

## Crystallography Newsletter

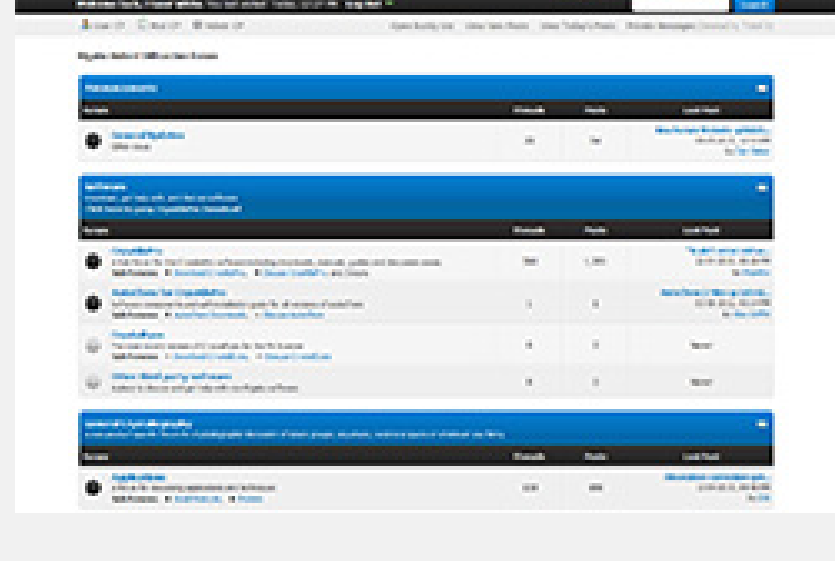
Volume 9, No. 5, May 2017

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### Rigaku Oxford Diffraction invites all users of Rigaku equipment to join us on our X-ray forum



[www.rigakuxrayforum.com](http://www.rigakuxrayforum.com)

Here you can find discussions about software, general crystallography issues and more. It's also the place to download the latest version of Rigaku Oxford Diffraction's CrysAlis<sup>Pro</sup> software for single crystal data processing.

We look forward to seeing you on there soon.

### Rigaku Reagents: Wizard TIME - 96-well block plate



Membrane proteins require detergent solubilization for purification and crystallization. The Wizard TIME, or Total Integral Membrane Protein Extraction, screen consists of 84 different formulations designed identify detergent reagents that will successfully extract a membrane protein from a membrane preparation. Each detergent formulation consists of a detergent at 2% (w/v) concentration, the stabilizing co-detergent cholesterol hemisuccinate and a buffer. One membrane protein target can be screened per kit. For a limited time, try the TIME kit with your membrane preparation at 25% off.

**Wizard TIME promotion: 25% off, expires 06/01/2017. Code: TIME**

Contact [ReagentOrders@Rigaku.com](mailto:ReagentOrders@Rigaku.com)

For more information, visit the [Rigaku Reagents website](#).

### Survey of the month



May 17 SCX Survey

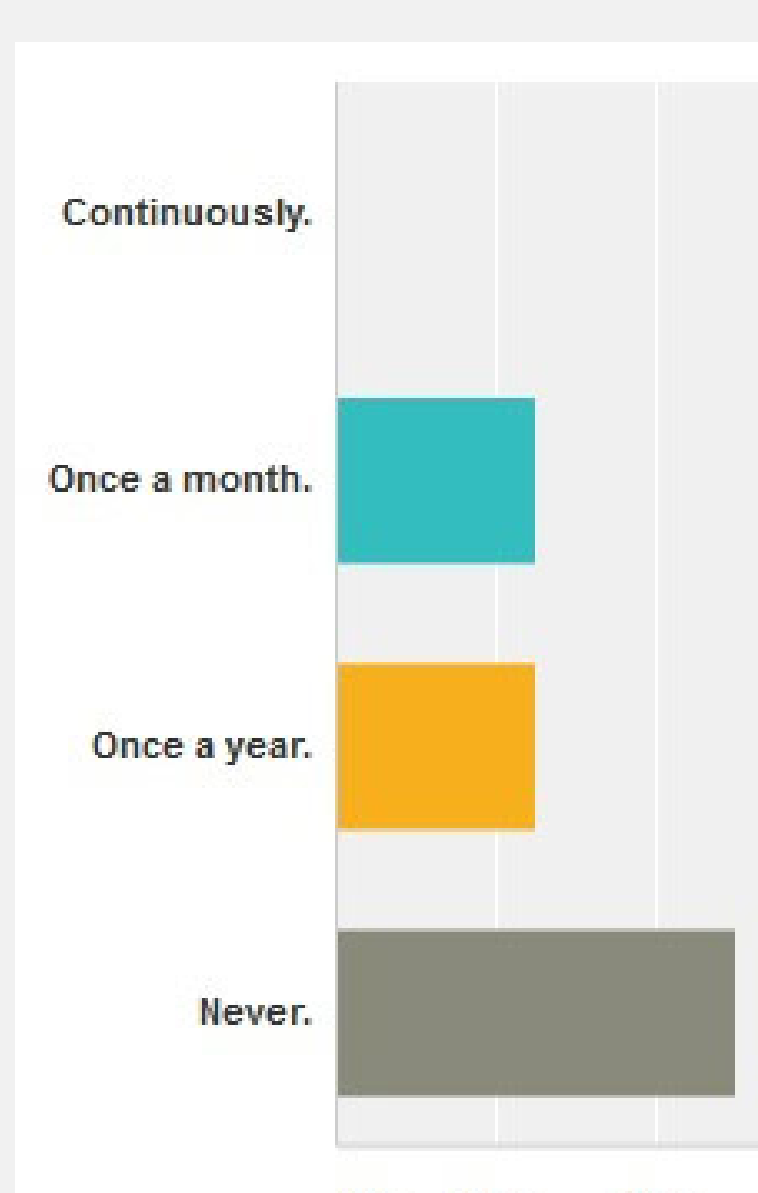
**What do you think is the biggest cause for decreased attendance at scientific conferences?**

- ☐ I don't know because I really like scientific conferences.
- ☐ It is just as easy to network and follow advances using the internet.
- ☐ They take too much time.
- ☐ They are too expensive.
- ☐ Scientific conferences were better suited to a time when the pace of life was slower.

**Take the Survey**

### Last month's survey

Data collection today often requires multiple PCs running 24 hours a day, 7 days a week, meaning your data collection software is stored on a hard drive constantly spinning at 7200 rpm. Unfortunately, hard drives have an annoying tendency to fail when you need them the most. Restoring all of the software can be real pain, unless you have a reliable backup copy. How often do you back up the software on your data collection machines?



### Video of the month

**Healing Crystals? The Development and Characterization of Pharmaceutical Solids**

Prof. Chris Frampton  
Brunel University



*You might want to skip the first 5 minutes of intro, but don't miss the first 5 minutes of and thought-provoking lecture by Chris Frampton.*

"Alternative medicine has long promoted crystals as having 'mystical healing' properties, yet in reality crystalline materials come with their own unique set of challenges that play havoc with attempts to develop new drugs and medicines. One of these is polymorphism, where a single active ingredient can cause drastically different effects depending on whether it is in its liquid or solid form. Many major setbacks to new treatments have been caused by a lack of understanding of the solid-state properties of a key material.

As a consequence investigations into the pharmaceutical solid-form need to be conducted at an early stage of the drug development process. In this lecture, Brunel's Professor Christopher Frampton will outline the latest approaches to solid-form drug development including polymorphism, salt-selection and co-crystallization studies".

**Watch the Video**

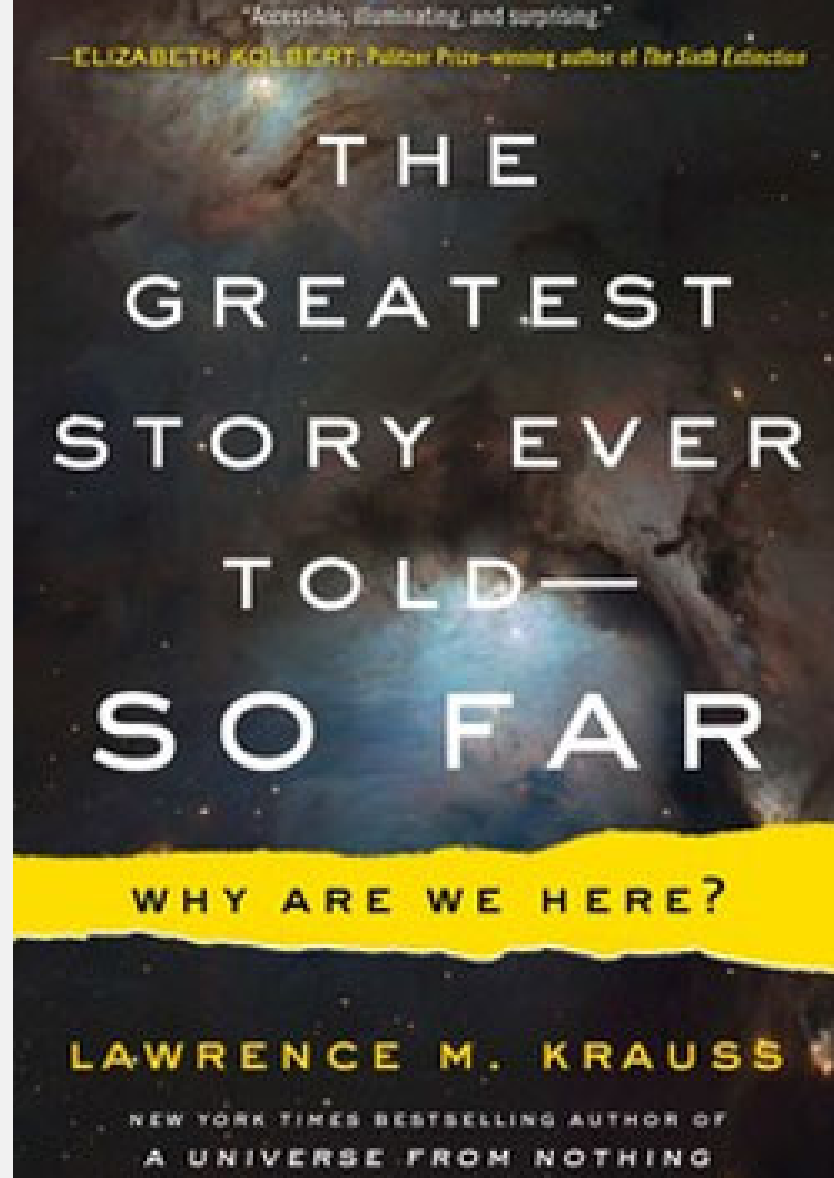
### Upcoming events

American Crystallographic Association (ACA) 2017, May 26 – 30, 2017 in New Orleans, LA, USA

47th Mid-Atlantic Macromolecular Crystallography Meeting, June 7 – 9, 2017 in Baltimore, MD, USA

5th Annual Symposium on Structural Biology at OU, June 15, 2017 in Norman, OK, USA

[See full list >](#)



### Join ROD on LinkedIn

The [Rigaku Oxford Diffraction LinkedIn group](#) shares information and fosters discussion about X-ray crystallography and SAXS topics. Connect with other research groups and receive updates on how they use these techniques in their own laboratories. You can also catch up on the latest newsletter or Rigaku Journal issue. We also hope that you will share information about your own research and laboratory groups.

### Crystallography in the news

**May 3, 2017.** Researchers from McGill University present in atomic detail [how specific bacterial enzymes, known as kinases, confer resistance to macrolide antibiotics](#), a widely used class of antibiotics and an alternative medication for patients with penicillin allergies. The study shows for the first time how these kinases recognize and chemically destroy macrolide antibiotics.

**May 5, 2017.** Scientists have modelled the shape and movement of biomolecules to depict step-by-step [how nucleoside analogs and natural nucleosides are transported into cells](#). The findings could be used to design smarter, more specific anticancer and antiviral drugs.

**May 9, 2017.** A web-based [open-source program called ContaMiner](#) determines protein structure contamination. Researchers can submit their X-ray diffraction data to the program, which compares it with an updatable database of known contaminants.

**May 9, 2017.** [Berkeley Lab researchers used structural characterization](#) — both X-ray crystallography and small angle X-ray scattering (SAXS) — to show that many of the designs adopted the target oligomerization state and predicted structure.

**May 15, 2017.** An international team including researchers from MIPT has shown that [iodide phasing](#) — a long-established technique in structural biology — is universally applicable to membrane protein structure determination.

**May 17, 2017.** Wei Liu and his colleagues at The Biodesign Institute join an international team, led by Beili Wu from the Shanghai Institute of Materia Medica (SIMM), Chinese Academy of Sciences, to explore a central component in glucose regulation. Their findings shed new light on the [structure of the glucagon receptor](#), a highly promising target for diabetes drug development.

**May 18, 2017.** The Molecular Structure Laboratory of the UW-Madison Department of Chemistry just completed the [4th Wisconsin Crystal Growing Competition](#). The objective of the competition is to grow the biggest and highest quality single crystal.

**May 18, 2017.** Using neutron crystallography, a research team has mapped the three-dimensional [structure of a protein that breaks down polysaccharides](#), such as the fibrous cellulose of grasses and woody plants, a finding that could help bring down the cost of creating biofuels.

**May 18, 2017.** Researchers at the University of Illinois at Urbana-Champaign have developed a [novel way to determine crystal type](#) based on optics — by identifying the unique ways in which these crystals absorb light.

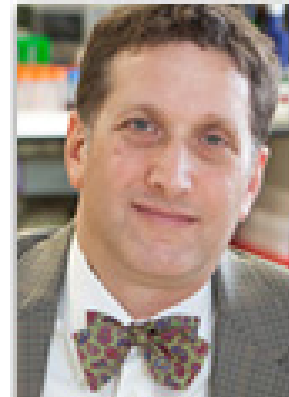
### Product spotlight: XtaLAB mini II Benchtop small molecule structure determination

The Rigaku XtaLAB mini II benchtop X-ray crystallography system is a compact single crystal X-ray diffractometer designed to produce publication-quality 3D structures. The perfect addition to any synthetic chemistry laboratory, the XtaLAB mini II will enhance research productivity by offering affordable structure analysis capability without the necessity of relying on a departmental facility. With the XtaLAB mini II, you no longer have to wait in line to determine your structures. Instead your research group can rapidly analyze new compounds as they are synthesized in the lab.



[For more about XtaLAB mini II](#)

### Lab in the spotlight



**Steven C. Almo, Ph.D.**

Professor, [Department of Biochemistry](#)

Professor, [Department of Physiology & Biophysics](#)

Chair, [Department of Biochemistry](#)

Wollowick Family Foundation Chair in Multiple Sclerosis and Immunology

Director, Einstein Macromolecular Therapeutics Developmental Facility

The Almo laboratory is interested in the development and application of strategies and technologies that enable the high-throughput/large-scale exploration of biological function. These efforts typically take advantage of automation and robotics to achieve the efficiencies and speed required to realize the desired rates of data generation and discovery. This cutting-edge infrastructure has been applied to a number of important biomedical areas to achieve new understanding and new therapeutic opportunities.

Their work on the large-scale annotation of enzyme function is helping to define the metabolic repertoire that exists in nature, and is providing new insights into the contributions of the gut microbiome to human health, the realization of new chemical processes for industry, and expanding our understanding of critical environmental issues, including global nutrient cycles and the evolution of complex microbial communities. Their high-resolution structural and functional analysis of the mammalian immune system has resulted in unprecedented understanding of the molecular mechanisms that control immunity and are guiding the development of novel strategies and reagents (e.g., biologics) for the treatment of infectious diseases, autoimmune diseases and cancers.

### Useful link: Crystal Growth, Evaluation and Handling

Alexander J. Blake, [The University of Nottingham, School of Chemistry](#)

This link contains excellent ideas for crystallization accompanied by useful diagrams.



### Selected recent crystallographic papers

**IP<sub>3</sub>-mediated gating mechanism of the IP<sub>3</sub> receptor revealed by mutagenesis and X-ray crystallography.** Kozo Hamada; Akiko Terauchi; Katsuhiko Mikoshiba; Hideyuki Miyatake. *Proceedings of the National Academy of Sciences of the United States of America*. 5/2/2017, Vol. 114 Issue 18, p4661-4666. 6p. DOI: [10.1073/pnas.1701420114](#).

**Room Temperature X-Ray Crystallography Reveals Conformational Heterogeneity of Engineered Proteins.** Szyperski, Thomas. *Structure*. May2017, Vol. 25 Issue 5, p691-692. 2p. DOI: [10.1016/j.str.2017.04.004](#).

**X-Ray Crystallography and Electron Microscopy of Cross- and Multi-Module Nonribosomal Peptide Synthetase Proteins Reveal a Flexible Architecture.** Tarry, Michael J.; Haque, Asfarul S.; Bui, Khanh Huy; Schmeing, T. Martin. *Structure*. May2017, Vol. 25 Issue 5, p783-793.e4. 1p. DOI: [10.1016/j.str.2017.03.014](#).

**A planar anthracene-imidazolium/anthracene-benzimidazolium cation system in a spherical polyoxometalate matrix: Synthesis, crystallography and spectroscopy.** Chatterjee, Tanmay; Kumar, N. Tanmaya; Das, Samar K. *Polyhedron*. May2017, Vol. 127, p68-83. 16p. DOI: [10.1016/j.poly.2017.01.049](#).

**Microstructure, texture, and crystallography in Ni-GDC and Co-GDC porous cermets obtained from directionally solidified eutectic ceramics.** Serrano-Zabaleta, S.; Larrea, A.; Larrañaga, A.; Dickey, E. *Journal of Materials Science*. May2017, Vol. 52 Issue 10, p5477-5488. 12p. 2 Black and White Photographs, 4 Diagrams, 1 Graph. DOI: [10.1007/s10853-016-0225-9](#).

**Non-contact luminescence lifetime cryothermometry for macromolecular crystallography.** Mykhaylyk, V. B.; Wagner, A.; Kraus, H. *Journal of Synchrotron Radiation*. May2017, Vol. 24 Issue 3, p636-645. 9p. DOI: [10.1107/S1600577517003484](#).

**Pepsi-SAXS: an adaptive method for rapid and accurate computation of small-angle X-ray scattering profiles.** Grudin, Sergei; Garkavenko, Maria; Kazennov, Andrei. *Acta Crystallographica Section D: Structural Biology*. May2017, Vol. 73 Issue 5, p449-464. 15p. DOI: [10.1107/S2059798317005745](#).

**Syntheses and Structures of New Rare-Earth Metal Tetracyanidoborates.** Falk, Fanni; Herkert, Lorena; Hackbarth, Liisa; Müller-Buschbaum, Klaus; Finze, Maik; Köckerling, Martin. *Zeitschrift für Anorganische und Allgemeine Chemie*. 5/4/2017, Vol. 643 Issue 9, p625-630. 6p. DOI: [10.1002/zaac.201700040](#).

**Syntheses, crystal structures and characterization of three alkaline metal borates.** Sambasivam, Sangaraju; Liu, Lili; Yang, Yun; Han, Guopeng; Bashir, Beenish; Yang, Zhihua; Pan, Shihue. *CrystEngComm*. 5/14/2017, Vol. 19 Issue 18, p2561-2569. 9p. DOI: [10.1039/c7ce00450h](#).

**Structural confirmation, single X-ray crystallographic behavior, molecular docking and other physico-chemical properties of gerberinol, a natural dimethyl dicoumarol from *Gerbera lanuginosa* Benth. (Compositae).** Brahmachari, Goutam; Das, Saktipada; Kumar, Abhishek; Misra, Neeraj; Sharma, Sakshi; Gupta, Vivek K. *Journal of Molecular Structure*. May2017, Vol. 1136, p214-221. 8p. DOI: [10.1016/j.molstruc.2017.01.062](#).

**Growth and characterization of L-Lysine adipate crystal.** Ramya, K.; Saraswathi, N.T.; Raja, C. Ramachandra. *Optics & Laser Technology*. May2017, Vol. 90, p222-225. 4p. DOI: [10.1016/j.optlastec.2016.12.002](#).

**Synthesis, structures and properties of three copper complexes with dibutylidithiocarbamate ligand.** Wang, Chen; Niu, Jiao; Li, Jun; Ma, Xiaoxun. *Journal of Molecular Structure*. May2017, Vol. 1135, p75-81. 7p. DOI: [10.1016/j.molstruc.2017.01.021](#).

**Solubility, potentiometric and thermodynamic studies on zinc-bosentan complex; synthesis and X-ray crystal structure.** Khandar, Ali Akbar; Mirzaei-Kalar, Zeinab; White, Jonathan M.; Hosseini-Yazdi, Seyed Abolfazl; Kebriaeezadeh, Abbas; Jouyban, Abolghasem. *Journal of Molecular Liquids*. May2017, Vol. 234, p64-72. 9p. DOI: [10.1016/j.molliq.2017.03.046](#).

**Synthesis and structural determination of 2D, ladder-like mononuclear coordinate (EnH<sub>2</sub>)[Nd<sup>III</sup>(Egta)(H<sub>2</sub>O)<sub>2</sub> · 6H<sub>2</sub>O and ten-coordinate (EnH<sub>2</sub>1.5[Nd<sup>III</sup>(Ttha)] · 5H<sub>2</sub>O.** Tian, F.; Liu, G.; Li, B.; Song, Y.; Wang, J. *Russian Journal of Coordination Chemistry*. May2017, Vol. 43 Issue 5, p304-313. 10p. DOI: [10.1134/S1070328417050074](#).

**Protein Immobilization onto Cationic Spherical Polyelectrolyte Brushes Studied by Small Angle X-ray Scattering.** Weihua Wang; Li Li; Henzler, Katja; Yan Lu; Junyong Wang; Haoya Han; Yuchuan Tian; Yunwei Wang; Zhiming Zhou; Lotze, L.; Gudrun; Narayanan, Theyencheri; Ballauff, Matthias; Xuhong Guo. *Biomacromolecules*. May2017, Vol. 18 Issue 5, p1574-1581. 8p. DOI: [10.1021/acs.biomac.7b00164](#).

**Comparison of X-ray crystal structures of a tetradecamer sequence d(CCCGGGTACCCGGG)<sub>2</sub> at 1.7 Å resolution.** Karthik, S.; Thirugnanasambandam, A.; Mandal, P. K.; Gautham, N. *Nucleosides, Nucleotides & Nucleic Acids*. 2017, Vol. 36 Issue 5, p343-354. 12p. DOI: [10.1080/15257770.2017.1287378](#).

**Synthesis, X-ray crystal structures, and antibacterial activities of Schiff base nickel(II) complexes with similar tetradentate Schiff bases.** Xu, Y.; Xue, L.; Wang, Z. *Russian Journal of Coordination Chemistry*. May2017, Vol. 43 Issue 5, p314-319. 6p. DOI: [10.1134/S1070328417050098](#).

**Synthesis, X-ray and Fluorescence Characteristics of Pyrimido[5,4-e]thiazolo[3,2-a]pyrimidine as a Novel Heterocyclic System.** Ebrahimpour, Zahra; Bakavoli, Mehdi; Shiri, Ali; Seyedi, Seyed; Asghari, Tayebe; Mague, Joel. *Journal of Fluorescence*. May2017, Vol. 27 Issue 3, p1183-1190. 8p. DOI: [10.1007/s10895-017-2055-9](#).

### The Greatest Story Ever Told – So Far: Why Are We Here? Lawrence M. Krauss, Simon and Schuster, Inc., New York, 2017, 336 pages, ISBN-13: 978-1476777610

I first learned of Professor Krauss when he published *The Physics of Star Trek* in 1996. I have read most of the books he has published since then. When Krauss was interviewed on Science Friday in March, I immediately pre-ordered my copy of this title.

This book is thought provoking. Its three divisions share titles with chapters of another book often referred to as "The Greatest Story Ever Told": Genesis, Exodus and Revelation. The prologue describes why Krauss chose this particular title and then uses the rest of the book to provide evidence for the secular version of The Greatest Story Ever Told.

The book is actually a history of modern physics. Krauss follows the timeline through the discovery of the forces of nature: gravity, electromagnetism, the weak nuclear and strong nuclear forces, and the theories that unify the forces, and the tools to validate the theories. The history ends with the experiments at the Large Hadron Collider and Laser Interferometer Gravitational-Wave Observatory. The last chapter attempts to answer the title question from the secular and non-secular point of view. You will have to decide which you choose.

The author artfully chooses a quotation to open each chapter. I particularly liked the opening for the chapter titled "More Questions than Answers": "A fool takes no pleasure in understanding, but only in expressing his opinion" – Proverbs 18:2.

Review by Joseph Ferrara  
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