporium* (Pc_Cel7D) . BAG: Uppsala (II)

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LS 1935

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Report:

Pc_Cel7D is the major cellobiohydrolase produced by the fungus *Phanerochaete chrysosporium*. Such enzymes are of great interest in terms of basic wood biology, as well as useful industrial tools. We have previously solved the structure of the catalytic domain of Pc_Cel7D by molecular replacement using the *Trichoderma reesei* CBHI structure as the search model.

Presently we are working to solve the structures complexed to different ligands. During this trip we collected 4 data sets on this enzyme, all in space group C2.

Data set 1: Pc_Cel7D crystallized with g3s (thio-linked oligosaccharide)

The data has been processed (resolution 1.85 Å, unit cell a= 85.964, b=46.655, c=98.844, beta=103.114, overall completeness 97.8 %, overall R merge 3%). But there was no density visible for the ligand in the initial electron density maps.

Data set 2: Pc_cel7D crystallized with cellobiose imidazole

The data has been processed (resolution 1.7 Å, unit cell a= 87.382, b=46.578, c=98.505, beta=102.585, overall completeness 97.4 %, overall R merge 3.4%). There is clear density for the ligand in the electron density maps and this structure is being refined.

Data set 3: Pc_cel7D crystallized with SVH486

The data have been processed (resolution 1.85 Å, unit cell a= 86.799, b=46.740, c=99.194, beta=103.222).

Data set 4: Cel7D complexed with R-propranolol, 1.2 Å resolution.