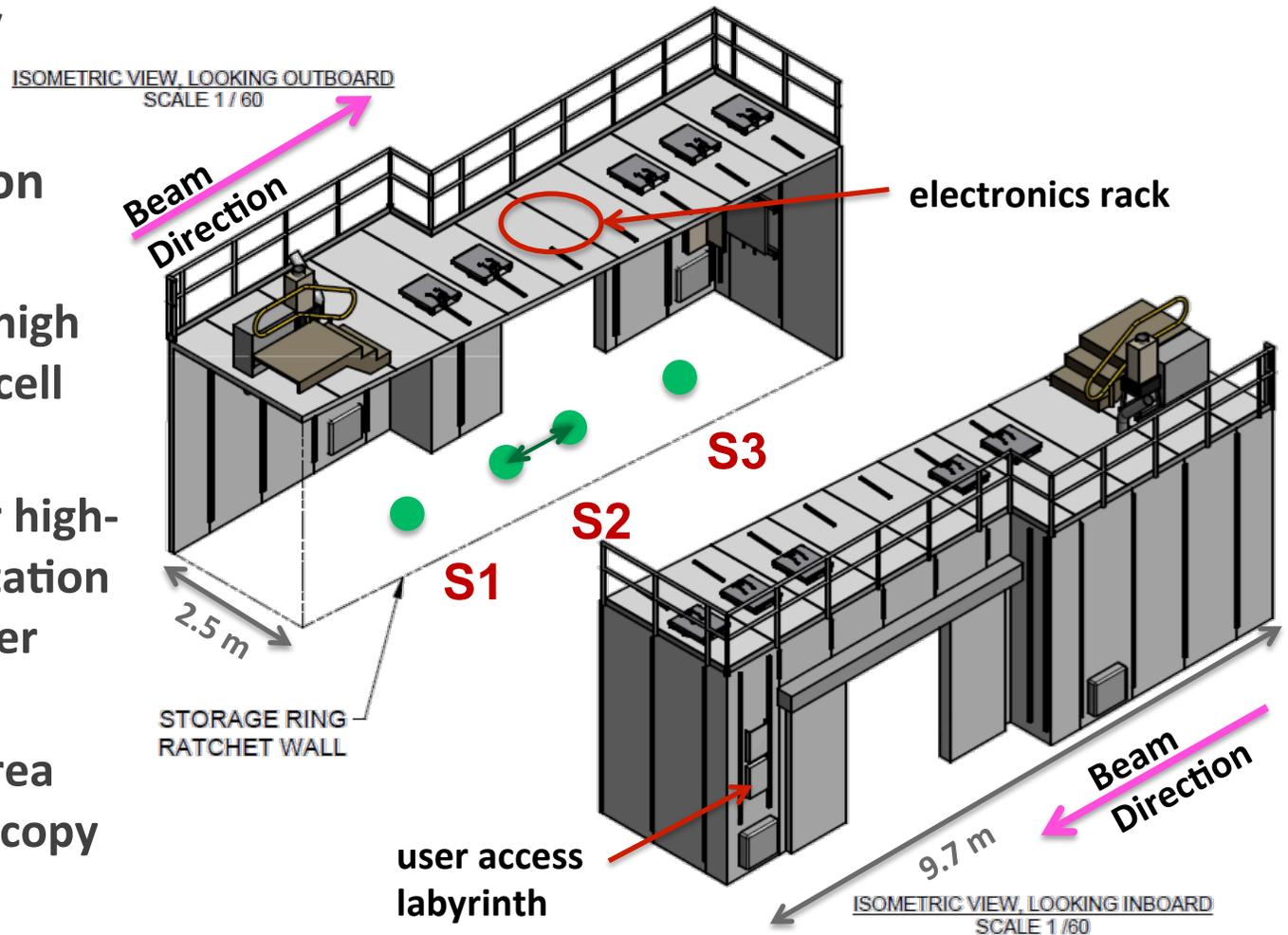


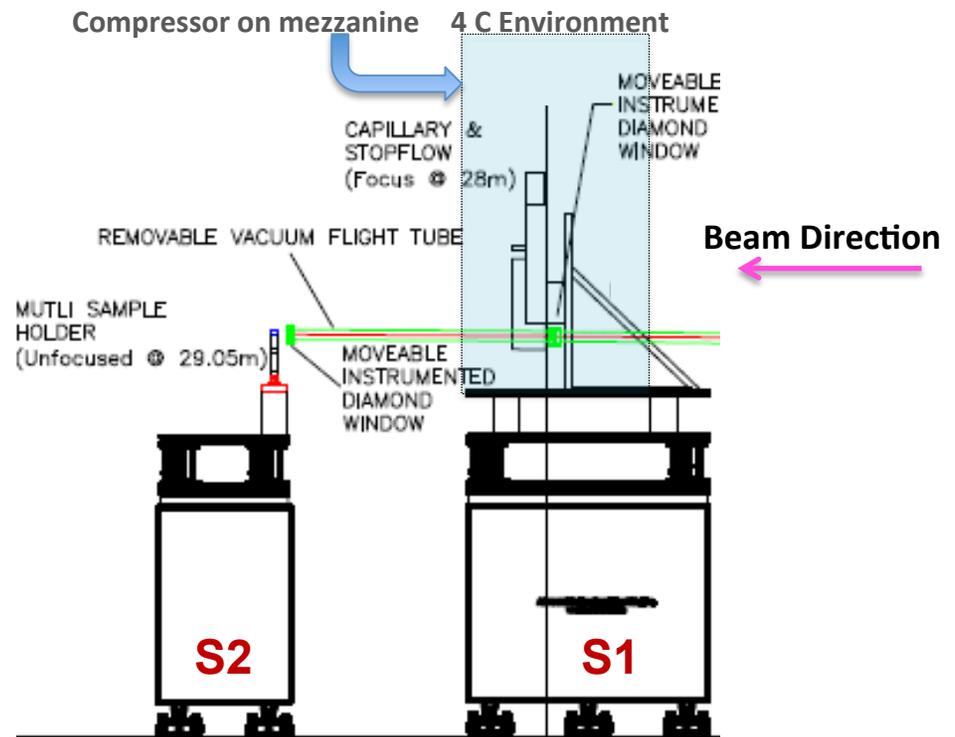
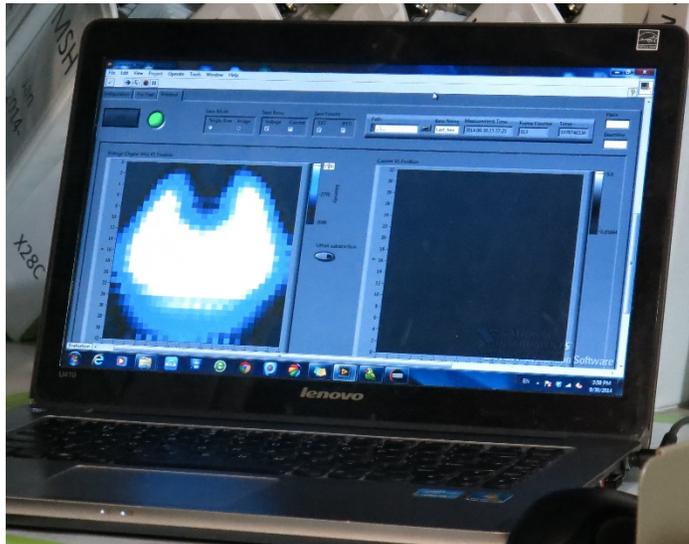
# XFP FOE/Hutch

- White-beam FOE/hutch
- Multiple endstation locations:
  - S1: Full focus for high flux density flow cell endstations
  - S2: Defocused for high-throughput endstation (movable for larger samples)
  - S3: Experiment area for x-ray spectroscopy



# Endstation

- Capabilities transferred from NSLS X28C: MSH, KinTek, capillary flow cell, *in-vivo* setup, local sample environment control
- New at XFP: global environmental control (temperature, humidity, 4C), in-line FPLC capability, instrumented diamond window (in progress, NSF)

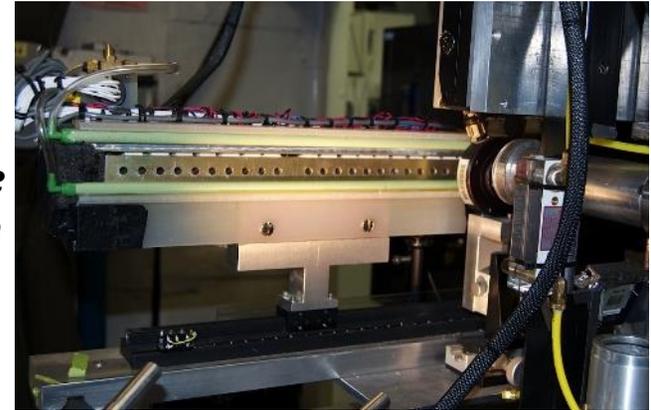


<http://www.bnl.gov/newsroom/news.php?a=25299>

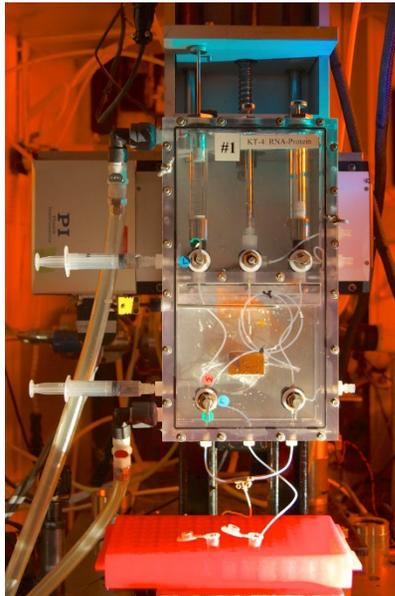
# Beamline Modes

## ➤ *Beamline Modes Enabled:*

- High Throughput
- High Flux Density
- Large ID Capillary/KinTek

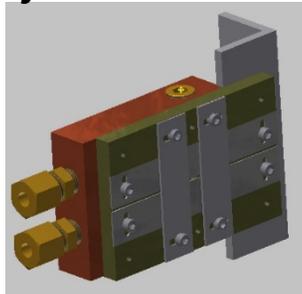


*Multi-sample holder – high throughput*

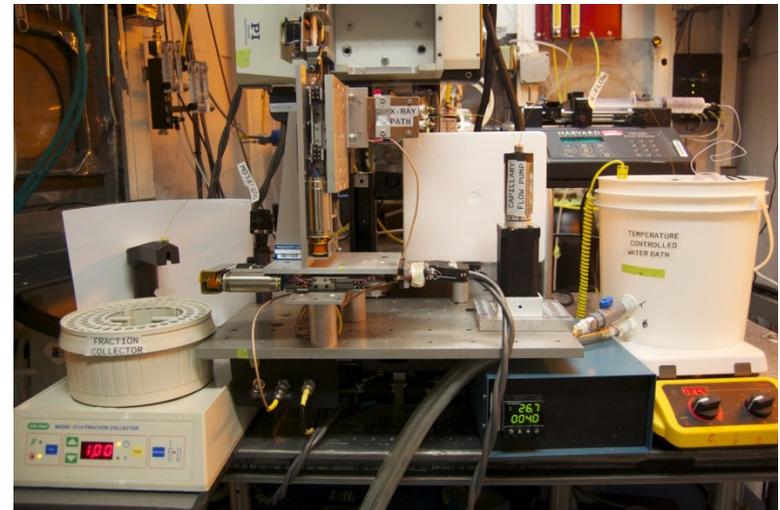


*KinTek quench – flow (time-resolved mixing)*

*100  $\mu\text{m}$  capillary flow cell*



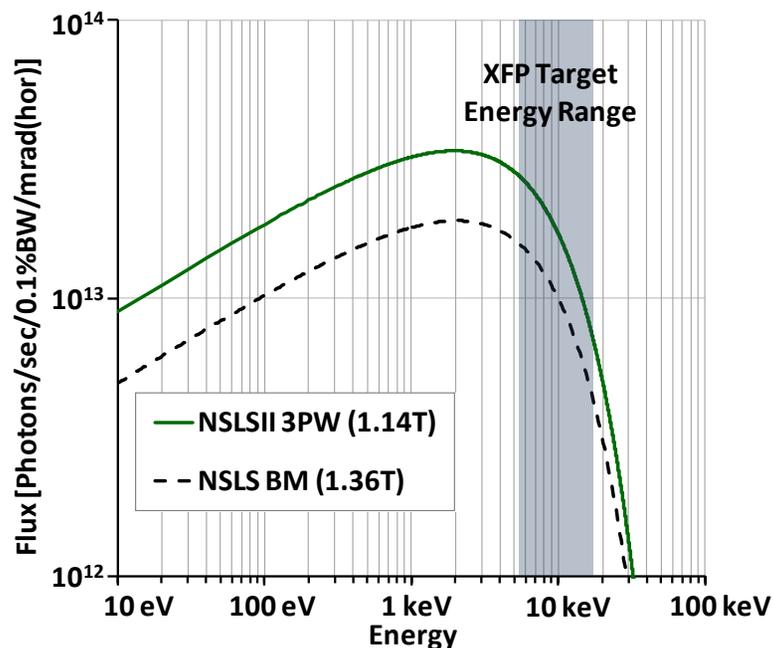
*Multi-pump in vivo*



# NSLS-II/XFP Source Properties

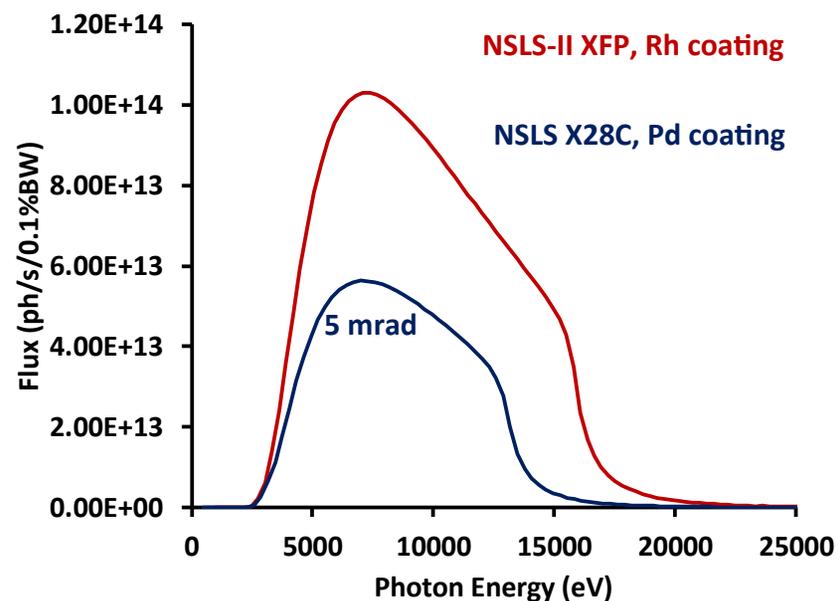
## 3-Pole Wiggler Source

Source	Hor. Size, Div. [ $\mu\text{m}$ , $\mu\text{rad}$ ]	Vert. Size, Div. [ $\mu\text{m}$ , $\mu\text{rad}$ ]
NSLS BM X28C	$\sigma_h = 260$ , $\sigma_h' = 300$	$\sigma_v = 57$ , $\sigma_v' = 11$
NSLS-II 3PW	$\sigma_h = 167$ , $\sigma_h' = 98$	$\sigma_v = 12.3$ , $\sigma_v' = 0.82$



## Spectral Flux

- 3 mrad H, 0.33 mrad V from 3PW
- Rh-coated toroidal mirror, 4.2 mrad angle
- 250  $\mu\text{m}$  Be window, 75  $\mu\text{m}$  diamond exit window
- $\sim 5 \times 10^{16}$  ph/s to sample

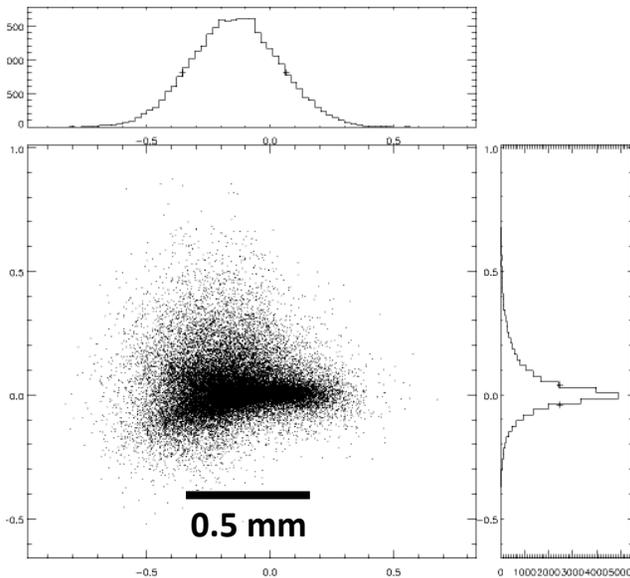


Note: assumes no rays lost, 500 mA beam current

# XFP Modes: Full Focus

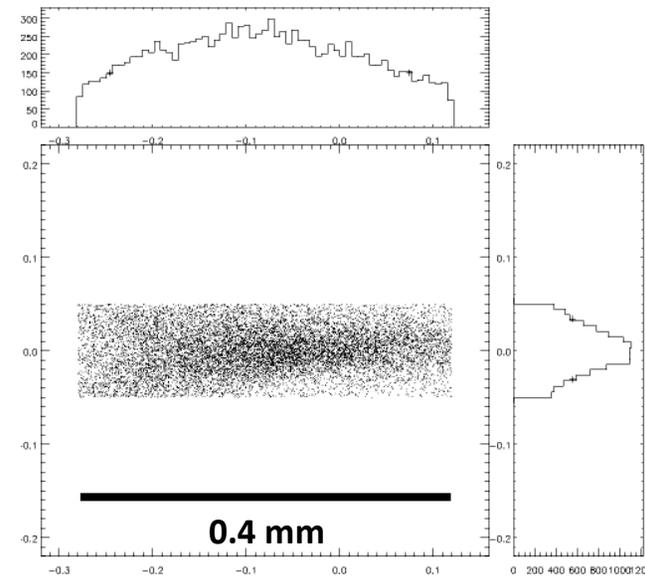
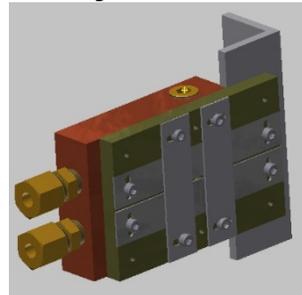
Major Radius: 3.3 km

FWHM V [mm]	FWHM H [mm]	Total Power in Spot [W]	Sample Morphology (V x H, mm)	Power Density on sample [W/mm <sup>2</sup> ]
0.08	0.43	46	0.1 x 0.4	1153



Full Focused Beam

100  $\mu\text{m}$  capillary flow cell



Sample: 100  $\mu\text{m}$  Capillary

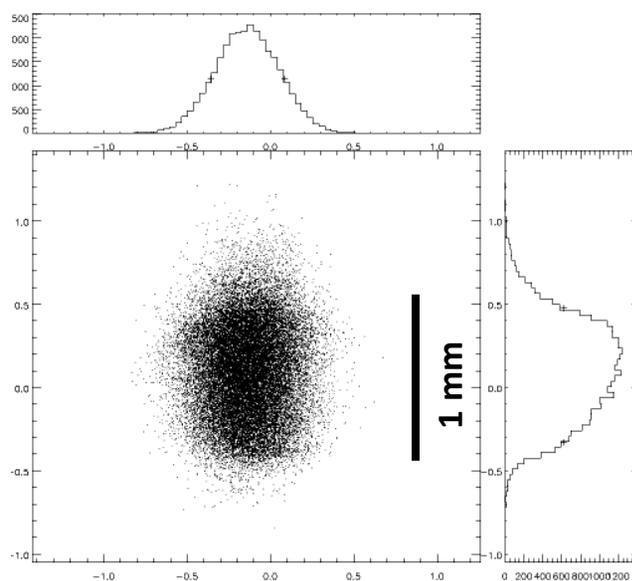
**Sample Position 1: 28.0 m from source**

Note: mirror figure error not included in calculations

# XFP Modes: Large Capillary (& Quench-Flow)

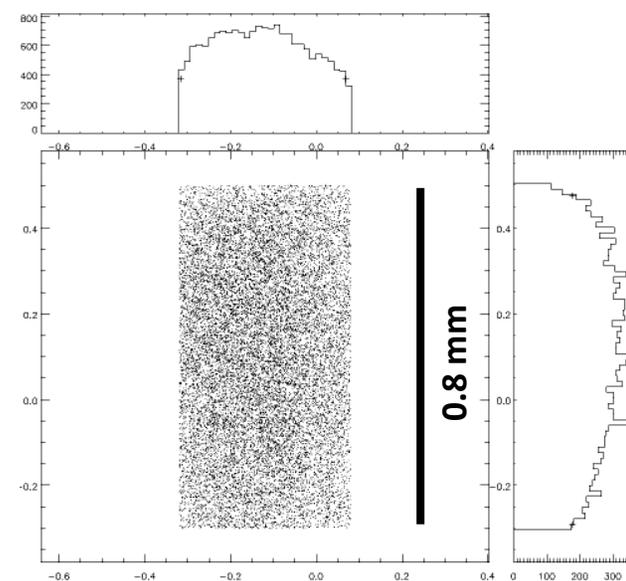
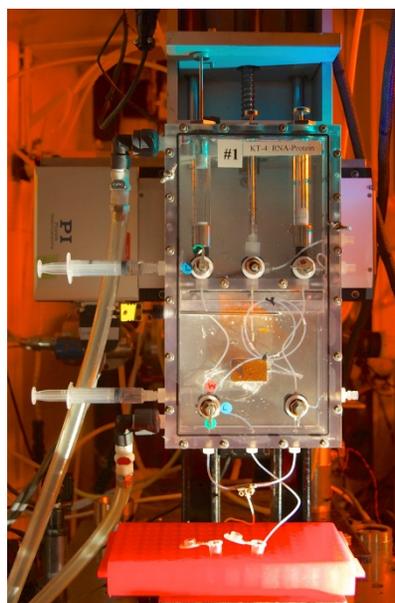
Major Radius: 3.7 km

FWHM V [mm]	FWHM H [mm]	Total Power in Spot [W]	Sample Morphology (V x H, mm)	Power Density on sample [W/mm <sup>2</sup> ]
0.8	0.46	59	0.8 x 0.4	185



**Full Beam**

*KinTek quench – flow  
(time-resolved mixing)*



**Sample: 800  $\mu$ m Capillary**

**Sample Position 1: 28.0 m from source**

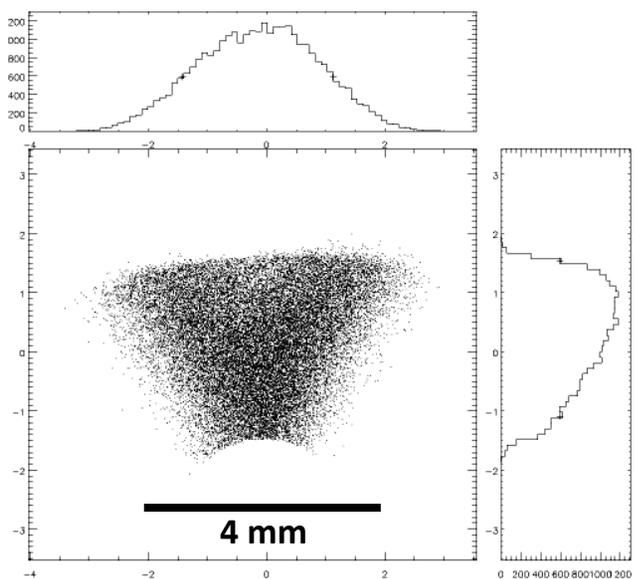
Note: mirror figure error not included in calculations

# XFP Modes: High Throughput & Large Samples

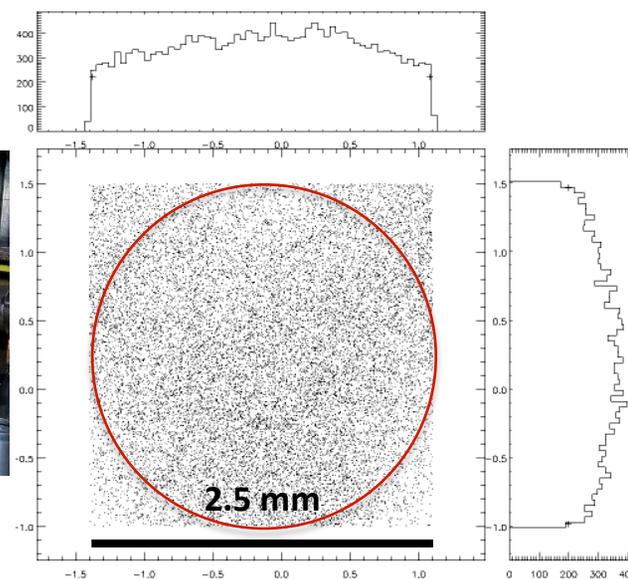
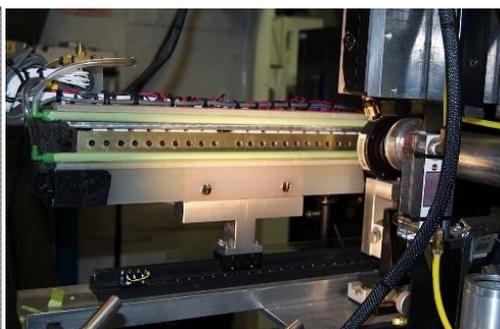
Major Radius: 5.7 km

FWHM V [mm]	FWHM H [mm]	Total Power in Spot [W]	Sample Morphology (Diameter, mm)	Power Density on sample [W/mm <sup>2</sup> ]
2.6	2.6	62	2.5	12.6

*Multi-sample holder – high throughput*



**Full Beam**



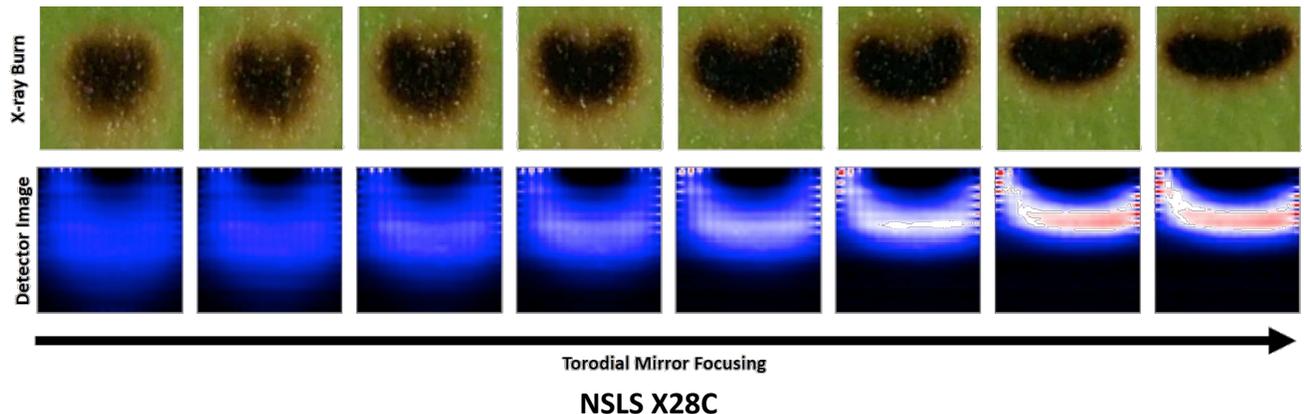
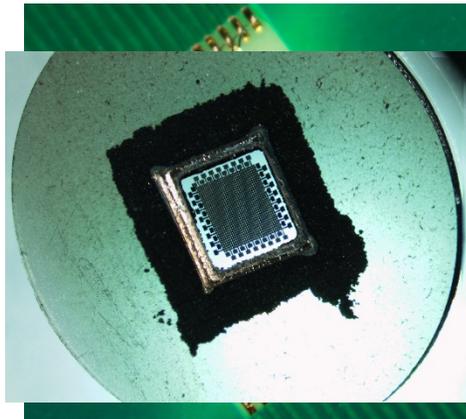
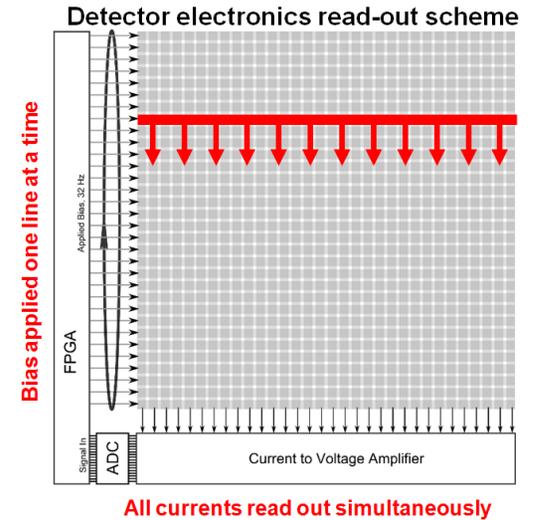
**Sample: 5  $\mu$ L Droplet in PCR Tube**

**Sample Position 2: 29.2 m from source**

Note: mirror figure error not included in calculations

# Instrumented Diamond Window

- *Beamline exit window (replaces standard Be window)*
- Transmission-mode diamond detector (no interconnects in beam)
  - Vertical lines measure current
  - Horizontal lines on opposite side sequentially biased
  - 40V Bias cycled at 1 kHz to generate images at 32 Hz
- Single crystal devices linear over >11 orders of magnitude in flux
- Diagnostic for alignment of mirror and/or sample motors
- Provides beam flux, position and morphology during experiment!
- Successfully tested 1024 “pixel” prototype detector (60 μm pixels)



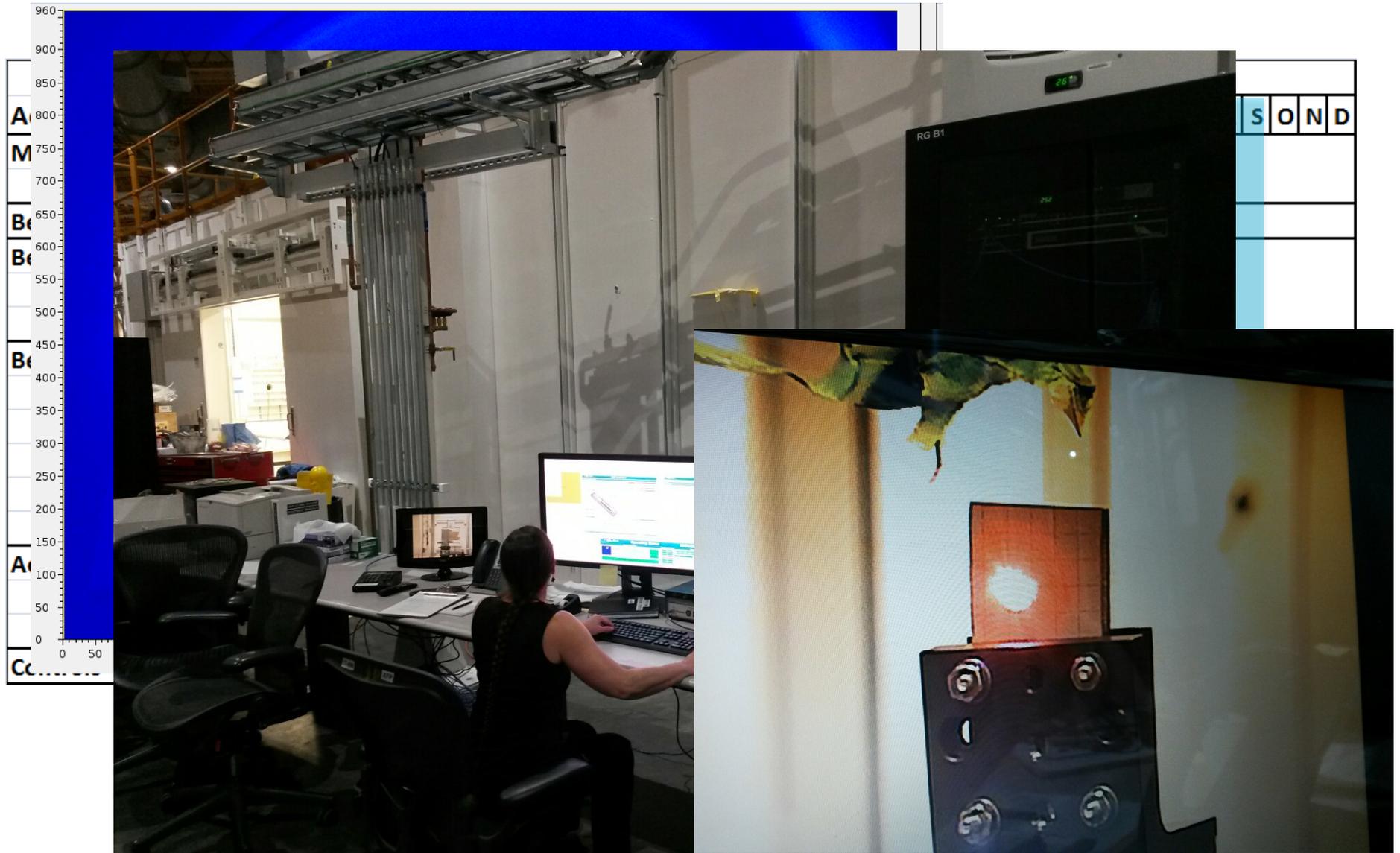
<http://www.bnl.gov/newsroom/news.php?a=25299>

# Sample Preparation Facility

- *Mass spectrometer*
- *High-pressure purification system (FPLC)*
- *Refrigerated Cabinet*
- *UV/Vis Spectrometer*
- *Fluorimeter*
- *-80 C Freezer*
- *Incubator*
- *Small-tube temp-controlled centrifuge*
- *Real-time PCR*
- **Work area, some chemical storage, no drain – waste will be contained and removed; will have emergency eye wash and shower, sprinklers**

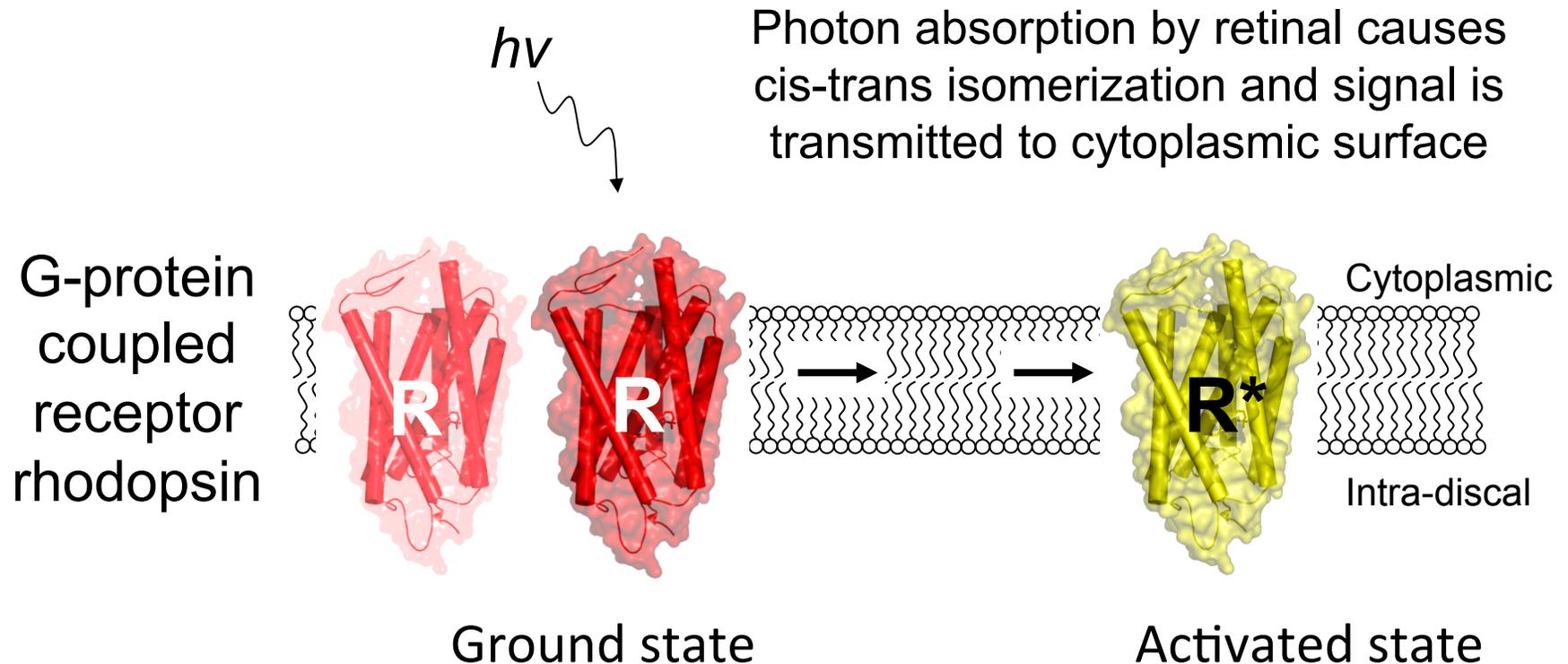


# XFP Timeline



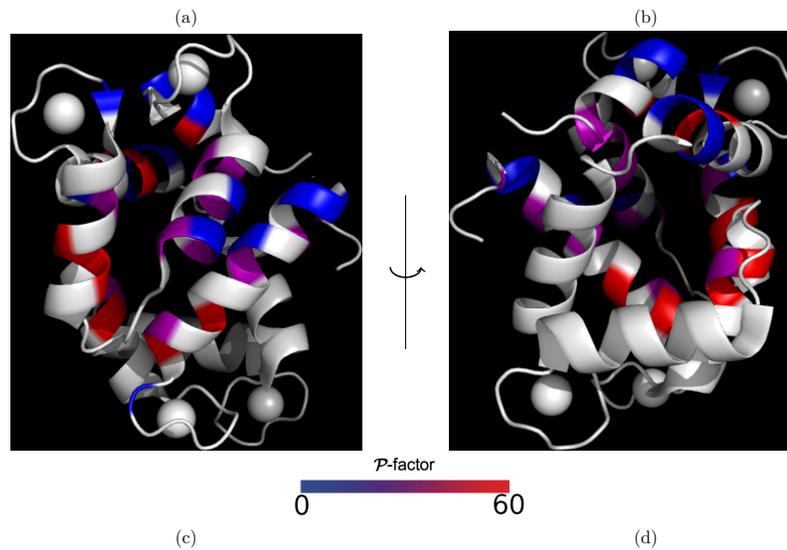
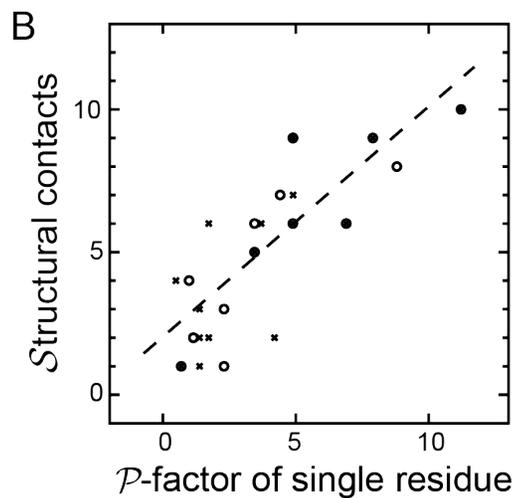
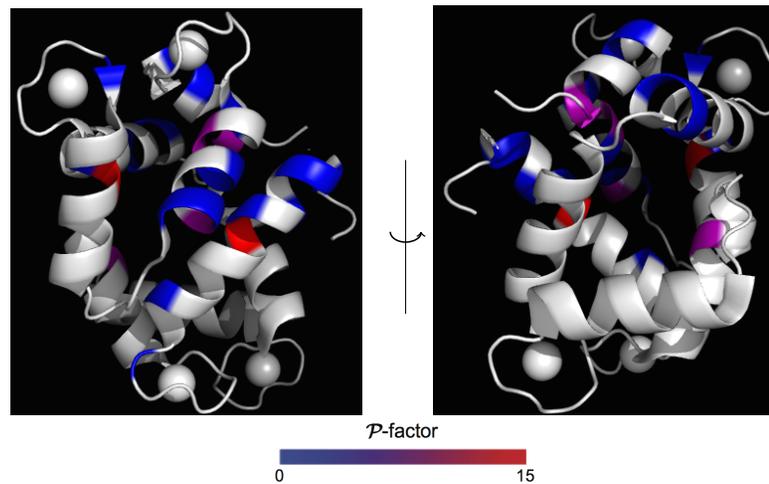
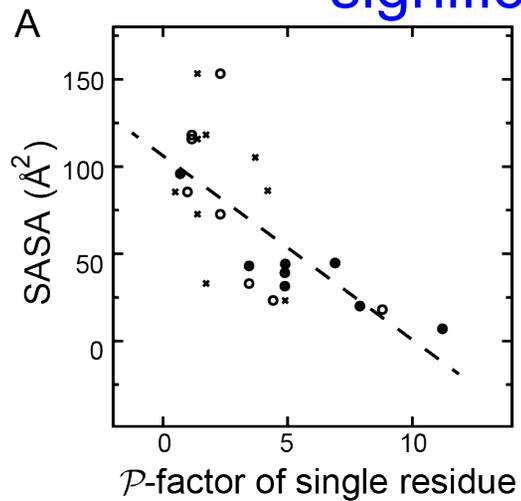
GPCRs (and 7TMRs) represent 50% of drug targets/market  
(outside antibiotics)

Understanding drug-GPCR interactions critical for drug development



What is the nature of the protein conformational changes?  
How is the signal transduced?  
Is Rho a good model for other GPCRs?

# Calmodulin Structure Assessment: PF provides statistically significant predictors of structure



Kaur et al., *Mol Cell Prot.*, 2015

# Acknowledgements

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Lilly, Amgen , Genentech, and Neo Proteomics