Workshop on NEUTRON MACROMOLECULAR CRYSTALLOGRAPHY AT THE SPALLATION NEUTRON SOURCE October 2-3, 2003 Argonne National Laboratory, Argonne, IL, USA

Background

Neutron macromolecular crystallography (NMC) can play a critical role in structural biology and functional genomics by providing accurate information on the positions of the protons and water molecules at active sites of enzymes that will enable the elucidation of the mechanistic details involved in their function. In order to exploit the high neutron flux that will become available by 2006 at the Spallation Neutron Source (SNS), and to leverage the enormous interest shown by the macromolecular crystallography community, it is proposed to develop a dedicated best-in-class high throughput and high resolution time-of-flight single crystal macromolecular neutron diffractometer (MaNDi) at the SNS high power target station (HPTS). Design calculations show that the data rates at the MaNDi instrument will be over 50 times greater than those for the best existing facilities. Furthermore, it will enable studies of crystals with larger lattice constants than is possible at the current facilities for NMC. It is expected that the unprecedented high data rates and resolution with MaNDi for the high resolution neutron macromolecular crystallography (NMC) will greatly advance the fields of structural biology and enzymology.

Objective

- To discuss the exciting opportunity that exists at the SNS for the development of a powerful facility for high resolution neutron macromolecular crystallography (NMC). NMC has been proven to provide accurate positions of hydrogens, protonation states of the atoms and the hydration in biological macromolecular crystals which are of interest to the scientific community in the fields of structural biology, enzymology, biochemistry, and macromolecular crystallography.
- To obtain input from the scientific community on the exciting scientific challenges that can be addressed by neutron macromolecular crystallography. Also, to obtain input on the design aspects of MaNDi with regard to the size of the unit cell, resolution, detectors, sample environment, and deuteration facilities, as well as any other requirements at the Spallation Neutron Source.
- To officially form an instrument development team (IDT) and to document a strong scientific case in order to obtain funding for the design and construction of the MaNDi instrument.

<u>Confirmed Speakers</u>

Ian Anderson (SNS) Robert Bau (USC) Gerry Bunick (ORNL) Dan Carter (New Century Pharmaceuticals, Inc.) Victor Davidson (U Of MS) Chris Dealwis (UTK) Martin Egli (Vanderbilt U) Petra Fromme (Arizona State U) Hong Guo (UTK) Leif Hanson (ORNL) John Helliwell (U of Manchester, UK) Andrzej Joachimiak (ANL-SBC) Michael E. Johnson (UIC) Anthony Kossiakoff (U of C) Paul Langan (LANL) J. Patrick Loria (Yale) Lee Makowski (ANL-BIO) Dean Myles (ORNL) Nobuo Niimura (JAERI, Japan) Alberto Podjarny (IGBMC-Strosborg, France) Benno Schoenborn (LANL) Geoffrey F. Stamper (Abbott Labs) Ichiro Tanaka (JAERI, Japan) Martha Teeter (Boston College) Peter Timmins (ILL, France) Alexander Wlodawer (NCI)

Organizing Committee:

Andrew Mesecar (UIC), Arthur Schultz (ANL) and P. Thiyagarajan (ANL) *Conference Site:*

Bldg. 360, Intense Pulsed Neutron Source (IPNS), Argonne National Laboratory <u>Workshop Website</u>: www.pns.anl.gov/events/conferences/mandi/flyer.pdf **Registration Deadline**: September 18, 2003

Fee: \$100.00 US cash or check payable to Carolyn Peters-Workshop Account 467290 **Accommodation:** Argonne Guest House

Conference Secretary: Carolyn Peters, IPNS, ANL (cpeters@anl.gov)





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