

**Third Biocenter Oulu Workshop on Enzymes**

**Title:** Structural enzymology: Experimental and theoretical approaches

**Duration:** 2 days

**Date:** Thursday, November 29 and Friday, November 30, 2007

**Place:** University of Oulu, Linnanmaa, L10

**Hosts:** André Juffer and Rik Wierenga

<i>Day 1</i>	<i>Lecturer</i>	<i>Title</i>
09.45 - 10.00h	<b>Opening words</b>	
10.00 - 11.00h	<b>Keynote lecture:</b> Mårten Wikström, Helsinki, Finland	The importance of proton wires for cytochrome oxidase
11.00 - 12.00h	<b>Keynote lecture:</b> Noam Agmon, Jerusalem, Israel	Switchable proton escape from a proton-wire within green fluorescence protein
12.00 - 13.00h	<i>Lunch</i>	
13.00 - 13.45h	<i>Lecture</i> Tamo Fukamizo, Nara, Japan	Enzymology of glycosyl hydrolases: chitinase and chitosanase
13.45 - 14:30h	<i>Lecture</i> Gunter Schneider, Stockholm, Sweden	Structural enzymology of the biosynthesis of polyketide antibiotics
14:30 - 15:00h	<i>Lecture</i> Petri Pihko, Helsinki, Finland.	Enolizing enzymes and their mimics
15.00 - 15.30h	<i>Coffee break</i>	
15.30 - 16.00h	Satyan Sharma, Oulu, Finland	Quantum simulation of the reaction mechanism of prostatic acid phosphatase.
16.00 - 16.30h	Antti Haapalainen, Oulu, Finland	The reaction mechanism of T2 thiolase

<i>DAY 2</i>	<i>Lecturer</i>	<i>Title</i>
09.00 – 09:45h	<i>Lecture</i> Antti Poso, Kuopio, Finland	Prediction of enzyme inhibitors and substrates: molecular modeling and chemoinformatics
09.45 – 10:30h	<i>Lecture</i> Santosh Panjekar, EMBL Hamburg, Germany	Auto-Rickshaw: An online automated crystal structure determination platform (BIOXHIT)
10.30 - 11.00h	<i>Coffee break</i>	
11.00 - 11.45h	<i>Lecture</i> Eugene Krissinel, EBI, Hinxton, UK	Web-tools for protein structure analysis from <u>MSD@EBI</u> (BIOXHIT)
11.45- 12.30h	<i>Lecture</i> Kimmo Mattila, CSC, Espoo, Finland	CSC's tools for structural enzymology.
12.30 - 13.30h	<i>Lunch</i>	
13.30 - 16.00h	<i>Tutorials:</i> <ol style="list-style-type: none"> <li>1. Auto-Rickshaw</li> <li>2. Web-tools for protein structure analysis from MSD@EBI</li> <li>3. The structural biology toolkit of CSC.</li> </ol>	Biochemistry Linux class room  ATK Linux class room or in L10.

The precise organization of the tutorials will be decided later. The participants can specify which tutorial they would like to follow when registering for the meeting.