SM3: SPECTROSCOPY + CRYSTALLOGRAPHY

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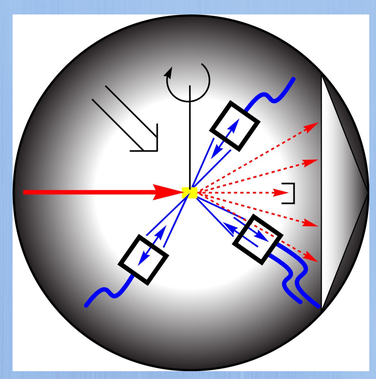
NATIONAL SYNCHROTRON LIGHT SOURCE II approved beamline

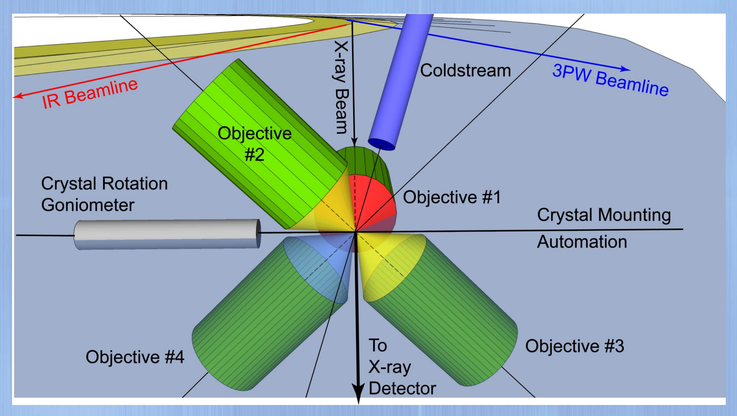
MULTIDISCIPLINARY STUDIES OF MACROMOLECULAR CRYSTALS

The SM3 missions are aligned with those of the NIH and the DOE.

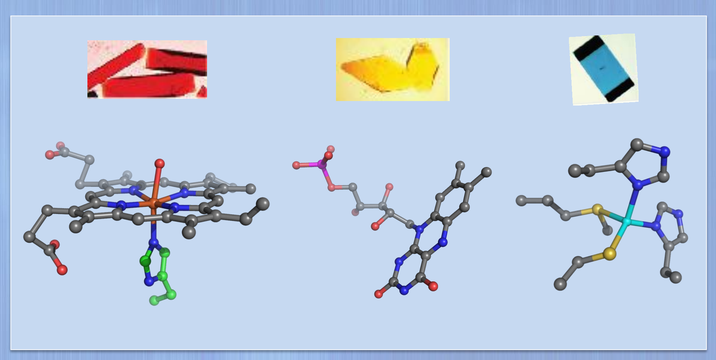
We will build an integrated infrastructure at the NSLS-II to support the nearly simultaneous, correlated measurements of data for:

- X-ray diffraction to high resolution (through objective #1)
- UV/Vis optical absorption (with objectives #2 and 3)
- Steady-state and time-resolved fluorescence spectroscopy (with objectives #2, 3, and 1 or 4)
- Non-resonance & resonance Raman spectroscopy (with lasers and backscatter mode through objectives #1, 3 and/or 4)
- FTIR spectroscopy from an adjacent IR beamline (e.g. with objectives #2 and 3)
- XAS/XANES/EXAFS viewing a 3PW and spectroscopy access through regions 1 and 3 or 4)

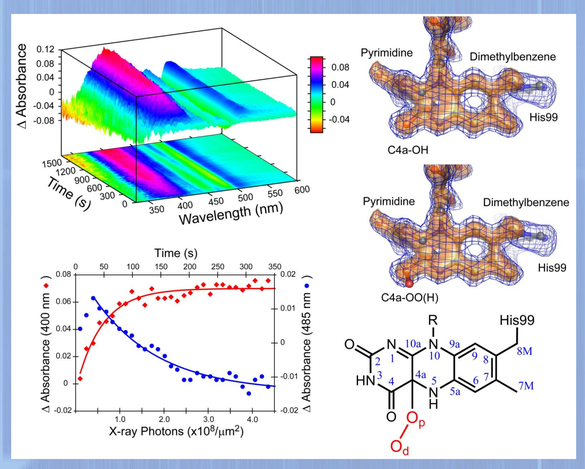




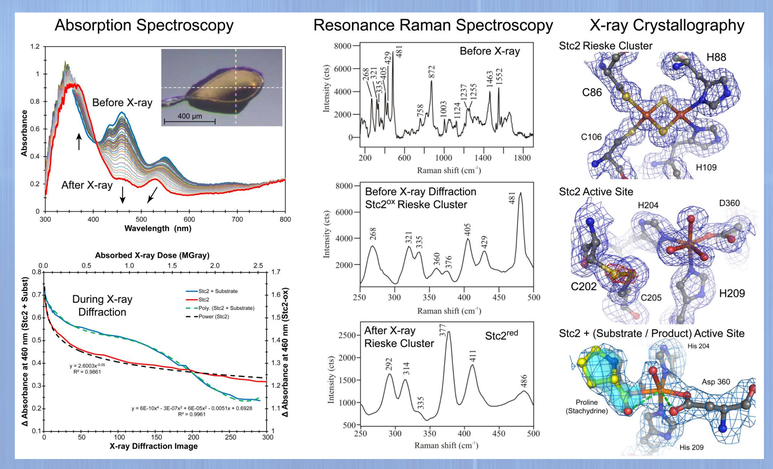
APPLICATIONS



- About ½ of all enzymes contain cofactors and/or metal ions.
- The electronic properties of these types of cofactors provide more strategies to achieve catalysis than H, C, N, O, P, or S atoms.
- Therefore, fundamental mechanistic insights into biology will come from understanding the relationship between atomic and electronic structure.

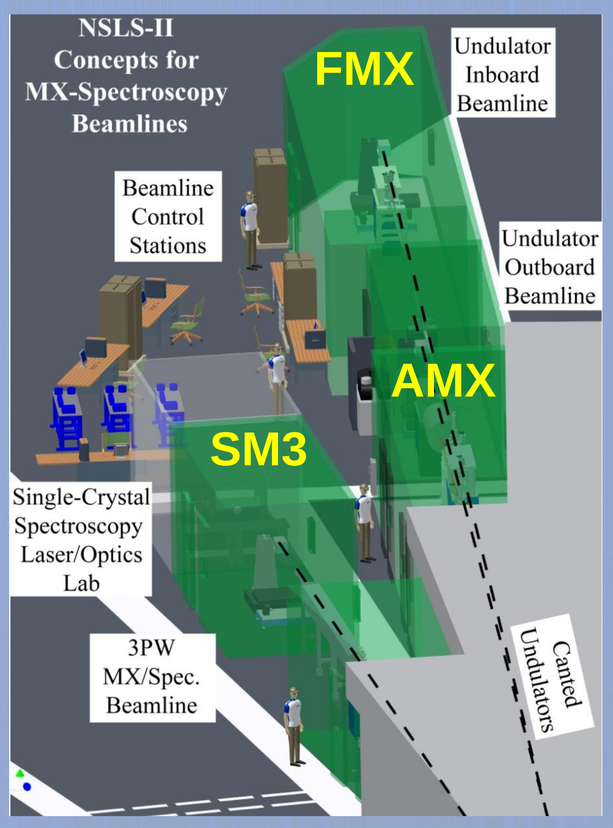


- Complementary data from choline oxidase (CHO) crystals
- Spectroscopic changes in a CHO crystal of upon X-ray exposure at 100 K
- Crystal structure of possible reactive oxygen species
- The electronic and atomic structures correlate well
- If only one type of data, then the interpretation remains uncertain



- Stachydrine demethylase (Stc2) impacts plant-microbe symbiosis
- Absorption spectra after each X-ray diffraction image show that the sample changes (left)
- Resonance Raman spectra (center) before and after X-ray diffraction indicates that the Rieske cluster is reduced
- Crystal structures (right) reveal X-ray promoted catalysis *in situ*

SM3 WILL INTERACT WITH NEIGHBORING BEAMLINES



- FMX: Frontier macromolecular crystallography (undulator, to produce a micro-beam in the 1 – 50 μm range)
- AMX: Highly automated macromolecular crystallography (undulator, to produce a mini-beam in the 5 – 300 μm range)
- Photons may also come from a nearby IR beamline
- **SM3 Techniques**: Macromolecular crystallography (MX) with spectroscopy integrated into the beamline and an off-line laser optics lab (UV/Vis Absorption, Fluorescence, FTIR, Raman, XAS/XANES/EXAFS)
- Source: Three-pole wiggler
- Flux: 10^{11} ph/s at 12 keV
- Energy Range: 5 – 20 keV
- Beam Size: 25 – 300 μm
- Dedicated to full-time correlated studies of spectroscopy with MX

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