Diffraction structural biology – introductory overview

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This issue of *Acta Crystallographica Section D* presents articles submitted in the context of the 5th International Symposium on Diffraction Structural Biology (ISDSB) 2016. The ISDSB series of symposia was initiated in 2003 by the Japan Society for the Promotion of Science (JSPS) and specifically by the University–Industry Cooperative Research Committee (#169) chaired by Professor Noriyoshi Sakabe. The fifth conference, the second outside of Japan, was held in Knoxville, Tennessee, USA, close to the Oak Ridge National Laboratory (ORNL) neutron user facilities, the High Flux Isotope Reactor (HFIR) and Spallation Neutron Source (SNS), on 7–10 August 2016.

The original purpose of this series of symposia was to bring together structural biology researchers using X-ray, neutron and electron diffraction techniques, and to facilitate interactions between academic and industrial research. Over the years the scope of the series has grown to include a wide variety of additional techniques used to study biological structure and dynamics including various microscopies, spectroscopies and computational methods. In some respects, the motivation for the ISDSB series anticipates the recent growth in integrative structural biology approaches. The evolution of the programme of the symposia has reflected the broader range of complementary techniques becoming available, the constant need for improved communication and collaboration across disciplines, and the growing recognition that more advanced mathematical and computational techniques are needed to integrate experimental data from a growing number of different experimental techniques as they are applied to address increasingly complex biological problems and emerging challenges.

At ISDSB 2016, the discoveries in structural biology using X-ray, neutron and electron diffraction, and complementary techniques such as small-angle scattering, nuclear magnetic resonance spectroscopy, electron microscopy and advanced computational approaches were reported. A total of 89 participants, with many young scientists and PhD students, from five countries took part. The speakers included four plenary lecturers (Jack Johnson, Michael Crowley, Peter Moody and Greg Hura), 31 invited session speakers and 30 poster presentations. Scientific session topics included Bioenergy, Drug Design, Enzyme Mechanism and Allostery, Macromolecular Complexes, Membranes and Membrane Proteins, New Instruments and Methods, and Sources and Facilities. A dinner seminar was held on prospects for biology at the SNS Second Target Station (STS), which represents a next-generation neutron scattering user facility that will provide new capabilities for structural biology.

A new feature of this ISDSB was two preceding one-day satellite workshops focused on introductory tutorials. The construction of MaNDi and IMAGINE neutron protein crystallography beamlines at ORNL provide new opportunities for neutron macromolecular crystallography to become a more accessible structural tool for enzymology and structural biology for understanding enzyme mechanisms and ligand binding. In the Computational Tools for Neutron Protein Crystallography workshop, organized by Leighton Coates, current and future neutron macromolecular crystallography users were introduced to the new beamlines, and provided lectures and practical instruction on neutron structure refinement using *PHENIX*. In the Small Angle Neutron Scattering workshop, organized by Shuo Qian, a combination of lectures and tutorials was used to introduce basic techniques and related computational tools to integrate molecular simulations with small-angle scattering data. Both workshops were well attended and highly appreciated, especially by early career scientists.

The symposium further included tours of the two nearby neutron user facilities and the TITAN supercomputing operated by ORNL.

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