



# The SER-CAT SPECTRUM

A Biannual Newsletter of the Southeast Regional Collaborative Access Team • Spring 2006

## Director's Message

Bi-Cheng Wang



Welcome to the spring 2006 issue of *The SER-CAT Spectrum*. It is a pleasure to share with you some of our accomplishments in 2005 and our plans and activities moving forward. With springtime comes “spring cleaning” and preparation for the new growth that we all look forward to during the season. At SER-CAT we are doing similar preparations, streamlining the tools at our facility and preparing for more growth in outreach, memberships and scientific productivity.

SER-CAT participated in several scientific conferences in 2005, beginning with our annual symposium at St. Jude Children's Research Hospital in March. A report on this event was included in the last issue of *The SER-CAT Spectrum* and also in the summer 2005 issue of the ACA newsletter. Other 2005 conferences included our annual exhibit and presentations at the ACA meeting in Orlando, poster presentations at the IUCr Congress in Florence, Italy, and invited talks and a remote access demonstration at the First Annual UK-Southeast USA Symposium held at the University of Georgia.

For 2006, our symposium series will continue with the third annual SER-CAT symposium, entitled, “Interesting Structures, Methods & Advances in SER-CAT Facilities,” planned at Georgia State University on Friday, March 10, 2006. We would like to thank Irene Weber for volunteering to host this event. Online registration has been set up at [www.ser-cat.org](http://www.ser-cat.org). In addition, we will participate in the annual ACA Meeting, in Honolulu, Hawaii, this summer, which should prove to be a fun-filled event for all.

We will host a booth in the exhibit hall for the fourth consecutive year and present some exciting features available at SER-CAT as well.

Our program continues to flourish each year, and we began 2006 by welcoming in two new members – University of Pittsburgh and Wyeth Research. This brings our total membership to 25 entities using SER-CAT as a significant tool for groundbreaking research. Our strong membership has placed our facility in the forefront of productive beamlines, and now the APS General Users are contributing to our productivity as well.

Please read on for details behind all of these events and more, including an update on robotics and a few comments from our new members. We have reached a mature stage in our program and are moving in a new direction. Now that construction of our facility is behind us, we are looking forward to continually increasing our capabilities for the users and increasing our activities in the crystallographic community. We are here to provide the best resources and the best service possible for our Members. Please feel free to contact us with any comments or suggestions on how we might better serve you. Thank you for reading and best wishes for a prosperous 2006!

**Symposium at GSU**

## Symposium at GSU



Our third annual symposium, entitled “Interesting Structures, Methods and Advances in SER-CAT Facilities,” will be held at Georgia State University, Friday, March 10, 2006. This year's program will combine stimulating structural discoveries with practical methods and aspects of tools at the SER-CAT beamlines from the user's perspective. The program lineup includes speakers from both inside and

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**Symposium at GSU**, from Page 1

outside of SER-CAT's membership.

In addition to the scheduled talks, the SER-CAT Young Investigator and Outstanding Science Awards will be presented for the second consecutive year. These awards are designed to recognize scientific achievements accomplished during the previous year that are related to SER-CAT. More information regarding the awards, and registration information for our symposium, may be found at [www.ser-cat.org](http://www.ser-cat.org). The registration deadline is Friday, February 24. We hope to see you in Atlanta!

## SER-CAT Board Meeting

The next SER-CAT Board meeting will be held at the Westin Atlanta Airport Hotel on Saturday, March 11, 2006. Information on accommodations has been forwarded to Board members in a previous email. The hotel reservation deadline has now been extended to February 23. If you have any questions regarding the Board meeting or agenda, please contact the SER-CAT Administrative Office.

## Robotics Update

The robotics program is now in the commissioning stage on the BM beamline, and the SER-CAT Operations Staff is offering free trial runs to our members. A few of our members have used the robot successfully, but we are still seeking more testing and feedback. To facilitate participation, a few extra sets of hardware have been purchased, allowing our members to use the robot before making an investment. BM mail-in crystallography for robotics work can be assigned upon request for members that have ID time during the following week, in effect, letting them screen on the BM before their ID trip.

The SER-CAT robot is based upon a design from the Advanced Light Source in Berkeley, California. The Operations staff has been working diligently on construction and improvements on the initial design to make it as user-friendly as possible. Sample alignment with an automatic cryogenic mounting system on BM-22 is simplified through the SERGUI software interface. However, the system still allows for mounting by hand, if the user desires.



SER-CAT robot located at BM-22 endstation. Visible features from left to right: cryogenic sample changer, auto-mounter and computer display of crystal centering simplified by SERGUI. Mounting a crystal takes less than 5 seconds.

The auto-mounter has random access to 96 samples, mounted in a precision engineered cryogenic dewar of liquid nitrogen.

Mounting of a crystal takes less than five seconds, during which the crystal temperature is maintained well below 120 K. Centering of a crystal can be done by the user through the remote-controlled xyz goniometer and SERGUI. The auto-mounter transfers all protein crystals at liquid nitrogen cryogenic temperatures very efficiently. To minimize icing during the transfer step and also in the liquid nitrogen of the dewar, the auto-mounter is heated and air dried during each transfer. The cool down stop to cryogenic temperature is rapid before the mount or demount stages of sample transfer.

There are specific hardware requirements for the use of the SER-CAT robot. These are listed in detail along with ordering instructions at [www.ser-cat.org](http://www.ser-cat.org). For additional information about using the robot during your next visit to SER-CAT, please contact Sector Manager, John Chrzas.

## Welcome New Members University of Pittsburgh and Wyeth Research



SER-CAT welcomed two new members in 2005, The University of Pittsburgh and Wyeth Research. This brings our current membership to 25, as shown on the back of this publication. Prior to joining, both members were able to test the facility in order to justify their needs for scientific access and for institutional support. It is a great source

of pride for SER-CAT that researchers are continuing to recognize our strong capabilities, both in terms of new memberships and steady activity from our current members and the APS General User program.

**Wyeth**

*The SER-CAT Spectrum* recently contacted Lidia Mosyak, Head of Crystallography at Wyeth Research, for an update on how they have benefited from their membership. When asked about Wyeth's experience, Dr. Mosyak responded, "Having about half-a-year experience with SER-CAT, we found both beamlines quite reliable and efficient in use, including software upgrades that ease crystallographic computing. The staff is exceptionally helpful and quite knowledgeable."

Wyeth Research chose SER-CAT over other member-based beamlines due to the "fast and convenient access to one of the world's brightest sources of x-ray beams," explained Mosyak. "Operating at two beamlines, ID and BM, gives flexibility in scheduling for data collection and in planning data collection experiments. Another very appealing factor is SER-CAT efforts in automation, such as robotic crystal mounting and robotic alignment capabilities, which will allow for high throughput crystallography. In addition, we have a significant savings in travel time as our previous beamline usage was in California."

Another advantage for Wyeth Research is the very high energy flux on the ID beamline. Dr. Mosyak stated that this feature

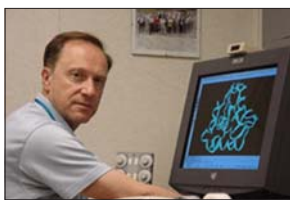
**Welcome New Members**, from Page 2

“makes previously impossible studies possible.” This along with other features has made their use of beamtime extremely productive. “From the data collected so far at SER-CAT, we have solved approximately 30 co-crystal structures; two of them represent exciting protein de-novo structures,” Mosyak proclaimed.

The SER-CAT staff is pleased that our new members are getting the best use of their beamtime, and we want to be sure that all users have the ability to be as productive as possible at our facility. The scientific excellence of the facility will always be the top priority for the SER-CAT program. We welcome any comments regarding your experience at our beamlines so that we may better serve you.

**Kudos!****Congratulations to Alex Wlodawer for Academy Membership**

The following article was originally published in the Volume 13, Number 2, 2005, edition of the IUCr Newsletter. *The SER-CAT Spectrum* would like to thank the author and the IUCr for allowing us to include this reprint to congratulate one of our active SER-CAT members. Kudos to Alex Wlodawer for this esteemed achievement! Please let us know of any awards or recognitions that you or your colleagues have received by contacting the SER-CAT Administrative Office. We hope to highlight other accomplishments within our membership in future issues.

**Academy Membership for Alexander Wlodawer**

Alexander Wlodawer in his laboratory at NCI-Frederick

Alexander Wlodawer, who was born in Poland and maintains very active collaborative links with Polish science, has been elected a foreign member of the Polish Academy of Sciences (PAN). PAN has 350 national members (full and corresponding) and about 200 foreign members. Alex was elected by the

vote of the General Assembly of the Academy, after a very competitive nomination by the Division of Biological Sciences. The membership was awarded by Andrzej Legocki, President of the Academy, on June 25, 2005, during the opening ceremony of the Inhibitors of Protein Kinases conference held in Warsaw. This honorable distinction recognizes his contribution to the advancement of structural biology, including discoveries fundamental for the development of drugs against AIDS and cancer and for our understanding of enzyme action. His accomplishments are linked to his research at the National Cancer Institute Frederick (USA), where he heads the Macromolecular Crystallography Laboratory.

■ The preceding was originally submitted to the IUCr Newsletter by Mariusz Jaskolski, Poznan, Poland.

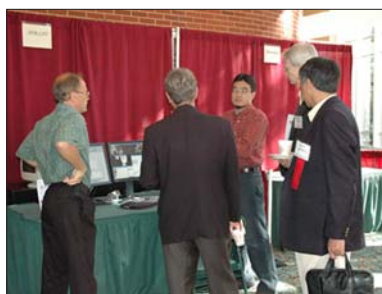
**SER-CAT at Outside Conferences**

SER-CAT participated in several scientific conferences in 2005, with scientific talks, poster presentations and our annual exhibit at the ACA meeting. The 2005 ACA was held at Walt Disney World, giving participants the opportunity to combine an interesting meeting with a family-friendly vacation. We enjoyed the opportunity to converse with SER-CAT users, both from our membership and the General User program, as well as those eager to try out our beamlines after hearing feedback from colleagues. Program Chair Ed Collins of UNC, also a SER-CAT member, organized a series of great scientific talks and workshops for participants to learn from and enjoy. SER-CAT staff members Andy Howard, Jim Fait and John Chrzas also contributed to the talks at the meeting. The 2006 ACA meeting will be held July 22-27 in Honolulu, Hawaii. This great location should draw in a lot of participants, so we hope to have a chance to say “Aloha!” to all of our SER-CAT users!



ACA meeting participants take a break between talks at the SER-CAT booth. From left to right: Andy Howard, Gary Newton, Leif Hansen and Joel Harp.

Other scientific meetings include the IUCr Congress held in Florence, Italy, where SER-CAT Assistant Director John Rose gave a talk on high-throughput structure determination at the SER-CAT beamlines. SER-CAT also participated in the poster session at the IUCr Congress.



SER-CAT Remote Access demonstration at the UK-Southeast USA Symposium on Structural Genomics and Proteomics

In October 2005, SER-CAT contributed to the First Annual UK-Southeast USA Symposium on Structural Genomics and Proteomics at the University of Georgia. Sector Manager John Chrzas presented a talk on the SER-CAT facility with SER-CAT Director B.C. Wang. John also presented a successful demonstration of remote access through Access Grid, along with SER-

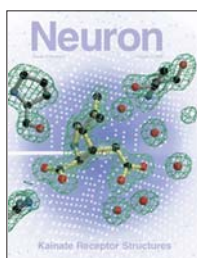
CAT Crystallographer Zhongmin Jin. The three-day symposium, designed to encourage large-scale international collaboration in the fields of structural genomics and proteomics, was chaired by Bi-Cheng Wang. A summary of the program was published in the winter 2006 ACA newsletter and is also available online at [www.bmb.uga.edu/uk-seusa](http://www.bmb.uga.edu/uk-seusa). The Second Annual UK-Southeast Symposium is to be held in August 2006 at the University of St. Andrews, St. Andrews, Scotland.

**SER-CAT at Outside Conferences**, from Page 3

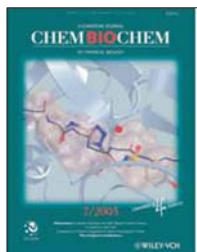
If you would like SER-CAT to participate in a conference at your institution, or if you would like to provide information on our facility to your participants, please contact the SER-CAT Administrative Office.

**Publications for 2005**

The results are still coming in for structures and publications in 2005, but we are pleased to report that it has been another productive year for SER-CAT. As of February 14, SER-CAT's 22-ID beamline is acknowledged in 65 publications for the 2005 year – a higher number of publications than any other ID beamline at the APS. The overwhelming majority of 2005 publications were submitted by member institutions, but the APS General Users are now contributing to our scientific productivity as well.



Two of the 2005 publications made the cover of their respective journals, and both were published by members at NIH. The full references for the articles are as follows: Mark L. Mayer, "Crystal Structures of the GluR5 and GluR6 Ligand Binding Cores: Molecular Mechanisms Underlying Kainate Receptor Selectivity," *Neuron* 45 (4), February, 539-552 (2005) and Ashraf Brik, Jerry Alexandratos, Ying-Chuan Lin, John H. Elder, Arthur J. Olson, Alexander Wlodawer, David S. Goodsell, Chi-Huey Wong, "1,2,3-Triazole as a Peptide Surrogate in the Rapid Synthesis of HIV-1 Protease Inhibitors," *ChemBioChem* 6, June, 1167-1169 (2005). SER-CAT would like to congratulate all of the users that published in 2005 and thank them for acknowledging our facility.



Please be sure to include the proper acknowledgements in your PDB submissions and published work, including theses, as this is vital to the productivity of our beamlines and our privilege to operate our facility at the Advanced Photon Source. Instructions on how to acknowledge SER-CAT in your PDB submissions and publications are available at [www.ser-cat.org](http://www.ser-cat.org).

**Staff Departures and Additions**

As many of our users know, Stephen Foundling departed from the Operations Team in 2005 to go back to work in industry. A search has been conducted to find the right person to provide user support, and a new staff member will be in place at the SER-CAT facility in approximately one month. In the meantime, Andy Howard and staff members from the Illinois Institute of Technology have been helping part-time to ensure a smooth transition. John Gonczy, who began his service with the SER-CAT Construction Team, is also contributing to user support and will continue this service after the new hire.



Lisa Horanyi

This issue is ending on a personal note for me, your Assistant Editor, as I am now departing from the SER-CAT program after three years of service. It has been a pleasure meeting all of the members and getting to know you both scientifically and personally during this time. I would like to take this opportunity to thank all of the SER-CAT staff for being so supportive and wonderful to work with. I must especially thank Kathy Morris and Bi-Cheng Wang at the Administrative Office for recognizing my strengths and allowing me to be creative and build on my skills while promoting the SER-CAT program.

I have seen a lot happen during my three years at SER-CAT. The facility has gone from construction to full operations with robust features allowing for the best data collection conditions. Our scientific productivity has put SER-CAT in the forefront of X-ray beamline research. We greatly increased our outreach efforts, establishing this newsletter, an annual exhibit at the ACA meeting, and the annual SER-CAT symposium, which has shown increased attendance each year. It was an honor to be a part of these exciting activities, and I hope I have left an impact on the program that can be expanded on in the future. The Administrative Office is searching now for a capable individual to organize future outreach activities for SER-CAT, and I know this new person will also have a great opportunity to learn and grow.

I will be relocating to Charlottesville, Virginia, along with my husband, Peter, also an X-ray crystallographer, who earned his Ph.D. in Bi-Cheng Wang's laboratory at the University of Georgia. Peter will be working at the University of Virginia, another SER-CAT member institution. Therefore, I hope to be able to keep in touch with many of the friends I have made during my service with SER-CAT. Best wishes to you all.

*Note from B.C. Wang* – Lisa, on behalf of SER-CAT members and staff, I would like to thank you for your exceptional services to SER-CAT in the last three years. Best wishes to you and Peter in your new careers.

*The SER-CAT Spectrum* is the biannual newsletter of the SER-CAT group. Additional information about SER-CAT and the Advanced Photon Source at Argonne National Laboratory can be found at our website [www.ser-cat.org](http://www.ser-cat.org) or by contacting the SER-CAT Administrative Office at 706-542-3384.

SER-CAT is supported by the Member Institutions shown on the back cover of this publication, including the National Aeronautics and Space Administration under Grant Number NCC8-233, the Department of Health and Human Services under Contract Numbers N01-CO-56000 and 2515145M and the Georgia Research Alliance. The contents of this publication do not reflect the views or policies of any of the supporting entities nor does mention of trade names, commercial products or organization imply endorsement by Member Institutions or the U.S. Government.

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