The Cairns SAXS-SANS-NMR Workshop -- Combining Small-Angle X-ray and Neutron Scattering with Biomolecular NMR - August 21, 2010

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Open Remarks (Wang)

Part One: Fundamentals and Experimental Aspects of Small Angle X-ray Scattering (Zuo and Grishaeve)

1. Fundamentals of solution x-ray scattering (Zuo)

   A. General aspects of x-ray scattering
      - History
      - Why x-ray scattering
      - Study scope
      - X-ray interference pattern
      - Solution x-ray scattering experiments

   B. Physics of X-ray Scattering
      - Scattering and interference phenomena
      - Momentum transfer and phase change
      - X-ray form factor and structure factor

   C. Solution x-ray scattering calculations from atomic coordinates
      - Solvent contribution and x-ray contrast
      - Debye equation
      - Fast calculation methods

2. Experimental Aspects of Solution Scattering (Grishaev)
      - Instruments (X-ray generators and detectors; exp. setups)
      - Data Acquisition (Synchrotron and bench-top based SAXS exp)
      - Scattering sample preparation

3. Data Processing (Grishaev)
      - 2D-> 1D data conversion
      - Background subtraction
      - Data quality evaluation

Part Two: Data Interpretation and Applications in Structural Biology (Zuo and Grishaev)

1. X-ray scattering profile and embedded structural information (Zuo)
      - d-spacing / resolution
      - Hierarchical structural information

- SAXS vs. WAXS
- Guinier plot & radius of gyration
- Molecular weight determination
- Porod's law, Porod invariant and Porod volume
- Kratky plot
- Pair distance distribution function (PDDF) and PDDF calculations

2. Structural analysis from SAXS data (Grishaev)
- Structure-data relationship
- Ab initio low-resolution model/shape reconstruction form SAXS data
- Multi-subunit systems: rigid body refinement against SAXS data
- Flexible and unfolded systems
- Multi-component systems, micelle-embedded proteins

Part Three: Neutron scattering (Whitten)

1. Neutron instrumentation (highlight differences to neutron scattering)
2. Theory of neutron scattering Comparison of X-ray and neutron scattering (how is the information different and   how is it similar)
3. Contrast and contrast variation (how contrast is achieved, how it can be exploited for biomolecular complexes)
4. SANS experiment design (concentration requirements, choice of contrast points,   deuteration levels)
5. Data collection and processing (normalisation, incoherent scattering, smearing effects)
6. Analysis of SANS data (stuhrmann plots etc, modelling)
7. Discussion of published examples of contrast variation

Part Four: Refinement of Structures restrained by SAXS and NMR restraints (Schwieters)

1. Computing SAXS/SANS curves during a structure calculation
- approximate calculation of I(q)
- calculation of the bound-solvent contribution
- determination of solvent parameters
2. Protocol strategies for SAXS/SANS structure determination
3. Overview of elements of an Xplor-NIH script
4. Examples
- refinement of NMR structures – use of SANS with the protein L11
- "docking" (with covalent bond) – structure of EI dimer from SAXS and RDCs
- characterization of hetereogeneity of DNA using NMR and SAXS data.
5. Stand-alone tools for computation of SAXS/SANS curves given one or more structures.