Crystallography Times

Protein Crystallography Newsletter
Volume 1, No. 7, August 2009

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Continuing Education Webinar

Small Angle X-ray Scattering Analysis Techniques for Proteins
Presenter: Tom McNulty
September 30th at 3:30 PM EDT
(19:30 GMT)

FR-E+ DW SuperBright dual wavelength rotating anode X-ray generator.

Crystallography in the news

August 20, 2009. A team of researchers, lead by Prof. Jamie Cate at UC Berkeley, have for the first time captured elusive nanoscale movements of ribosomes at work, shedding light on how these cellular factories take in genetic instructions and amino acids to churn out proteins.

August 19, 2009. Case Western Reserve University School of Medicine has received a $4 million grant from the National Institute of Biomedical Imaging and Bioengineering, a division of the National Institutes of Health (NIH), to fund the Case Center for Synchrotron Biosciences.

August 17, 2009. Researchers at the University of Virginia Health System, led by Prof. Wladek Minor, determined the structure of the enzyme protein BA2930, which is produced by the bacteria responsible for anthrax.

August 13, 2009. Presearchers at the European Molecular Biology Laboratory (EMBL) in Heidelberg, Germany, have identified a whole family of proteins capable of a direct response to the activation of PARP1 by DNA damage.

August 3, 2009. Led by crystallographer Eric Gouaux of the Vollum Institute at Oregon Health & Science University, a team of researchers solved the structure of an ion channel membrane protein in the closed conformation.

Synchrotron quality data in your home laboratory

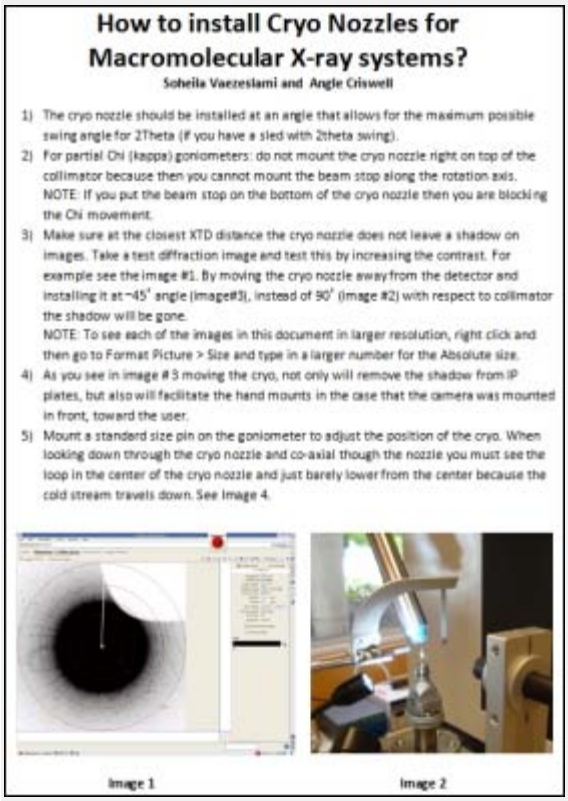
When you need to collect data immediately, the Rigaku FR-E+ SuperBright™ X-ray generator delivers the flux of a 2nd generation beam line in your home lab, allowing you to examine crystals at home that previously required a trip to the synchrotron. Extremely high flux in a small beam enables screening of poor crystals, where no diffraction would be observed with a conventional X-ray generator or sealed tube source. The FR-E+ can collect full data sets on difficult samples and solve previously intractable structures.

Why wait for beam time at the synchrotron? The unique anode design, combined with a patented 70 micron anode focal spot, provides unrivaled intensities. Owners routinely collect high resolution data on their FR-E+ and have often reported collecting better data on their FR-E+ than they have from a synchrotron beamline. One customer even told us that the FR-E+ has "changed the way we do crystallography". As the only commercially available rotating anode X-ray generator with a dual wavelength (DW) option, FR-E+ DW users employ longer wavelengths (like Cr or Co) to collect phasing information for rapid *de novo* structure determinations. For maximum performance, a VariMax optic has been designed for each available wavelength to provide a beam with ideal properties for unparalleled performance.

Request a copy of the FR-E+ SuperBright brochure.

SAXS analysis techniques for proteins

Rigaku Life Sciences Webinar Series continues on September 30th. In this webinar presented by Tom McNulty, we will explore the application of small angle X-ray scattering (SAXS) techniques to study non-crystalline macromolecular samples in



How to install Cryo Nozzles for Macromolecular X-ray systems?

Soheila Vaezeslami and Angie Criswell

1) The cryo nozzle should be installed at an angle that allows for the maximum possible swing angle for 2Theta (if you have a sled with 2theta swing).
2) For partial Chi (kappa) goniometers: do not mount the cryo nozzle right on top of the collimator because then you cannot mount the beam stop along the rotation axis. NOTE: If you put the beam stop on the bottom of the cryo nozzle then you are blocking the Chi movement.
3) Make sure at the closest XTD distance the cryo nozzle does not leave a shadow on images. Take a test diffraction image and test this by increasing the contrast. For example see the image #1. By moving the cryo nozzle away from the detector and installing it at ~45° angle (image#3), instead of 90° (image #2) with respect to collimator the shadow will be gone.
NOTE: To see each of the images in this document in larger resolution, right click and then go to Format Picture > Size and type in a larger number for the Absolute size.
4) As you see in image # 3 moving the cryo, not only will remove the shadow from IP plates, but also will facilitate the hand mounts in the case that the camera was mounted in front, toward the user.
5) Mount a standard size pin on the goniometer to adjust the position of the cryo. When looking down through the cryo nozzle and co-axial though the nozzle you must see the loop in the center of the cryo nozzle and just barely lower from the center because the cold stream travels down. See Image 4.

Dr. Garib Murshudov of the University of York presenting a paper about BALBES at ecm25 (top) and ecm25 participants enjoying the street life of Istanbul (bottom).

solution, including proteins, DNA and RNA, viruses and biological fibers.

Useful links for crystallography

BALBES - a system for solving protein structures from molecular replacement. A unique feature is that it contains a specifically designed internal database tailored from the PDB. All entries of the PDB have been analyzed according to sequence identities and three dimensional similarity; only non-redundant sets of protein structure are stored with entries clustered into hierarchical trees based on sequence alignment. The internal database is updated from the PDB on a monthly basis. BALBES can be downloaded or you can run it on the BALBES server. Long, F., Vagin, A., Young, P., Murshudov, G. N. " BALBES: a molecular replacement pipeline" *Acta Cryst*, **D64**; 125-134 (2008).

Selected recent crystallographic papers

BioXTAS RAW, a software program for high-throughput automated small-angle X-ray scattering data reduction and preliminary analysis. S. Nielsen, K. Toft, D. Snakenborg, M. Jeppesen, J. Jacobsen, B. Vestergaard, J. Kutter and L. Arleth. *J. Appl. Cryst.* **42** (2009).

Characterization of gadolinium complexes for SAD phasing in macromolecular crystallography: application to CbpF. R. Molina, M. Stelter, R. Kahn and J. Hermoso. *Acta Cryst.* **D65**, 823-831 (2009).

Cross-linking of protein crystals as an aid in the generation of binary protein-ligand crystal complexes, exemplified by the human PDE10a-papaverine structure. O. Andersen, D. Sch?nfeld, I. Toogood-Johnson, B. Felicetti, C. Albrecht, T. Fryatt, M. Whittaker, D. Hallett and J. Barker. *Acta Cryst.* **D65**, 872-874 (2009).

Handling cell-parameter errors in crystallographic data. J. Haestier. *J. Appl. Cryst.* **42** (2009).

Simulation of small-angle X-ray scattering from thylakoid membranes. J. Kirkensgaard, J. Holm, J. Larsen and D. Posselt. *J. Appl. Cryst.* **42**, 649-659 (2009).

Slow cooling of protein crystals. M. Warkentin and R. Thorne. *J. Appl. Cryst.* **42** (2009).

To scavenge or not to scavenge: that is the question. E. Nowak, A. Brzuszkiewicz, M. Dauter, Z. Dauter and G. Rosenbaum. *Acta Cryst.* **D65**, 1004-1006 (2009).

Book review:

The End of Overeating:
Taking Control of the Insatiable American Appetite

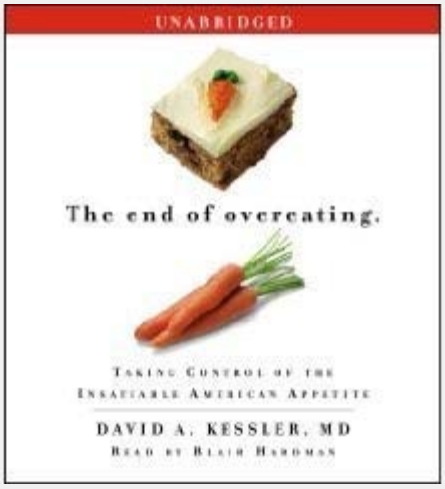
by David Kessler

I came across this book just before hitting the road for the summer conferences. The author was the commissioner of the FDA under Bush (41) and Clinton. What I found most interesting about *The End of Overeating* is how well the author mapped out my own personal journey with the problem of overeating.

Basically, this book describes how the American food industry has found that a combination of fat, sugar and salt in the right proportions is nearly as addictive to all mammals as cocaine. If you like Chili's you better not read the book. By mixing these three natural ingredients in ways that do not occur in nature, Americans have created a diet that is unsustainable and addictive. Furthermore, Kessler contrasts the American style of eating, often in a car, to the French and Japanese, where meals are based on quality food, presentation and often lengthy affairs. Of course, the portions are also usually somewhat smaller in these foreign countries.

What finally made me decide to recommend this book is that I was at a conference with

SURVEY QUESTION What is your typical crystal size for data collection at home?	
◉	25-50 µm
○	50-100 µm
○	100-200 µm
○	> 200 µm
Submit	
Use this link if the form above doesn't work.	



The End of Overeating: How to Curb the Insatiable American Appetite by David Kessler.

nearly unlimited food, breakfast buffet, pastries at mid-morning, lunch buffet, afternoon snacks, dinner buffet and late night snacks. At lunch a young, German student asked me "do Americans always eat like this?" All one had to do was look around at the other students and visitors to know the answer was that the majority do. Ironically, by the end of the week the German student had adopted our bad habits, several plates piled with food and a muffin at every break. In the end the author suggests that - unlike other addictions - food is one we cannot do without. In order to deal with it, we have to realize food is not our friend. That is not to say we can't we enjoy a piece of cake once in a while ... but that is just it, once in a while.

For further reading:

The Big Oyster: History on the Half Shell by Mark Kurlansky. This book provides a history of New York City from the point of its estuaries oyster beds. An interesting side story is how the abundance of cheap food became the American way.

In Defense of Food by Michael Pollan. A great book that first defines "food" and some simple rules for finding "food".

I promise to review a book relevant to structural biology next month.

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