



NIGMS East Coast Structural Biology Research Facility

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

Science Advisory Committee meeting
01 February 2013



Vivian Stojanoff

Our Mission

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.

This goal includes:

- 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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NIGMS metrics review requirement

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- Scientific Productivity
 - user number
 - quality of science
 - comparison with similar beam lines
- User satisfaction
- Beamline performance
- Technical and infrastructure development
 - quality
 - importance
 - relevance to user program
- Resource allocation
- Interaction with other programs at the NSLS

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The X6A Operation Timeline

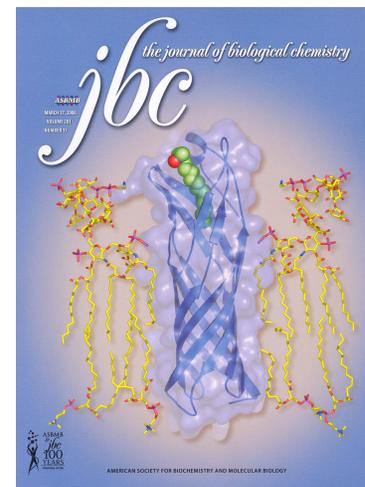
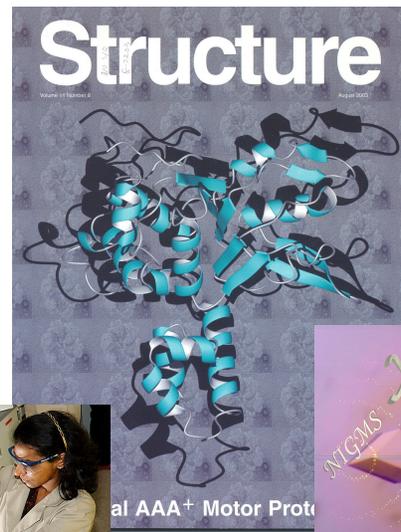
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2001



03



2002



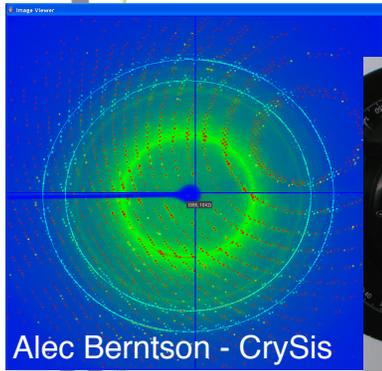
1Q72

2004

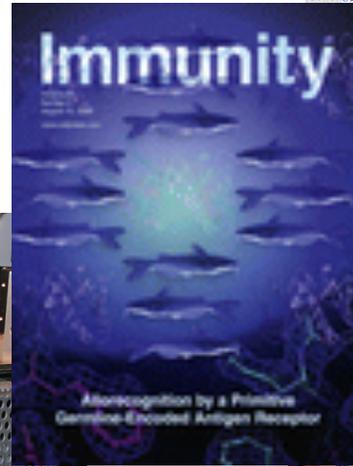
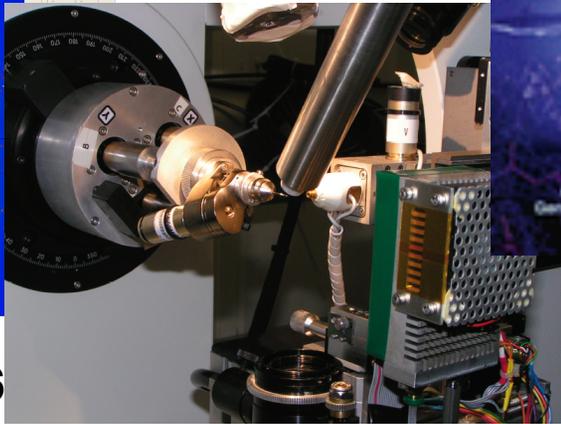


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The X6A Operation Timeline



2006

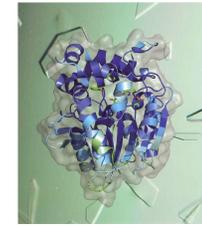


2008

November 2012						
Sun	Mon	Tue	Wed	Thu	Fri	Sat
Available From 08:00	Available	Available	Available	Available	Available	Available
Available From 08:00						
Available From 08:00						
Available From 08:00						
Available From 08:00						
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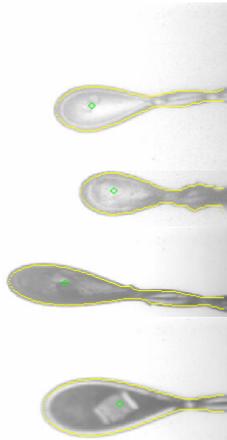


2010

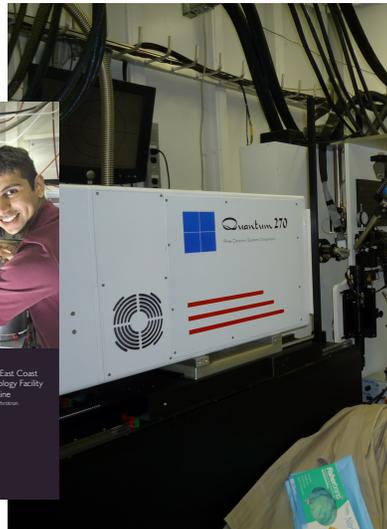


JB
Journal of Bacteriology

2007



Anubhav Jain - CrysCen



2009



ProteinXpress
Your protein structure one shipment away

RemoteAccess

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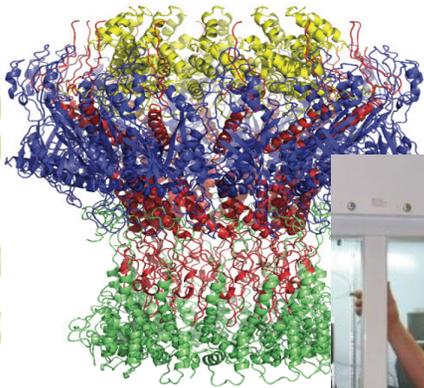
The NIGMS Facility is funded by the NIGMS (1-04-0000) by NIGMS and supported by NIGMS (04-0000) NIGMS (04-0000) NIGMS (04-0000)

BROOKHAVEN
NATIONAL LABORATORY

The NIGMS East Coast Structural Biology Facility X6A Beam Line at Brookhaven National Laboratory

The X6A Operation Timeline

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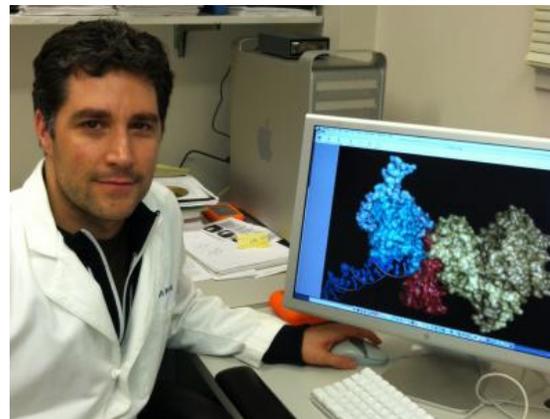
2011



2013



2012



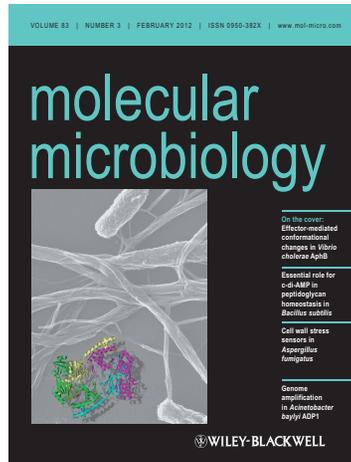
2014

01Feb2013

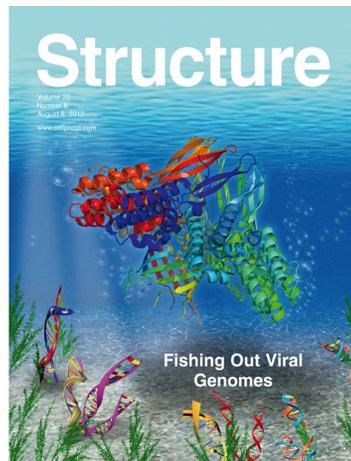
Science Advisory Committee Meeting

A vibrant user community

65 Publications in 2012 with 20 in premier journals.



<IMPACT>= 5.9



- Pascal **Science** 336:728-732
- Marmorstein **Angew.Chem.Int.Edit** 51:5244-46
- Aggarwal **Nat. Struct. Mol. Biol.** 19:628-32
- Loll **Acta Cryst. D** 68:497-504
- Rudino **Acta Cryst. D** 68:564-577
- Berg **Plos Biol.** 10:e1001242
- Schilbach² **Proc.Natl.Acad.Sci.USA** 109: 2308-13
- Ostrov² **Proc.Natl.Acad.Sci.USA** 109: 9959-645
- Garman **Proc.Natl.Acad.Sci.USA** 109: 17400-405
- Boggon **Proc.Natl.Acad.Sci.USA** 109: 16107-112
- Sunddberg¹ **Adv. Funct. Mater.** 22:3191-3201
- Loll **J. Am. Chem. Soc.** 134:4637-45
- Zhang **Nat. Commun.** 3:1021
- Rudino **Plant Physiol.** 158:1570-82

¹The X6A Workbench ²ProteinXpress
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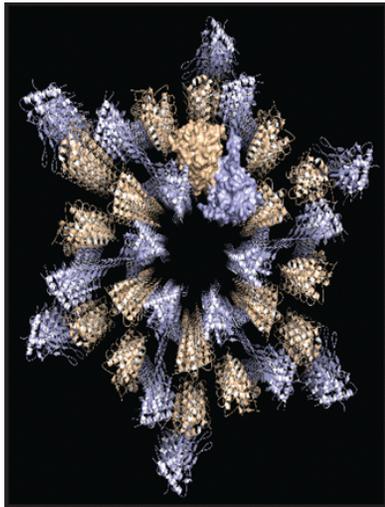
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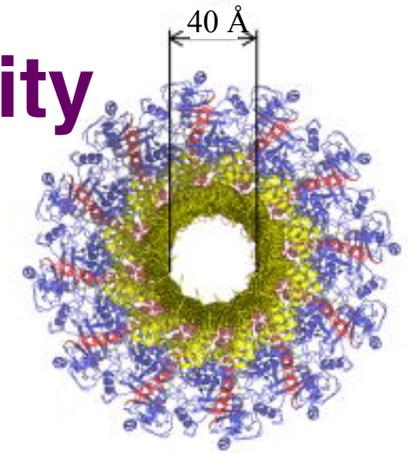
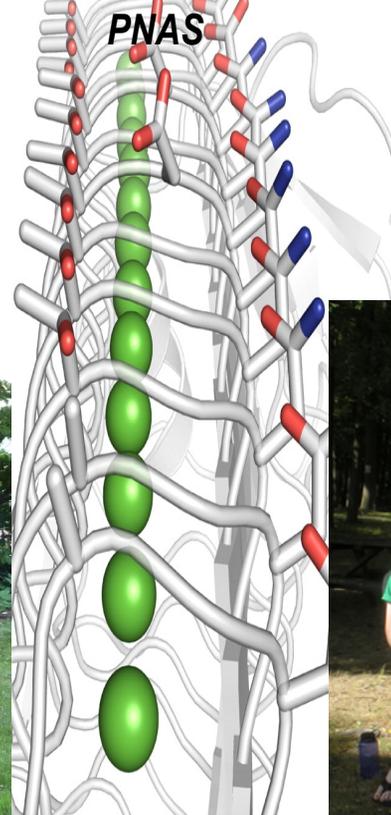
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An engaged user community



Skordalake's team, Wistar
Telomere length regulation
Mol. Cell. Biol.

Davies's team Queen's
University
Anchored Clathrate Waters
Bind Antifreeze Proteins to Ice



Cingolani's Lab, Thomas Jefferson
3D structure of a viral genome-
delivery portal vertex
Nat. Struct. Biol.



Hardy's Group, UMASS
Substrate-Induced Conformational Changes Occur in Caspase-6
J. Mol. Biol.



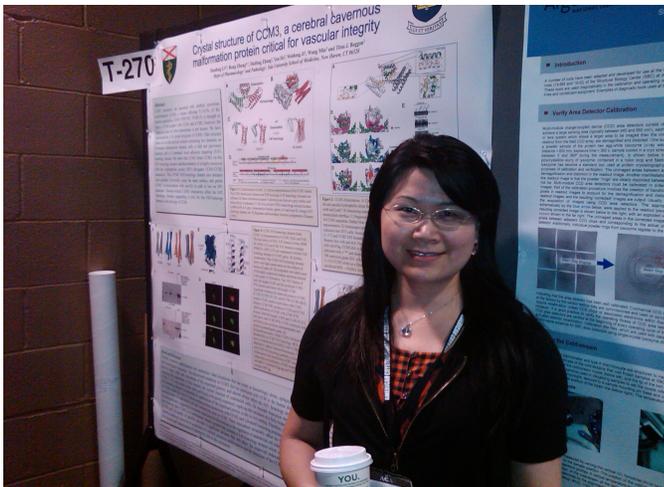
Marmorstein's team, Wistar
MYST protein acetyltransferase activity
requires active site lysine autoacetylation
EMBO J.

A dynamic user community

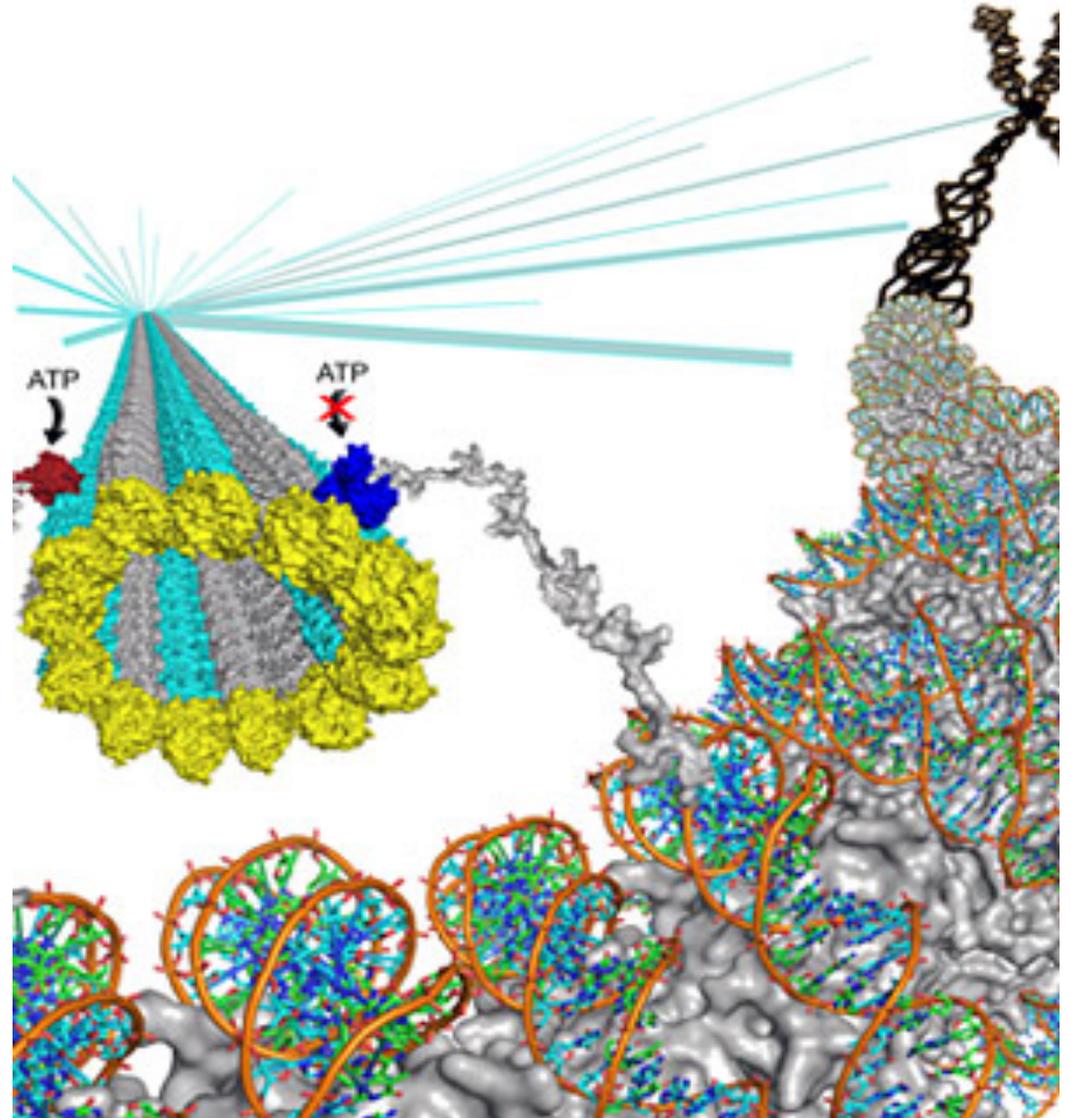
Jon Kull Group, Dartmouth College
Cell 136,110-122



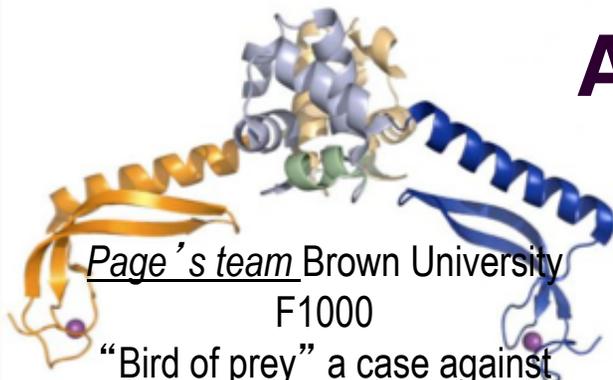
Patrick Loll Group, Drexel
'Non-trivial' Crystallization Reveals Antibiotic's
Molecular Mode of Action



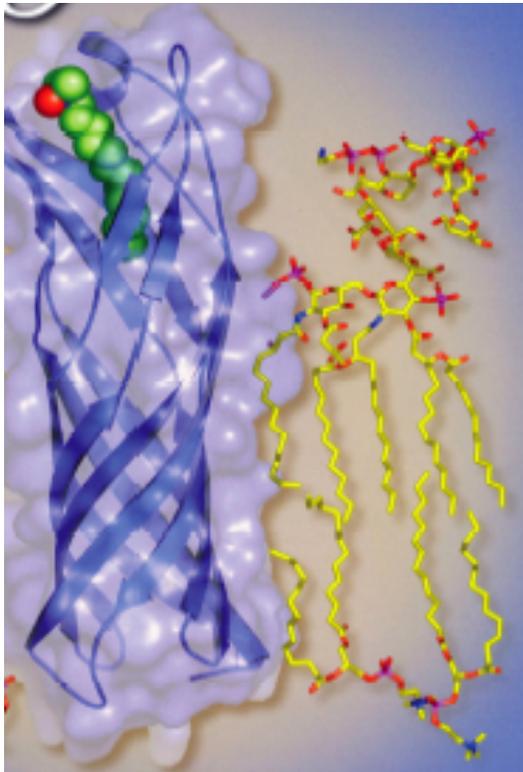
Boggon's Lab, Yale University
CCM3, a cerebral cavernous malformation protein
critical for vascular integrity
J Biol. Chem.



A dynamic user community

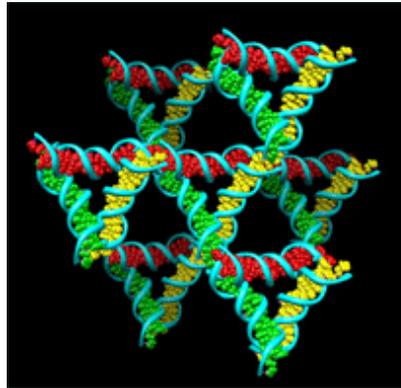


Page's team Brown University
F1000
"Bird of prey" a case against
drug-resistant biofilms;
J Biol. Chem.

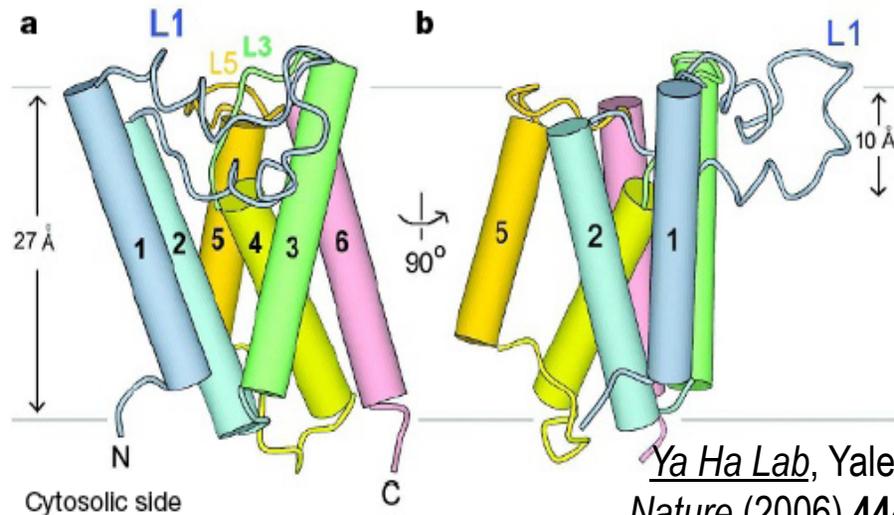
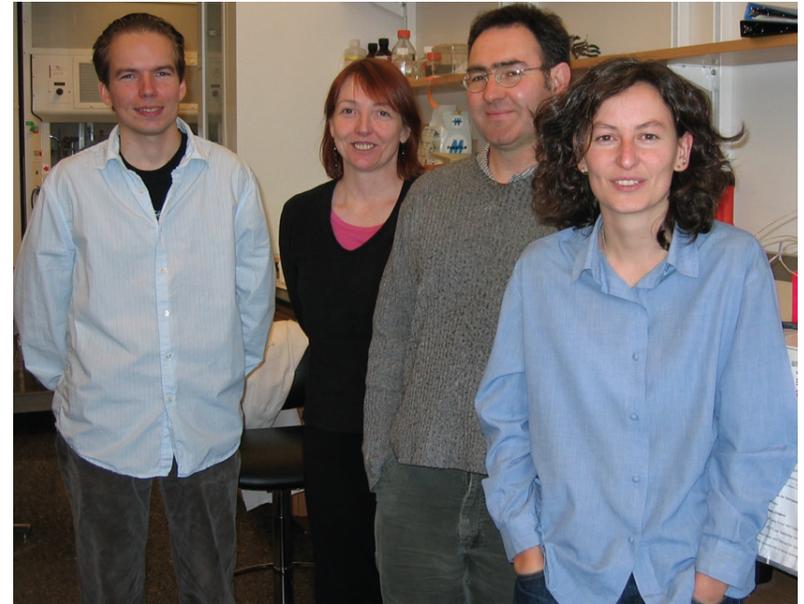


Van den Berg, UMASS Worcester
J. Biol. Chem (2006) 281, 7568 -7577

Seeman, Lab, NYU
Nature, 458, 367-370



Regan Lab, Yale University
J. Am. Chem. Soc. (2005) 127, 10188-10190.



Ya Ha Lab, Yale University
Nature (2006) 444, 179-180



Staff

Organizational Chart



Qun Shen *1
Photon Science Division

Scientific Advisory
Committee

Mario Amzel
John Hopkins
chair

Hao Wu
Weil Medical

Craig Ogata
GM/CA CAT

Vivian Stojanoff
Project Director

Jean Jakoncic
Associate Scientist

Kun Qian
IT Associate

Edwin Lazo
Science Associate

Lisa Miller *1
Photon Science Associate
Life Science Div Head

Marc Allaire *2
Associate Scientist

Scientific, Technical,
ES&H, Administrative *1
Support as required

*1 PS Directorate scientific staff

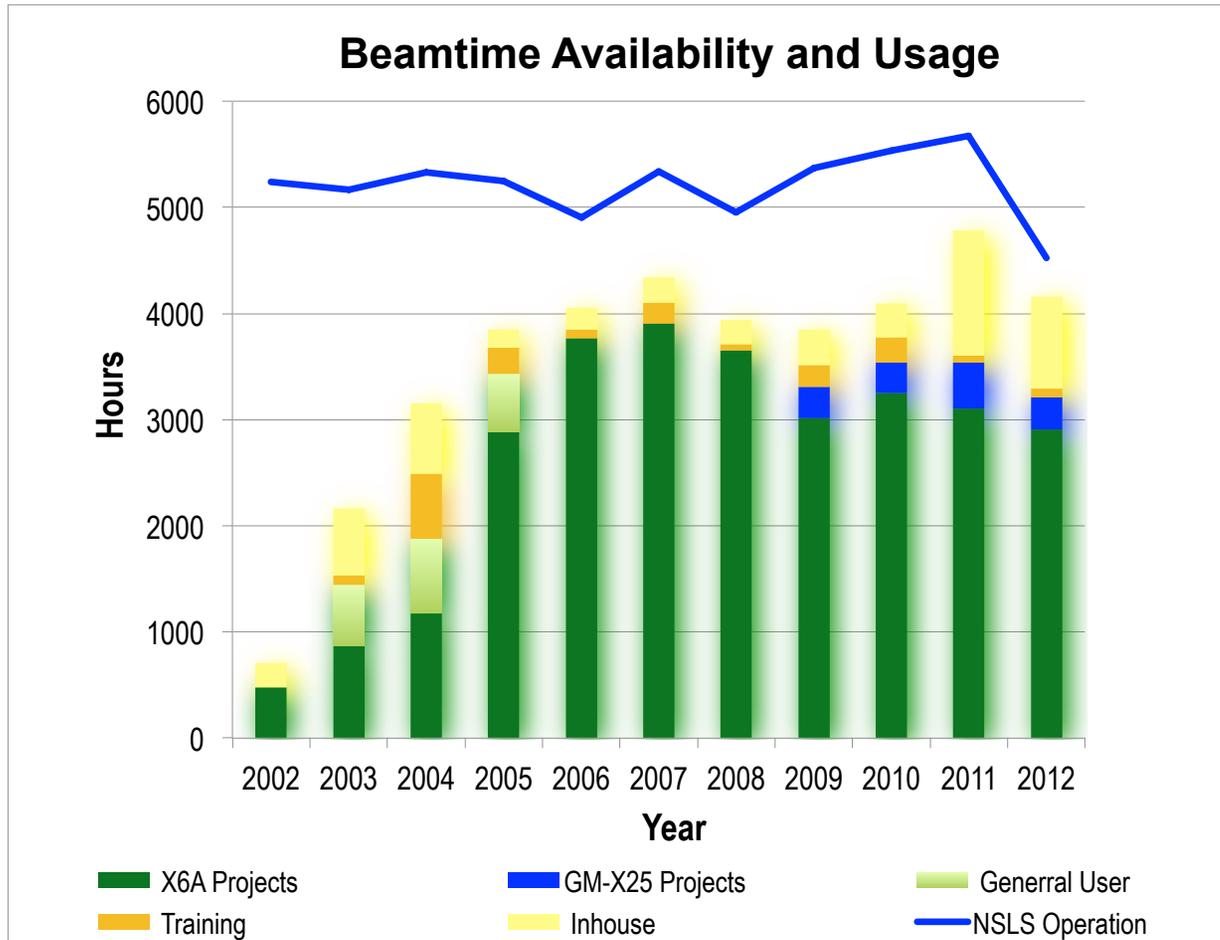
Science Advisory Committee Meeting

*2 1/4 FTE



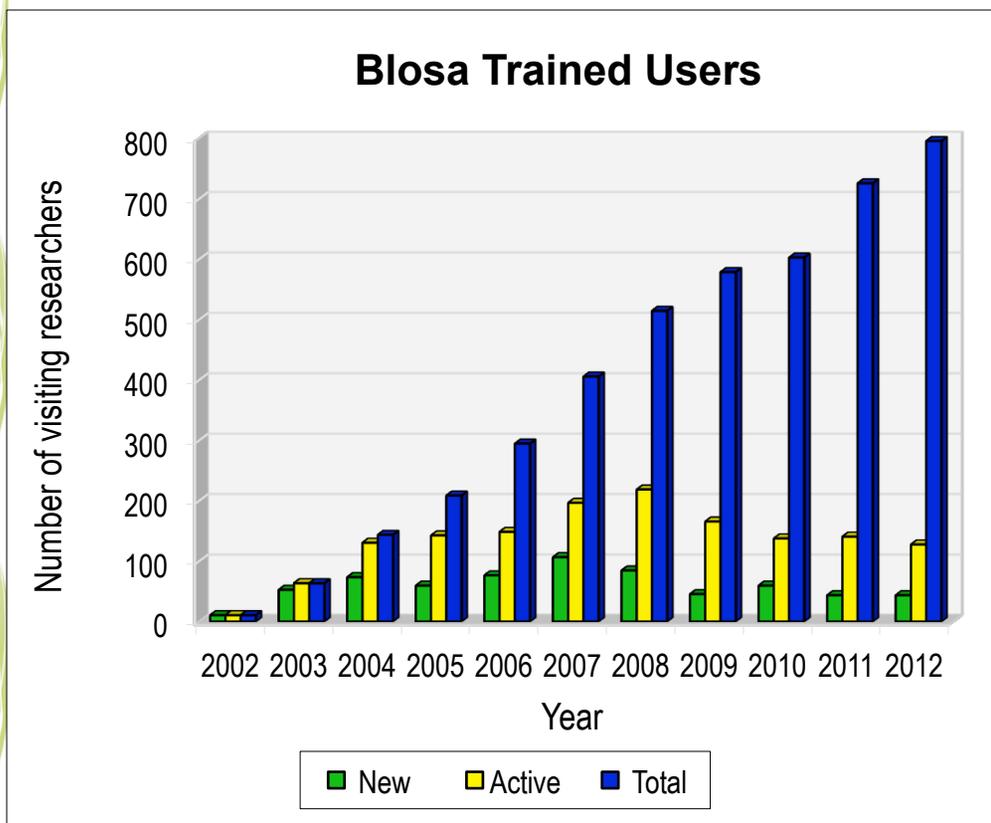
User Program

Available beam time



In the past 10 years ~70% of the NSLS user available beam time at the Facility was dedicated towards external research and collaborations.

(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.

*Source NSLS PASS System December 2012

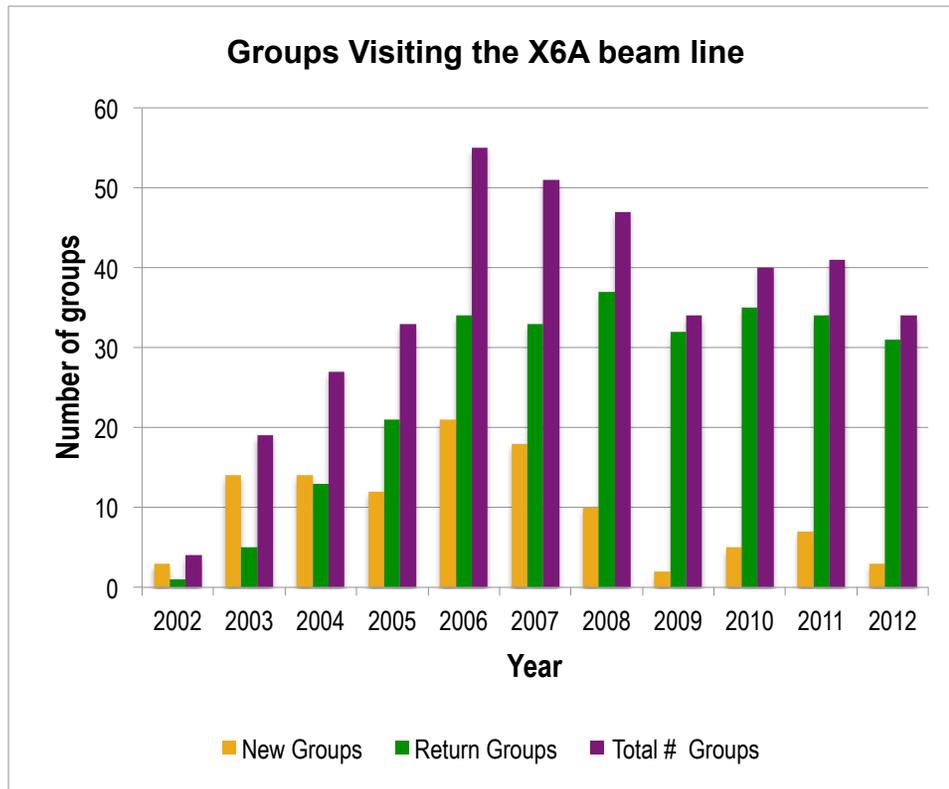
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Consolidation of the user community*



New groups: scheduled their projects only once in 2012.

Return groups: scheduled their projects at least 2x in 2012.

*Source X6A Survey December 2012

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Over the last seven years the number of user groups visiting the beam line remained nearly constant (~ 33 groups/year) .

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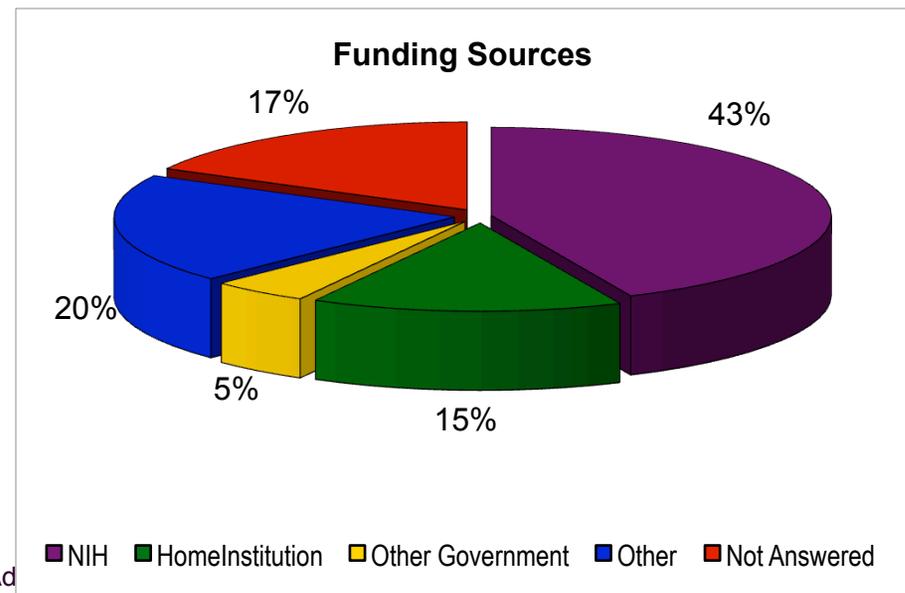
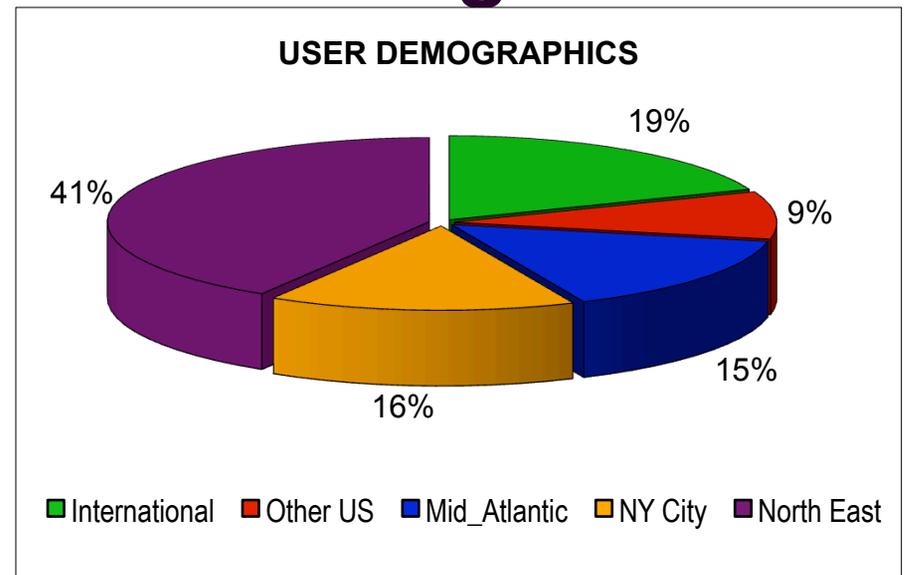
User demographics and funding*

- Primary usage by academic institutions located in the Northeast;
- Registered researchers are mostly expert crystallographers but less than 54% provide this information. Most non-expert crystallographers do not register on the X6A webpages.
- Funding for projects developed at X6A is provided by NIH institutes, with start up funds accounting for 15% of the projects.

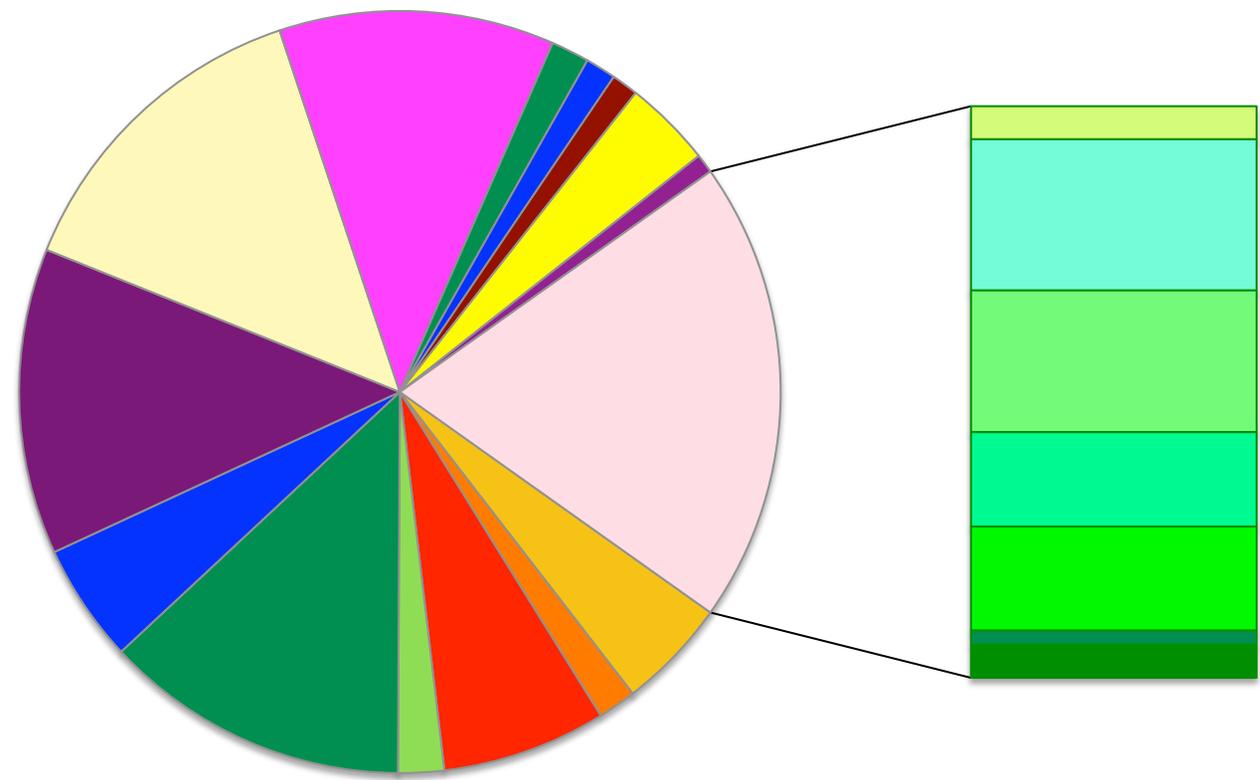
*X6A survey Dec2012

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X6A User Community Profile 2002-2012



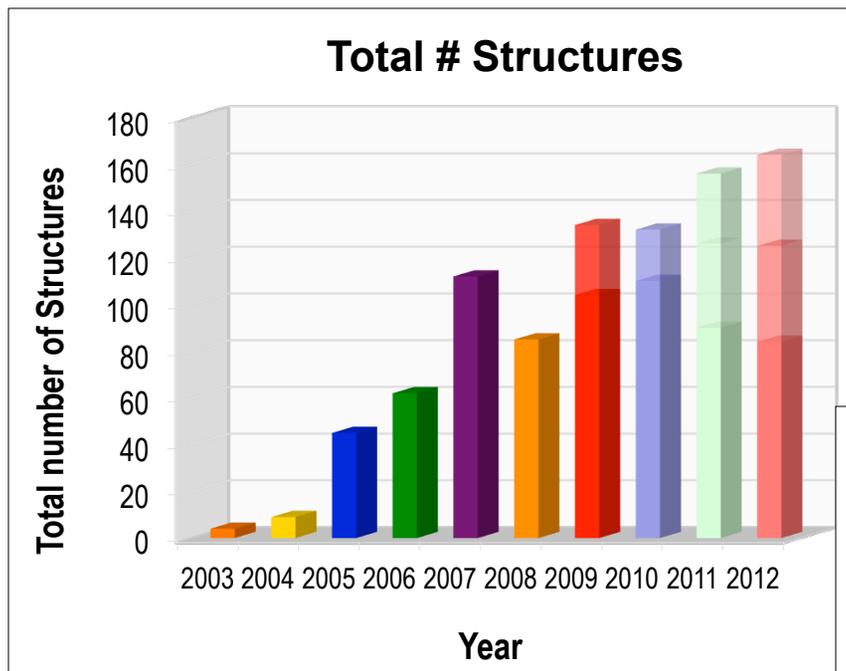
- New Hampshire
- Rhode Island
- Connecticut
- New Jersey
- Pennsylvania
- Maryland
- Massachusetts
- NY
- NYC
- Virginia
- Florida
- Southeast
- California
- West Coast
- South West
- MidWest
- Canada
- Mexico
- Europe
- South America
- Asia

Source: NSLS/ X6A Survey



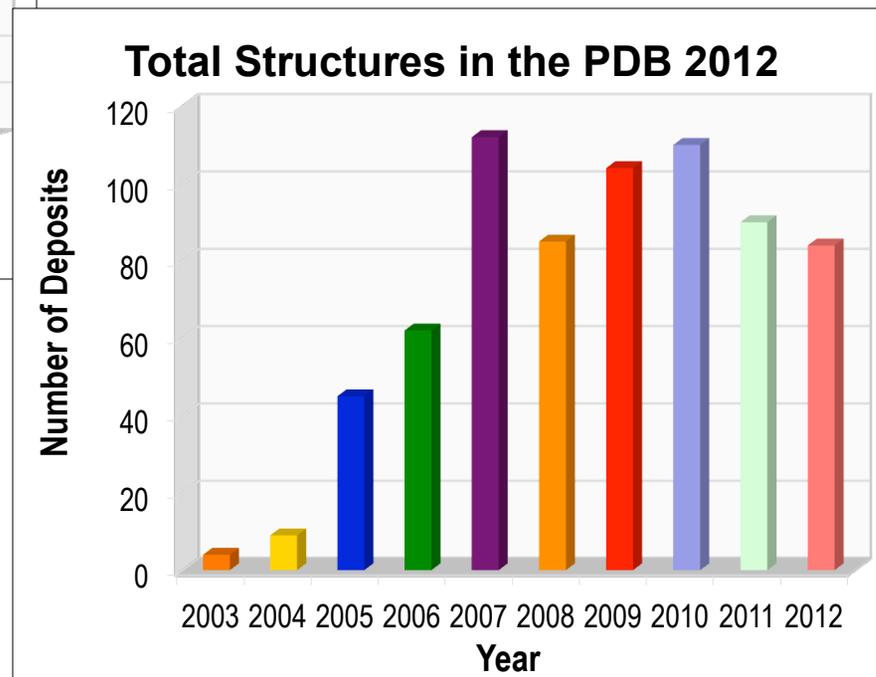
Impact

Protein Data Bank Deposits*



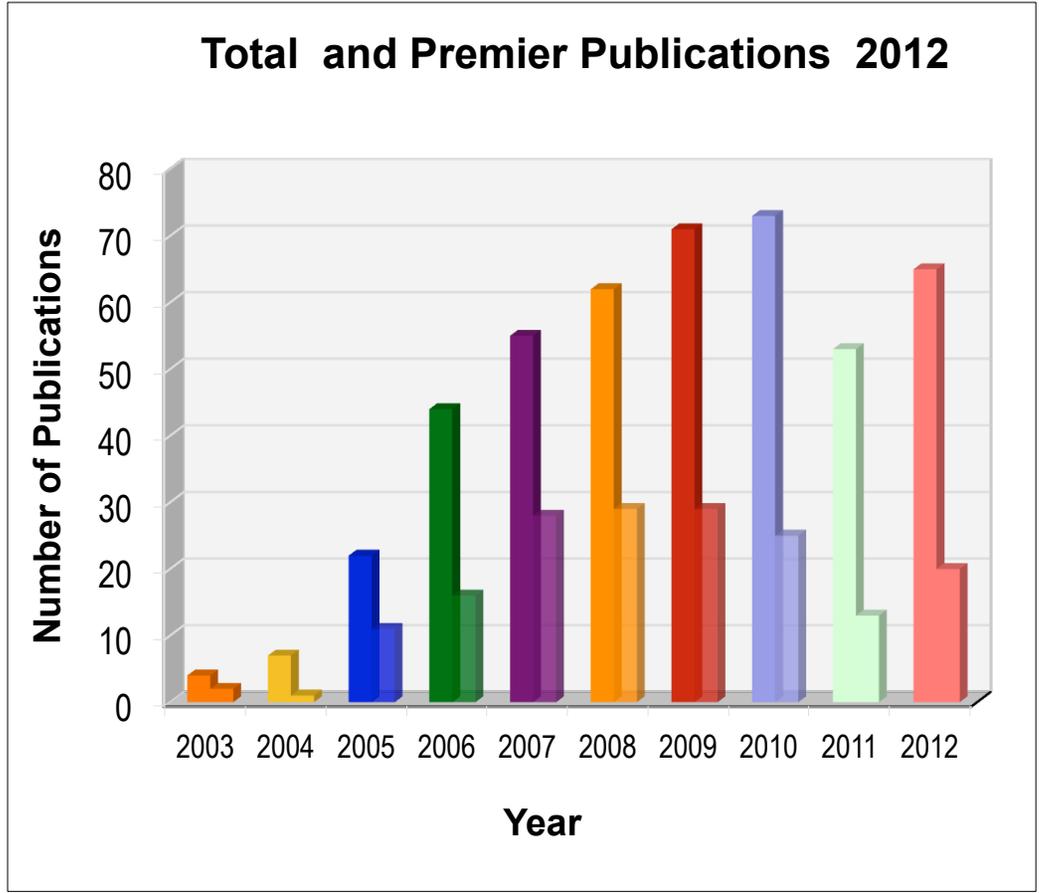
Total number of structures include proprietary and high throughput research center results. These groups take advantage mostly of the automounter.

The number of structures deposited in the protein data bank has stabilized in the last 5 years.



*Source X6A Survey December 2012

Publications*



Publications*	
Total	High Impact**
456	174
2012	
65	20

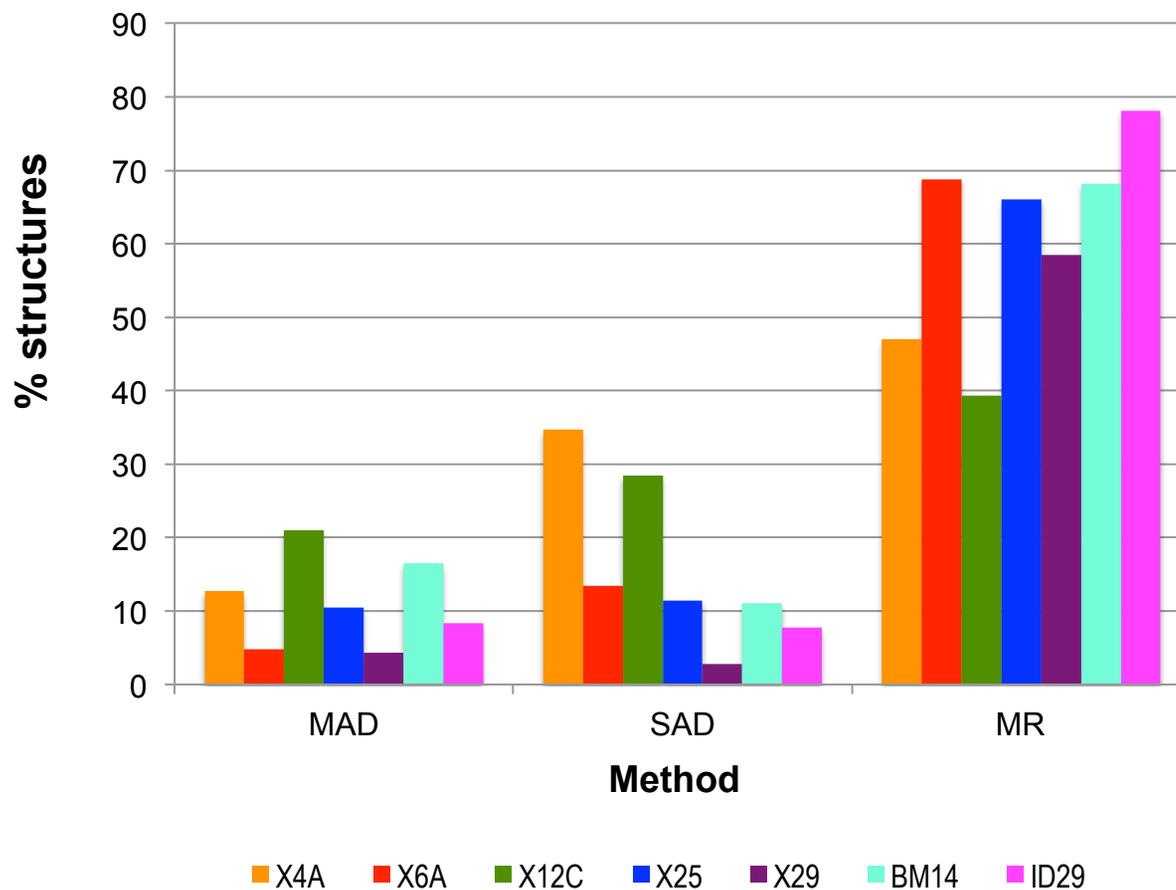
*Source X6A Survey December 2012

** Journals with an impact of 6.0 or greater. Source BNL Library Service

Research published in premier journals account for 37% of the publications from the Facility.

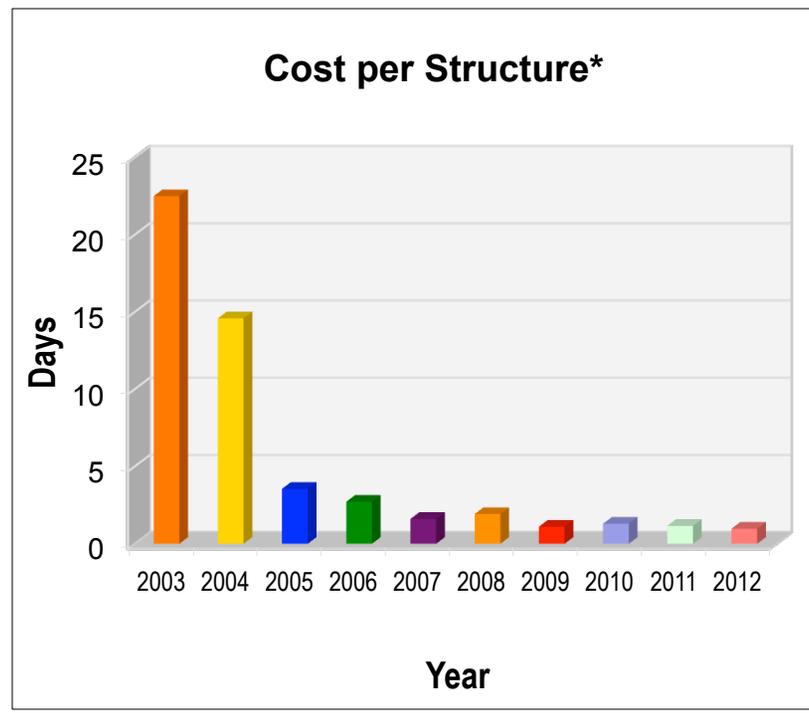
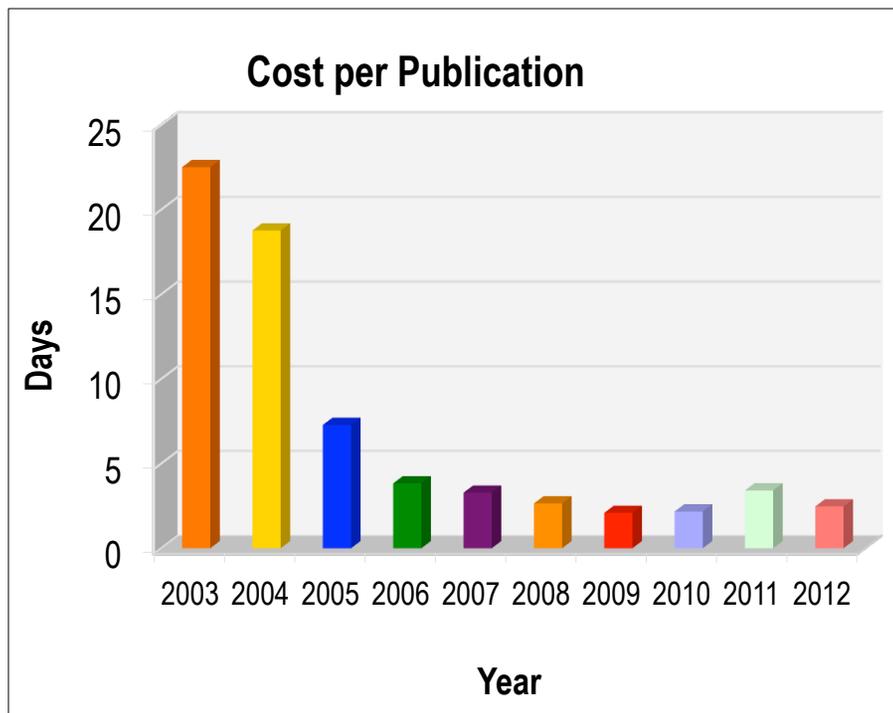


METHODS



Other impact factors*

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



* Includes proprietary and SG structures

The cost per structure as a function of scheduled user hours decreased if proprietary and SG data are taken into account

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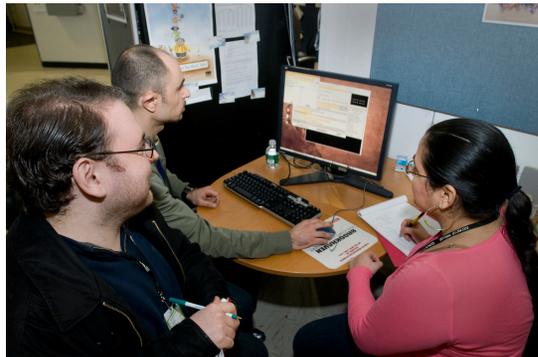
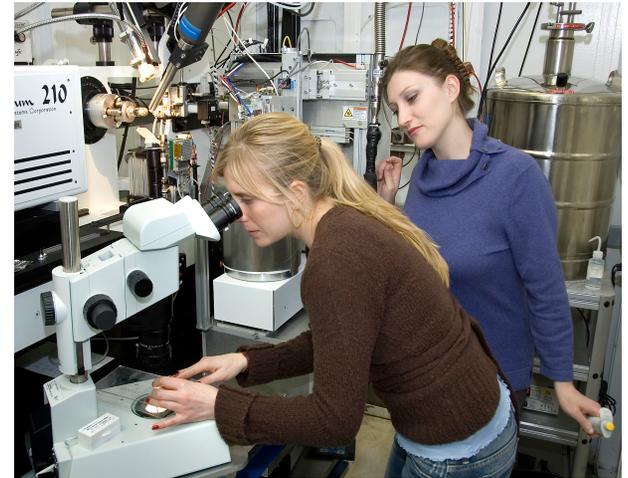


Education and Outreach

Education and outreach

X6A team members and interns participate in courses and workshops. This is an important activity to attract new users.

- Workbench
- Crystallization workshop
- DOE summer internship program
- NSLS Summer Sunday
- CCNY Summer Program
- Graduate Course



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Summary

- FOCUS on the USER.
- Junior Faculty User base
- USER RESEARCH ALIGNED with NIGMS Road Map
- One of the most productive beam lines at the NSLS.
- Continued upgrade of instrumentation assures optimal beam time usage.
- Expect to operate through summer/fall 2014

aaahhhh...personal attention! I love it!
CM

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Beam time usage

Beam time Utilization

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X6A Program 2012*

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- X6A user projects 66%
- Available 7%
- X6A beam line 27%
 - ✓ X6A commissioning 11%
 - ✧ Instrumentation upgrade
 - ✧ Instrumentation failure (alignment, automounter)
 - ✓ X6A inhouse projects 6%
 - ✧ Scientific staff research and external collaborations
 - ✧ Student training and mentoring

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*percentages are calculated relative to NSLS total available time for operation

User beam time usage 2012

Total # images	354674
Total # images screened	29993
Total # data sets*	1126
Total # crystals screened and collected	8741
Automated Sample Changer	
Total # images screened	7166
Total # data sets*	105
Total # crystals screened and collected	3645
usage	49d 21h

*data set 40 or more images

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The 1999 NIGMS Initiative at the NSLS

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Bending magnet source recommended by NIGMS

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- 2000 procurement slits, mirror, detector
- 2001 construction and installation, monochromator NSLS design
- 2001, two FTE' s hired for operation support
- X6A program includes support for four FTE' s
- 2002 operation start
- 2003 \$1,200K supplement for detector upgrade
- 2008 End-station upgrade (November, 2008)
- 2009 End-station commissioned (March 2009)

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