



Operation: Present and Future

<http://protein.nsls.bnl.gov>

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2008 Highlights

This year our user community was very productive with 57 publications, 20 in premier journals of which 14 were developed at X6A only

Nature, **456**, 409-412 (Davies)

Nature, **455**, 633-637 (Skordalakes)

Nature, **451**, 846-850 (Marmorstein)

Nat. Rev. Cancer, **8**, 665-669 (Amzel)

Science, **322**, 1369-1373 (Schwartz)

Immunity, **29**, 228-237 (Ostrov)

Nat. Struct. Mol. Biol., **15**, 738 (Marmorstein)

Curr. Opin. Struct. Biol., **18**, 507-515 (Regan)

Proc Natl Acad Sci USA, **105**, 5465-5470 (Murali)

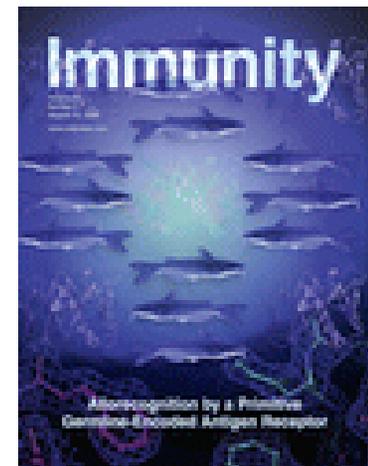
Proc Natl Acad Sci USA, **105**, 8601-8606 (van den Berg)

Proc Natl Acad Sci USA, **105**, 12206-12211 (Marmorstein)

J. Am. Chem. Soc., **130**, 14324-14328 (Ismagilov)

J. Am. Chem. Soc., **130**, 17254-17255 (Christianson)

Plant Physiol., **146**, 455-467 (Noel)





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Mission

The East Coast NIGMS Structural Biology Facility mission is to provide first class resources to the biological- biochemical-, and biophysics- communities to explore all aspects of structural biology. It is the goal of this facility to provide assistance to expert and non-expert crystallographers.

These goals include:

- Beam line access to a structural biology community at large.
- Fast access to beam time for the user community.
- Crystal screening and high-throughput data collection.
- Assistance and training for academic and professional users.

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Background



NIGMS Initiative in 1999*

- Beamline upgrades for benefit of general users
- Reports on increasing demand for user access and beamline needs
- Estimate of doubling of capacity for crystallographic experiments from staff increases and equipment upgrades
- Letter to synchrotron facility directors inviting informal proposals
- NIGMS synchrotron advisory group
- FY99 funding of \$7M from NIGMS

* source Norvell, Aug1999



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The NIGMS support at the NSLS

Supplement to the PSI

- construction of bending magnet beamline
- including beamline optics, monochromator, detector, crystallography station
- four beamline scientists/technicians
- \$2,372K equipment/construction
- 2003 \$1,200K supplement for detector upgrade
- \$839K annual (inclusive overhead) – staff and operation > Flat since 2005

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Technical Upgrades and Developments



Hardware - *Upgrade*

Required careful planning to minimized user beam down time.

End-Station Upgrade - mid November 2008

- Diffractometer
- In line sample viewing
- Detector
- Computer workstations

Development

- Beam position monitor

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Hardware - *Diffractometer*

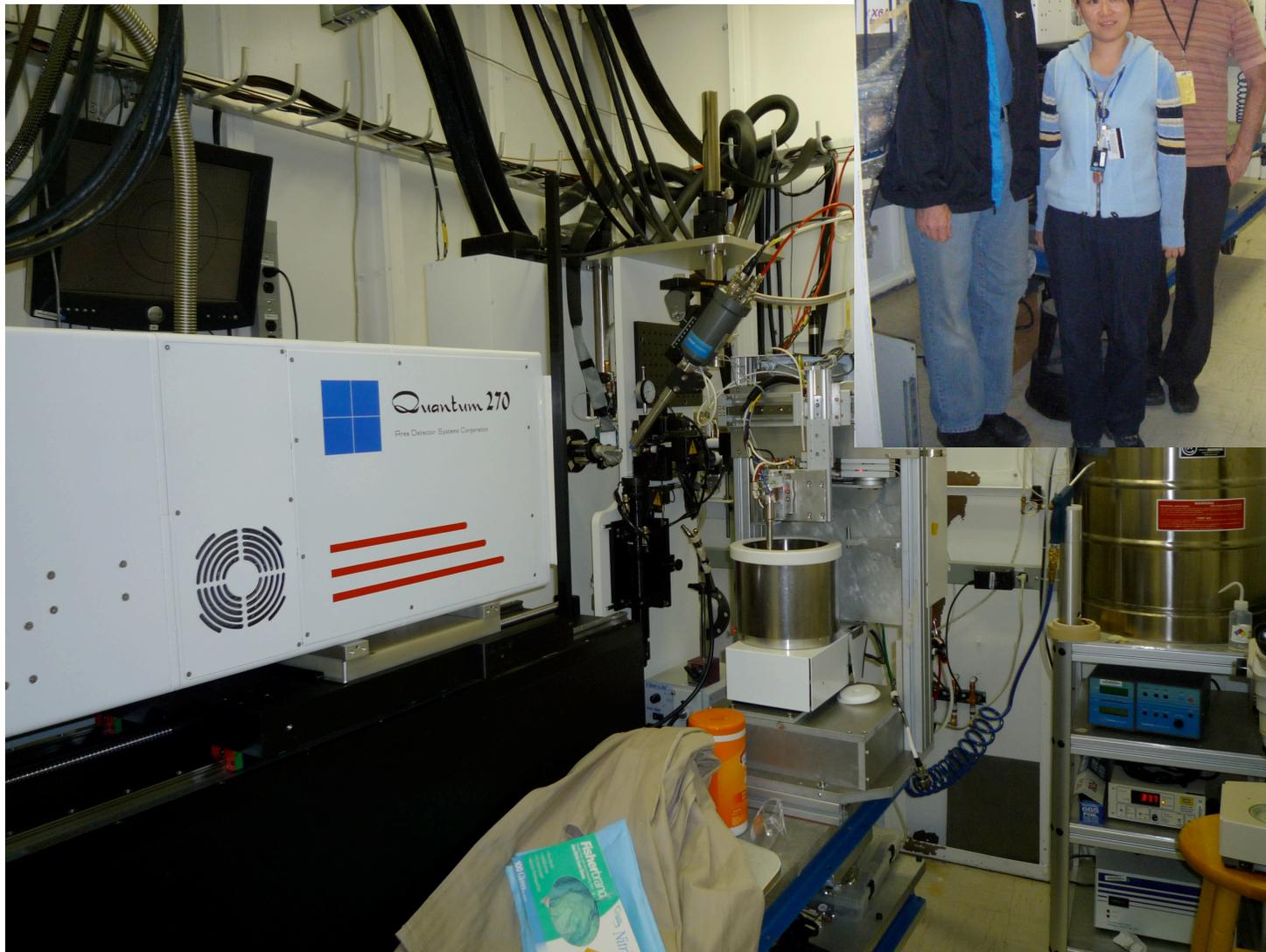
Crystallog

- ❖ Rotation axis: from step motor to an air-bearing
- ❖ Slit assembly: augmented opening
- ❖ In line sample viewer



Hardware - *Detector*

ADSC from the Q210 to the Q270

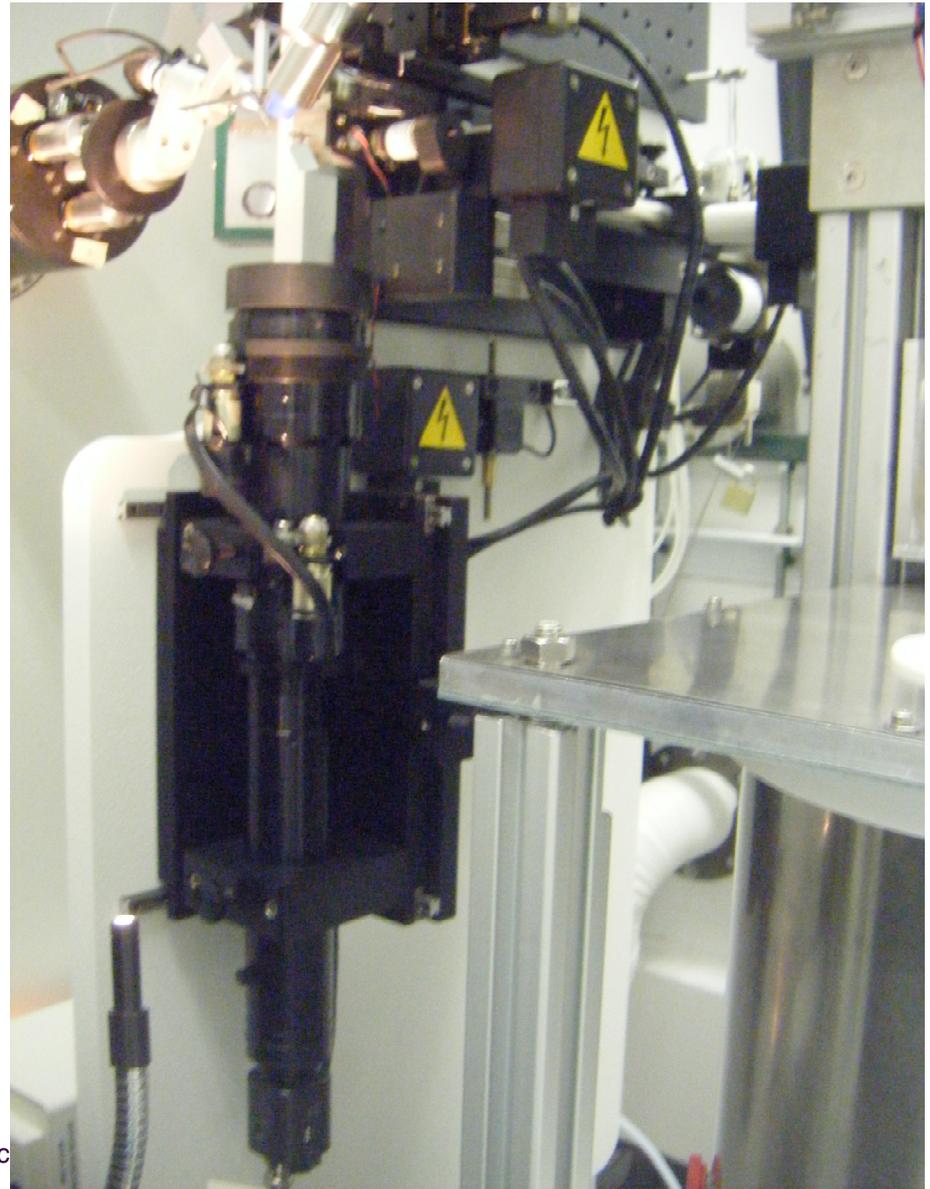


VS



Hardware - *“In-line”* sample viewer

In line sample viewer (Crystallogic) allows for x-y translations which facilitate the initial alignment of the camera. A stable setup is imperative for automated sample centering.





Hardware - Workstations

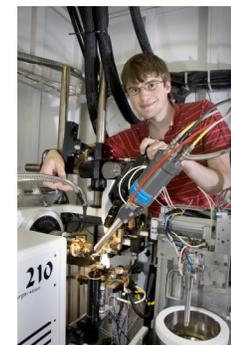
	Old configuration	New configuration
Data collection / Beamline control	2 x 1.8 GHz CPUs 4 Gb RAM Base 100 Network 1 TB RAID 10	4 x 2.2 GHz CPUs 4 Gb RAM GiBit Network 1 TB RAID 10
Data processing / Storage	4 x 2.2 GHz CPUs 4 Gb RAM GiBit Network 1 TB RAID 10	4 x 2.8 GHz CPUs 4 Gb RAM GiBit Network 1 TB RAID 10
	4 x 1.6 GHz CPUs 2 Gb RAM GiBit Network 1 TB RAID 5	4 x 3 GHz CPUs 4 Gb RAM GiBit Network 3.6 TB RAID 10
Storage		Inhouse Storage GiBit Network 1.8 TB RAID 1
Increase of data storage and processing power	3 TB 18.8 GHz Mixed Network	7.4 TB 32 GHz All GigaBit

Hardware - *Development*

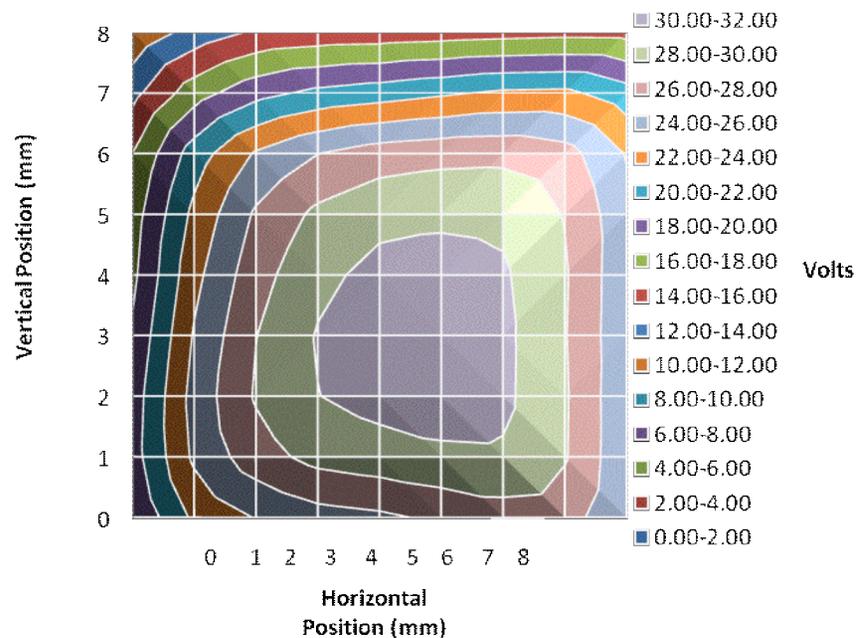
Beam position monitor

Collaboration with Detector group, Peter Siddons

Project Champion: Christopher Owen - Summer Intern
SUNY Buffalo, Chemical Engineering



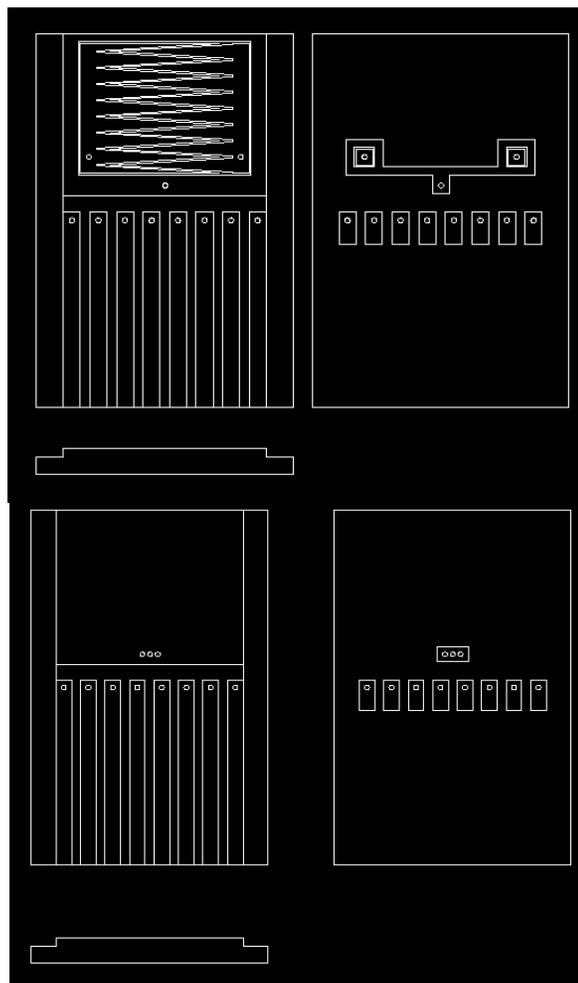
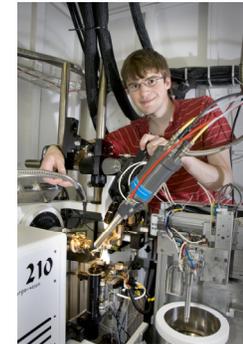
Total Voltages Across BPM Chamber Area



Hardware - *Development*

Beam position monitor

Collaboration with Detector group, Peter Siddons



- Chevron pattern (zig-zag)
 - Negates varying charge gradient along the Z axis
- Grounding rings
 - No capacitance charge build up
- More gradient field strips
 - More uniform electric field gradient
- Gold plating instead of copper
 - No oxidation to impede charge collection
- Notched wafers
 - Easy assembly of chamber that is square
- Increased charged pad size
 - Electric field extends over entire chamber

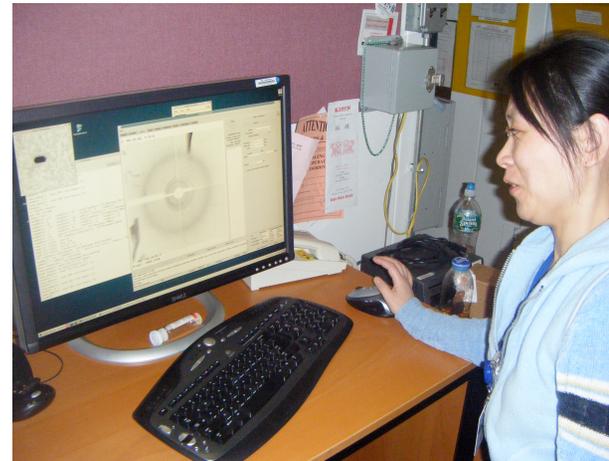


Hardware - *Future Developments*

- Sample illumination
- Beam stop (SSRL like)
 - ❖ dose limited experiments
- Improved He flight path
 - ❖ for improved signal
- Sensors for improved remote access
 - ❖ smart magnets (for automounter operation)
- KB mirrors
 - ❖ for improved intensity

Software - *Upgrade*

Blulce/DCS upgrades focused on the hardware upgrade





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Software - *Blulce/DCS*

Is Beam Line Specific!

- Major changes transparent to the user
 - ❖ related to diffractometer control
 - all parts are now controlled through Galil controllers
 - ❖ related to the detector
 - data collection in bin/unbin modes,
 - remote start-up
 - ❖ preparation for improved sample throughput, ie. CrysCent

- Minor improvements
 - ❖ increased user friendliness
 - detector shield (up/down button),
 - beam sense threshold control



Software - *Future Developments*

Small implementations

- Integrate further CrysCent to allow for fully automated sample screening
- Integrate sensors

Long term implementations

- Automated beamline alignment

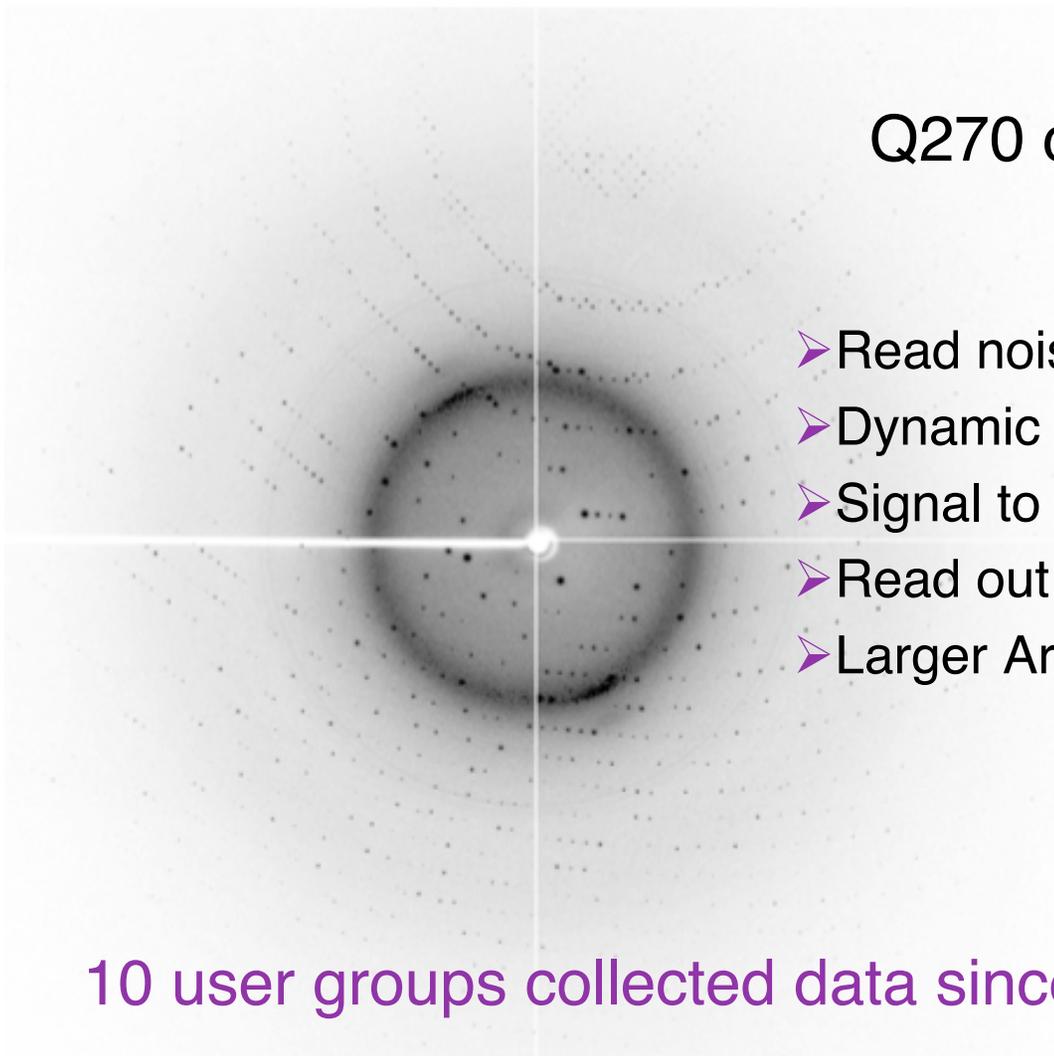
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Commissioning

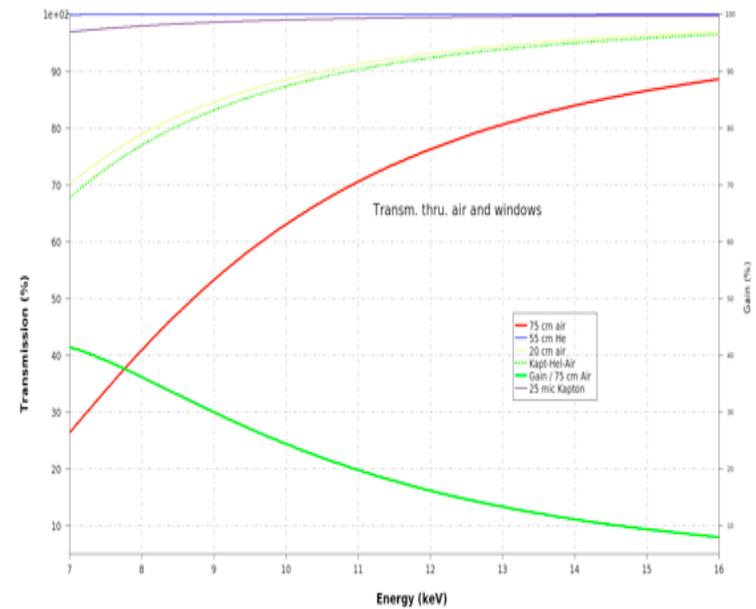
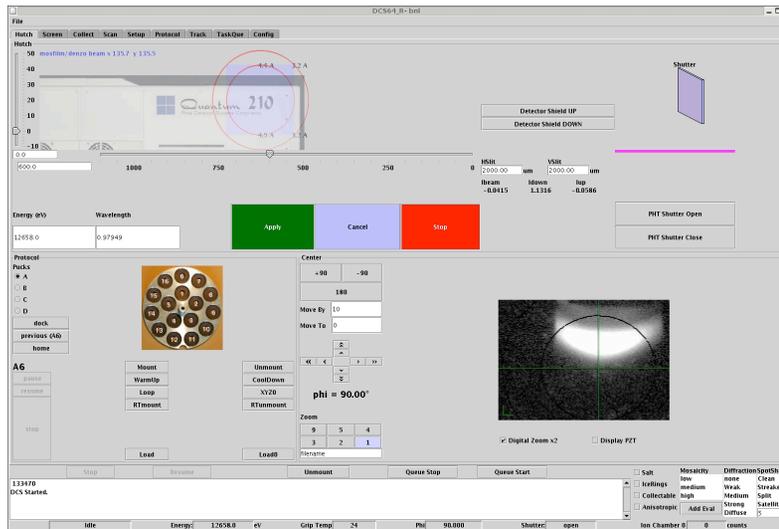
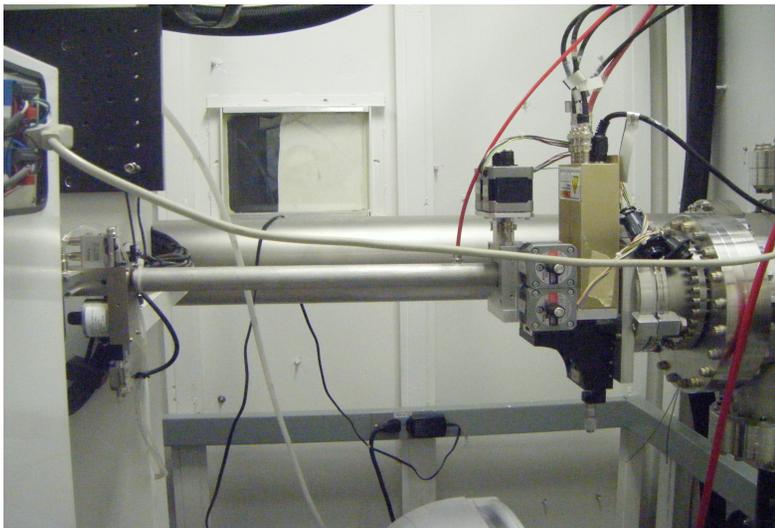


Q270 characteristics

- Read noise ~3x better @12.5 keV
- Dynamic range 4X better
- Signal to noise >3X better
- Read out time about the same 1.10s
- Larger Area 270mm

10 user groups collected data since last December

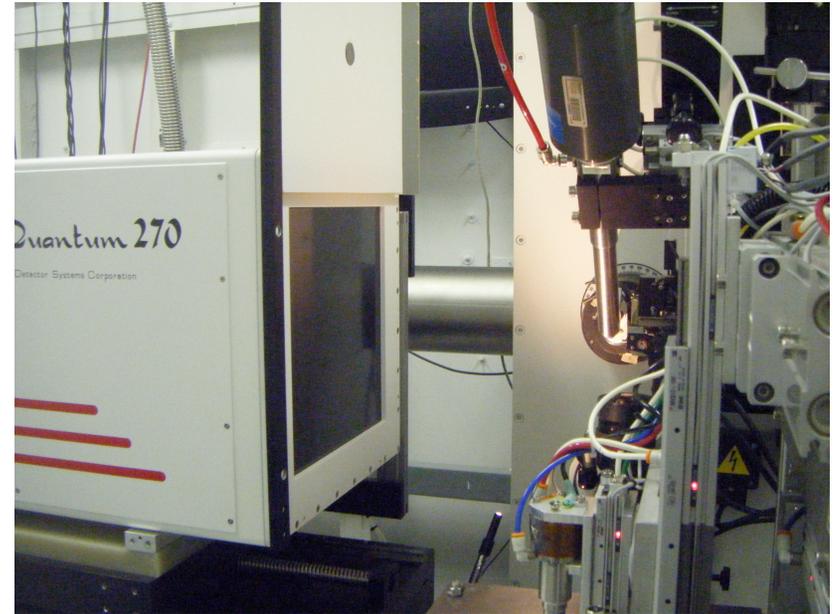
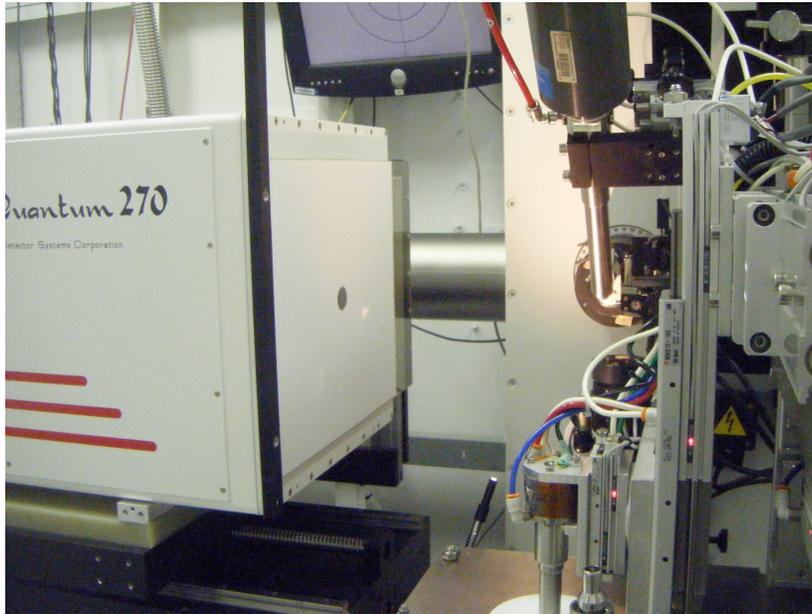
Commissioning



Helium path (prototype)
 Wide opening slits
 Q270 improved I/sigI

Allow for improved signal-to-noise
 >>> shorter exposure times

Commissioning

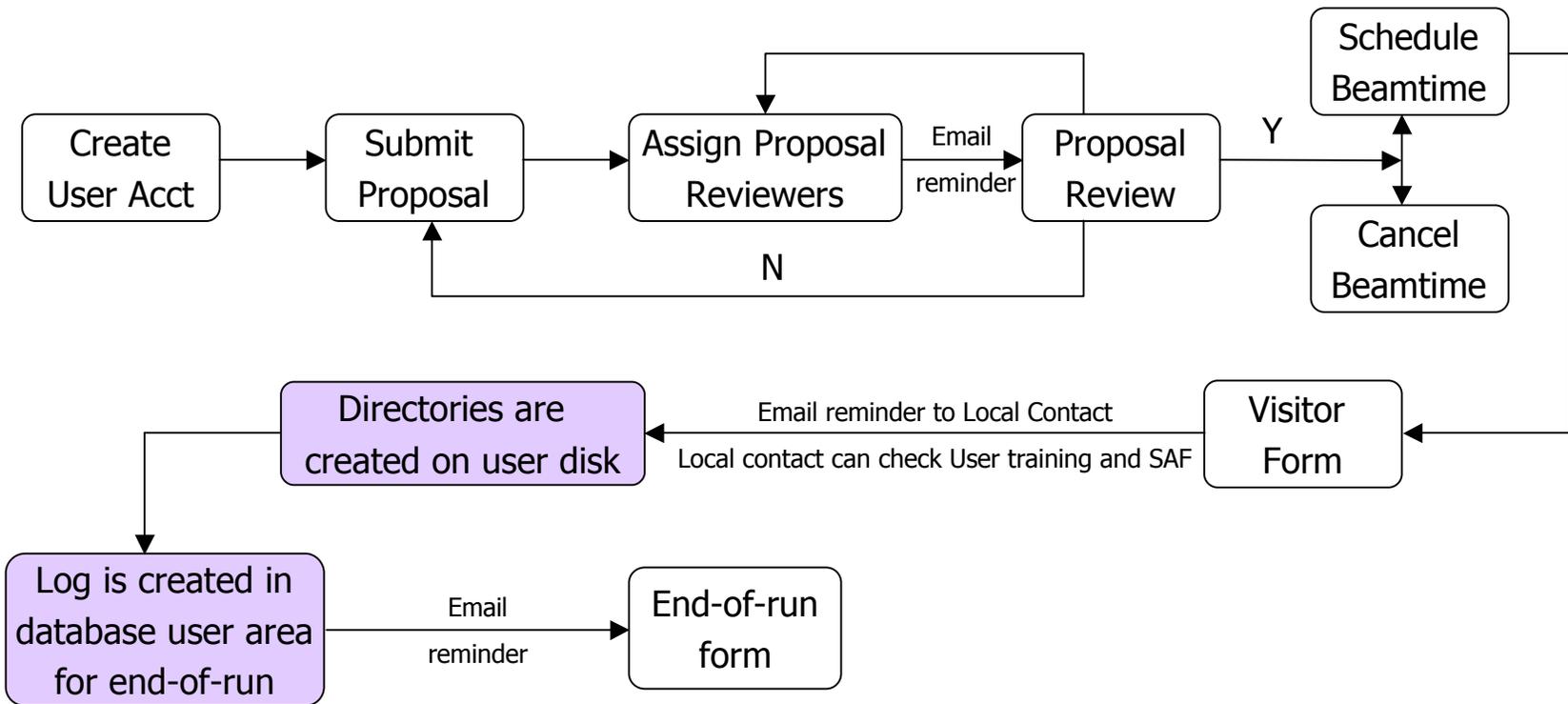


Rick Greene

Detector shield was improved with leaded plexiglass. When starting an energy scan the shield comes down automatically.



The X6A Web and Data Base Environment



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The X6A Web and Data Base Environment

X6A

Welcome To X6A Beamline

Main Page

X6A Home

- News
- PDB deposits
- X6A Publications
- Collaboration Policy
- X6A People

User Corner

- User Login
- X6A Schedule
- Safety Approval Form
- Dry Shipper Shipments
- Smooth Arrival
- Smooth Departure

Beam Line Facilities

- Optics
- End Station
- Automounter
- Crystallization Lab

User Guide

- Use Lab Facilities
- Preparation
- Run Experiment: Manual
- Run Experiment: Automounter
- Data Analysis
- Data Back Up
- FAQ

X6A Team

- X6A SAC Login
- SAC Members Only

MISSION

The NIGMS East Coast structural biology facility at National Synchrotron Light Source has been established to provide first-class resources to a growing community of life scientists to explore all aspects of structural biology. Our goal is to offer rapid access to beam time and high sample throughput.

- Beam line access to a structural biology community at large.
- Fast access to beam time for the user community.
- Crystal screening and high-throughput data collection.
- Assistance and training for academic and professional users.

ACKNOWLEDGEMENTS

Research carried out (in whole or in part) at X6A beam line, funded by the National Institute of General Medical Sciences, National Institute of Health under agreement GM-0080. The National Synchrotron Light Source, Brookhaven National Laboratory is supported by the U.S. Department of Energy under contract No. DE-AC02-98CH10886.

News and Events

Next Beamtime Available on **February 16, 2007**

X6A launched the new web site, [more >>](#)

X6A Automounter Featured on Take 5, [more >>](#)

[View all the X6A news >>](#)

New User Register

User & Reviewer Login

View X6A Schedule

Search

Go Search

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Media Wiki

- Improve communication

User and Experimental Control Databases

- Communication between databases

User Database

- Improve User Access
- Improve Beam Line Management
- Real time Statistical Analysis of beam time usage

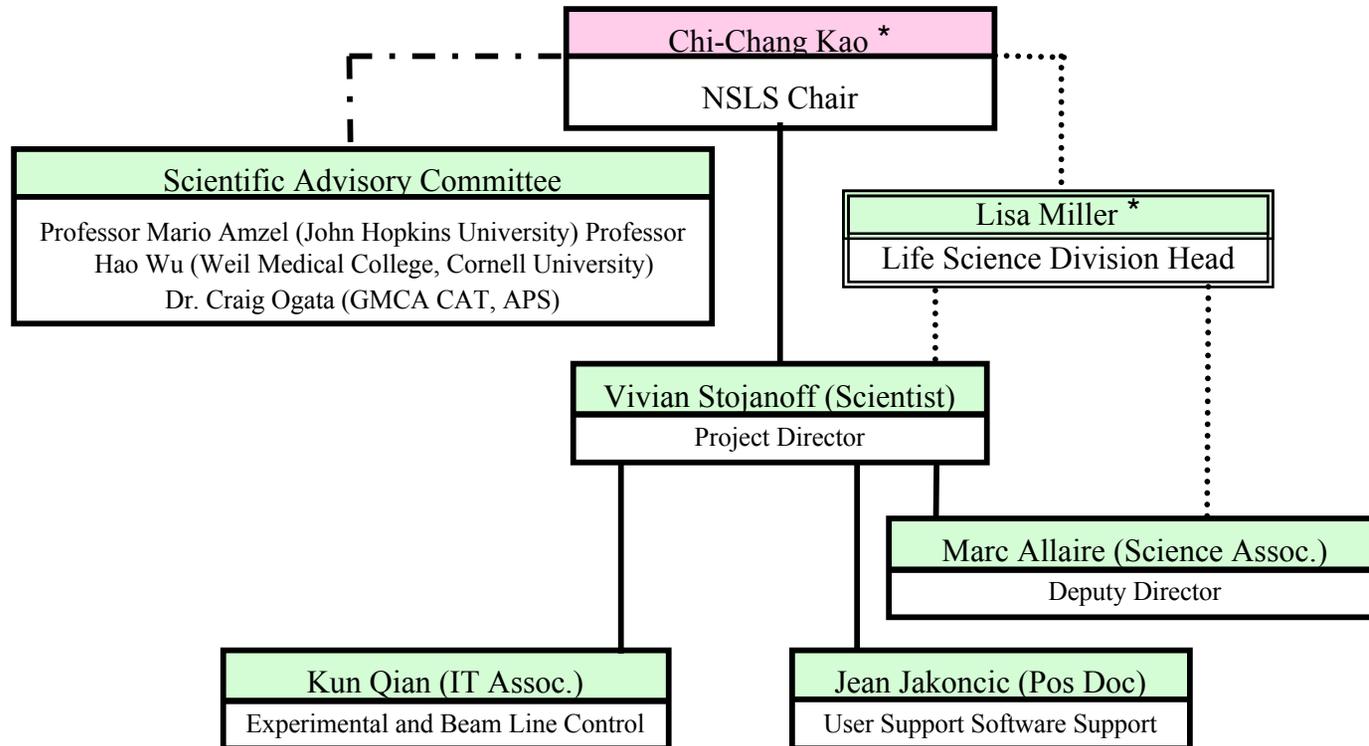


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Staff



Organizational Chart



* NSLS scientific staff



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NSLS staff contributing to the operation

Technical support provide by the NSLS as needed

Peter Siddons Detectors

(T. Kuczewski)

Steve Hulbert Beamline Support

(S. Cheung, R. Greene, T. Lenhard)

Z. Yin Computer & Control

Wayne Rambo Electrical Support

(B. Clay, D. Poshka)

Administrative support provide by the NSLS as needed

Brian Boyle Budget Administration

(W. Morrin)

Eileen Morello Secretarial Support

(A. Bowden)

Katheleen Nasters User Administration

(G. Cisco, L. Flynn, M. Baez)

A. Ackerman EH&S

(J. Aloï, K. Klaus)

B. Kiss Building Management



User Program

...in many instances we choose X6A over other beamlines because of the great help and support we obtain



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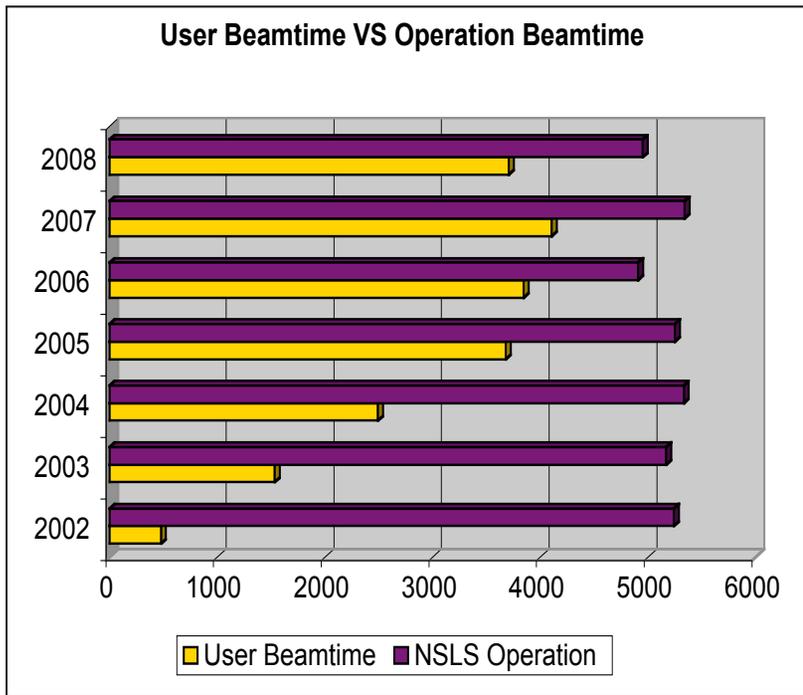
User access

Two modes are available to users for beam time application:

- X6A Fast Access (<http://protein.nsls.bnl.gov>)
 - ❖ Projects submitted through the X6A application form
 - ❖ Single Projects (1Protein = 1Project)
 - ❖ Easy, simple and fast (3 days to a week review process)
 - ❖ Multiple visits
 - ❖ User schedules own beam time
- General User proposals submitted through the PASS system
 - ❖ Two modes of application:
 - ✓ general users beam time: 4 month in advance valid for 2Y
 - ✓ rapid access (valid for current cycle only)
 - single visit within a cycle
 - ❖ Multiple projects in one single proposal
 - ❖ Beam line scheduler has to schedule beam time with user

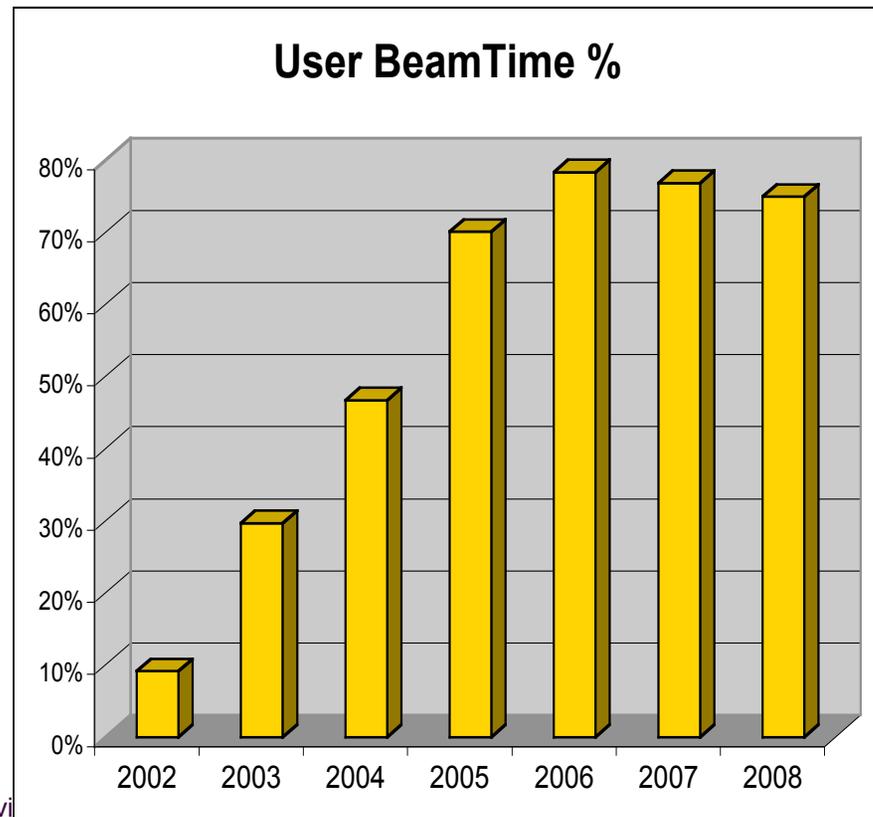
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Available beam time



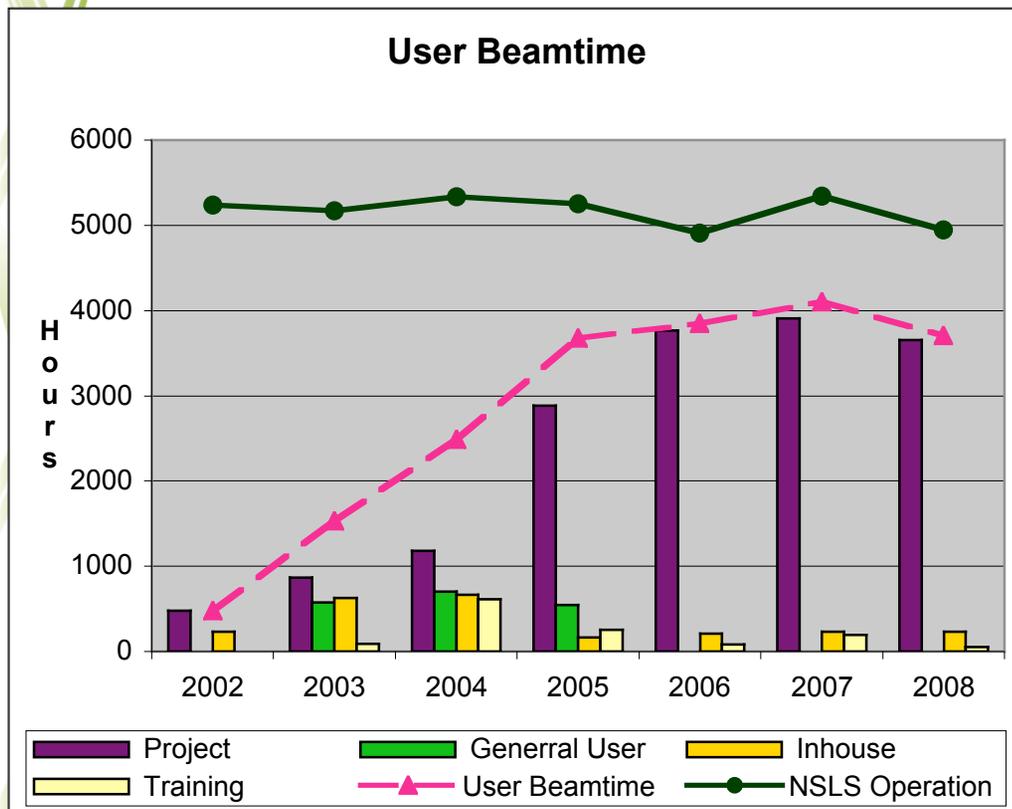
User scheduled beam time still increasing but reaching saturation.

The beam line continued to be oversubscribed. 100% of the beam time available to users has been scheduled in 2008.



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User beam time



X6A operation

- X6A user projects 75%
- X6A beam line 18%
 - ✓ X6A commissioning 68%
 - ✓ X6A inhouse projects 32%
- Unused 8%

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User beam time usage

Total # images	240044
Total # images screened	16001
Total#data sets*	772
Total # crystals screened and collected	5075
Automated Sample Changer	
Total #images screened	2106
Total # data sets*	58
Total # crystals screened and collected	967
usage	21d 10 h 30m

*data set 40 or more images

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On site users

Most of the X6A projects are carried out by users who visit the facility

- Groups are in average composed of two individuals
- Average schedules are 1.5 days
- Mostly leave with image files and scaled data
- Some also leave with an electron density map

Automounter usage

- ~ 8 groups
- ~ 967 samples were screened
- ~ 58 data sets collected



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Virtual users

Virtual Users are required to have visited the beam line once

- Not present during the measurement
- Leave behind or send in their samples
- Receive image files and scaled data
- Receive an electron density map

A special type of Virtual Users: Remote Users

- Control the experiment with limited staff assistance (NoMachine technology)
- To become effective still waiting for the development of sensors

may become impossible due to Lab policies

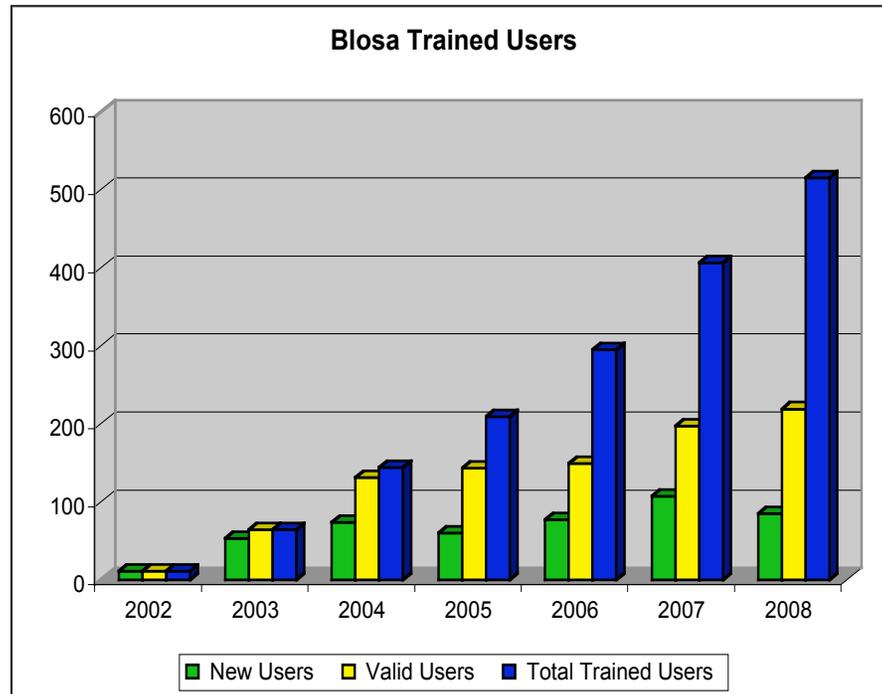


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BLOSA (Beam Line Operation and Safety Awareness) trained users



BLOSA training is valid for two years.

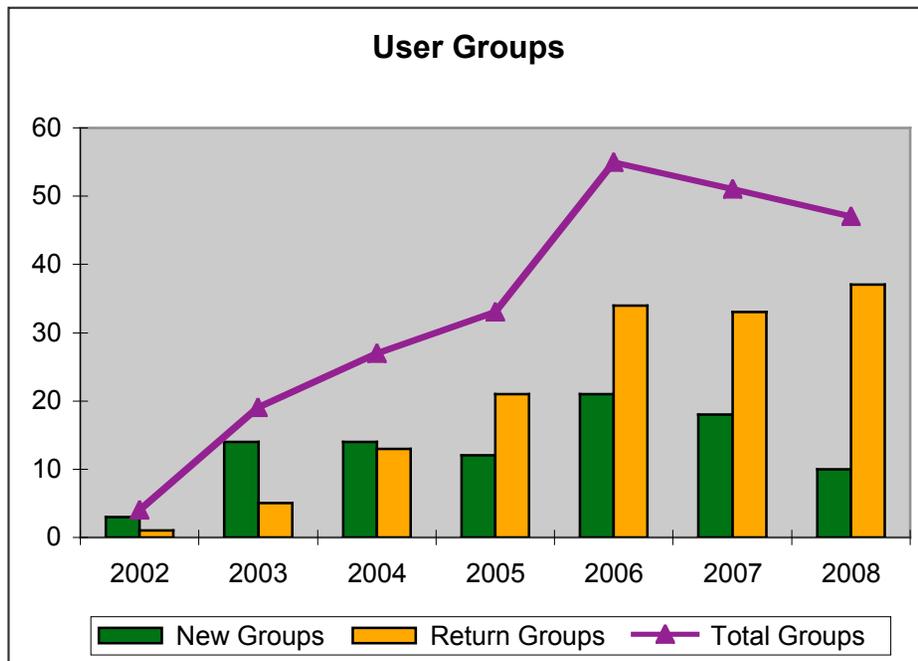
**New Users*: are experimenters who got trained in a specific year and were never BLOSA trained in previous years.

**Valid Users*: are experimenters who keep a valid BLOSA Training Status in a specific year.

**Total Trained Users*: are experimenters who trained in that year or before (accumulated number). Numbers include new and returning users.

In the past calendar year 85 new users were welcomed at the beam line; with 219 showing active user status.

Consolidation of the user community*



*Source X6A Survey December 2008

New groups: scheduled their projects only once in 2008.

Return groups: scheduled their projects at least 2x in 2008.

The number of user groups returning to the beam line is leveling off with 37 groups scheduling at least twice their projects in 2008.

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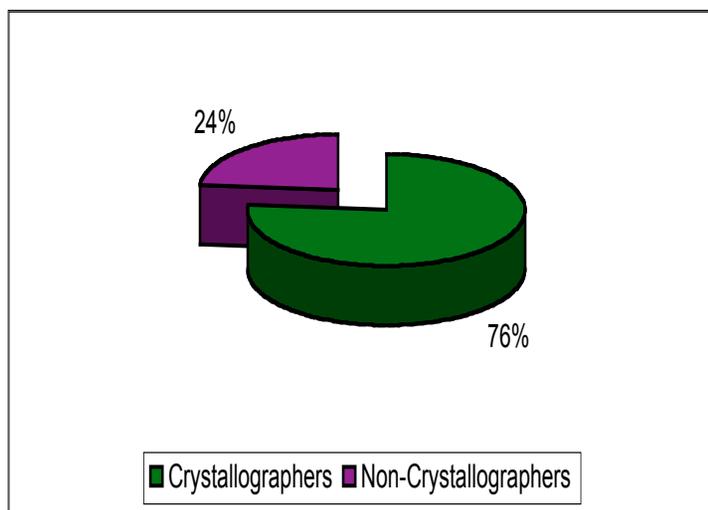
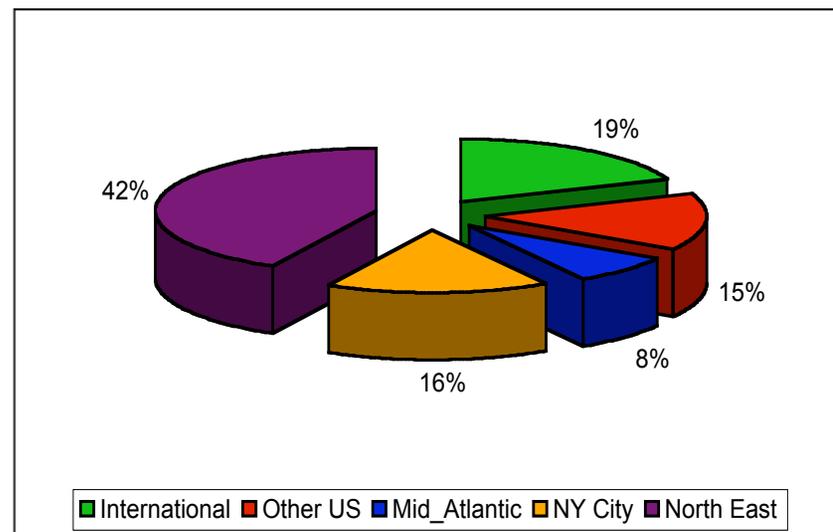
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User demographics*

The number of user groups from academic institutions located in the northeast region of the US increased by 4%.



Expert and Non-Expert user groups. Only 59% of the users answered this line item in the survey.

*x6a survey Dec2008

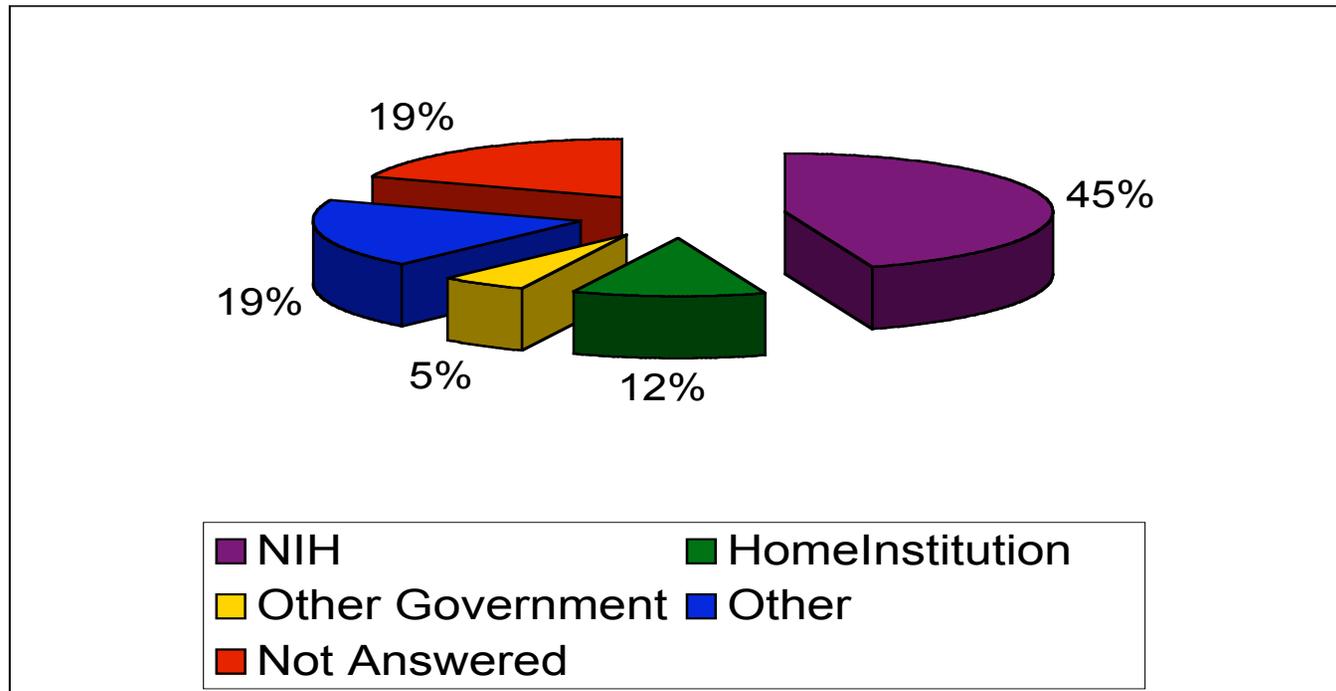
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User Funding Sources



Over the last two years the number of groups supported by the NIH and by home institutions fluctuated +/- 1%, and funding by other sources decreased.

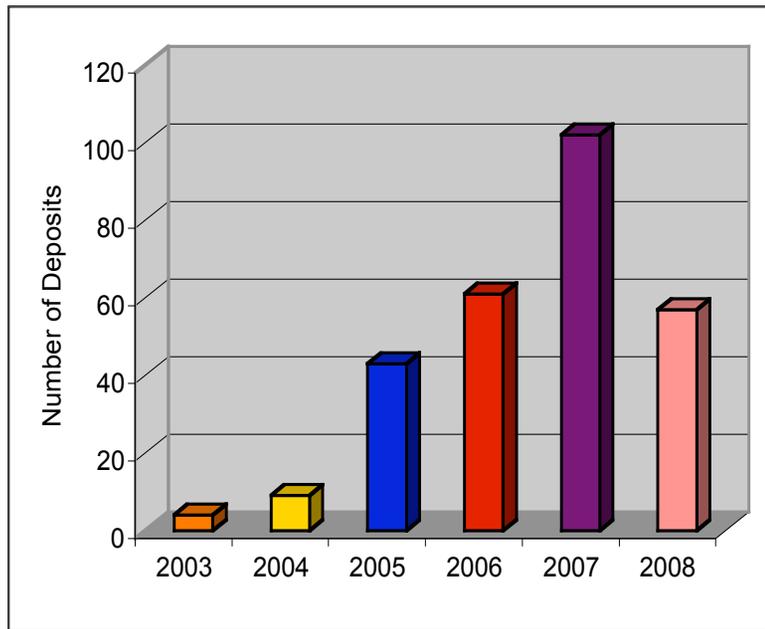


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Impact

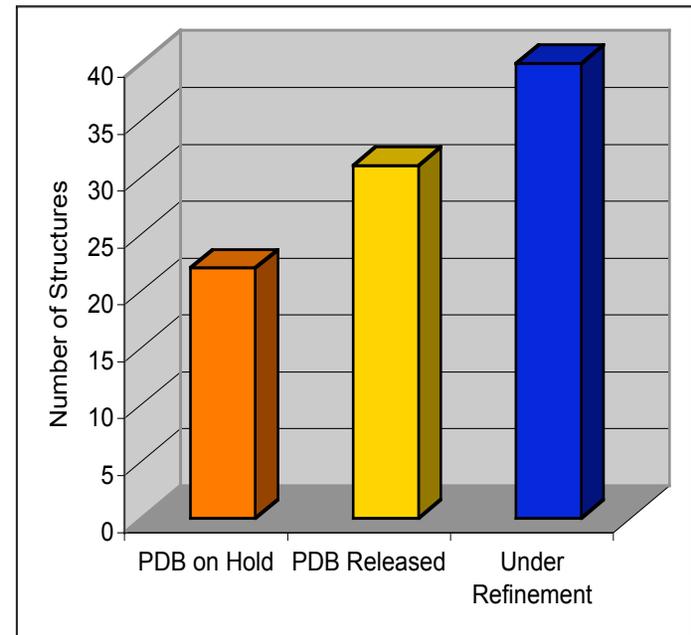


Protein Data Bank Deposits*



Number of deposits (released and on hold) is leveling off as the beam line matures.

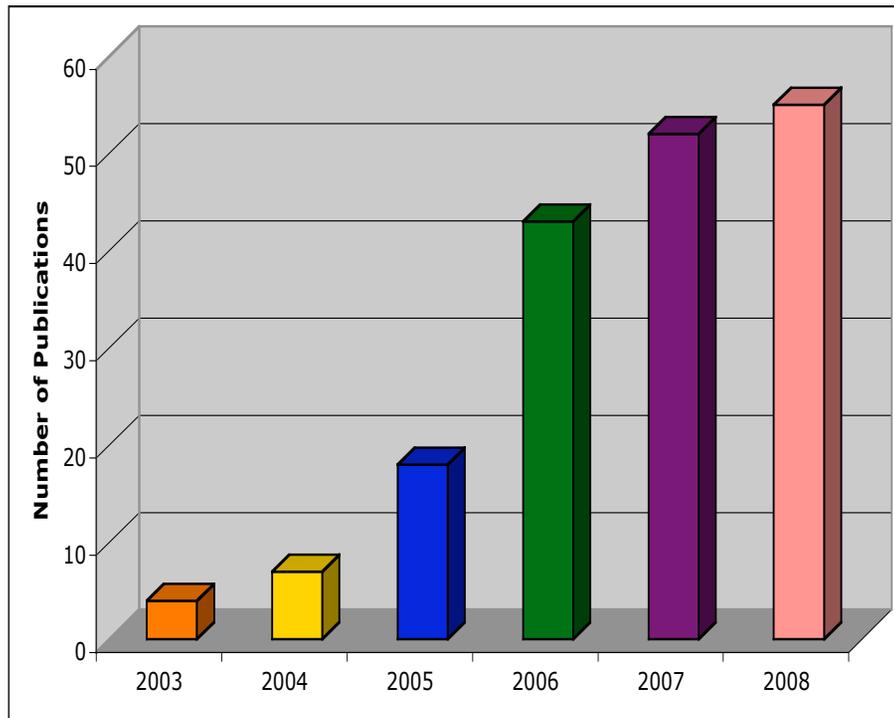
The number of structures deposited in the PDB has increased for each of the past years. More so for 2007 were according to the Dec2007 survey only 61 structures were reported.



*Source X6A Survey December 2008



Publications*



Publications*	
Total	High Impact**
179	75
2008	
57	20

*Source X6A Survey December 2008

** Journals with an impact of 6.0 or greater. Source JCR 2007

In spite of a thorough survey the total number of publications in a given year are not completely captured. An overall increase in publication numbers was observed for the last two years. As expected for a maturing beam line the number of publications/year seems to be leveling at about 53 pub/year.

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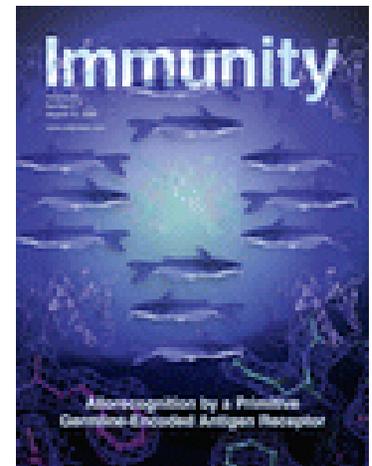
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Publications - *Highlights*

This year our user community was very productive with 57 publications, 20 in premier journals of which 14 were developed at X6A only

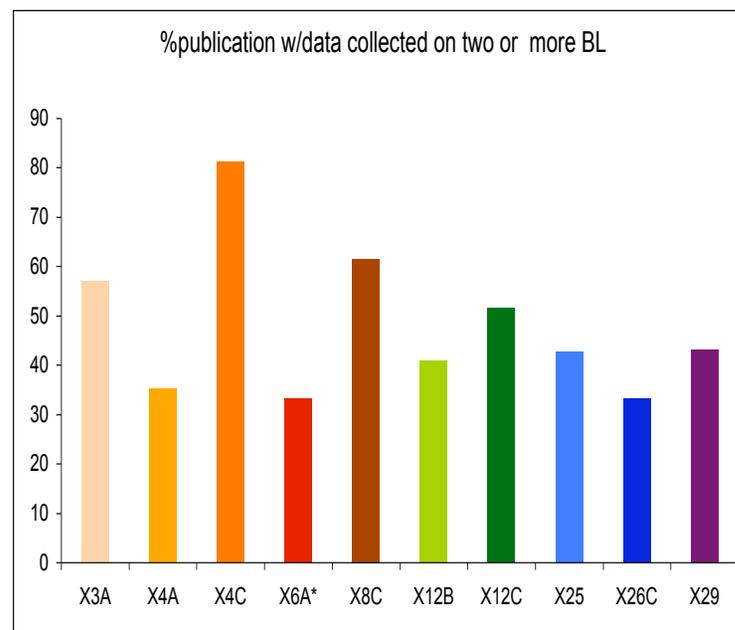
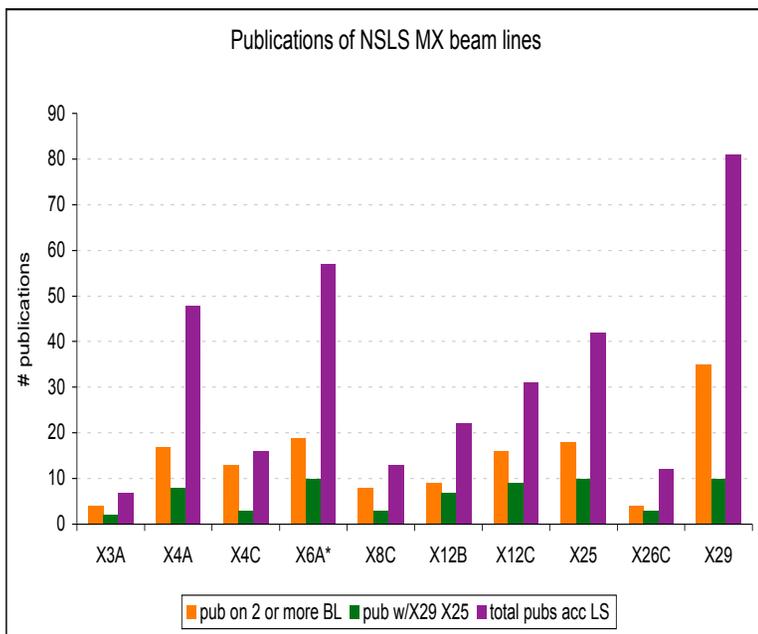
Projects developed by the user community also appeared in a broader impact media.

- Three projects were recognized by the Faculty of 1000
- At least four projects were cited in editorials and broad impact media





Facility Shared Publications*



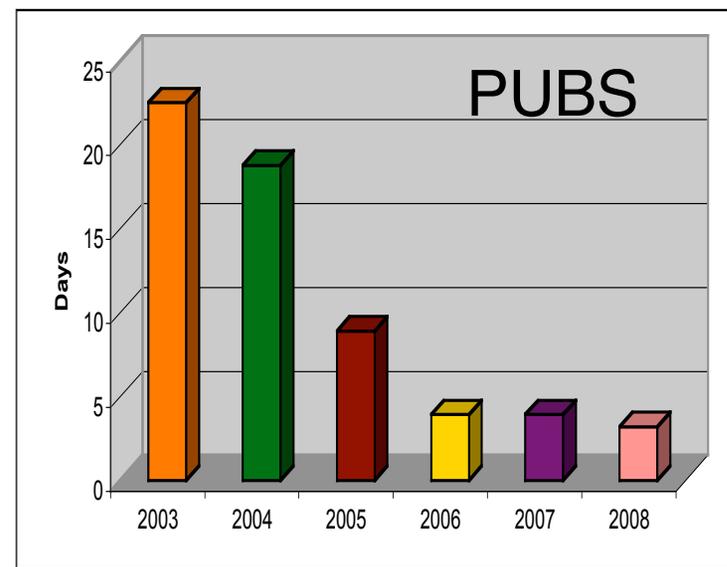
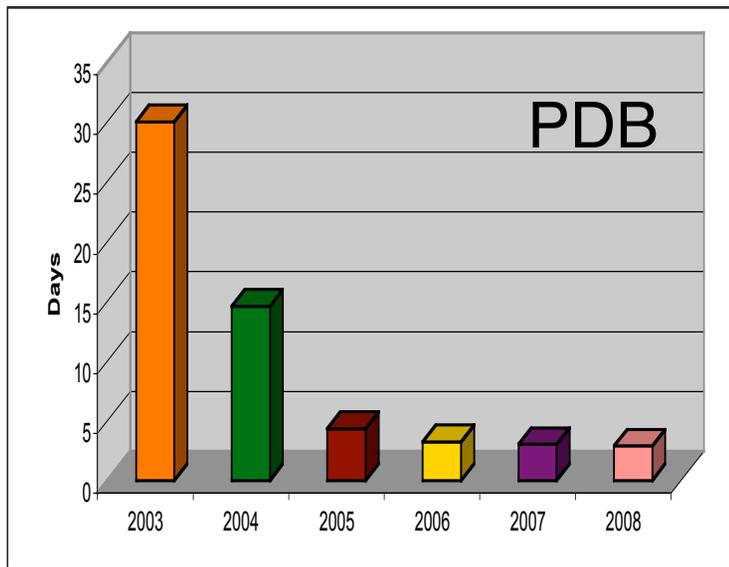
Compared to other user communities at the NSLS the X6A community is very active and loyal. According to the NSLS publication survey only ~ 33% of the X6A publications were shared with other Facilities.

*Source NSLS website 2008



Other impact factors*

It is common to refer to the cost per structure, per paper.....



The cost per paper per structure as a function of scheduled user hours continues to decrease.



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Education and outreach

The beam line has participated in the NSLS and BNL Education and Outreach programs

Education

- Crystallization: focus on **membrane proteins**
- CUNY, Queen's, Chemistry Department, Chem315
 - ❖ a three day course over several weeks
 - ❖ students bring the crystals grown at school
 - ❖ crystals are screened and data collected at the beamline
- Interns

Outreach

- Summer Sundays
- NSLS tours

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Education and outreach

The beam line has participated in the NSLS and BNL Education and Outreach programs

Education

➤ Interns



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Synergy



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Synergy

The X6A team continues to make the facility available to user groups from other communities and promotes complementary methods between its user community. In specific:

❖ X4 PRT

- User beam time re-allocation
- Technical and scientific approaches to crystallography
- Educational outreach

❖ PXRR

- X6A users in need of insertion device beam time has been allocated beam time on X29 or X25 during their X6A beam time
3 groups took advantage, 2 for X29 and 2 for X25



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Summary

Upgrades did not interfere with available user beam time and Overall productivity.

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- FOCUS on the USER.
- Young Faculty User base.
- USER RESEARCH program ALIGNED with NIGMS Road Map
- Increased beam line productivity.
- Continued upgrade of instrumentation assures optimal beam time usage.

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The X6A Team

Kun Qian
Jean Jakoncic
Marc Allaire
Vivian Stojanoff

... we choose X6A over other beamlines because of the great help and support we obtain



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