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Calendar of events

Rigaku will be attending the following conferences in the coming months:

- [SouthWest Macromolecular Symposium](#), The Woodlands, TX, October 24-26
- [XV PSDI Workshop](#), Autrans, France, October 28-30
- [NIH RoadMap Membrane Protein Technology Meeting](#), La Jolla, CA, November 1-2
- [Asian Crystallographic Association](#), Taipei, Taiwan, November 4-7
- [MRS](#), Boston, MA, November 26-29
- [Fragment-based Lead Discovery Conference](#), San Diego, CA, February 18-20, 2008

Training Sessions

Newsletter Vol. 5, No. 2, Fall 2007

A word from our president: Providing tools

The analytical instrument business is really about providing people with tools that help them achieve success in their work. Tool usage is typically considered to be a sign of higher intelligence and, for those of us involved with analytical instruments, there may be a tendency to think of ourselves as pretty high up the intelligence ladder. But there are many examples of tool usage by primates other than humans and when you examine their use of tools you have to wonder how far we have really come; the problems we are trying to solve might be more complicated but the type of questions we are trying to answer are very similar.

The accompanying photo captures a gorilla using a stick to measure the depth of a pond that it is wading into; the depth of the water is of critical interest as the gorilla does not want to drown. Depth, distance, or length: aren't these the same questions many of us ask in our use of analytical instruments? From the person working in a semiconductor fab who uses XRF to measure thin-film depth, the structural biologist who uses X-ray analysis to measure the geometry of the active site in an important enzyme, or the gorilla crossing the pond—fast, accurate knowledge of critical parameters can mean the difference between success and failure. At Rigaku we are dedicated to helping you predict your success by giving you the tools you need to cross your own river.



Paul N. Swepston

NANOHUNTER wins R&D 100 Award

Rigaku Americas Corporation is pleased to announce that the NANOHUNTER benchtop total reflection X-ray fluorescence (TXRF) spectrometer has won the 2007 R&D 100 Award. Presented annually for 44 years by R&D Magazine, the R&D 100 Award is a mark of excellence known to industry, government, and academia as proof that the winner is one of the most innovative products of the year.

The NANOHUNTER was specifically designed to offer comprehensive trace element and materials characterization analysis capabilities to a broader range of research disciplines, and in more diverse analytical settings, than was possible with previous technology. Whether for geologists, chemists, biochemists, biologists, materials scientists and engineers, non-destructive trace element analysis is attainable, with minimal to no sample preparation, for applications that span from metallo-protein research to environmental assessment and semiconductor wafer metrology.

Providing both trace-level elemental analysis and evaluation of the physical nature of the sample, NANOHUNTER uses a patented switchable wavelength and automated variable X-ray incidence angle excitation design. The instrument can analyze the full range of elements, from aluminum (Al) to uranium (U), in solids, liquids, and powders. It also provides chemical information as a function of analysis depth for profiling surface characteristics of materials. As an example, for researchers involved in nanotechnology, this ability allows surface layers to be characterized as particles on a substrate, a homogenous thin film, or as something in between.



With sensitivity on par with inductively coupled plasma optical emission spectroscopy (ICP-OES), NANOHUNTER provides part-per-billion (PPB) level detection limits for liquid samples in a fully automated tool. Halogens can be analyzed with high reproducibility. Organic liquids may also be measured without sample preparation and sample volumes as small as 50 microliters may be analyzed.

Direct measurement of solids and powders provides freedom from complex sample digestion or preparation and makes this spectrometer suitable for replacing or supplementing traditional atomic spectroscopy methods. Compared to other trace level atomic spectroscopy techniques, the revolutionary aspect of NANOHUNTER is in the minimal level of sample preparation required. It liberates the operator from ancillary equipment—like fume hoods and microwave

Rigaku is pleased to announce the following training sessions:

- Macromolecular
 - March 26-28, 2008
 - September 17-19, 2008
- XRD (MiniFlex II):
 - October 23-24, 2007
 - December 4-5, 2007
 - February 19-20, 2008
 - September 23-24, 2008
- XRD (
 - December 11-12 (13), 2007
 - January 8-9 (10), 2008
 - May 20-21 (22), 2008
 - November 4-5 (6), 2008

All classes are held at Rigaku's applications laboratory in The Woodlands, TX.



UK service help desk

In Rigaku Europe's continuing effort to sustain high-quality customer service through personal accountability and professional commitment to you and your research, we are pleased to announce a new, dedicated phone number and e-mail address for our customers in Europe.

Phone: +[44] 1732 765 008
E-mail: ServiceEurope@Rigaku.com

Targeted at resolving your service issues promptly and accurately, our dedicated Service Helpdesk will put you in contact with the correct Rigaku professionals when you need them.

SWMS 2007

There's still time to register for the [SouthWest Macromolecular Symposium](#), which is being held at the Shenandoah Conference & Visitors Center near The Woodlands, TX from October 24-26, 2007.

The keynote speaker is Dr. Stephen K. Burley, SGX Pharmaceuticals

>>> [Click here for more information](#)

Limestone analysis with the Primini®

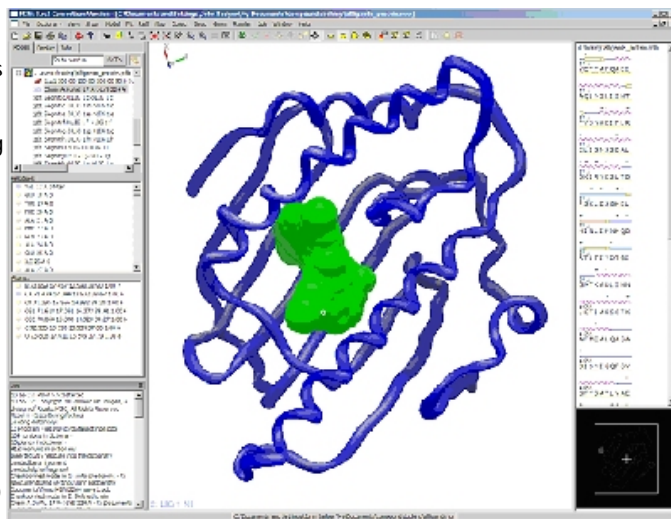
Limestone quarry lab technicians are required to take samplings frequently and respond quickly to certify product

digesters—associated with trace element analysis in a wet laboratory environment.

FBLD 2008 Conference: Perspectives on drug discovery and X-ray crystallography's increasing role

ActiveSight® and Rigaku are organizing a Fragment-based Lead Discovery (FBLD) Conference February 2008 in San Diego. FBLD is a technique that utilizes smaller compounds and libraries to screen drug lead chemical space more thoroughly, leading to more tightly binding compounds than traditional high-throughput screening. Fragment libraries can be screened using biochemical assays, surface plasmon resonance, NMR, or X-ray crystallography. Advances in high-throughput crystallization, data collection, and structure determination have made crystallographic screening much more achievable. X-ray crystallographers can now have an even greater impact on drug discovery programs by creating lead compounds using FBLD.

The conference's agenda has been put together by a scientific advisory board comprised of FBLD pioneers from ActiveSight, Astex Therapeutics, Novartis, Sunesis, and Vernalis. The opening plenary speaker will be Stephen Fesik from Abbott Labs, creator of the "SAR by NMR" method. The closing plenary speaker will be Christopher Lipinski, formerly of Pfizer, who determined the "Rule of 5" which is used universally as a guide for druglike compounds. Along with speakers from Plexikon, SGX Pharmaceuticals, UCSF, and University of Washington, among others, the conference will provide a forum to discuss the status and future of lead discovery and optimization, and FBLD's role.



ActiveSight and Rigaku have been instrumental in the emergence of FBLD as a Lead Discovery ActiveSight's Vicki Nienaber did groundbreaking work at Abbott to establish that crystallography could be automated for fragment screening, and was co-inventor of Rigaku's ACTOR™ crystal-mounting system robot. Rigaku's ACTOR and powerful in-house generators facilitate the rapid data collection needed for screening the large number of crystals needed. ActiveSight uses the Ultimate HomeLab™ to screen their Fragment library in-house. The data are then processed by MIFit+ Rigaku's automated structural determination software that was based on ActiveSight President Duncan McRee's popular Xfit software. ActiveSight collaborates with its pharmaceutical and biotech partners to screen their drug targets, and they also have internal drug discovery programs. Rigaku's innovation in high-throughput crystallization and crystallography has also enabled FBLD at Astex Therapeutics, who have put several lead compounds into clinical trials.

FBLD 2008 will take place at Paradise Point Resort & Spa, a 44 acre private island in San Diego. Emphasis will be placed on creating an atmosphere that is conducive to scientists interacting. Exhibitors will also provide information on complementary technologies such as surface plasmon resonance, calorimetry, and NMR. An FBLD methods and implementation workshop is also planned. For more information, e-mail ActiveSight.

Two advanced CCD X-ray detectors announced at ECM24

Rigaku Americas Corporation introduced two new high-performance CCD-based X-ray area detectors at the 24th European Crystallographic Meeting (ECM24) in August. Optimized for macromolecular and small molecule X-ray crystallography respectively, the Saturn 944+ and Saturn 724+ were internally designed, developed and manufactured by Rigaku as part of an on-going commitment to providing the most advanced tools for structural biology and chemistry research and development.

Bringing a new dimension to high-throughput data collection, with a 4-fold increase in readout speed (to 8 MHz total) and improved signal-to-noise and dynamic range, the Saturn+ line of third generation Rigaku CCD X-ray detectors is optimized for high performance X-ray crystallography applications where maximum productivity is essential. This new generation of CCD detectors delivers extremely high readout speeds without any significant increase in read noise compared to the previous generation of CCD based X-ray detectors. Both detectors employ the advanced Kodak® KAF-4320E CCD sensor, incorporating transparent indium tin oxide (ITO) technology for superior sensitivity. A large format front illuminated sensor, optimized for high dynamic range and superior spatial resolution, is coupled with a state-of-the-art high speed 18-bit analog-to-digital converter and 4 port parallel readout to deliver low noise, a true 17,500:1 dynamic range and ultra fast readout times simultaneously for the first time in such a detector.

The full-frame CCD sensor uses proprietary 2-phase architecture with large pixels for wide dynamic range. To increase the sensitivity of the chip, one of the two polysilicon gates used in conventional CCD sensors has been replaced with the transparent conductor indium-tin-oxide (ITO). This architecture eliminates the need to resort to backside illumination and provides the intrinsically superior dark current characteristics needed to generate the highest quality data.

With a large 94 mm x 94 mm (133 mm diagonal) image area, the Rigaku Saturn 944+ is the definitive CCD X-ray detector specifically optimized for the high throughput and spatial resolution needs of protein and macromolecular crystallography. For small molecule crystallography, the Saturn 724+ features a 72 mm x 72 mm image area (102 mm diagonal). Both detector systems employ an extremely reliable closed loop Joule-Thompson cooling system (no water required) and an in-camera LCD status display panel.

ready to release by truck or trainload. The demand for limestone is increasing due to legislation requiring sulfur dioxide flue gas scrubbers to be installed in oil- and coal- burning power generating plants.

Rigaku's low-powered Primini benchtop WDXRF spectrometer is ideal for limestone analysis using a pressed pellet technique. The analysis of light elements such as Na and Mg can be performed with better sensitivity and improved element resolution compared to similar EDXRF units and without the need of higher-powered WDXRF systems.

A new application byte is available on our web site that describes applicable concentration ranges, sample preparations, calibration and analysis results.

Testimonials

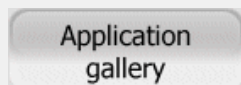
You may have noticed that we've added video content to our website. Some of it is to enhance product descriptions, as in the videos found on the ACTOR product page.

We hope that you find these videos informative and interesting. If you feel inspired to share your thoughts with us, either in print or by video, we'd love to hear from you.

Do you want to brag about something you've accomplished using a Rigaku instrument or pay tribute to a Rigaku employee who helped you through a difficult situation. If so: please [contact Bev Vincent](#).

Application bytes

Rigaku's application specialists are constantly using Rigaku instruments to test and demonstrate their use and capabilities.



We recently decided to make the results of these experiments available on our web site. To that end, we are developing application galleries for many of our products. The galleries themselves (for example, the MiniFlex II gallery) are accessed by clicking on a button like the one above in the right-hand margin of the product page.

The gallery lists available application bytes by title. We call them bytes because they are brief and to-the-point. They usually consist of a description of the importance of the study, a snapshot of the experimental details and the major results.

Complementing the Saturn+ line is the Rigaku Saturn A200, the first "next generation" large area CCD detector to be offered. Incorporating a 2 x 2 array of the Kodak KAF-4320E CCD chips, with a 203 x 203 mm active area, the Saturn A200 brings a new dimension to both synchrotron and home laboratory data collection.

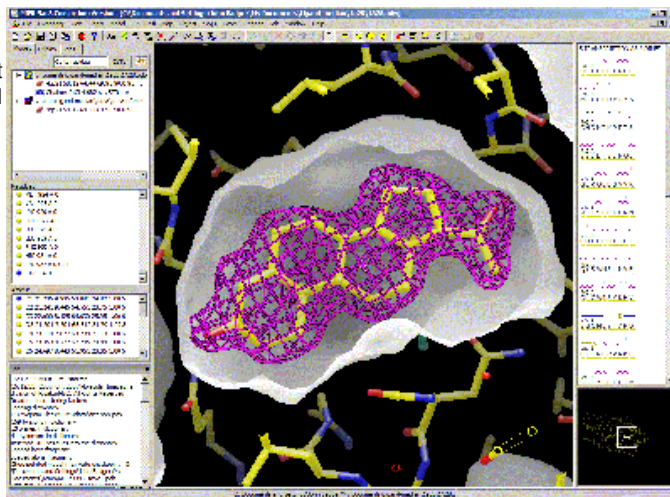
MIFit+ software released

The protein crystal structure solution software, MIFit+, is now available for download. MIFit+ contains a new and updated version of the MIFit model fitting and molecular display program and MIEExpert, a robust expert system for running molecular replacement and refinement applications.

MIEExpert includes a pipeline automation system for analyzing the data obtained from high-throughput co-crystallography and fragment screening projects.

MIFit+ is the software used by the crystallographers at ActiveSight for protein structure solution, crystallographic fragment screening and to create structure reports for project partners.

This software runs on Windows® and LINUX® operating systems; it is free to academic users and a demo version is also available.



ActiveSight and CHDI leverage fragment-based lead discovery for Huntington Disease therapies

ActiveSight announced recently that it will collaborate on a Fragment-based Lead Discovery (FBLD) Project with CHDI, Inc.

FBLD involves the binding of small compounds, "fragments," to the active sites of protein drug targets. The fragments are much smaller than the compounds used in traditional high-throughput screening (HTS), allowing a more extensive sampling of chemical space with a smaller screening library. Utilizing a Huntington Disease (HD) target chosen by CHDI, ActiveSight will screen fragment libraries using X-ray crystallography to visualize fragments that bind to the target. The fragments will then be linked or grown into larger, drug-like compounds that are thought to be more efficiently binding than compounds resulting from HTS methodologies.

Several compounds based on Fragment-based Lead Discovery (FBLD) methodologies are currently in clinical trials, and the technology is thought to shorten the time from drug target selection to an investigational new drug (IND) filing. The two companies hope that the FBLD collaboration will lead to HD therapies in shorter time periods than conventional lead discovery methods such as HTS.

ActiveSight's high-throughput structural biology capabilities will facilitate rapid screening of CHDI's HD target with hundreds of drug-like fragments. Automated data collection and structural determination will be facilitated by Rigaku's tools for high-throughput X-ray crystallography, including the ACTOR crystal-mounting system and MIFit+ automated structural determination software. ActiveSight has leveraged these capabilities to screen several drug targets with their proprietary fragment libraries, and is pursuing lead development on promising fragment hits. The CHDI project will be overseen by Vicki Nienaber, Ph.D. at ActiveSight, a pioneer in the utilization of X-ray crystallography for Fragment-based screening and lead development.

"We are pleased to have the opportunity to work with CHDI to discover new treatments for Huntington Disease," said Duncan McRee. "We will work closely with CHDI's drug discovery team to turn the results of our high-throughput FBLD screens into tightly binding lead compounds."

Rigaku congratulates...

Congratulations to the winners of the Rigaku Fun Run at the 2007 ACA meeting in Salt Lake City.

Left: Jason Bischof, University of North Carolina

Right: Olga Virillova, University of Virginia

Want to know the difference between chocolate and cocoa? We have a MiniFlex II app byte for that. Want to see how we can handle twinned samples? There's an R-AXIS SPIDER app byte for that.

We currently have over seventy bytes on the web site, with more being added each week. If you see one you think a friend would be interested in, click the button at the bottom of the page to forward a link to it.

Send this page
to a friend

What's new?

What's new at www.Rigaku.com:

- 08/28/2007 Rigaku introduces the Ultima IV X-ray diffractometer featuring cross beam optics and a small footprint design
- 08/23/2007 2008 XRD training sessions announced
- 08/15/2007 Job postings updated
- 07/23/2007 July 23, 2007: NANO HUNTER™ wins 2007 R&D 100 Award
- 07/11/2007 The first Rigaku international distributors' meeting, May 21-25, 2007
- 07/09/2007 What can the NitroGen™ do for you? See our slideshow presentation

Congratulations to Jianhua Li from Rigaku, who won the award for Best Poster at the Denver X-ray Conference for his presentation: "Reciprocal space mapping of epitaxial nanowires."

Front, left to right: Kenichi Yaoita, George Stone, George Fischer, Sean Bird

Back row: Joe Ferrara, Jianhua Li, Jeff Weller, Tom Concolino



Rigaku awarded several \$500 conference travel bursaries to post-doctoral fellows who provided compelling explanations about how they intend to pursue careers in structural biology. The recipients of these bursaries were Dr. Ganapathy N. Sarma (UCSD); Eric Ortlund (University of North Carolina); Peter Horanyi (University of Virginia); Bernhard Loll (Max Planck Institute); Natalie Borg (Monash) and Charles Dann III (UT Southwestern).



Eric Ortlund

Peter Horanyi

Charles Dann III

ACTOR User Meeting

The ACTOR User Meeting on September 6-7, 2007 was attended by users from 12 ACTOR sites and members of the Rigaku ACTOR team, ActiveSight and OSS.

To date, there are 42 ACTOR installations worldwide, representing the highest number of sample mounting robots from all commercial, government and academic endeavors combined.

The success of the ACTOR system results from the flexibility for integration, many software advancements, and a continued commitment for development. In keeping with this spirit, the goal of the meeting was to facilitate free discussion among ACTOR users and with the Rigaku ACTOR team to identify bottlenecks, common user problems, and directions for future development. The meeting included presentations from ACTOR



users and open discussion sessions.

The Rigaku ACTOR team also presented new hardware and future development projects. An immediate outcome from the meeting included the creation of a moderated e-mail list available to ACTOR users. Information will be sent out in the coming week describing how ACTOR users can gain access to meeting summaries, presentations, and the ACTOR user bulletin board. We thank those who were able to attend the meeting this year for fruitful discussions and hope to see all ACTOR users at future meetings.



To subscribe to this newsletter or cancel your subscription, [e-mail the webmaster](#).

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[survey](#)