Crystallography Times

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Crystallography Newsletter
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Crystallography in the news

November 1, 2017. Scientists at the Department of Energy's Oak Ridge National Laboratory have performed neutron structural analysis of a vitamin B6-dependent protein, potentially opening avenues for new antibiotics and drugs to battle diseases such as drug-resistant tuberculosis, malaria, and diabetes.

November 1, 2017. Genetic alphabet expansion technology is the introduction of artificial base pairs into DNA. Researchers from the Institute of Bioengineering and Nanotechnology (IBN) of the Agency for Science, Technology and Research in Singapore have created a DNA technology with two new genetic letters that could be used in the detection of infectious diseases, such as dengue and Zika.

November 1, 2017. According to a new study from scientists at The Scripps Research Institute (TSRI), the common practice of growing influenza vaccine components in chicken eggs disrupts the major antibody target site on the virus surface, rendering the flu vaccine less effective in humans.

November 3, 2017. A newly developed set-up tremendously reduces background scattering in X-ray structure analysis of biomolecules like proteins at synchrotron X-ray sources. To achieve this, the X-ray beam is enclosed in thin metal capillaries shortly before and behind the sample and the air immediately surrounding the sample is replaced by a stream of helium gas.

November 8, 2017. Professor Paul Workman, Chief Executive at The Institute of Cancer Research (London), and Dr Rob van Montfort, a structural biologist at the ICR, have guest edited a special edition of the journal *Essays in Biochemistry* focusing on structure-based drug design. It features 10 articles from specialists in the field.

November 10, 2017. Michael Gerken and his colleagues at the University of Lethbridge in Canada snared elusive chemical intermediates by running the parent reactions in baths of highly corrosive acid. The reactions created products including solid deposits of a compound that pairs acetone – a widely used industrial solvent – with an extra proton. Using spectroscopy and X-ray crystallography, the team worked out the 3D shape of the molecules, which are intermediate products in reactions used to create complex organic molecules, such as pharmaceuticals.

November 10, 2017. The Pistoia Alliance, a global, not for profit alliance that works to lower barriers to innovation in life sciences R&D, has announced today that its project to increase knowledge of antibody (Ab) structures has reached its first major milestone – 12 antibody structures have been deposited into the European Bioinformatics Institute's (EMBL-EBI) Protein Data Bank (PDB).

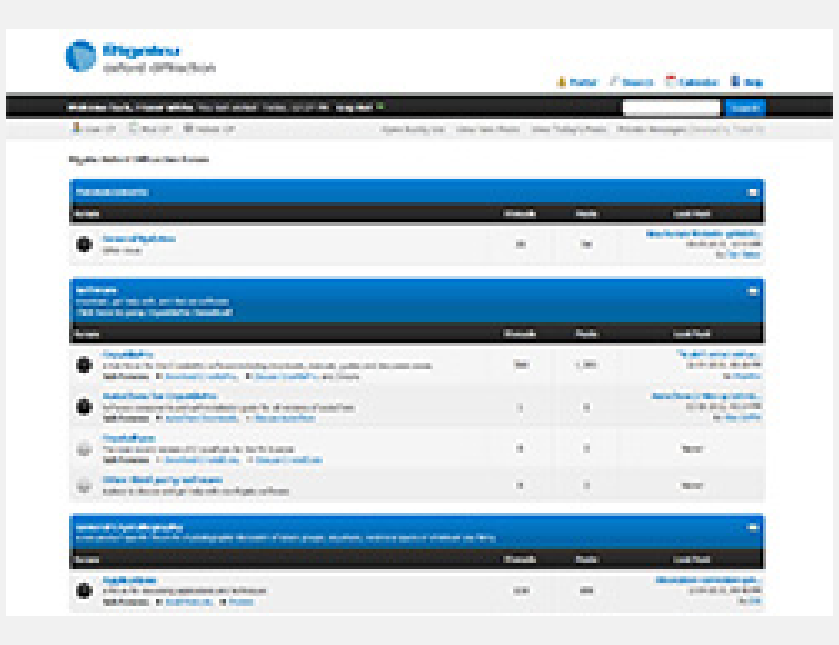
November 15, 2017. Researchers from The Scripps Research Institute (TSRI) and PATH's Malaria Vaccine Initiative (MVI) have shed light on how the human immune system recognizes the malaria parasite though investigation of antibodies generated from the RTS,S malaria vaccine – work that could boost the development of a more potent vaccine against the global killer. X-ray crystallography was employed to analyze how two functional antibodies from RTS,S-vaccinated individuals latched onto the CSP protein target.

November 16, 2017. Scientists are hoping to learn more about the structure of the LRRK2 protein, implicated in Parkinson's disease, as it returns from the gravity-free environment of the International Space Station. "The Michael J. Fox Foundation has put in over a hundred million dollars into research on LRRK2 beginning around 2005," said Marco Baptista, PhD, a principal investigator of the study and a director of the foundation's research programs.

Join ROD on LinkedIn

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.

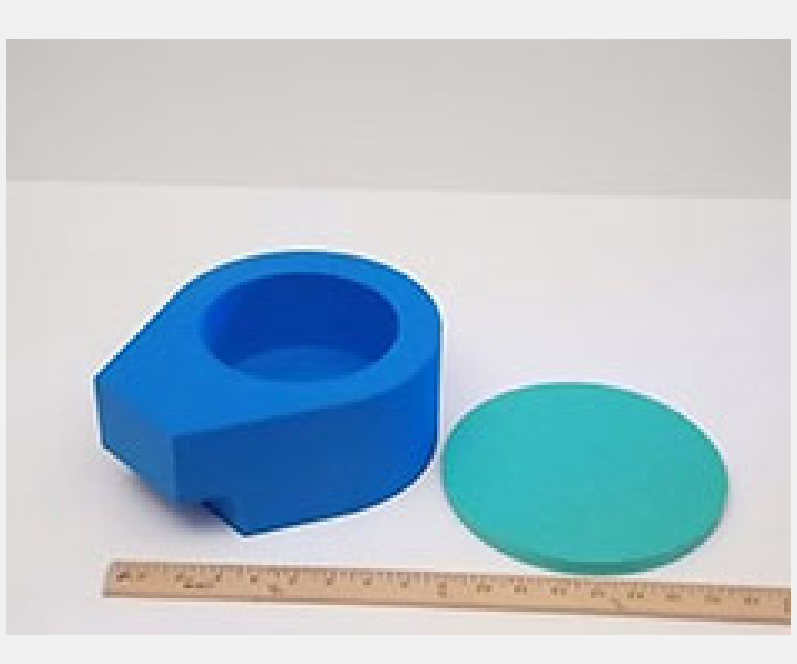
Rigaku Oxford Diffraction Forum



The Rigaku Oxford Diffraction Forum just passed the 2500 member mark! We have received over 2800 posts in 830 threads over the 9 years since its inception. Congratulations all! If you haven't signed up and would like to do so, please register:

www.rigakuxrayforum.com

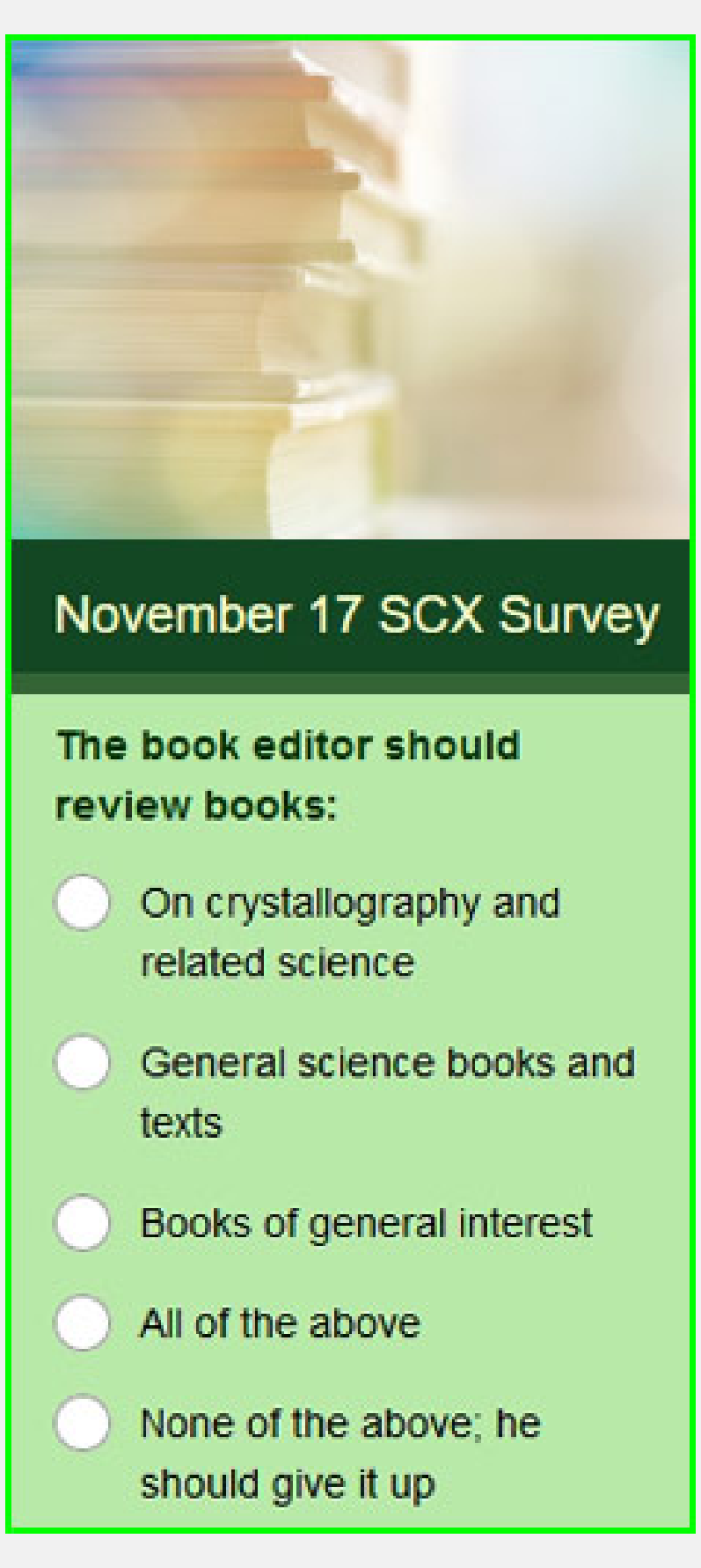
Rigaku Reagents: Spearlab foam dewars



Rigaku Reagents is now offering the popular Spearlab foam dewars. These polyethylene foam dewars are an effective way for handling liquid nitrogen and cryogenic materials. They are easy to handle, safe and durable!

Contact ReagentOrders@Rigaku.com
For more information, visit the Rigaku Reagents website.

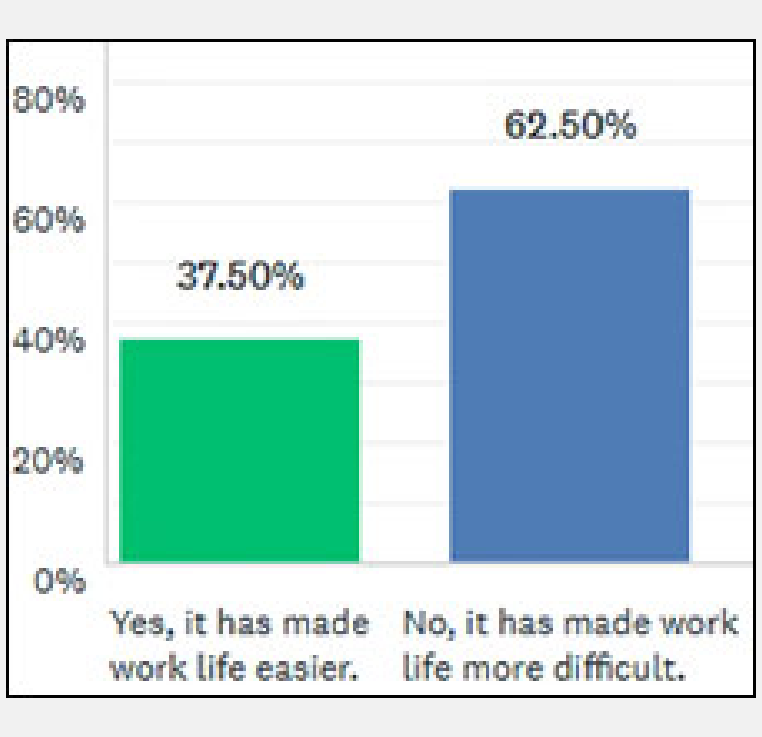
Survey of the month



Take the Survey

Last month's survey

Do you find social media has enhanced your scientific career?



Video of the month

The Rosalind Franklin Lecture 2016, with Dame Anne Glover | Why evidence really matters

Here is the inaugural Rosalind Franklin Lecture sponsored by Humanists UK and presented by Dame Anne Glover titled "Why evidence really matters".

Watch the Video

Upcoming events

CRYSTAL 31
Dec 3 – 7, 2017 in Bunker Bay, Western Australia

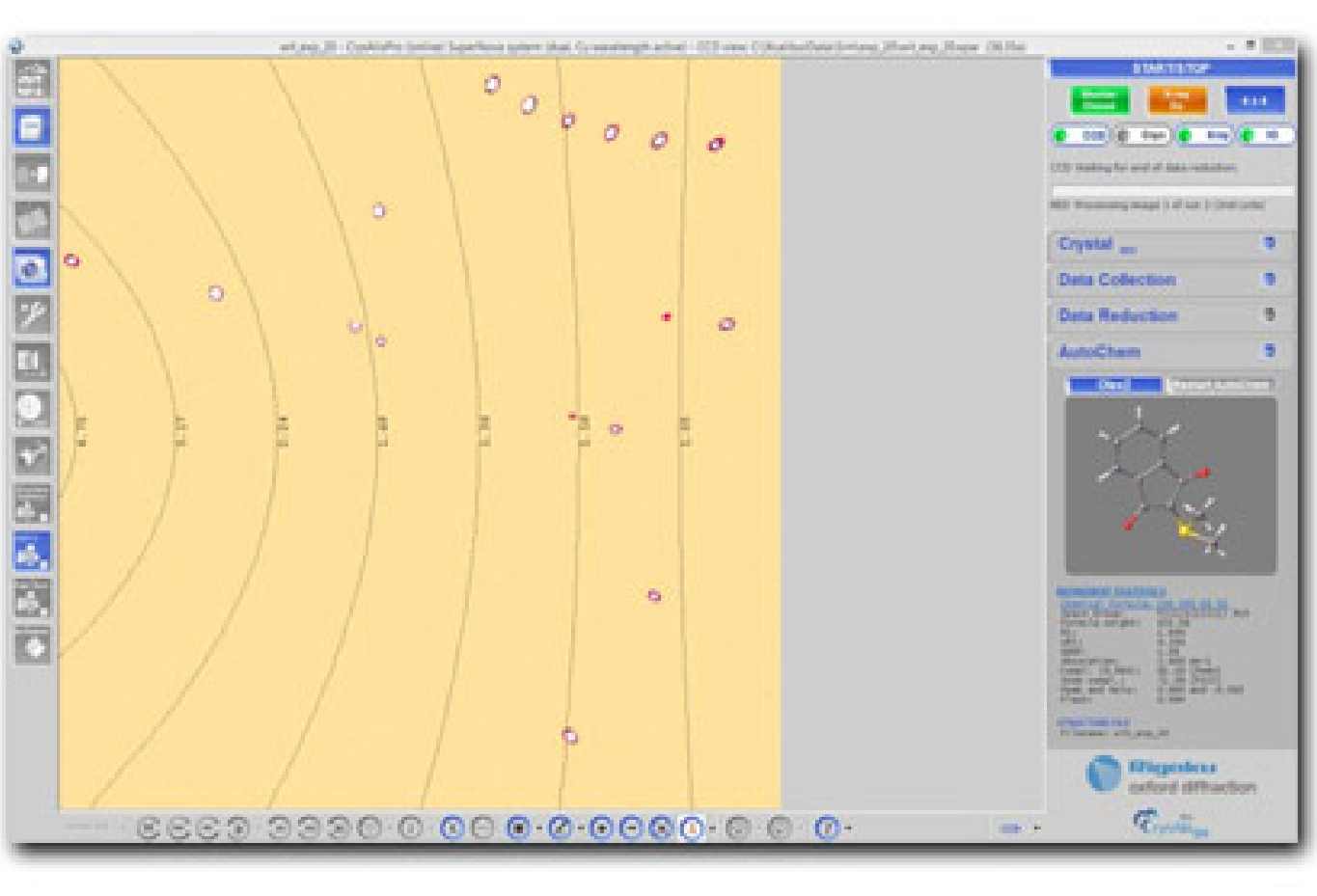
OpenLab Costa Rica
Dec 4 – 9, 2017 in San José, Costa Rica

See full list >

Product spotlight: AutoChem

AutoChem is the ultimate productivity tool for chemical crystallography, offering fast, fully automatic structure solution and refinement during data collection. Developed exclusively for Rigaku Oxford Diffraction by the authors of Olex2 (Durham University and OlexSys), AutoChem builds upon the success of the original AutoChem software. Seamlessly integrated as an optional plug-in for CrysAlis^{Pro}, AutoChem offers an advanced approach for automatic structure determination, with an even higher rate of success.

AutoChem can work with or without a chemical formula, intelligently using multiple solution programs and typically requiring only partial completeness to solve routine structures. In more difficult cases, AutoChem will make attempts in multiple space groups. A number of refinement options are available; atoms are modeled anisotropically where the data supports it and hydrogen atoms are included in calculated geometric positions. The structure is then re-labeled and refined to completion before a final structure report is generated. For more >



CrysAlis^{Pro} displays the structure and key refinement parameters, and provides a link to a full Rigaku Oxford Diffraction edition of Olex2 — complete with AutoChem plug-in — which can be launched at any time. Here the user can review all aspects of the refinement, step back to any stage of the process and apply changes as necessary.

For more about AutoChem and CrysAlis^{Pro} >

Lab in the spotlight

The Strynadka Lab
Dr. Natalie Strynadka
Dept. of Biochemistry and Molecular Biology
University of British Columbia

Dr. Natalie Strynadka has been chosen as the 2018 Fellow of the Biophysical Society of Canada. Dr. Strynadka received this recognition for her pioneering studies in determining the structural mechanisms underlying microbial diseases. Dr. Strynadka will give the National Lecture at BSC2018 in Vancouver. Infectious diseases account for a third of deaths worldwide, and are the third leading cause of death in Canada. Bacterial resistance to standard antibiotic therapies is a critical health problem worldwide, and has led to increased morbidity, mortality, and health-care costs in the clinic and community.

The research in her laboratory aims to address the antibiotic crisis in two ways:

- Understand at the molecular level how antibiotic resistance mechanisms work in bacteria
- Characterize and design inhibitors for entirely novel antibiotic targets found in a wide range of pathogenic bacteria

To illuminate the molecular basis of antibiotic resistance and viability/pathogenicity afforded by the proteins involved, her lab uses a multidisciplinary structural biology approach that relies on X-ray crystallography, NMR, and electron microscopy, complemented by phenotypic analysis in vitro and in vivo. Many of the bacterial proteins and protein complexes her lab studies are membrane associated, adding to the challenge of achieving their structural, biochemical, and in vivo characterization. Her lab is equipped with state of the art equipment for protein purification, biophysical analysis, high-throughput crystallization and X-ray data collection. In addition, her lab has access to world-class facilities at UBC including the bioimaging suite and NMR facility.

The Strynadka Lab >

Useful links

AAAS Statement on Scientific Freedom & Responsibility >

How to downgrade your iPhone or iPad from iOS 11 >

Selected recent crystallographic papers

On the state of crystallography at the dawn of the electron microscopy revolution. Higgins, Matthew K; Lea, Susan M. *Current Opinion in Structural Biology*. Oct2017, Vol. 46, p95-101. 7p. DOI: 10.1016/j.sbi.2017.06.005.

Complementary uses of small angle X-ray scattering and X-ray crystallography. Pillon, Monica C.; Guarné, Alba. *BBA – Proteins & Proteomics*. Nov2017 Part B, Vol. 1865 Issue 11B, p1623-1630. 8p. DOI: 10.1016/j.bbapap.2017.07.013.

Combining NMR and small angle X-ray scattering for the study of biomolecular structure and dynamics. Mertens, Haydyn D.T.; Svergun, Dmitri I. *Archives of Biochemistry & Biophysics*. Aug2017, Vol. 628, p33-41. 9p. DOI: 10.1016/j.abb.2017.05.005.

Synergy among phase-refinement techniques in macromolecular crystallography. Burla, Maria Cristina; Cascarano, Giovanni Luca; Giacovazzo, Carmelo; Polidori, Giampiero. *Acta Crystallographica Section D: Structural Biology*. Nov2017, Vol. 73 Issue 11, p877-888. 11p. DOI: 10.1107/S2059798317014590.

Small-angle X-ray scattering study of conditions for the formation of growth units of protein crystals in lysozyme solutions. Dyakova, Yu.; Ilina, K.; Konarev, P.; Kryukova, A.; Marchenkova, M.; Blagov, A.; Volkov, V.; Pisarevsky, Yu.; Kovalchuk, M. *Crystallography Reports*. May2017, Vol. 62 Issue 3, p364-369. 6p. DOI: 10.1134/S1063774517030051.

Using crystallography, topology and graph set analysis for the description of the hydrogen bond network of triamterene: a rational approach to solid form selection. Hughes, David S.; Delori, Amit; Rehman, Abida; Jones, William. *Chemistry Central Journal*. 7/13/2017, Vol. 11 Issue 1, p1-19. 19p. DOI: 10.1186/s13065-017-0293-1.

Insights on the structural dynamics of Leishmania braziliensis Hsp90 molecular chaperone by small angle X-ray scattering. Seraphim, Thiago V.; Silva, Kelly P.; Dores-Silva, Paulo R.; Barbosa, Leandro R.S.; Borges, Júlio C. *International Journal of Biological Macromolecules*. Apr2017, Vol. 97, p503-512. 10p. DOI: 10.1016/j.ijbiomac.2017.01.058.

Substituted 4-Acyl-5-methyl-2-phenyl-pyrazol-3-one-phenylhydrazones with Antioxidant Properties: X-Ray Crystal and Spectroscopic Studies. Idemudia, Omoruyi G.; Okoh, Anthony I.; Sadimenko, Alexander P.; Hosten, Eric C.; Okoh, Omobola O. *Journal of Chemistry*. 11/13/2017, p1-10. 10p. DOI: 10.1155/2017/7943051.

Topological Structure Determination of RNA Using Small-Angle X-Ray Scattering. Bhandari, Yuba R.; Fan, Lixin; Fang, Xianyang; Zaki, George F.; Stahlberg, Eric A.; Jiang, Wei; Schwieters, Charles D.; Stagno, Jason R.; Wang, Yun-Xing. *Journal of Molecular Biology*. Nov2017, Vol. 429 Issue 23, p3635-3649. 15p. DOI: 10.1016/j.jmb.2017.09.006.

Deciphering Structural Photophysics of Fluorescent Proteins by Kinetic Crystallography. Bourgeois, Dominique. *International Journal of Molecular Sciences*. Jun2017, Vol. 18 Issue 6, p1-19. 19p. 5 Diagrams, 4 Graphs. DOI: 10.3390/ijms18061187.

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

Biochemical analysis and the preliminary crystallographic characterization of D-tagatose 3-epimerase from *Rhodobacter sphaeroides*. Zhengliang Qi; Zhangliang Zhu; Jian-Wen Wang; Songtao Li; Qianqian Guo; Panpan Xu; Fuping Lu; Hui-Min Qin. *Microbial Cell Factories*. 11/9/2017, Vol. 16, p1-9. 9p. 2 Diagrams, 2 Charts, 4 Graphs. DOI: 10.1186/s12934-017-0808-4.

Small-angle X-ray scattering study of the influence of solvent replacement (from H_2O to D_2O) on the initial crystallization stage of tetragonal lysozyme. Boikova, A.; D'yakova, Yu.; Il'ina, K.; Konarev, P.; Kryukova, A.; Marchenkova, M.; Blagov, A.; Pisarevskii, Yu.; Koval'chuk, M. *Crystallography Reports*. Nov2017, Vol. 62 Issue 6, p837-842. 6p. DOI: 10.1134/S1063774517060074.

Neutron Crystallography for the Study of Hydrogen Bonds in Macromolecules. Oksanen, Esko; Chen, Julian C. H.; Fisher, Suzanne Zoë. *Molecules*. Apr2017, Vol. 22 Issue 4, p1-26. 26p. 1 Color Photograph, 15 Diagrams, 1 Chart. DOI: 10.3390/molecules22040596.

Nanobodies targeting norovirus capsid reveal functional epitopes and potential mechanisms of neutralization. Koromyslova, Anna D.; Hansman, Grant S. *PLoS Pathogens*. 11/02/2017, Vol. 13 Issue 11, p1-33. 33p. DOI: 10.1371/journal.ppat.1006636.

Cross-Validation of Data Compatibility Between Small Angle X-ray Scattering and Cryo-Electron Microscopy. Kim, Jin Seob; Afsari, Bijan; Chirikjian, Gregory S. *Journal of Computational Biology*. Jan2017, Vol. 24 Issue 1, p13-30. 18p. DOI: 10.1089/cmb.2016.0139.

Long-wavelength macromolecular crystallography – First successful native SAD experiment close to the sulfur edge. Aurelius, O.; Duman, R.; El Omari, K.; Mykhaylyk, V.; Wagner, A. *Nuclear Instruments & Methods in Physics Research Section B*. Nov2017, Vol. 411, p12-16. 5p. DOI: 10.1016/j.nimb.2016.12.005.

Improving virtual screening of G protein-coupled receptors via ligand-directed modeling. Coudrat, Thomas; Simms, John; Christopoulos, Arthur; Wootten, Denise; Sexton, Patrick M. *PLoS Computational Biology*. 11/13/2017, Vol. 13 Issue 11, p1-40. 40p. DOI: 10.1371/journal.pcbi.1005819.

Protein metalation by metal-based drugs: X-ray crystallography and mass spectrometry studies. Messori, L.; Merlino, A. *Chemical Communications*. 11/4/2017, Vol. 53 Issue 85, p11622-11633. 12p. DOI: 10.1039/c7cc06442j.

Biological evaluation, docking and molecular dynamic simulation of some novel diaryl urea derivatives bearing quinoxalindione moiety. Sadeghian-Rizi, Sedighe; Khodarahmi, Ghadam Ali; Sakhteman, Amirhossein; Jahanian-Najafabadi, Ali; Rostami, Mahboubeh; Mirzaei, Mahmoud; Hassanzadeh, Farshid. *Journal of Research in Pharmaceutical Sciences*. Nov/Dec2017, Vol. 12 Issue 6, p500-509. 10p. DOI: 10.4103/1735-5362.217430.

Nuclear Magnetic Resonance and X-ray Crystallography to Improve Struvite Determination. Witty, Michael; Dingra, Nin N.; Abboud, Khalil A.; Felts, Ashley C.; Ayudhya, Theppawut Israsena Na. *Analytical Letters*. 2017, Vol. 50 Issue 16, p2549-2559. 11p. 9 Graphs. DOI: 10.1080/00032719.2017.1302459.

Determination of the Molecular Structures of Ferric Enterobactin and Ferric Enantioenterobactin Using Racemic Crystallography. C. Johnstone, Timothy C.; Nolan, Elizabeth M. *Journal of the American Chemical Society*. 10/25/2017, Vol. 139 Issue 42, p15245-15250. 6p. DOI: 10.1021/jacs.7b09375.

Ferrocene derivatives of liquid chiral molecules allow assignment of absolute configuration by X-ray crystallography. Holstein, Philipp M.; Escudero-Adán, Eduardo C.; Echavarren, Antonio M.; Holstein, Julian J.; Baudoin, Olivier. *Tetrahedron: Asymmetry*. Oct2017, Vol. 28 Issue 10, p1321-1329. 9p. DOI: 10.1016/j.tetasy.2017.09.002.

Cationic and Anionic Disorder in CZTSSe Kesterite Compounds: A Chemical Crystallography Study. Bais, Pierre; Caldes, Maria Teresa; Paris, Michaël; Guillot-Deudon, Catherine; Fertey, Pierre; Domengès, Bernadette; Lafond, Alain. *Inorganic Chemistry*. 10/2/2017, Vol. 56 Issue 19, p11779-11786. 8p. DOI: 10.1021/acs.inorgchem.7b01791.

A zigzag path through quantum crystallography. Massa, Lou. *Structural Chemistry*. Oct2017, Vol. 28 Issue 5, p1293-1296. 4p. DOI: 10.1007/s11224-017-0960-9.

Guest Editorial: A path through quantum crystallography: a short tribute to Professor Lou Massa. Matta, Chérif. *Structural Chemistry*. Oct2017, Vol. 28 Issue 5, p1279-1283. 5p. DOI: 10.1007/s11224-017-0961-8.

X-ray Scattering Studies of Protein Structural Dynamics. Meisburger, Steve P.; Thomas, William C.; Watkins, Maxwell B.; Ando, Nozomi. *Chemical Reviews*. 6/28/2017, Vol. 117 Issue 12, p7615-7672. 58p. DOI: 10.1021/acs.chemrev.6b00790.

Towards a compact and precise sample holder for macromolecular crystallography. Papp, Gergely; Rossi, Christopher; Janocha, Robert; Sorez, Clement; Lopez-Marrero, Marcos; Astruc, Anthony; McCarthy, Andrew; Belrhali, Hassan; Bowler, Matthew W.; Cipriani, Florent. *Acta Crystallographica Section D: Structural Biology*. Oct2017, Vol. 73 Issue 10, p829-840. 11p. DOI: 10.1107/S2059798317013742.

Synthesis of a new pyridinyl thiazole ligand with hydrazone moiety and its cobalt(III) complex: X-ray crystallography, *in vitro* evaluation of antibacterial activity. Bera, Pradip; Brandão, Paula; Mondal, Gopinath; Jana, Harekrishna; Jana, Abhimanyu; Santra, Ananyakumari; Bera, Pulakesh. *Polyhedron*. Sep2017, Vol. 134, p230-237. 8p. DOI: 10.1016/j.poly.2017.06.024.

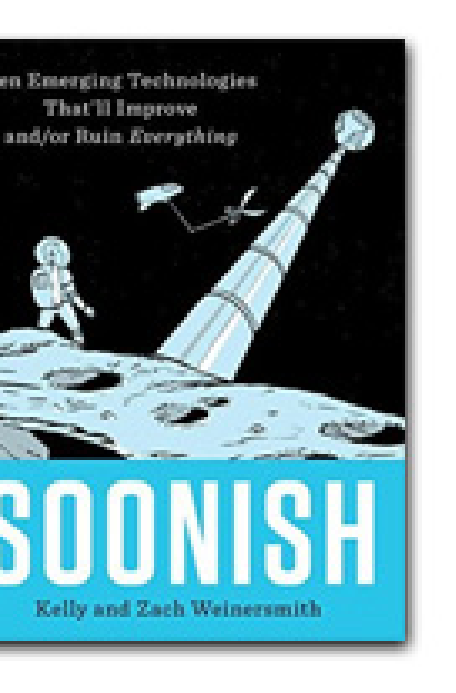
Recent advances in racemic protein crystallography. Yan, Bingjia; Ye, Linzhi; Xu, Weiliang; Liu, Lei. *Bioorganic & Medicinal Chemistry*. Sep2017, Vol. 25 Issue 18, p4953-4965. 13p. DOI: 10.1016/j.bmc.2017.05.020.

Covalent inhibitors for eradication of drug-resistant HIV-1 reverse transcriptase: From design to protein crystallography. Chan, Albert H.; Won-Gil Lee; Spasov, Krasimir A.; Cisneros, José A.; Kudalkar, Shalley N.; Petrova, Zaritza O.; Buckingham, Amanda B.; Anderson, Karen S.; Jorgensen, William L. *Proceedings of the National Academy of Sciences of the United States of America*. 9/5/2017, Vol. 114 Issue 36, p9725-9730. 6p. DOI: 10.1073/pnas.1711463114.

Pitfalls in metal–organic framework crystallography: towards more accurate crystal structures. Øien-Ødegaard, S.; Shearer, G. C.; Wragg, D. S.; Lillerud, K. P. *Chemical Society Reviews*. 8/21/2017, Vol. 46 Issue 16, p4867-4876. 10p. DOI: 10.1039/c6cs00533k.

Solution structure of human steroidogenic acute regulatory protein STARD1 studied by small-angle X-ray scattering. Sluchanko, Nikolai N.; Tugaeva, Kristina V.; Maksimov, Eugene G. *Biochemical & Biophysical Research Communications*. Aug2017, Vol. 489 Issue 4, p445-450. 6p. DOI: 10.1016/j.bbrc.2017.05.167.

Book review



***Soonish: Ten Emerging Technologies That'll Improve and/or Ruin Everything* by Kelly and Zach Weinersmith, Penguin Press, New York, 2017, 368 pages, ISBN: 978-0399563829**

Soonish is a marriage of science fact and science humor, which makes sense, given that the authors, a scientist and a comic strip creator, are married.

They divided the book into three sections: the universe, stuff, and you. Translation: space exploration, gadgets and robots, and human biology.

In *The Universe, Soonish*, the authors detail everything from the impracticalities of a space elevator, to the pitfalls and potential struggles of asteroid mining, to Elon Musk and his SpaceX program. Aside from the practicality of execution, the main roadblock on the highway to space exploration is cost. Although, as the authors casually observe: if you stopped worrying about getting explorers back to Earth alive, you could cut a lot of the costs.

Next, in *Stuff, Soonish*, fusion power, augmented reality, and robots take the lead, along with programmable matter (it's exactly what it sounds like: both perplexing and riveting) and synthetic biology (CRISPR!*). Fusion power seems a long way off for practical reasons but, if it could be achieved, what a way to power your microwave (and fridge and toaster and pretty much everything else). Augmented reality—anyone who has been run over by an overeager Millenial or Gen Z teenager playing Pokémon Go knows the pitfalls—has numerous applications, and not all of them involve playing app-based phone games. Robots, the authors somewhat jokingly posit, are going to take over in 2027. The sooner you accept that inevitability, the sooner you can be open to the incredible advances in robotics and how they can help you in the next decade.

Finally, in *You, Soonish*, the human body takes the stage—namely precision medicine and bioprinting. Every person's body processes prescription medication and treatments in a different way. Two people with Stage 3 cancer can be given the exact same drug regimen: one might survive while the other does not. The idea behind precision medicine is that by studying a patient's DNA—and even potentially modifying it—you can cure someone of a chronic condition before they even present symptoms. And, as for bioprinting, it presents a possible solution for a real problem. Roughly one person dies every hour in the United States waiting for an organ—liver, heart, lung, kidney, take your pick. That's over 8,000 people per year, just in the U.S. The U.S. only accounts for 4.4% of the world population—you can do the math. 3D-printing of cells, and, eventually, whole organs, means dying people around the world won't have to wait for someone to donate an organ (whether by generosity or death) to survive.

The intermittent comics add a colorful and playfully sardonic tone to a book that covers emergent technologies with a combined sense of wonder, skepticism, and even a healthy dose of fear. *Soonish* is a fun look at the future of technology, which like the present and the past, isn't always fun.

*The authors deserve some serious bonus points for giving Jennifer Doudna and Emmanuelle Charpentier their due credit for developing CRISPR. There is an ongoing patent battle between these phenomenal women in science and their mostly male collaborators at the Broad Institute of MIT and Harvard.

Review by Jeanette S. Ferrara, MA

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