

Crystallography Newsletter
Volume 12, No. 6, August 2020

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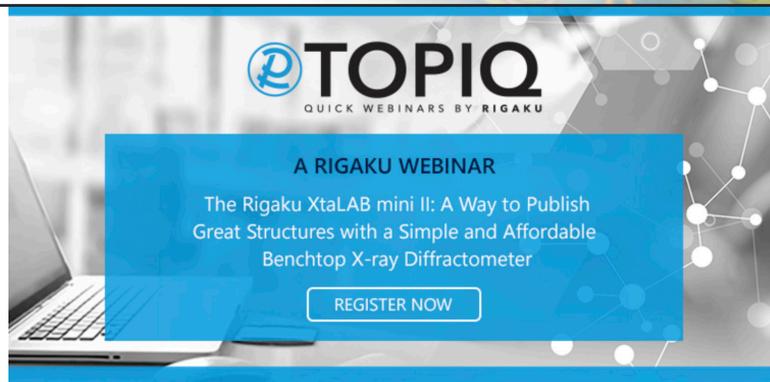
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Rigaku School for Practical Crystallography

If you missed our summer event and want to watch the recordings or download course material from the Rigaku School for Practical Crystallography, please go to www.rigakuxrayforum.com and register as a user. In the instruments field enter "Rigaku School" to indicate you wish to partake of the school benefits. You will not receive a notification when you've been approved so please check periodically.

Rigaku TOPIQ Webinars

Rigaku has developed a series of short, 20-30 minute training webinars that cover a broad range of topics in the fields of X-ray diffraction, X-ray fluorescence, and X-ray imaging. You can register [here](#) and also [watch](#) recordings if you can't attend the live session.



A lot has happened since the last eNewsletter. We completed the exams and certifications for the Asia-Pacific edition of the Rigaku School for Practical Crystallography. The American Crystallographic Association held its Annual Meeting virtually, and in my humble opinion, it was a resounding success. We also held the Rigaku Virtual Analytical X-ray Convention and participated in the virtual Denver X-ray Conference and Microscopy and Microanalysis annual meetings. Lastly, we just completed our first Online Rigaku Oxford Diffraction Users' Meeting, which saw more participants than any in-person users' meeting we've held. I want to give a special thank you to the users who gave presentations on some fascinating research.

What is coming up? Today and tomorrow we will be holding a webinar on our benchtop single crystal diffractometer, the XtaLAB mini II. The two sessions will cover the same topics but at different times of the day so we can provide more convenient viewing times for different parts of the world. You can register by clicking [here](#). We will continue to provide webinars on various aspects of single crystal diffraction. If there is a specific topic that interests you, please let me know.

In this edition of *Crystallography Times*, we are introducing XtaLAB Synergy Flow, a product that was designed to enhance your workflow and provide much needed social distancing. We are also spotlighting the laboratory of Dr. Kovalevsky of ORNL. You will find the usual useful information and videos of the month. Finally, this month's review is on *Science Fictions*, a book about how fraud, bias, negligence, and hype negatively impact the scientific enterprise.

Crystallography in the News

July 24, 2020: Researchers in South Korea, the U.K. and the U.S. have developed [functionalized metal-organic frameworks](#) that capture CO₂ from humid air and are regenerated by steam.

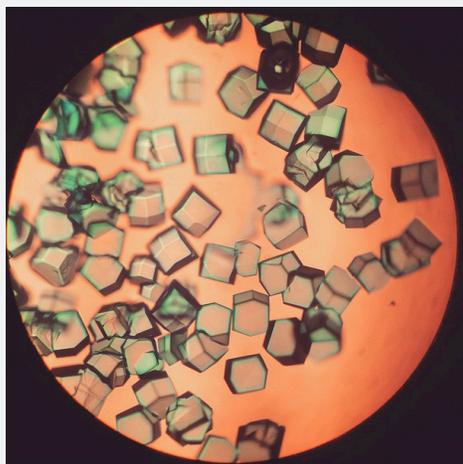
July 24, 2020: Researchers in the Czech Republic have completed a structural analysis of the [SARS-CoV-2 methyltransferase complex](#)

Rigaku Reagents



The Lysozyme Crystallography Kit

This kit is designed to grow cryoprotected hen egg white lysozyme crystals that can be used for protein crystallography. The crystallographic space group is usually primitive tetragonal $P4_32_12$ with unit cell dimensions of $78 \text{ \AA} \times 78 \text{ \AA} \times 38 \text{ \AA}$. The crystals may grow to be as large as 0.5 mm on an edge. The mosaicity of the crystals will vary depending on the handling, flash-cooling, and mounting techniques used.



[Order Here](#)

involved in RNA cap creation bound to sinefungin which adds to the list of possible drug candidates to mitigate the ongoing COVID-19 pandemic.

August 7, 2020: Researchers in Germany and The Netherlands have used *in silico* and home laboratory X-ray structures to design better [protein-protein interaction inhibitors](#).

August 12, 2020: Researchers from Genentech and Stanford have elucidated the [structure of the essential inner membrane lipopolysaccharide–PbgA complex](#) in order to understand better how antibiotics pass through the *E. coli* outer membrane.



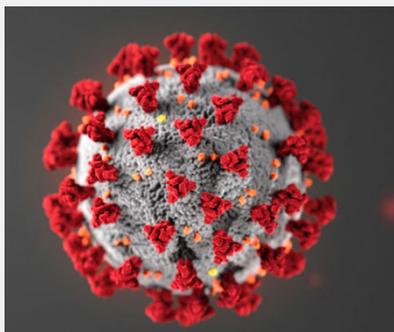
Product Introduction Rigaku Oxford Diffraction [The XtaLAB Synergy Flow](#)

Rigaku Oxford Diffraction is proud to announce a new diffractometer system with integrated sample-changing automation designed to improve the workflow of your X-ray laboratory. The XtaLAB Synergy Flow system incorporates a 6-axis UR3 Universal Robot into our popular XtaLAB Synergy diffractometer, providing unattended data acquisition, enhanced productivity and standardized workflow to your research environment.

Today's COVID-19 workplace environment requires a minimization of human interaction and potential viral contamination. A XtaLAB Synergy Flow system can be used as part of a sample submission protocol that minimizes human contact. With automated sample mounting, potential contamination of the diffractometer by human contact is eliminated. A crystal capacity of 48 samples means that unattended data collection can be easily performed, thus minimizing the time required to be in the X-ray laboratory.

Survey of the Month

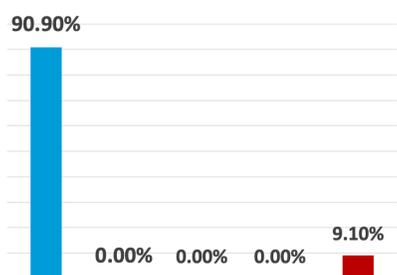
When do you expect an effective vaccine for COVID-19 to be available?



Take the Survey

Last Issue's Survey Results

What best describes your face mask usage?



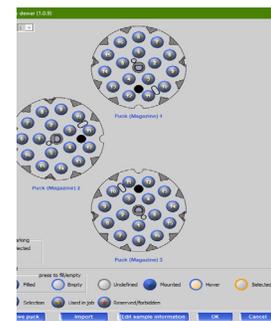
- I wear one anytime I'm in a public place because I don't want to risk getting sick or making someone else sick.
- I wear one anytime I'm in a public place because I don't like people giving me the evil eye.
- I never wear one because I don't believe they are effective.
- I never wear one because I don't like looking like a bank robber.
- I never wear one because nobody can tell me what to do.



A negative aspect of existing automated diffractometers is that data collection must be halted in order to open the enclosure and add more samples. The XtaLAB Synergy Flow system avoids that problem by incorporating a unique X-ray safe dewar-drawer

system that can be accessed from the side of the cabinet while data collection continues unimpeded.

The XtaLAB Synergy Flow is controlled by *CrysAlis^{Pro}* for frustration-free operation including sample addition, experiment queuing and sample sorting. Samples can be sorted into “good” pucks that can then be queued up for long experiments or removed and stored for transport to a synchrotron. A judgment on good samples can be made automatically or by the user on inspection of the results later.



The XtaLAB Synergy Flow system utilizes the Intelligent Goniometer Head (IGH), a motorized marvel with fast response and intelligence built in. Automated sample centering can be as fast as 6 seconds on dual-camera systems, the standard for our robotic instruments. Manual and point-and-click control are also available for fine-tuning centering or targeting a specific feature or part of the sample.



Samples are stored in an LN2 dewar, with a capacity of 48 samples stored in three UNI-PUCKS. Dewar accessories include a bar code reader, a defrost system, rotatable lid, level sensor and automatic LN2 dosing system. Accepted pins include the

ALS standard from ALS and the SPINE standard from EMBL.

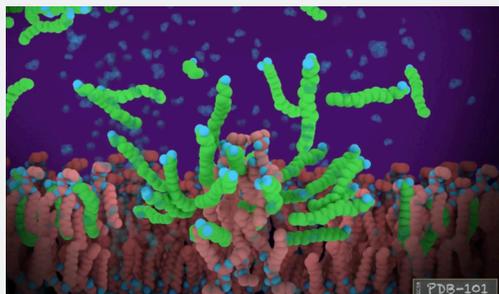
The XtaLAB Synergy diffractometers are known for high-performance X-ray sources and direct X-ray detection detectors, a combination that means amazing throughput potential. The XtaLAB Synergy Flow system was designed to take full advantage of the high performance by minimizing the time that an instrument might sit idle due to lack of human interaction. In the current climate of minimizing human interaction and maximizing efficiency and productivity, the [XtaLAB Synergy Flow](#) provides a transformational instrument for today's single crystal X-ray laboratories.

Videos of the Month

Fighting Coronavirus with Soap

RCSBProteinDataBank

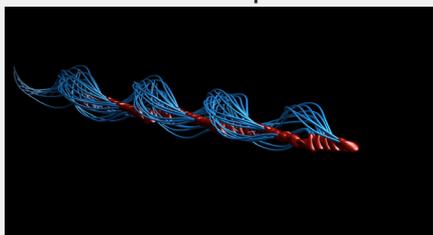
Always use soap when you wash your hands! Soap molecules break up the outer layer of enveloped viruses stopping infection. Watch at the molecular level how soap breaks up coronavirus by using series of hydrophilic and hydrophobic interactions.



Watch the Video

Watch a 3D video reveal how sperm really swim

Watch a human sperm under a microscope and it will appear to swim like an eel wiggling its tail through the water. But a new study reveals that sperm actually swim in a much more chaotic manner—one they've been able to harness for maximal speed.



Watch the Video

Researcher in the Spotlight

Andrey Kovalevsky

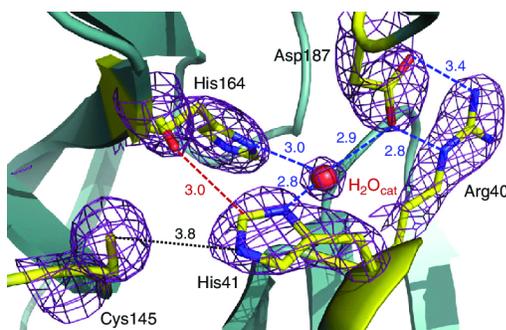


Dr. Kovalevsky is a macromolecular crystallographer, biochemist and instrument scientist on the ORNL IMAGINE neutron crystallographic instrument, HFIR beam line CG-4D. His current research focuses on the atomic level understanding of enzyme function, drug binding, and drug resistance, including the effects of molecular dynamics, utilizing macromolecular X-ray and neutron crystallography, X-ray and neutron

scattering, and other biophysical methods in combination with QM/MM and MD simulations. Dr. Kovalevsky is using macromolecular neutron crystallography to study enzyme mechanisms uncovering atomic-level details about enzymatic reactions not recognized previously; he was the first to observe a hydronium ion and proton complexation in a protein, and to detect proton transfer in an enzyme active site. His neutron structures of protein-drug complexes provide an exact picture, virtually impossible to achieve with any other technique, of how inhibitors bind to their targets, aiding structure-based drug design.

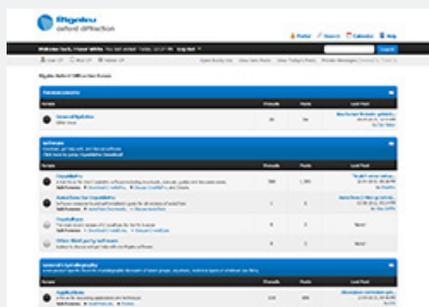
Andrey and his colleagues have been publishing a lot of Main Protease structures recently determined on their in-house X-ray system. It has been a key capability in doing rapid COVID-19 related structural work due to the many travel restrictions in place. Here is an example of a recent publication:

Kneller, Daniel & Phillips, Gwyndalyn & O'Neill, Hugh & Jedrzejczak, Robert & Stols, Lucy & Langan, Paul & Joachimiak, Andrzej & Coates, Leighton & Kovalevsky, Andrey. Structural plasticity of SARS-CoV-2 3CL M^{pro} active site cavity revealed by room temperature X-ray crystallography. [Nature Communications. 11, 3202 \(2020\).](#)



Join Us on LinkedIn

Our [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 X-ray Forum
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^{Pro} software for single crystal data processing.



Subscribe to Rigaku eNewsletters
Each month, Rigaku distributes two eNewsletters: *The Bridge*, which focuses on Materials Analysis, and *Crystallography Times*, which concentrates on X-ray crystallography.
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Useful Links



[MoProSuite : Crystallographic software for charge density refinement](#)

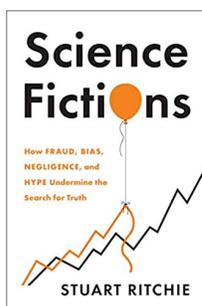
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[Retraction Watch](#)

Retraction Watch is a blog that reports on retractions of scientific papers and on related topics. The blog was launched in August 2010 and is produced by science writers Ivan Oransky and Adam Marcus. Its parent organization is the Center for Scientific Integrity.

Book Review



[Science Fictions: How Fraud, Bias, Negligence, and Hype Undermine the Search for the Truth](#)

By Stuart Ritchie
ISBN 9718-1-250-22269-5

Stuart Ritchie's *Science Fictions* is a well-crafted and compelling work about the critical importance of reproducibility in scientific research and studies. Ritchie dives into both historical and recent examples of science gone wrong—ranging from papers published under false pretenses to those published with entirely fabricated results.

Ritchie begins with an eloquent preface in which he elucidates very clearly what he hopes to accomplish over the course of his book, and offers a brief introduction to the nature of his work.

He then jumps right in with Part I, titled "Ought and Is." In it, he explains how science works, or rather how it is supposed to, versus the reality of many scientific endeavors. He defines the so-called "Replication Crisis," in which numerous scientific papers published in the past decades contain irreproducible results. He mentions Retraction Watch, a website started in part by one of my former journalism professors at NYU, Ivan Oransky. The goal of the site is to flag retracted papers in scientific publications across disciplines and dig deeper into the cause of the retraction.

Part II is the crux of Ritchie's work, in which he details the four main "Faults and Flaws" of scientific research and discovery as it

is conducted today, and how those issues lead to irreproducible results, which in turn can lead to a retracted paper. These four faults and flaws are listed in the subtitle of the book: fraud, bias, negligence, and hype. Each has its own set of causes and effects in the sphere of scientific discovery, and Ritchie illustrates each with several memorable and colorful anecdotes, highlighting instances in recent and less recent history where these four factors had a negative impact on the respective field of its offending researcher.

Part III, “Causes and Cures,” digs a little more deeply into the “why” of irreproducible scientific studies. The most recurrent theme is money—whether it’s institutional pressure to produce tangible results and churn out papers in order to secure grant money, or even drawing out a single study into multiple papers to maximize the numbers of publications and the subsequent income. But Ritchie’s approach is not at all pessimistic. He simply diagnoses a pressing issue across all disciplines of scientific inquiry, addresses the symptoms and the underlying disease, and then prescribes a solution for “Fixing Science,” which he elaborates upon in his final chapter.

Perhaps the most helpful part of the whole book indeed comes at the very end in an appendix titled “How to Read a Scientific Paper.” Ritchie provides his reader with a list of critical questions to ask oneself when reading a paper in any science publication to ensure that their understanding of the research and results described is not misleading, and prevent the potential spread of misinformation following a reading of such a paper.

Overall, the book is a quick, well-written, and enlightening read.

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