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| ESRF | Experiment title: Oligosaccharide-binding to family 11 xylanases: both covalent intermediate and mutant-product complexes display $^{2,5}B$ conformations at the active-centre. | **Experiment number**: LS-1532 |
| **Beamline**: ID14-4 | **Date of experiment**: from: 09/09/99 to: 11/09/99 | **Date of report**: 30/08/01 |
| **Shifts:** 1 | **Local contact(s)**: Sean McSweeney | *Received at ESRF:* |


**Names and affiliations of applicants** (* indicates experimentalists):

Elisabetta Sabini[a,b], Keith S Wilson[a], Steffen Danielsen[c], Martin Schülein[c] & Gideon J Davies[a,*]

a. Department of Chemistry, Structural Biology Laboratory, University of York, Heslington, York, YO10 5DD, United Kingdom

b. Current address: The Scripps Research Institute, MB-31, 10550 North Torrey Pines Road, La Jolla, California 92037, USA

c. Novozymes A/S, Smoermosevej 25, DK 2880 Bagsvaerd, Denmark.


## Report:

### *Abstract of published paper*


The glycoside hydrolase sequence-based classification reveals two families of enzymes which hydrolyse the β-1,4 linked backbone of xylan, xylanases, termed families GH-10 and GH-11. Family GH-11 xylanases are intriguing in that catalysis is performed *via* a covalent intermediate adopting an unusual $^{2,5}B$ (boat) conformation, a conformation which also fulfils the stereochemical constraints of the oxocarbenium-ion like transition-state. The 1.9Å structure of a nucleophile, E94A, mutant of the Xyn11 from *Bacillus agaradhaerens* in complex with xylotriose was solved using data collected on ESRF beamline ID14-4. Intriguingly this complex also adopts the $^{2,5}B$ in the –1 subsite with the vacant space provided by the Glu-Ala mutation allowing the sugar to adopt the α-configuration at C1. The structure of the covalent 2-deoxy-2-fluoro xylobiosyl-enzyme intermediate has been extended to atomic (1.1Å) resolution.


**References**


Sabini, E., Wilson, K.S., Danielsen, S., Schülein, M. & Davies, G.J. (2001). Oligosaccharide-binding to family 11 xylanases: both covalent intermediate and mutant-product complexes display $^{2,5}$B conformations at the active-centre. *Acta Crystallogr. D***57,** 1344-1347.