Crystallography in the news

July 1, 2013. There’s not much difference between what makes a man and what makes his beer—at least at the molecular level—according to a new study led by Professor John Schwabe at the University of Leicester. They discovered that a family of complexes that switch off gene expression is regulated by small signaling molecules called inositol phosphates.

July 13, 2013. UK scientists plan to build a chromosome for the world’s first synthetic yeast. Once all parts of the genome are complete, scientists can design new strains of the yeast Saccharomyces cerevisiae to make products including chemicals, vaccines and biofuels. Minister for Universities and Science David Willetts announced nearly £1M in funding for the UK arm of an international consortium attempting to build a synthetic version of the yeast genome by 2017.

July 16, 2013. A group of researchers led by Witold K. Surewicz of Case Western Reserve University studying the crystal structure of a snippet of the human prion has found clues to how oligomers of the proteins could coax others to misfold.

July 16, 2013. Chemists of Radboud Univ. Nijmegen have found that a uniquely shaped enzyme that has never been seen before in biology is real: two interlocked ring structures, known as catenanes. This locked protein structure is maintained via weak non-covalent interactions.

July 17, 2013. An international team led by scientists at The Scripps Research Institute (TSRI) has determined and analyzed the three-dimensional atomic structure of the human glucagon receptor. The receptor, found mainly on liver and kidney cells, helps regulate glucose levels in the bloodstream and is the target of potential therapeutic agents for type 2 diabetes.

July 25, 2013. Google celebrated the life and legacy of Rosalind Franklin on the anniversary of her 93rd birthday with a special doodle on their search engine homepages. Born in 1920 in London, Franklin earned a Ph.D. in physical chemistry from Cambridge University. She learned crystallography and X-ray diffraction, techniques that she applied to DNA fibers.

Product spotlight: HKL-3000R

HKL-3000R represents a new approach in crystallographic software that integrates data collection, data reduction, phasing and model building into a single package. This approach significantly accelerates the process of structure determination and on average minimizes the number of crystals, data sets and time required for structure solution.

- HKL-3000R controls the data collection instrument.
- Data collection strategy calculation for single and multiple axes goniometers.
- Raw image data reduction and analysis by industry standard HKL-2000.
- Structure solution pipeline uses industry standard software packages (CCP4, shelx, Arp/Warp, COOT, SOLVE/RESOLVE, etc.).
- Communication with standard databases (PDB, SwissProt).

Ask for more information.
Upcoming Event

The 71st Annual Pittsburgh Diffraction Conference will be being held in Buffalo, NY at the Hauptman-Woodward Medical Research Institute from the evening of the 18th of September to the afternoon of the 20th. Preliminary details are now available. Program topics include crystalization approaches for recalcitrant proteins and protein complexes, structural biology from an industrial perspective, macromolecular design and DNA nanotechnology, technology developments for diffraction methods and a small molecule diffraction session. Meeting registration and discount hotel reservation deadlines are the 16th and 21st of August. For more information contact the organizers.

Lab in the spotlight: Wolberger lab

Professor Cynthia Wolberger
Department of Biophysics and Biophysical Chemistry
Johns Hopkins Univ. School of Medicine, Baltimore, MD
Investigator, HHMI

The Wolberger lab is interested in the structural and mechanistic basis for transcriptional regulation and ubiquitin signaling. Protein function is dynamically regulated in the cell by the attachment and subsequent removal of covalent posttranslational modifications. The modifications can be small, as in the case of acetylation, or quite large, as in the case of a polyubiquitin chain. Acetylation and ubiquitination both occur in chromatin, the nucleoprotein complex into which eukaryotic DNA is packaged.

Acetylation of the histone proteins in chromatin is associated with activation of transcription, whereas ubiquitination can be either an activating or a repressive mark, depending on which histone protein is modified. Ubiquitination of chromatin also plays a role in the response to DNA double-strand breaks, helping to recruit proteins that are required for DNA repair. The Wolberger group is interested in the molecular basis for these events, which ensure the integrity and expression of the genome. The lab uses X-ray crystallography, enzymology, and a variety of biophysical tools to gain insights into the mechanisms underlying these essential cellular processes.

Useful links: CHAPTER TWENTY-NINE


Selected recent crystallographic papers


Last Month’s Survey Results

When was the last time you backed up your data?

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Science Video

The Structures of Life

The NIH/NIGMS video reveals how structural biology provides insight into health and disease and is useful in developing new medications.

Crystallographers in the News

The Protein Society Meeting in Boston

Professor Sheena Radford of the University of Leeds received the Carl Brändén Award, which honors a protein scientist who has made significant contributions to the science and/or education. Rigaku sponsors the award each year. Two crystallographers


Crytallographers reports are the backbone of Acta Cryst. F, but do they have any spine? Newman, Janet; Burton, Denis R.; Caria, Sofia; Desbois, Sebastien; Gee, Christine L.; Fazio, Vincent J.; Kvansakul, Marc; Marshall, Bevan; Mills, Grant; Richter, Viviane; Seabrook, Shane A.; Wu, Mingbo; Peat, Thomas S. Acta Crystallographica: Section F. Jul2013, Vol. 69 Issue 7, p712-718. 7p. http://dx.doi.org/10.1107/S1744309113013152.

Book review:

Visualizing the Invisible

By Peter B. Moore


This book is devoted to using scattering of waves by physical objects to generate images of those objects. It is by no means complete, but covers just about everything relevant to structural biology. The scales measured range from a few microns (cells) down to an Ångström or so (molecules).

Many years ago, I listened to a dynamic lecture by Peter Moore at a conference at CCNY. I was riveted by the presentation of the work done at Yale on the ribosome. The preface indicates that this book was created from the course the author teaches on instrumentation at Yale. As I read, I tried to imagine Professor Moore as he lectured at CCNY. I thought this would capture the essence of the course itself and give a better picture of the use of the book as a textbook. I think Moore accomplished his goal.

There are a few typos in this first edition, but I did not find any mistakes in the equations—and there are a lot of equations. Some are derived and some are merely presented as fact, but ample information is provided to derive results on one’s own if so inclined. The end of each chapter contains a problem set and a series of appendices for those interested in detailed derivations of some of the concepts.

The book is divided into five parts. Part One covers the basics of scattering from electrons, atoms, and then molecules. The concept of how the Fourier transform applies to scattering is introduced in Chapter 2. The final chapter of the first part covers the process of scattering by solid materials and brings forth the concepts of phase, velocity changes, absorption and dispersion. Finally, that particles can scatter like waves is introduced.

Part Two covers crystallography and provides a good description of the basics of
shared the Dorothy Hodgkin Award this year, Professor Chris Hill of the University of Utah and Professor Cynthia Wolberger of Johns Hopkins University Medical Center.

Part Two covers crystallography and provides a good description of the basics of lattices and the resulting diffraction pattern. Once diffraction is described, the author covers the various solutions to the phase problem as applied to macromolecular crystallography. Chapter 7 provides a good description of electron density maps and their interpretation. Part Three covers scattering from materials that are not crystalline. Two topics are treated in detail: coherent diffraction imaging and small angle scattering, with the latter receiving the most attention.

Part Four is devoted to the light microscope. The author covers the basics of lenses and how they form images. Next, Moore describes how light microscopes work and their limitations. This provides a natural segue into the higher resolution electron microscope, which is covered in Part Five. Here the author covers how electron lenses work, how electron microscopes create images from the hardware itself, and how refinements from downstream processing improve the images. The very last chapter covers three dimensional reconstruction and electron diffraction.

Here is a quick overview of my summer reading list:

For entertainment I recommend Joyland by Stephen King and NOS4A2 by Joe Hill, King’s son. I picked up Bad Monkey by Carl Hiaasen for some laughs and Inferno by Dan Brown. Jeanette says the latter wasn’t as entertaining as the author’s previous books so I have put off starting it. Jared Diamond’s latest The World Until Yesterday was enlightening and suggests we might all be a little happier and little healthier in a simpler world. I have Cooked by Michael Pollan and Plutocrats by Chrystia Freeland in my to-read stack. I really enjoyed Our Inner Ape by Frans De Waal a few years ago, so I picked up The Bonobo and the Atheist when I heard his interview on SciFri. So far, it is quite interesting. I am also working on Antifragile by Nicholas Taleb, author of The Black Swan, a book I reviewed here a couple of years ago.

Joseph D. Ferrara
Chief Science Officer

Rigaku Corporation
e-mail: rinttyo@rigaku.co.jp
Tel: +(81) 3-3479-0618

Rigaku Americas
e-mail: info@Rigaku.com
Tel: (281) 362-2300