

Crystallography Newsletter
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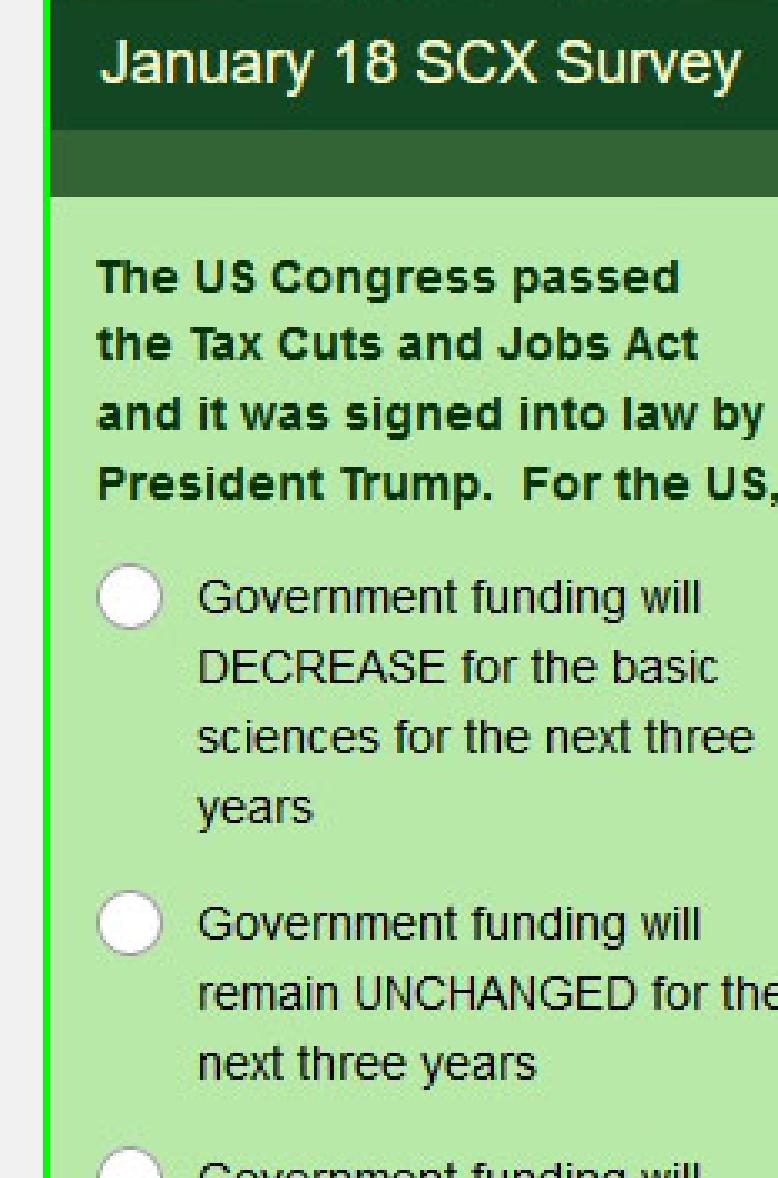
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Join ROD on LinkedIn

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



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^{Pro} software for single crystal data processing.

We look forward to seeing you on there soon.

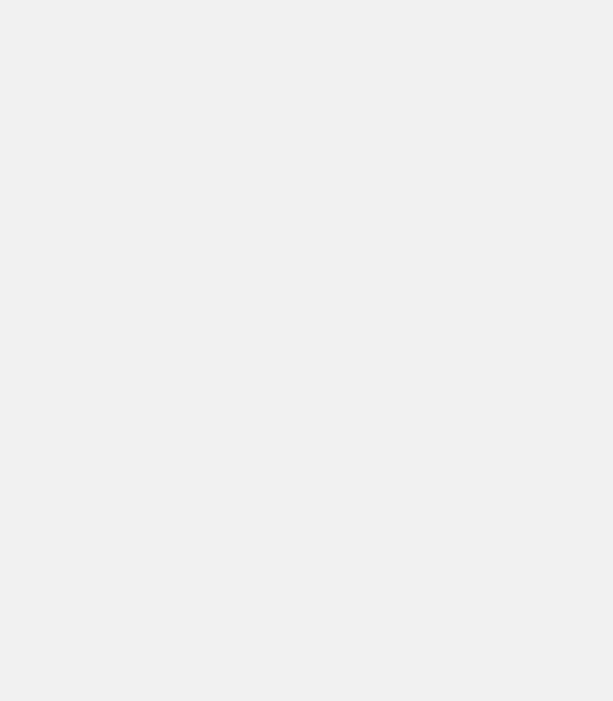
Survey of the month



Take the Survey

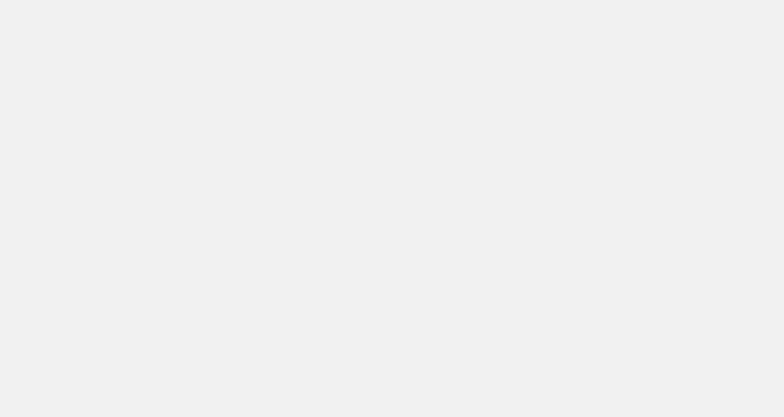
Last month's survey

Sexual harassment has come out of the shadows and we are beginning to come to terms with this unacceptable behavior:



Video of the month

Here is *Science Magazine's* top ten breakthroughs of last year.



Watch the Video

Upcoming events

Biophysical Society 2018

Feb 17 – 21, 2018 in San Francisco, CA, USA

Texas Society for Microscopy 2018

Feb 22 – 24, 2018 in Denton, TX, USA

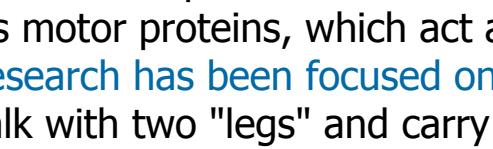
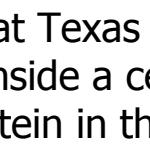
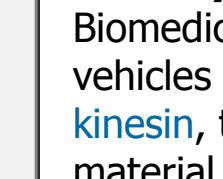
26th Annual Meeting of the German Crystallographic Society (DGK 2018)

Mar 5 – 8, 2018 in Essen, Germany

NESBA: The Resolution Revolution in cryoEM: Potential for Drug Discovery

Mar 16, 2018 in Waltham, MA, USA

[See full list >](#)



Crystallography in the news

January 2, 2018. Dr. Wonmuk Hwang, associate professor in the Department of Biomedical Engineering at Texas A&M University, researches motor proteins, which act as vehicles to carry cargo inside a cell in the body. His latest [research](#) has been focused on *kinesin*, the smallest protein in the human body that can walk with two "legs" and carry material throughout the body on intracellular filaments called microtubules.

January 3, 2018. In order to identify the [exact receptor on the pollen tube for the LURE peptide](#), Tetsuya Higashiyama, a professor at Nagoya University and his collaborators at Tsinghua University, who have expertise in structural biology of plant ligands and receptors, performed analyses of the complexes by X-ray crystallography. The team examined the protein that binds to LURE peptide.

January 4, 2018. An international team of scientists that includes top researchers at the Bridge Institute at the USC Michelson Center for Convergent Bioscience captured the [crystal structure of the kappa opioid receptor](#) — critical for providing pain relief — in action on the surface of human brain cells. The researchers also made another important discovery: a new opioid-based compound that, unlike current opioids, activates only the kappa opioid receptor, raising hopes that they may develop a painkiller that has no risk of addiction and, therefore, none of the devastating consequences and side effects that accompany it.

January 4, 2018. Osaka University researchers develop [new green fluorescent protein that can withstand low pH](#) environment for imaging of acidic organelles. Visualizing cellular components and processes at the molecular level is important for understanding the basis of any biological activity. Fluorescent proteins (FPs) are one of the most useful tools for investigating intracellular molecular dynamics.

January 8, 2018. Crystallographer Dr. Claire Murray tells Elaine Burke how she [found her love for art through science](#), and unearthed untold stories on the way. She is actively involved in outreach activities with Diamond and the British Crystallographic Association, promoting science and crystallography to the public.

January 16, 2018. Mysterious microbes that thrive in hot and super-salty brine lakes at the bottom of the Red Sea could yield a treasure trove of [new enzymes for industrial applications](#)—if only scientists had access to their biological bounty. A new study led by KAUST scientists now spells out a way to exploit this vast untapped resource.

January 18, 2018. A team of Yale University researchers has discovered an anti-aging protein, named after a Greek goddess, which may play an important role in the treatment of multiple diseases ranging from diabetes to cancers. The findings indicated that the three-dimensional [X-ray crystal structure of one of the so-called Klotho proteins](#) has a big role in the regulation of longevity and metabolism.

Product spotlight

XtaLAB Synergy Custom

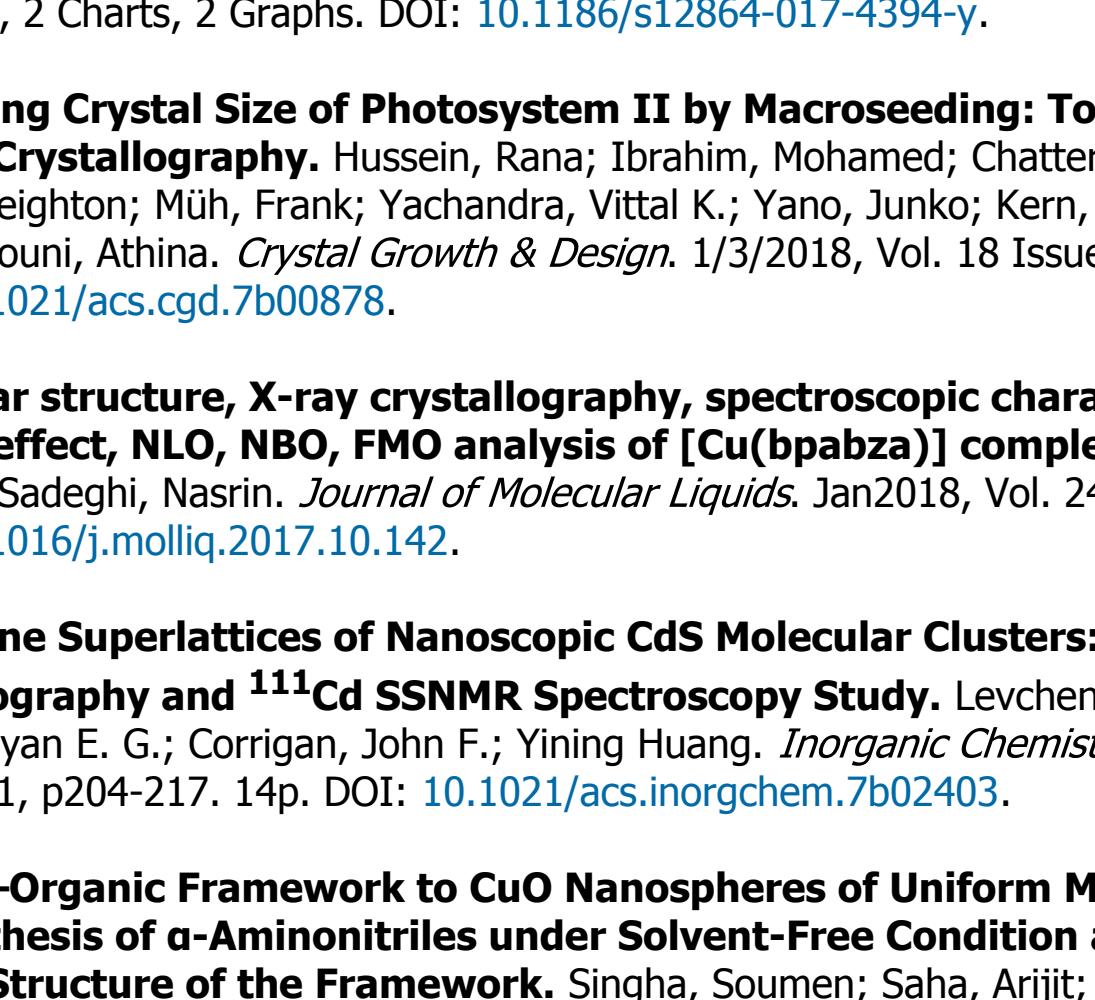
We realize that standard systems may not fit the needs for every lab, so we offer XtaLAB Synergy Custom single crystal X-ray diffractometers for those labs who want to take advantage of dual ports or want to integrate special components, such as [ACTOR sample changers](#). Additionally, for laboratories that want even greater flux we offer the FR-X based diffraction systems.

HPC detector

XtaLAB Synergy Custom systems are configured with a Hybrid Photon Counting (HPC) X-ray detector, such as the HyPix-6000HE, PILATUS or ELGER. HPC detectors are ideal for macromolecular crystallography experiments because they are photon counting detectors that directly detect X-ray photons without the need for the intermediate step of converting X-ray photons to light with a phosphor or scintillator. As a result, HPCs have high dynamic range, fast readout speed and extremely low noise. Additionally, HPC X-ray detectors have a top-hat point spread function of a single pixel. These combined features, along with shutterless data collection, mean that you can collect more accurate diffraction data, faster. As a result, the XtaLAB Synergy Custom systems offer outstanding performance for your single crystal X-ray diffraction experiments.

Dual Port Capability

The XtaLAB Synergy Custom system includes a dual port, microfocus rotating anode X-ray generator. With XtaLAB Synergy Custom systems, you can have two single crystal end stations or you can configure the second port with a small angle X-ray scattering system, such as the BioSAXS-2000^{nano}. Additionally, the XtaLAB Synergy Custom comes in a custom-designed enclosure with your choice of table size, to accommodate accessory equipment, such as an ACTOR system or microscope close to the goniometer. Thus, the versatility offered by the XtaLAB Synergy Custom system provides the most flexibility possible for your structural biology program.

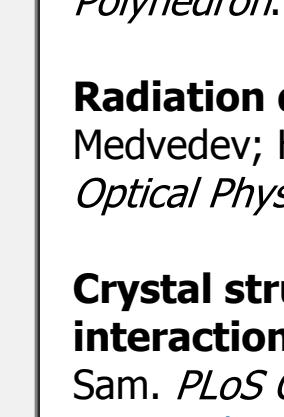


Features:

- Customized systems for structural biology and chemical crystallography utilizing a high flux microfocus source
- Your choice of VariMax™ confocal double-bounce optics for better spectral purity and beam size to match your sample types
- Four-circle goniometer to provide completeness and redundancy for your data sets
- HPC detector with single pixel point spread function and true shutterless data collection
- Dual ports allow for various combinations of crystallography and SAXS ports
- Options for *in situ* crystallography and automated mounting for cryo-protected samples

[For more about XtaLAB Synergy Custom >](#)

Lab in the spotlight



Alexander Wlodawer, Ph.D.

Chief, Macromolecular Crystallography Laboratory

Head, Protein Structure Section

Center for Cancer Research

National Cancer Institute

Dr. Wlodawer is a structural biologist investigating the relationship between protein structure and function, mainly by high-resolution X-ray diffraction. Some of his areas of interest include elucidating structural features of macromolecules that could explain their importance to understanding cancer and AIDS. Examples include proteases, viral glycoproteins and enzymes, and proteins that are part of cell signaling systems, in particular cytokines and their receptors. He is also active in the development of crystallographic methods.

The Protein Structure Section investigates the relationship between protein structure and function, mainly by the technique of high-resolution X-ray diffraction. Some of the areas of interest are directly involved in elucidating structural features of the molecules that could explain their importance to understanding cancer and AIDS, but the group is also active in the development of methods for protein crystallography.

Additional projects investigated by the Protein Structure Section include crystallographic studies of proteases and their inhibitors, cytokines and cytokine receptors, and lectins with antiviral activity.

[For more about the Macromolecular Crystallography Laboratory >](#)

Useful link



Open Access Crystallography Resource Portal

I was poking around the IUCr website and found this useful link: a long list of crystallographic databases maintained by Portland State University's Nano-Crystallography Group.

Selected recent crystallographic papers

Crystallography and the liquid crystal phase: a new approach to structural studies on a thermo-tropic smectic Schiff base. Piro, Oscar Enrique; Echeverría, Gustavo Alberto; Cukiernik, Fabio Daniel. *Crystallography Reviews*. Jan2018, Vol. 24 Issue 1, p3-21. 19p. DOI: [10.1080/0889311X.2017.1320550](https://doi.org/10.1080/0889311X.2017.1320550).

Papain-like cysteine proteases in *Carica papaya*: lineage-specific gene duplication and expansion. Juan Liu; Sharma, Anupma; Niewiara, Marie Jamille; Singh, Ratnesh; Ray Ming; Qingyi Yu. *BMC Genomics*. 1/6/2018, Vol. 19, p1-12. 12p. 3 Diagrams, 2 Charts, 2 Graphs. DOI: [10.1186/s12864-017-4394-y](https://doi.org/10.1186/s12864-017-4394-y).

Optimizing Crystal Size of Photosystem II by Macroseeding: Toward Neutron Protein Crystallography. Hussein, Rana; Ibrahim, Mohamed; Chatterjee, Ruchira; Coates, Leighton; Mühl, Frank; Yachandra, Vitali K.; Yano, Junko; Kern, Jan; Dobbek, Holger; Zouni, Athina. *Crystal Growth & Design*. 1/3/2018, Vol. 18 Issue 1, p85-94. 10p. DOI: [10.1021/acs.cgd.7b00087](https://doi.org/10.1021/acs.cgd.7b00087).

Molecular structure, X-ray crystallography, spectroscopic characterization, solvent effect, NLO, NBO, FMO analysis of [Cu(bpbabz)] complex. Khajehzadeh, Mostafa; Sadeghi, Nasrin. *Journal of Molecular Liquids*. Jan2018, Vol. 249, p281-293. 13p. DOI: [10.1016/j.molliq.2017.10.142](https://doi.org/10.1016/j.molliq.2017.10.142).

Crystalline Superlattices of Nanoscopic CdS Molecular Clusters: An X-ray Crystallography and ¹¹³C SSNMR Spectroscopy Study. Levchenko, Tetyana I.; Lucier, Bryan E. G.; Corrigan, John F.; Yining Huang. *Inorganic Chemistry*. 1/2/2018, Vol. 57 Issue 1, p204-217. 14p. DOI: [10.1021/acs.inorgchem.7b02403](https://doi.org/10.1021/acs.inorgchem.7b02403).

A Metal–Organic Framework to CuO Nanospheres of Uniform Morphology for the Synthesis of α-Aminonitriles under Solvent-Free Condition along with Crystal Structure of the Framework. Singha, Soumen; Saha, Arjita; Goswami, Somen; Dey, Sanjoy Kumar; Payra, Soumen; Banerjee, Subhash; Kumar, Sanjay; Saha, Rajat. *Crystal Growth & Design*. 1/3/2018, Vol. 18 Issue 1, p189-199. 11p. DOI: [10.1021/acs.cgd.7b01085](https://doi.org/10.1021/acs.cgd.7b01085).

Design of Bulk Protein Crystallization Based on Phase Diagrams Accounting for the Presence of Interfacial Water. Kolodziej, Michal; Poplewska, Izabela; Piatkowski, Wojciech; Antos, Dorota. *Crystal Growth & Design*. 1/3/2018, Vol. 18 Issue 1, p393-401. 9p. DOI: [10.1021/acs.cgd.7b01398](https://doi.org/10.1021/acs.cgd.7b01398).

Control of Polymorphism of Metal–Organic Frameworks Using Mixed-Metal Approach. Tanasaro, Thanadporn; Adpakpong, Kanyaporn; Itisanronnachai, Somlak; Faungnawakij, Kajornkij; Butburee, Teera; Wannapaiboon, Suttipong; Ogawa, Makoto; Bureekaew, Sareeya. *Crystal Growth & Design*. 1/3/2018, Vol. 18 Issue 1, p16-21. 6p. DOI: [10.1021/acs.cgd.7b01193](https://doi.org/10.1021/acs.cgd.7b01193).

Crystallographic and enzymatic insights into the mechanisms of Mg-ADP inhibition in the A₁ complex of the A₁A₀ ATP synthase. Singh, Dhirendra; Grüber, Gerhard. *Journal of Structural Biology*. Jan2018, Vol. 201 Issue 1, p26-35. 10p. DOI: [10.1016/j.jsb.2017.10.008](https://doi.org/10.1016/j.jsb.2017.10.008).

Cyclic olefin copolymer as an X-ray compatible material for microfluidic devices. Denz, Manuela; Brehm, Gerrit; H?monnot, Cl?ment Y.; Spears, Heidi; Wittmeier, Andrew; Cassini, Chiara; Saldaña, Oliva; Perego, Eleonora; Diaz, Ana; Burghammer, Manfred; Köster, Sarah. *Lab on a Chip – Miniaturisation for Chemistry & Biology*. 1/7/2018, Vol. 18 Issue 1, p171-178. 8p. DOI: [10.1039/c7lc00824d](https://doi.org/10.1039/c7lc00824d).

Structural and biophysical characterization of Rv3716c, a hypothetical protein from *Mycobacterium tuberculosis*. Gopalan, A.; Deka, G.; Prabhavathi, M.; Savithri, H.S.; Murthy, M.R.N.; Raja, A. *Biochemical & Biophysical Research Communications*. Jan2018, Vol. 495 Issue 1, p982-987. 6p. DOI: [10.1016/j.bbrc.2017.11.093](https://doi.org/10.1016/j.bbrc.2017.11.093).

Synthesis, cytotoxic activity and DNA-binding properties of copper(II) complexes with terpyridine. Glisić, Biljana D.; Nikodinović-Ruric, Jasmina; Ilic-Tomic, Tatjana; Wadeholt, Hubert; Veselinovic, Aleksandar; Ospenski, Igor M.; Djuranić, Miloš I. *Polyhedron*. Jan2018, Vol. 139, p313-322. 10p. DOI: [10.1016/j.poly.2017.11.008](https://doi.org/10.1016/j.poly.2017.11.008).

Radiation damage free ghost diffraction with atomic resolution. Zheng Li; Nikita Medvedev; Henry N Chapman; Yanhua Shih. *Journal of Physics: B Atomic Molecular & Optical Physics*. 1/28/2018, Vol. 51 Issue 2, p1-1. 1p. DOI: [10.1088/1361-6455/aa9737](https://doi.org/10.1088/1361-6455/aa9737).

Crystal structure of huanan NLRP12 PYD domain and implication in homotypic interaction. Jin, Tengchuan; Huang, Mo; Jiang, Jiansheng; Smith, Patrick; Xiao, Tsan Sam. *PLoS ONE*. 1/2/2018, Vol. 13 Issue 1, p1-11. 11p. DOI: [10.1371/journal.pone.0190547](https://doi.org/10.1371/journal.pone.0190547).

Alcoholysis of Al₂(OBu)₆ - Synthesis and Crystal Structure of Al₉O₃(OEt)₂₁. Nachtigall, Olaf; Hirsch, Tobias; Spandl, Johann. *Zeitschrift für Anorganische und Allgemeine Chemie*. 1/17/2018, Vol. 644 Issue 1, p2-5. 4p. DOI: [10.1002/zaac.201700327](https://doi.org/10.1002/zaac.201700327).

X-ray crystal structures and anti-breast cancer property of 3-*tert*-butoxycarbonyl-2-arylhiazolidine-4-carboxylic acids. Jagtap, Rohidas M.; Thorat, Shridhar H.; Gonnade, Rajesh G.; Khan, Ayesha A.; Pardeshi, Satish K. *New Journal of Chemistry*. 1/15/2018, Vol. 42 Issue 2, p1078-1086. 9