

The Cairns ICMRBS SAXS-SANS-NMR Workshop

Combining Small-Angle X-ray and Neutron Scattering with Biomolecular NMR

Organizers:

Terry Mulhern and Yun-Xing Wang

Lecturers:

Ad Bax (NIDDK, NIH)

Andrew Byrd (NCI, NIH)

Charles Schwieters (DCIT, NIH, USA)

Xiaobing Zuo (NCI, NIH, USA)

Alex Grishaev (NIDDK, NIH, USA)

Andrew Whitten (Univ. of Queensland, Australia)

Yun-Xing Wang (NCI, NIH, USA)

Venue Location: the Sebel Hotel, Cairns

Time and Date: 9:00 AM - 5:00 PM, Saturday, August 21, 2010

Registration: Please register with the ICMRBS conference first at the web site:

http://www.icmrbs2010.org/index.php?option=com_content&task=view&id=41&Itemid=67

This is an intensive tutorial workshop. The topics covered (listed on the next page) range from the fundamental principles of scattering phenomena to the practical applications of scattering experiments with a focus on the combined use of scattering and solution NMR. The course is modeled on the 1st NIH Workshop on Small Angle X-ray Scattering and its Application in Biological Studies, which was held in Oct 28, 2009 in NCI-Frederick, NIH (<https://ccrod.cancer.gov/confluence/display/public/SBL+Workshop+2009>).

The workshop will be sponsored by NCI (USA), The Australian Synchrotron and Anton Paar (GmbH). Registration is required (\$25), and will be accessible as part of the ICMRBS registration process. The lecture notes will be available for download prior to the workshop. Please note, the workshop is on the day before the main ICMRBS meeting commences and the attendees are responsible for arranging their additional lodging.

Deadline for applications: June 1, 2010. Applications after this date can be considered only if space still available. Strong applications from overseas participants may be confirmed long before the deadline to help with visa and flight ticket arrangements.

We are looking forward to seeing you in Cairns,

Terry Mulhern and Yun-Xing Wang

The tentative topics are listed in the next page.

Part One: Fundamentals and Experimental Aspects of Small Angle X-ray Scattering

1. Fundamentals of x-ray scattering
 - a. Scattering phenomenon and interference
 - b. From crystal and fiber diffraction to solution scattering
 - c. Form factor and object shapes
 - d. X-ray scattering contrast
 - e. Theory on solution scattering calculations
2. Experimental Aspects of Scattering
 - a. Instruments
 - i. X-ray generators (bench-top, synchrotron) and detectors
 - ii. Synchrotron-based setups
 - b. Data acquisition
 - i. Synchrotron based SAXS experiments
 - ii. Bench-top x-ray source based SAXS experiments
 - iii. Neutron scattering
 - c. Scattering sample preparations
3. Data Processing
 - a. 2D-> 1D data conversion
 - b. Background subtraction
 - c. Data quality evaluation

Part Two: Data Interpretation and Applications in Structural Biology

1. X-ray scattering profile and embedded information
 - a. d-spacing / resolution
 - b. Hierarchical structural information
 - c. SAXS vs. WAXS
 - d. Guinier plot & radius of gyration
 - e. Molecular weight
 - f. Porod's law & Porod invariant
 - g. Pair distance distribution function

2. Statistical validation of structural models
 - a. Molecular envelope and shape
 - b. Low-resolution model/shape reconstruction
 - c. Molecular conformation and flexibility
 - d. Contrast variation and matching (SAXS and SANS)
3. SAXS in combination with other techniques for high resolution structure determination and conformational ensemble optimization
 - a. Single-structure refinement with NMR and SAXS data using Xplor-NIH
 - b. Ensemble refinement using SAXS and Xplor-NIH
 - c. Using SAXS to determine global structures of complexes
 - d. Combined use of NMR data and SAXS for structure determination of large RNAs in solution