Crystallography Times

Rigaku

Protein Crystallography Newsletter

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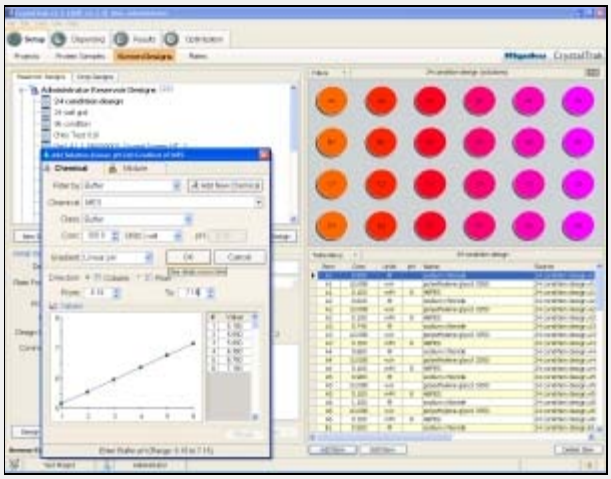
In this issue:

Continuing Education Webinar

How to collect exceptional diffraction data from your crystals

Presenter: Dr. Angela Criswell

June 24 at 12:00 PM EDT (16:00 GMT)



Crystallography in the news

May 21, 2009. Long-awaited structure of AADase solved: discovery heralds new approaches to protein-engineered biofuels.

May 22, 2009. A research team, led by Che Alex Ma, an assistant research fellow at Academia Sinica's Genomics Research Center, has successfully developed a complete three-dimensional model structure of an Escherichia coli *membrane protein*.

May 20, 2009. European biotechnologists unravel life's big cellular factories. Prospects for progress obtaining the structure of important molecular machines involved in critical cellular activities were discussed at a recent meeting co-organised by the EUROCORES programme EuroSCOPE (Science of Protein Production for Functional and Structural Analysis) of the European Science Foundation (ESF).

CrystalTrak™ - automated crystallization software

A complete relational database application for crystallization is now available for all labs as a stand-alone software application: CrystalTrak. Based on an Oracle® platform, the software tracks all of the necessary information used in crystallization trials, such as chemicals, screens, protein samples, images, and annotations. CrystalTrak simplifies the crystallization process by providing tools that enable greatly improved productivity, efficient use of protein samples and the design of reproducable targeted experiments.

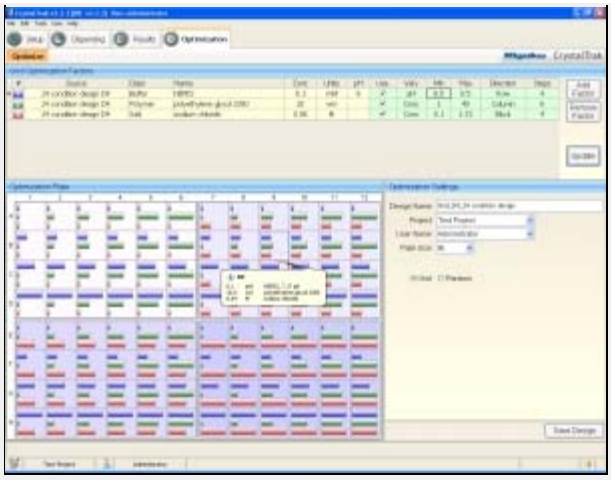
Rigaku CrystalTrak provides simple, graphical tools to easily design coarse and optimization crystallization screens using an extensive library of pre-loaded chemicals and commercially available screens. The built-in database includes information such as solubility, pKa, CAS, aliases and molecular weight for thousands of chemicals used in protein crystallization. pH gradients are automatically calculated using Henderson-Hasselbach interpolation or pH curves may be imported for complex buffer systems.

CrystalTrak automatically generates optimization strategies with a single mouse click, using initial hit conditions to create a grid of similar conditions around an initial hit (or combine multiple hits to create a random sparse matrix of conditions). Based on stock concentrations and buffer pH, all required dispense volumes are automatically calculated, and formatted into a printable recipe, for easy hand setup. CrystalTrak also seamlessly integrates Rigaku crystallization instruments, such as the Alchemist™ II for producing crystallization matrices, the Minstrel™ series imaging systems, for capturing crystallization images, and the Phoenix™ RE for the preparation of crystallization trials, offering labs a complete end-to-end solution for crystallization.

Request a copy of the CrystalTrak brochure.

How to collect exceptional diffraction data

Rigaku Life Sciences Webinar Series continues on June 24th with a discussion of



CrystalTrak gradient screen (top) and optimization (bottom). Click through for larger image.

Summer Travel Bursary Application

Rigaku Americas Corporation will award summer travel bursaries (to be used for travel to a scientific conference) in the amount of U.S. $500 each to the five (5) post-doctoral fellows who provide the most compelling explanation as to how they intend to pursue a career in structural biology.

SURVEY QUESTION What software do you use to process your home lab data?	
( )	HKL 2000
( )	d*Trek
( )	MOSFLM
( )	XDS
( )	DPS
( )	Other
[Submit]	
Use this link if form does not work	

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the diffraction experiment in terms of best practices and providing tools both for identifying diffraction quality samples and for collecting exceptional data. Hosted by Angela Criswell, Ph.D., this complementary continuing education seminar is recommended viewing for students or as a refresher for routine users and their staff.

Useful links for crystallography

Looking for a New Job? - Links to crystallographic jobs around the world, and websites that maintain links to job openings, are indexed on the protein crystallographic portal PXuniverse.

The Global Protein Crystallographic Community - A directory of links to protein crystallographic laboratories around the world is being created. Each entry contains contact information for the PI, a link to the lab website, and photos of the PI, the research group or a structure of particular interest. Labs are being added in a random walk approach; if you would like to have your lab added, please use this submittal form.

50 Years of Protein Structure Determination - An in-depth interactive NIH slideshow, with historical navigation, in Adobe® Flash® format.

Selected recent crystallographic papers

Re-refinement from deposited X-ray data can deliver improved models for most PDB entries. R. P. Joosten, T. Womack, G. Vriend and G. Bricogne. *Acta Cryst.* **D65**, 176-185 (2009).

Nothing about protein structure classification makes sense except in the light of evolution. Ruben E Valas, Song Yang and Philip E Bourne. *Current Opinion in Structural Biology* **19**, 1-6 (2009).

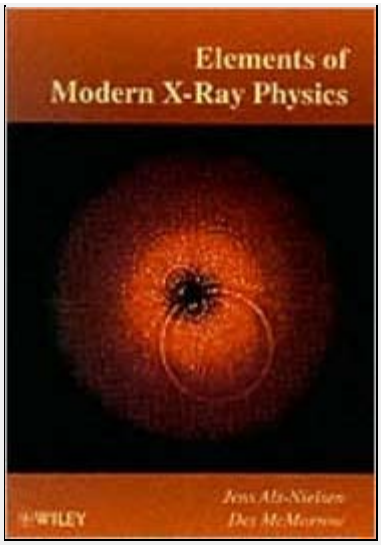
Model-building strategies for low-resolution X-ray crystallographic data. A. M. Karmali, T. L. Blundell and N. Furnham. *Acta Cryst.* **D65**, 121-127 (2009).

Combining solution wide-angle X-ray scattering and crystallography: determination of molecular envelope and heavy-atom sites. Xinguo Honga and Quan Hao. *J. Appl. Cryst.* **42**, 259-264 (2009).

Book review: *Elements of Modern X-ray Physics*

by Jens Als-Nielsen and Des McMorrow

Hendrickson about the difficulties in sorting out resonance scattering for a presentation I had given at an ECM because different authors use different notation



for the same parameters, or worse the same notation for different parameters. Wayne told me he was using "Elements of Modern X-ray Physics" by Jens Als-Nielsen and Des McMorrow for his X-ray diffraction course so I bought a copy. I don't often read textbooks cover to cover, but the book is well written, and worth the time and effort.

The book starts with an excellent introduction to X-ray interactions and sources. Next, refraction and reflection are discussed. I should point out that the text explains clearly the relationship between absorption and f" here, useful for understanding concepts in the last chapter. The next two chapters are devoted to diffraction. The penultimate chapter reviews photoelectron absorption and EXAFS.

The final chapter on resonance scattering is a must read for young macromolecular crystallographers. This chapter provides a lucid explanation of "anomalous scattering", the phase problem, the breakdown of Friedel's law and MAD phasing.

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