Experimental Report

Proposal: **8-01-365** **Council:** 4/2010

Title: The Catalytic Mechanism of xylose isomerase

This proposal is a new proposal

Researh Area: Biology

Main proposer: **KEEN David A.**

Experimental Team: SAWADA Daisuke
HANSON Leif
KEEN David A.
KOVALEVSKY Andrey
MASON Sax Anton
BLAKELEY Matthew
FORSYTH Trevor

Local Contact: MASON Sax Anton
FORSYTH Trevor

Samples: xylose isomerase amino acid

Instrument	Req. Days	All. Days	From	To
D19	21	16	12/07/2010	20/07/2010

Abstract:

Xylose isomerase (XI) is the most abundantly applied industrial enzyme, with major applications in the production of biofuels and value-added products from cellulosic biomass. Engineering efforts to improve the performance of XI will be significantly aided by understanding the enzyme's catalytic mechanism. Our goal is to use neutron crystallography to reveal the catalytic mechanism by determining the location and movement of H over the course of the multistep reaction. This involves determining a large number of neutron structures of XI in complex with different metals and substrates.In order to make this possible we have assembled an international consortium of scientists from ISIS, ILL, Fox Chase Cancer Center and LANSCE to collect these data sets on different beam lines. This consortium will not only be involved in determining the enzyme's mechanism but also in supporting the development of TOF protein crystallography at LMX at ISIS.

Following a successful experiment on D19, the work is about to be published as a communication in the journal "Angewandte Chemie". The title, author list, abstract and doi are reproduced below.

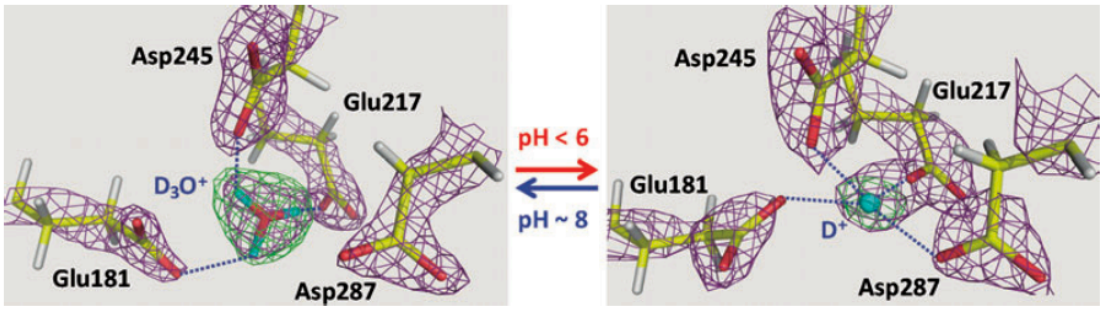
Identification of the elusive hydronium ion replacing a proton in an enzyme at lower pH values

A. Y. Kovalevsky,[1] B. L. Hanson,[2] S. A. Mason,[3] T. Yoshida,[4] S. Z. Fisher,[1] M. Mustyakimov,[1] V. T. Forsyth,[3,5] M. P. Blakeley,[3] D. A. Keen,[6] P. Langan[1]

1 Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM 87544, USA.
2 Chemistry Department, University of Toledo, Toledo, OH 43606, USA.
3 Institut Laue Langevin, Grenoble, 38042, France.
4 Chemistry Division, Los Alamos National Laboratory, Los Alamos, NM 87544, USA.
5 EPSAM/ISTM, Keele University, Staffordshire, ST5 5BG, UK.
6 ISIS Facility, Rutherford Appleton Laboratory, Harwell Science and Innovation Campus, Didcot OX11 0QX, Oxon, UK.

Summary

Visible to Neutrons: Although thought to be involved in biological processes, hydronium ions had never been identified in biomacromolecular crystallographic structures. A hydronium ion has now been found by neutron and X-ray crystallography to interchange with metal cofactors in the active site of an enzyme. Under more acidic conditions, the hydronium ion is dehydrated to a proton, and the binding site collapses (see picture).



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