

**Conference on New Frontiers in Neutron Macromolecular Crystallography**  
**Research Support Center, Oak Ridge National Laboratory**  
**July 12-13, 2005 (Agenda draft – July 1)**

**Monday, July 11**

5 – 8 p.m. Registration & ORNL Site Access Badge Pick Up for ORNL (Comfort Inn)

**Tuesday, July 12**

7:30 a.m. Buses depart Comfort Inn

8:00 Coffee

8:30 Thom Mason, Oak Ridge National Laboratory /Spallation Neutron Source  
*"Overview of the SNS"*

9:00 P. Thiyagarajan, Argonne National Laboratory /Intense Pulsed Neutron Source  
*"Design and Expected Performance of the next generation Macromolecular Neutron Diffractometer (MaNDi) for the Spallation Neutron Source"*

9:30 Anthony Kossiakoff, University of Chicago  
*"Back to the basics, what neutrons can tell us about protein structure that X-rays can't"*

10:00 Dean Myles, Oak Ridge National Laboratory  
*"Current status of macromolecular neutron crystallography"*

10:30 Coffee break

11:00 Andrzej Joachimiak, Argonne National Laboratory  
*"Structural genomics – exploring protein structure and function"*

11:30 Alberto Podjarny, University of Strasburg  
*"Complementary neutron and subatomic resolution X-ray studies of Aldose Reductase"*

Noon Lunch; discussions continue

1:30 p.m. Wayne Hendrickson, Columbia University  
*"Impact of radiation damage in biological crystallography"*

2:00 Dagmar Ringe, Brandeis University  
*"Pushing the limits of protein structure"*

2:30 Brian Matthews, University of Oregon, Institute of Molecular Biology  
*"Flash-freezing: It's cool but is it kosher?"*

3:00 Coffee break and poster session

4:00 SNS tour [**Note: extensive walking is required. Some of the tour is in a construction area; shorts and skirts are not permitted in these areas.**]

6:00 Continuing discussions at Doubletree Hotel

7:00 Dinner with Talk by Ian Anderson on *SNS as a Science Facility*

8:30 Return to Comfort Inn

Wednesday, July 13

- 7:30 a.m. Depart Comfort Inn via bus
- 8:00 Coffee
- 8:30 Herbert A. Hauptman, Hauptman-Woodward Medical Research Institute  
*"Neutrons break the low resolution barrier to direct methods"*
- 9:00 B.C. Wang, University of Georgia  
*"If You Build It "We" Will Come: Past Experiences and Predictions"*
- 9:30 Gerald Stubbs, Vanderbilt University  
*"Fiber diffraction in biology: new opportunities from neutron scattering"*
- 10:00 Jenny Glusker, Fox Chase Cancer Center  
*"Time-of-flight neutron diffraction as an aid to elucidating enzyme mechanisms: D-xylose isomerase."*
- 10:30 Coffee
- 11:00 Andrew Mesecar, University of Illinois at Chicago  
*"The future of macromolecular neutron crystallography in enzymology & drug discovery"*
- 11:15 Dean Myles, ORNL  
*"Infrastructure at ORNL"*
- 11:30 Panel discussions  
Scientific direction, infrastructure & funding strategies for MaNDi
- 12:30-1:30 pm Lunch and continuing discussions
- 1:30 -3:30 Full Instrument Development Team session
- 3:30 Depart ORNL