

# Workshop on "Neutron Macromolecular Crystallography at the SNS"

October 2-3, 2003

Intense Pulsed Neutron Source, Bldg. 360, Room A-224

Thursday, October 2, 2003

8:15 AM Continental Breakfast

## General Introduction

8:45 AM Ray Teller Welcome

8:50 AM Andy Mesecar Introduction and Objective

## Morning Session Chair, Andy Mesecar

### Challenges in Structural Biology

9:00 AM Anthony Kossiakoff Picking the Right Systems for the Right Problems

9:40 AM Alex Wlodawer What Can We Learn From Neutron Crystallographic Studies of Enzymes and Other Proteins?

10:20 AM Coffee

## Neutron Diffraction in Biology

10:45 AM Dean Myles Recent Trends and Advances in Neutron Macromolecular Crystallography

11:15 AM Ian Anderson The Spallation Neutron Source: Project Update

11:45 AM P. Thiyagarajan MaNDi - Design of the Proposed Instrument at SNS

12:15 PM Lunch

## Afternoon Session Chair, Anthony Kossiakoff

### Hydrogens and Water in Macromolecular Systems

1:30 PM Alberto Podjarny The Aldose Reductase Case: Ultra High Resolution X-Ray Structure and Preliminary Neutron Diffraction Results

2:10 PM John Helliwell Getting the Complete Protein (Crystal) Structure; Concanavalin A and beta-crustacyanin Case Studies at Current Capabilities and Beyond

2:40 PM Martin Egli Limits of XMC: DNA-Cation Interactions and Water-Nucleobase 'Stacking'

3:15 PM Coffee

3:45 PM Patrick Loria Enzyme Dynamics, Catalysis, and Water

4:15 PM Michael Johnson NMR, X-ray and Computational Analysis of Sickle Hemoglobin Aggregation Inhibitors -- Importance of Protonation States

4:45 PM Hong Guo Quantum Mechanical/Molecular Mechanical MD Simulations of Cytidine and Adenosine Deaminase: Importance of Proton Positions

## Drug Development

5:15 PM Chris Dealwis Towards Elucidating Catalytic Mechanism of Dihydrofolate Reductase Using Neutron and Ultra High Resolution X-ray Crystallography

5:45 PM Geoffrey Stamper Structure-Based Drug Design in the Pharmaceutical Industry: Is There a Role for NMC?

6:15 PM End of Session

7:00 PM Workshop Banquet (Argonne Guest House), Cash Bar Opens at 6:30 pm

## MaNDi Workshop Schedule - continued

**Friday, October 3, 2003**

8:00 AM Continental Breakfast

**Morning Session Chair, John Helliwell**

**Current Neutron Macromolecular Crystallography Research**

8:30 AM Martha Teeter Modeling Protein Dynamics with Neutron Crystallography at 1 Å Resolution

9:00 AM Peter Timmins Detergent Structures in Membrane Protein Crystals

9:30 AM Petra Fromme Neutron Diffraction on Membrane Protein Crystals

10:00 AM Coffee

10:30 PM Dan Carter Counter-diffusion Methods in the Growth of Macrocystals for Neutron Diffraction

11:00 AM Nobou Niimura Hydrogen and Hydration in Proteins and DNA Obtained by BIX-3 and BIX-4

11:30 AM Paul Langan Protein Crystallography with Spallation Neutrons: Results from the PCS at Los Alamos

12:15 PM Lunch

1:30 PM **Discussion of the Scientific Case and Formation of an Instrumentation Development Team**

**Discussion Chairs: Andy Mesecar, Alex Wlodawer, Art Schultz and Bernard Santarsiero**

**Discussion Topics:**

- MaNDi Capabilities
- Scientific Case
- IDT Formation
- Strategy for Securing Funding
- Development of Proposals

3:30 PM End of Workshop