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**Continuing Education Webinar**

**Scientific inquiry, inference and critical reasoning in the macromolecular crystallography curriculum**

**Presenter: Dr. Bernhard Rupp**

**October 21, 2010**

1PM EDT (18:00 GMT)

Dr. Rupp will expand on his recent *Journal of Applied Crystallography* article that discusses higher education curricula in the context of scientific analysis. Bernhard analyzes recent cases of high profile structure retractions and argues that “With the great power of modern crystallography comes great responsibility for its appropriate use.”

**Macromolecular Crystallography Training Class**

**March 23-25, 2011**

**October 26-28, 2011**

The Woodlands, Texas

This class is tailored towards the needs of macromolecular crystallographers and their staff. Course format will be a series of short lectures on theory followed by hands-on activities with detectors, X-ray generators, and software. Class will also feature a training session on processing data with HKL.

**Crystallography in the news**

**September 28, 2010.** Collaboration between Trinity Dublin College (TDC) and Oxford University used X-ray crystallography to discover how two proteins interact to guide connections between brain cells. As described by Dr. Kevin Mitchell, a senior lecturer at the Smurfit Institute of Genetics and the Institute of Neuroscience at TCD, the research examined the interaction between a “semaphorin” protein (known as Sema6A) and another protein, PlexinA2.

**September 27, 2010.** The National Institutes of Health (NIH) has awarded a prestigious EUREKA award to Prof. Robert Woods, at the University of Georgia Complex Carbohydrate Research Center, to develop a new method (diagnostic antibody specificity) for understanding how antibodies interact with large molecules known as glycans that are a major component of all cell surfaces. The EUREKA award, given to support “Exceptional, Unconventional Research Enabling Knowledge Acceleration,” will provide Woods with approximately $200,000 per year for four years.

**September 24, 2010.** Prof. Edward Yu and his colleagues at Iowa State University, in conjunction with Ames Laboratory researchers, have discovered the X-ray crystal structures of pumps that remove heavy metal toxins from bacteria, making them resistant to antibiotics. What these pumps do is “recognize and actively export these substances out of bacterial cells, thereby allowing the bugs to survive in extremely toxic conditions.”

**September 23, 2010.** The University of Arkansas Center for Protein Structure and Function, which includes the X-ray crystallography facility headed by Prof. Joshua Sakon, will receive more than $5.4 million over the next five years from the National Institutes of Health (NIH) to continue biomedical research in cancer, heart disease, osteoporosis, flu and other diseases and conditions.

**September 20, 2010.** Scientists at Rutgers, led by Prof. Eddy Arnold, employed X-ray crystallography to discover how HIV-1, the virus that causes AIDS, resists AZT, a drug widely used to treat the deadly disease. The results describe in atomic detail how the AZT-resistance mutations allow reverse transcriptase to recruit ATP to remove the AZT.

**September 16, 2010.** The Donald Danforth Plant Science Center in St. Louis, Missouri (USA) will be hosting its 12th annual Fall Symposium from September 29th to October 1st, 2010. This year’s symposium includes a wide range of topics with a focus, in part, on using X-ray crystallography to elucidate important biological problems, including virus structures, drug discovery, plant hormone receptors, photosynthetic complexes, engineering of plant metabolic pathways, membrane proteins, circadian rhythms, and DNA repair.

**September 6, 2010.** In two closely related studies, two teams of Scripps Research Institute scientists, led by Professors Wendy Havran and Ian Wilson, have discovered the underlying mechanisms that activate a type of immune cell in the skin and other organs. Together, the new research sheds light on γd (“gamma delta”) T cells, an immune cell found within epithelial tissues—the thin layer of cells that makes up the outermost layer of skin and organs like the intestines and lungs. The research identified a junctional adhesion molecule, JAML, as a new costimulatory receptor for γd T cells that binds to the ligand CAR (coxackie and adenovirus receptor) expressed on keratinocytes.
Rigaku Desktop Alchemist™ can make optimization screens directly into Linbro and Nextal plates, in addition to Deep Well Blocks for 96-well SBS plate preparation.

From the Waksman lab at the Institute of Structural Molecular Biology, Birkbeck and University College London: structure of the translocator domain of the Hia trimeric autotransporter.

Lab spotlight: Waksman Lab @ Birkbeck College

Introducing the "Quick Puck Loader"

The Quick Puck Loader, invented at Structural Genomics Consortium at Toronto, is designed to load crystal mounted pins into the Rigaku style puck quickly while
reducing the potential for mis-seating. This tool was designed to be used with both a Rigaku Puck and Puck Tong.

Just load pins directly into the Quick Puck Loader, and then fit the Rigaku Puck right on top... and use Puck tongs to firmly grasp and flip. Pins are perfectly seated. No more losing crystals. The device is currently used in labs from University Health Network (Canada), York University and the Structural Genomics Consortium.

The Quick Puck Loader is made of durable aluminum and comes with a 1-year warranty on the part. Colors available include red, blue and gold. Mixed colors are also available.

View more information on the new Quick Puck Loader.

Useful links for crystallography

ACMI - Automatic Crystallographic Map Interpreter uses a probabilistic approach, known as a Markov field, to automate tracing of the protein backbone in the electron density image. Testing of this method has shown that an accurate backbone model could be traced even with lower-resolution and poor-quality density maps. Principal author: George Phillips, University of Wisconsin.

Selected recent crystallographic papers


Crystal structure of a metal ion-bound oxoiron(IV) complex and implications for biological electron transfer. Fukuzumi, Shunichi; Morimoto, Yuma; Kotani, Hiroaki; Naumov, Pance; Yong-Min Lee; Wonwoo Nam. Nature Chemistry,


**Book reviews:**

*Cooking for Geeks*


I heard an interview with Mr. Potter on NPR's Science Friday a few weeks ago and immediately bought a copy of this book for myself. The author is a software developer who likes to cook. The book is published by O'Reilly Media, the company that has brought out so many software cookbooks. The "Geeks" in the title are software developers, but let's face it, most of us crystallographers are geeks too and a lot of us like to cook. My last argument for reviewing *Cooking for Geeks* is that cooking is really just applied chemistry.

The book pays due homage to *Mastering the Art of French Cooking* by Julia Child and *On Food and Cooking* by Harold McGee. The author treats cooking like running a program. Potter starts with a discussion on initializing your kitchen and calibrating your tools. Much attention is paid to heat and time and the interchangeability (to a degree) of the two. His favorite tool is an infrared thermometer for temperature calibration but he also describes the use of sugar to calibrate ovens to 365°F.

There are some useful discussions about the tasty products of chemical reactions that occur during the cooking process: Maillard reactions, caramelization and protein denaturation. Although the description of the last reaction was a little weak and the description of using alcohol to make aroma molecules lighter is obviously wrong, I found the rest enlightening. For example, I really liked the idea of replacing the glass window in my oven with Pyroceram® to make a proper 850°F pizza oven. All I have to do is convince my wife nothing will happen to the house.

The other "hack" I am interested in trying is sous vide (under vacuum) cooking. In this method the food item is placed in a sealed plastic bag brought to an exact temperature, 140°F for example, in a water bath and allowed to reach thermal equilibrium. The results are supposed to produce delicious and tender meat and fish. I am sure there are enough low temp controllers and pumps around here that I can cobble something together in a
few hours. Speaking of fish, did you know that if you brine salmon for 20 minutes in 5-10% saline solution and rinse, the albumin will set and won’t leach out during grilling? This works for mahi-mahi too.

Another interesting trick is to create a recipe by averaging a number of existing recipes for the desired product. However, I am sure it is the outliers that make for the interesting results. Throughout the book you will find sidebars with interviews from experts and recipes that demonstrate the topics being covered.

Joseph D. Ferrara, Ph.D.