



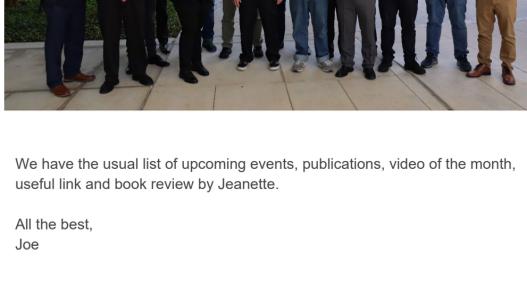
Volume 15, No. 4, April 2023

WELCOME

In March, I had the pleasure of visiting Aarhus University for an IUCr Finance Committee meeting, where I met Bo Brummerstedt Iversen for the first time. After a tour of his lab, I knew who would provide the Lab in the Spotlight for April.

I chose Rigaku Reagents as the Product in the Spotlight for several reasons, the most of which is that haven't done so before. Rigaku Reagents moved to The Woodlands in August and have increased capacity with a new Tecan liquid handler.

Last month, Rigaku Europe held an open house in conjunction with the DGK Meeting held in Frankfurt. This week we held two open houses in The Woodlands to celebrate the recently installed XtaLAB Synergy-ED. We had folks from Texas on April 11 and people from around the US on April 13. Todd Hudnall, Texas State University San Marcos, Chris Malliakas of Northwestern University, Jose Rodriguez of UCLA, and Jacob Brink of JEOL all gave excellent lectures on various aspects of the MicroED/3DED. You can watch the lectures and download the presentation slides [here](#). You can tell from the pictures everyone had a great time and sees a bright future for MicroED/3DED.



We have the usual list of upcoming events, publications, video of the month, useful link and book review by Jeanette.

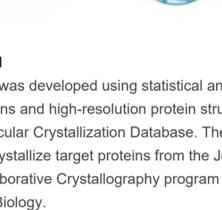
All the best,
Joe

PRODUCT IN THE SPOTLIGHT

Rigaku Reagents: Reagents, Crystallization Kits and Crystallography Tools

Crystallization of macromolecules is challenging and requires examining a large number of variables through crystallization space. Rigaku Reagents screens offer a broad range of conditions to give you the highest probability of crystallizing your proteins of interest.

Rigaku Reagents is a leading provider of protein science solutions. We develop and supply reagent kits, stock solutions, proteins, and accessories for protein researchers. An innovation leader, the team at Rigaku Reagents continues to create award-winning research tools that accelerate discovery and decision-making in protein labs worldwide. Our reagents and stock solutions are available individually, in convenient screens, and as custom products.



BERKELEY SCREEN

The Berkeley Screen was developed using statistical analysis of the crystallization conditions and high-resolution protein structures in the Biological Macromolecular Crystallization Database. The screen has been extensively used to crystallize target proteins from the Joint BioEnergy Institute and the Collaborative Crystallography program at the Berkeley Center for Structural Biology.

WIZARD JCSG+ SCREENS

JCSG Core Suite screens each contain 96 unique formulations delivered in a deep well block or 10 mL tubes. These screens were designed by analyzing over 500,000 high-throughput crystallization experiments performed at JCSG. These 384 formulations provided the highest hit rates.

The JCSG Top96 and JCSG Top96 Cryo screens were designed for proteins available in limited quantities where conservation of material is of high importance. These screens were designed based on over 1000 deposited protein structures from the JCSG.

WIZARD CLASSIC AND CRYO SCREENS

The Wizard Classic suite of sparse matrix method screens is biased towards, and selected from, well-established crystallization conditions for macromolecules. Different concentrations, components and pH values are used to narrow down favorable crystallization conditions. There are four versions of the Wizard Classic to offer a wider range of formulations for initial setup. Wizard 2 has many of the same components as Wizard 1, just different concentrations, pHs and pairings with other components. Wizard 3 and 4 were developed from proven, successful solutions from which others have grown crystals.

The Wizard Cryo screen is a sparse matrix screen whose formulations will flash-cool to a clear amorphous glass in liquid nitrogen or in the cryo-stream at 100K. Crystals grown in the Wizard Cryo screen can be flash frozen straight from the drop, thus avoiding the additional step of testing for cryoconditions.

WIZARD PRECIPITANT SYNERGY SCREEN

Use of this screen is advised for protein targets that have failed to yield hits with traditional random sparse matrix crystallization approaches. The Wizard Precipitant Synergy screen targets all types of soluble protein and protein complexes. Tests have shown that this screen can triple the number of unique crystals when compared with other screens. Each unique formulation is made available in three different concentrations, increasing the coverage of crystallization space.

WIZARD pH BUFFER SCREEN

The Wizard pH Buffer screen is an optimization screen that can be applied to your crystallization hit conditions to simultaneously explore the effects of pH and buffer composition on crystal growth.

WIZARD PEG ION SCREEN

The Wizard PEG Ion Screens combine the crystallizing power of polyethylene glycols (PEGs) with salts that are commonly found in crystallization conditions. Best used for coarse screening.

STOCK SOLUTIONS

Use our stock solutions directly or as a component in solutions you create in your own lab. Rigaku Reagents prepares its stock solutions using high-quality raw materials, ASTM Type 1 water, and sterile packaging. We offer a wide variety of salts, buffers and precipitants in a range of concentrations and pHs. These stock solutions are the same used to produce our crystallization screens. They can be used to set up crystallization experiments by hand or can be used on liquid-handling instrumentation.

Rigaku Reagents also provides complete stock solution libraries. Build your own customized solution library to maximize the reproducibility of your experiments with high-quality stock solutions.

Additionally, you can order fully customized screens in deep well or larger formats.

CRYSTALLIZATION TOOLS

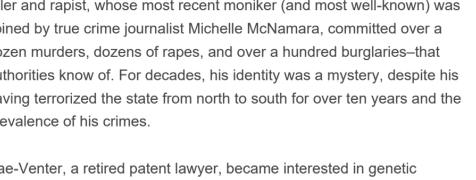
Cryo-crystallography is an invaluable technique for single crystal X-ray diffraction and provides many benefits including mitigation of radiation damage. The technique requires special tools and practical considerations to be successful.

Rigaku Reagents is pleased to offer a number of these tools for cryo-crystallography, including cryovial clamps, pin tongs and magnetic pin tools.

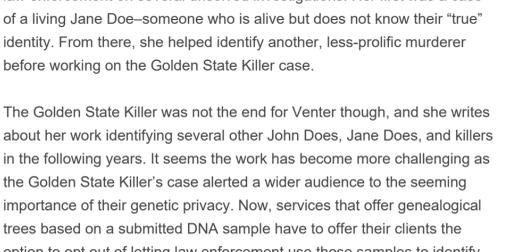
Additionally, Rigaku Reagents offers Unipucks and Unipuck tools for high-throughput crystallography. The pucks and tools are available individually or as kits. Pucks are supplied with unique IDs. Custom identifiers are available on request.

OPTIMIZATION

When initial screening produces small crystals or just promising hits, optimization around these conditions becomes necessary by adjusting the various parameters from initial crystallization trials. For example, one might vary salt or precipitant concentration, pH, biomolecule concentration or use additives.



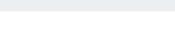
LAB IN THE SPOTLIGHT



Above is a very happy Bo Brummerstedt Iversen standing next to his XtaLAB Synergy-S.

Research in the [Brummerstedt Iversen Group](#) focuses on exploiting the tremendous power of structural studies to obtain a proper understanding of material properties. This involves materials synthesis and advanced property characterization, as well as first principles computations and includes diverse fields of study: thermoelectrics and semiconductors, battery materials, electron density and chemical bonding, nanomaterials, *in situ* studies, electrocatalysis, high-pressure and advanced crystallography. I was poking around the Department of Chemistry's website and found he has published 777 papers, an impressive tally.

BOOK REVIEW



Review: [I Know Who You Are: How an Amateur DNA Sleuth Unmasked the Golden State Killer and Changed Crime Fighting Forever](#)

By Barbara Rae-Venter
ISBN: 9780593358894

Barbara Rae-Venter's *I Know Who You Are: How an Amateur DNA Sleuth Unmasked the Golden State Killer and Changed Crime Fighting Forever* is an electrifying combination of memoir and mystery. Rae-Venter, who until the publication of her book had chosen to remain anonymous, is the retired lawyer turned amateur genetic genealogist whose research identified the Golden State Killer's identity back in 2018. The prolific serial killer and rapist, whose most recent moniker (and most well-known) was coined by true crime journalist Michelle McNamara, committed over a dozen murders, dozens of rapes, and over a hundred burglaries—that authorities know of. For decades, his identity was a mystery, despite his having terrorized the state from north to south for over ten years and the prevalence of his crimes.

Rae-Venter, a retired patent lawyer, became interested in genetic genealogy as a hobbyist. She submitted her own DNA to answer some questions about her family history, learning that some of her ancestral connections were not as family lore had long claimed. In *I Know Who You Are*, Venter details her initial intrigue and subsequent partnering with local law enforcement on several unsolved investigations. Her first was a case of a living Jane Doe—someone who is alive but does not know their "true" identity. From there, she helped identify another, less-prolific murderer before working on the Golden State Killer case.

The Golden State Killer was not the end for Venter though, and she writes about her work identifying several other John Does, Jane Does, and killers in the following years. It seems the work has become more challenging as the Golden State Killer's case alerted a wider audience to the seeming importance of their genetic privacy. Now, services that offer genealogical trees based on a submitted DNA sample have to offer their clients the option to opt out of letting DNA enforcement use those samples to identify criminals.

Regardless of where one stands on the issue of genetic privacy and the right to one's own DNA, *Know Who You Are* is impossible to put down. Venter's writing is open and accessible, and she brings an element of personal warmth and care to what can seem a very impersonal and cold pursuit of justice. Even if you follow the news or are a true crime enthusiast and already know the outcomes of every case outlined in Venter's book, it is still worth a read.

Jeanette S. Ferrara, MFA

RIGAKU TOPIQ WEBINARS

Rigaku has developed a series of 20–30 minute webinars that cover a broad range of topics in the fields of X-ray diffraction, X-ray fluorescence and X-ray imaging. You can watch recordings our past sessions [here](#).

UPCOMING WEBINAR

[TOPIQ | The New ACTOR 2 Sample Changer for Automating your Single Crystal Workflow.](#)

Wednesday, April 26, 9AM CDT.

UPCOMING EVENTS:

[PPXRD-17](#), Pharmaceutical Powder X-ray Diffraction Symposium, Newtown Square, PA, May 21-24, 2023

[CCCW23](#), 14th Canadian Chemical Crystallography Workshop, Vancouver, Canada, May 30-June 3, 2023

[CSC 2023](#), Canadian Chemistry Conference and Exhibition, Vancouver, Canada, June 4-8

[ACA Summer Course for Chemical Crystallography](#), Evanston, IL, June 19-26, 2023.

[ACA 2023](#), 73rd ACA Annual Meeting, Baltimore, MD, July 7-11, 2023.

[IUCr 2023](#), 26th Congress and General Assembly of the International Union of Crystallography, Melbourne, Australia, August 22-29, 2023.

CRYSTALLOGRAPHY IN THE NEWS

January 11, 2023

Scientists Australia, China, Italy, Switzerland, the UK and the US have synthesized and characterized an [electrically actuated molecular motor](#).

March 15, 2023

Researchers from the UK and US describe the synthesis and characterization of a chiral, non-racemic and stable molecule [in which an oxygen atom is the chiral center](#).

March 30, 2023

Researchers from École Polytechnique Fédérale de Lausanne used palladium (IV) catalysts to [convert alkyl and aryl olefins to ketones](#) via a modified Wacker oxidation.

USEFUL LINKS

It has been just over a year since Russia invaded Ukraine. This link is a year old but still provides useful information regarding relief efforts for Ukraine: [Here's how you can help the people of Ukraine](#) : NPR

Here is an interesting link that will help teach youngsters that they can't believe everything they find on the web: [Save The Pacific Northwest Tree Octopus](#) ([zapatopi.net](#))

VIDEO OF THE MONTH

Here is a [short video of the pale blue dot](#) from the second stage of a SpaceX rocket as it enters geosynchronous orbit.

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.

[JOIN HERE](#)

RIGAKU X-RAY FORUM

At [rigakuxrayforum.com](#) 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.

[JOIN HERE](#)

