NIH Data Science at NIH

HKL approach to handling Eiger images

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HDMRX, BNL, May 2016

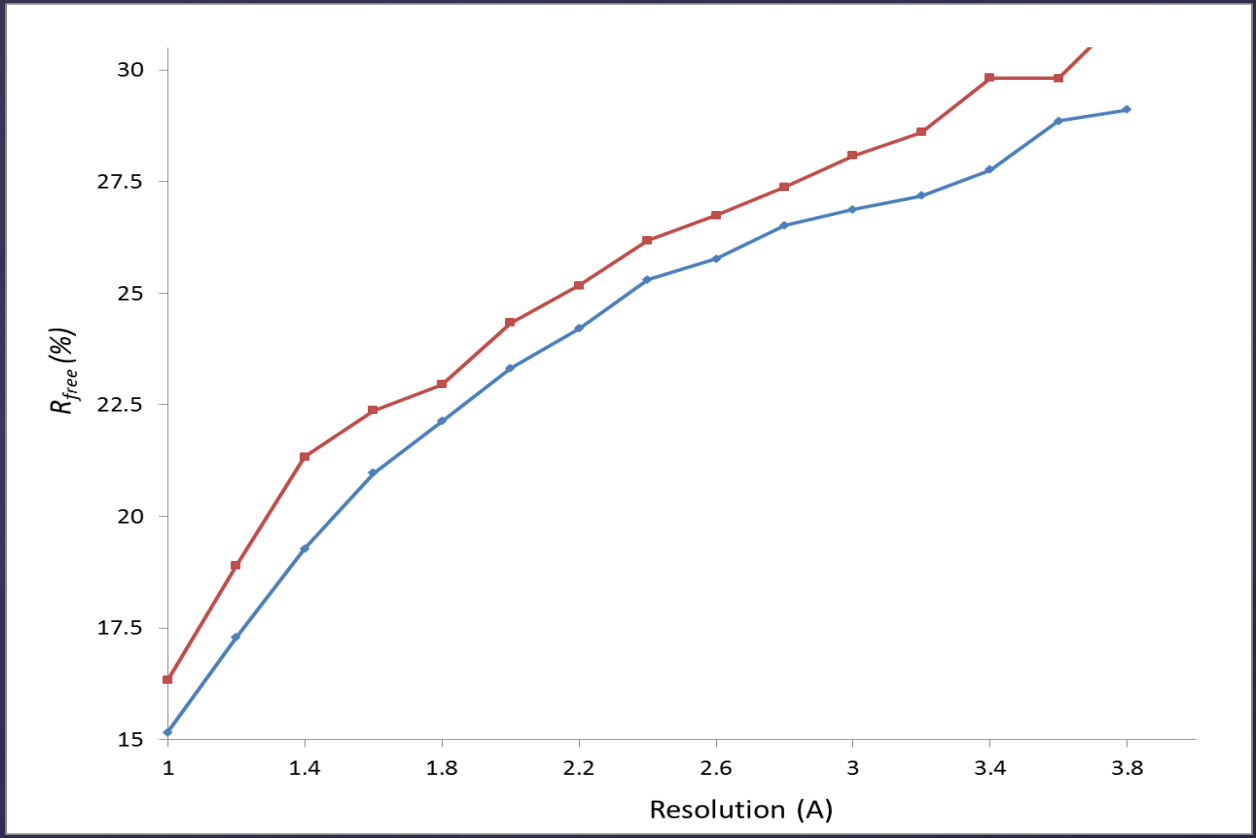
What experimenters know about data collection ?

```
REMARK   3  ESTIMATED OVERALL COORDINATE ERROR.
REMARK   3   ESU BASED ON R VALUE                            (A): NULL
REMARK   3   ESU BASED ON FREE R VALUE                       (A): NULL
REMARK   3   ESU BASED ON MAXIMUM LIKELIHOOD                 (A): NULL
REMARK   3   ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD (A**2): NULL
REMARK   3
REMARK   3  RMS DEVIATIONS FROM IDEAL VALUES.
REMARK   3   DISTANCE RESTRAINTS.                      RMS    SIGMA
REMARK   3    BOND LENGTH                     (A) : NULL  ; NULL
REMARK   3    ANGLE DISTANCE                  (A) : NULL  ; NULL
REMARK   3    INTRAPLANAR 1-4 DISTANCE        (A) : NULL  ; NULL
REMARK   3    H-BOND OR METAL COORDINATION    (A) : NULL  ; NULL
REMARK   3
REMARK   3   PLANE RESTRAINT                  (A) : NULL  ; NULL
REMARK   3   CHIRAL-CENTER RESTRAINT       (A**3) : NULL  ; NULL
REMARK   3
REMARK   3   NON-BONDED CONTACT RESTRAINTS.
REMARK   3    SINGLE TORSION                  (A) : NULL  ; NULL
REMARK   3    MULTIPLE TORSION                (A) : NULL  ; NULL
REMARK   3    H-BOND (X...Y)                  (A) : NULL  ; NULL
REMARK   3    H-BOND (X-H...Y)                (A) : NULL  ; NULL
REMARK   3
REMARK   3   CONFORMATIONAL TORSION ANGLE RESTRAINTS.
REMARK   3    SPECIFIED                 (DEGREES) : NULL  ; NULL
REMARK   3    PLANAR                    (DEGREES) : NULL  ; NULL
REMARK   3    STAGGERED                 (DEGREES) : NULL  ; NULL
REMARK   3    TRANSVERSE                (DEGREES) : NULL  ; NULL
REMARK   3
REMARK   3  ISOTROPIC THERMAL FACTOR RESTRAINTS.     RMS    SIGMA
REMARK   3   MAIN-CHAIN BOND                (A**2) : NULL  ; NULL
REMARK   3   MAIN-CHAIN ANGLE               (A**2) : NULL  ; NULL
REMARK   3   SIDE-CHAIN BOND                (A**2) : NULL  ; NULL
```

What experimenters know about data collection ?

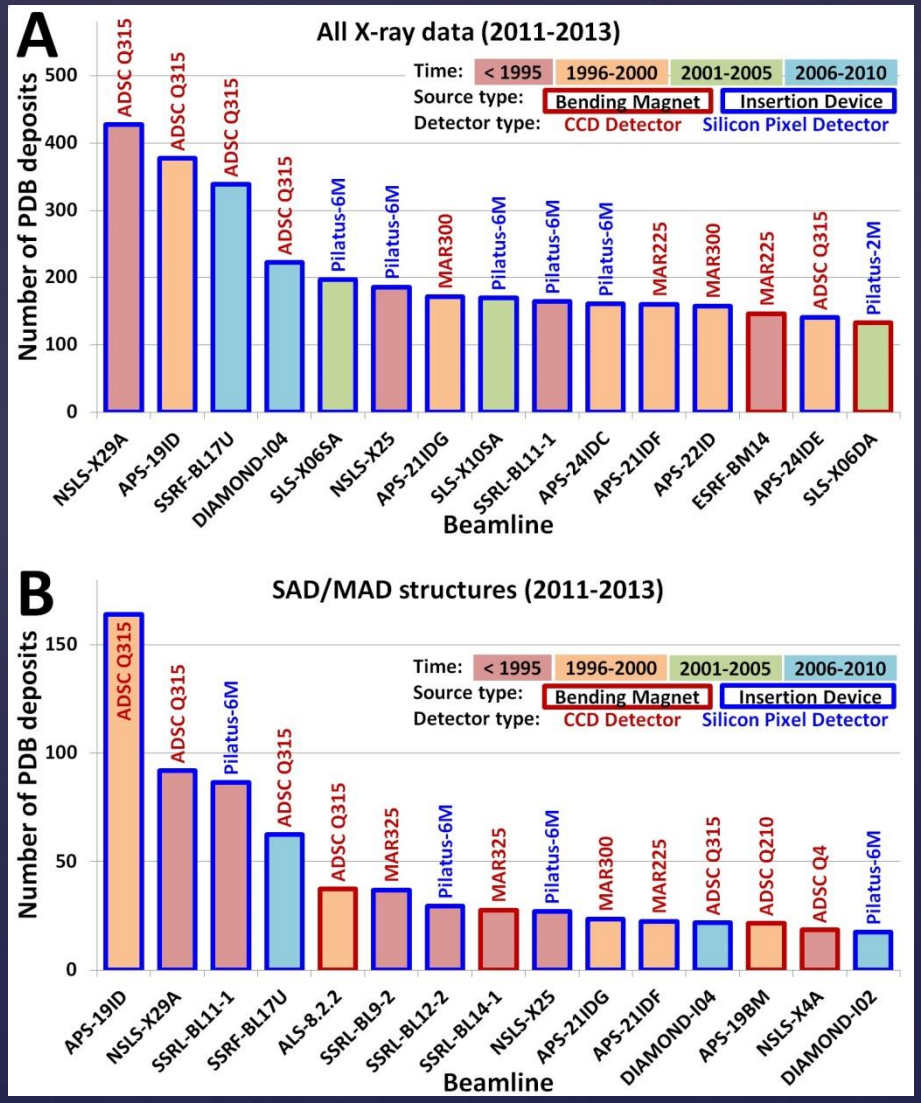
```
REMARK 200  DETECTOR TYPE                    : CCD
REMARK 200  DETECTOR MANUFACTURER            : ADSC QUANTUM 4
REMARK 200  INTENSITY-INTEGRATION SOFTWARE   : BLU-ICE
REMARK 200  DATA SCALING SOFTWARE            : MOSFLM, CCP4, SCALEPACK
REMARK 200
REMARK 200  NUMBER OF UNIQUE REFLECTIONS     : 17575
REMARK 200  RESOLUTION RANGE HIGH      (A)   : 2.950
REMARK 200  RESOLUTION RANGE LOW       (A)   : 47.870
REMARK 200  REJECTION CRITERIA  (SIGMA(I))   : NULL
REMARK 200
REMARK 200 OVERALL.
REMARK 200  COMPLETENESS FOR RANGE     (%)   : 94.3
REMARK 200  DATA REDUNDANCY                  : 3.200
REMARK 200  R MERGE                    (I)   : 0.07800
REMARK 200  R SYM                      (I)   : 0.08600
REMARK 200  <I/SIGMA(I)> FOR THE DATA SET    : NULL
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : 2.95
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE LOW  (A) : 3.03
REMARK 200  COMPLETENESS FOR SHELL     (%)   : 92.4
REMARK 200  DATA REDUNDANCY IN SHELL         : 2.80
REMARK 200  R MERGE FOR SHELL          (I)   : NULL
REMARK 200  R SYM FOR SHELL            (I)   : NULL
REMARK 200  <I/SIGMA(I)> FOR SHELL           : NULL
REMARK 200
REMARK 200 DIFFRACTION PROTOCOL: SINGLE WAVELENGTH
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: MAD SE-MET
REMARK 200 SOFTWARE USED: SNB, MLPHARE, CCP4, SOLVE, HKL, RESOLE
REMARK 200 STARTING MODEL: NULL
REMARK 200
REMARK 200 REMARK: NULL
REMARK 280
REMARK 280 CRYSTAL
REMARK 280 SOLVENT CONTENT, VS    (%): NULL
REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA): NULL
REMARK 280
```

Unexpected correlation?



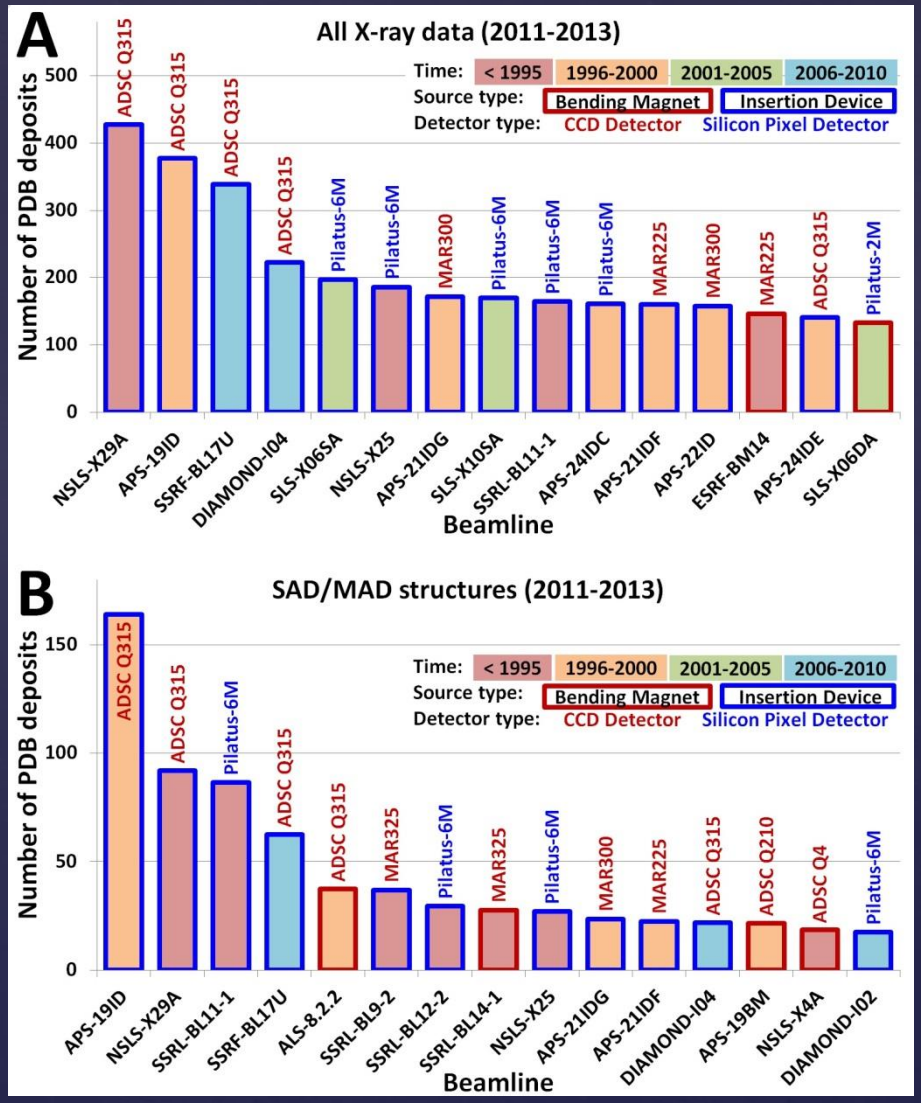
Average R_{free} by resolution bin (with a width of 0.2 Å for X-ray crystallography PDB structures deposited after January 1, 2001, divided into two groups by the number of missing data items ("NULLs") in the PDB file. The means for "high-completion" deposits (20 NULLs or less) are shown in blue, and the means for "low-completion" deposits (50 or more NULLs) are shown in red.

Where we should collect data ?



Zheng *et al*, *Expert Opinion on Drug Discovery(2014) 9: 125-37*

High Data-Rate?



Zheng *et al*, *Expert Opinion on Drug Discovery(2014) 9: 125-37*

Diffraction experiment - the last experiment before deposition to PDB

Dataset – 2minutes, sample change 2minutes -> 10minutes

6 datasets/hour -> 144 datasets/day

180 days -> 25920 datasets/day -> 2.5 PDB

125 synchrotron stations -> 324 PDB

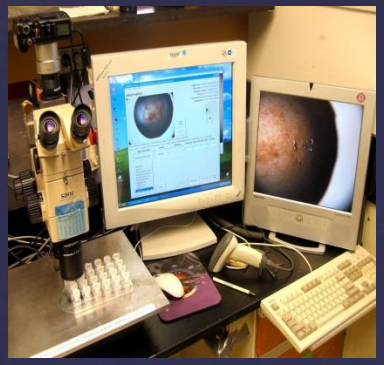
Efficiency -> 0.3%

HKL-3000 at SBC

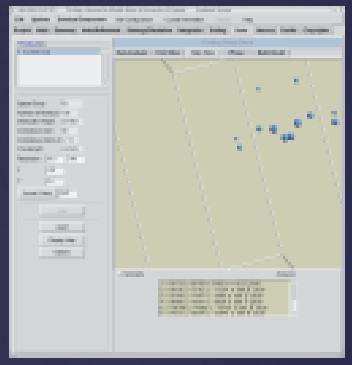
Database-controlled pipeline

lab e-book

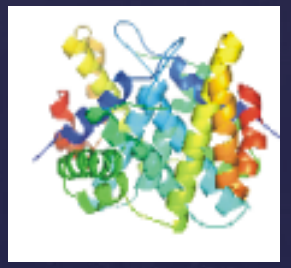
FPLC

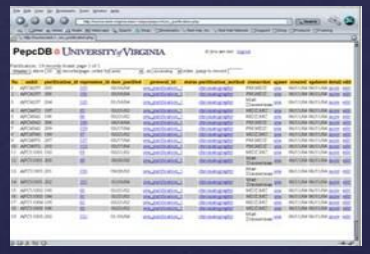


EQUIPMENT

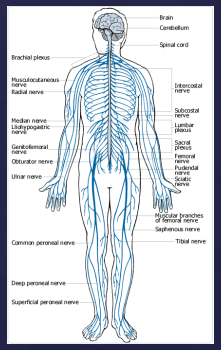


HKL-3000





DATABASES



Big brother?

Statistics / Progress in Minor Lab LIMS by researcher

Last week (17 Apr 2015 - 24 Apr 2015)

Person	Clones	Exprs	Purifs	Macro preps	Plates	Drops	Crystals	Datasets processed	Structure refs	Kinetic assays	Thermal shift assays
Cooper, David	0	0	0	0	0	0	23	18	0	0	0
Handing, Katarzyna	0	0	0	0	0	0	51	53	13	0	0
Hou, Jing	0	0	0	0	1	30	0	1	1	0	0
Kowiel, Marcin	0	0	0	0	0	0	1	8	3	0	0
Shabalin, Ivan	0	0	0	0	0	0	125	14	9	0	0
Shumilin, Igor	0	0	0	0	0	0	0	3	2	0	0
Szlachta, Karol	0	0	0	0	0	0	34	20	3	0	0

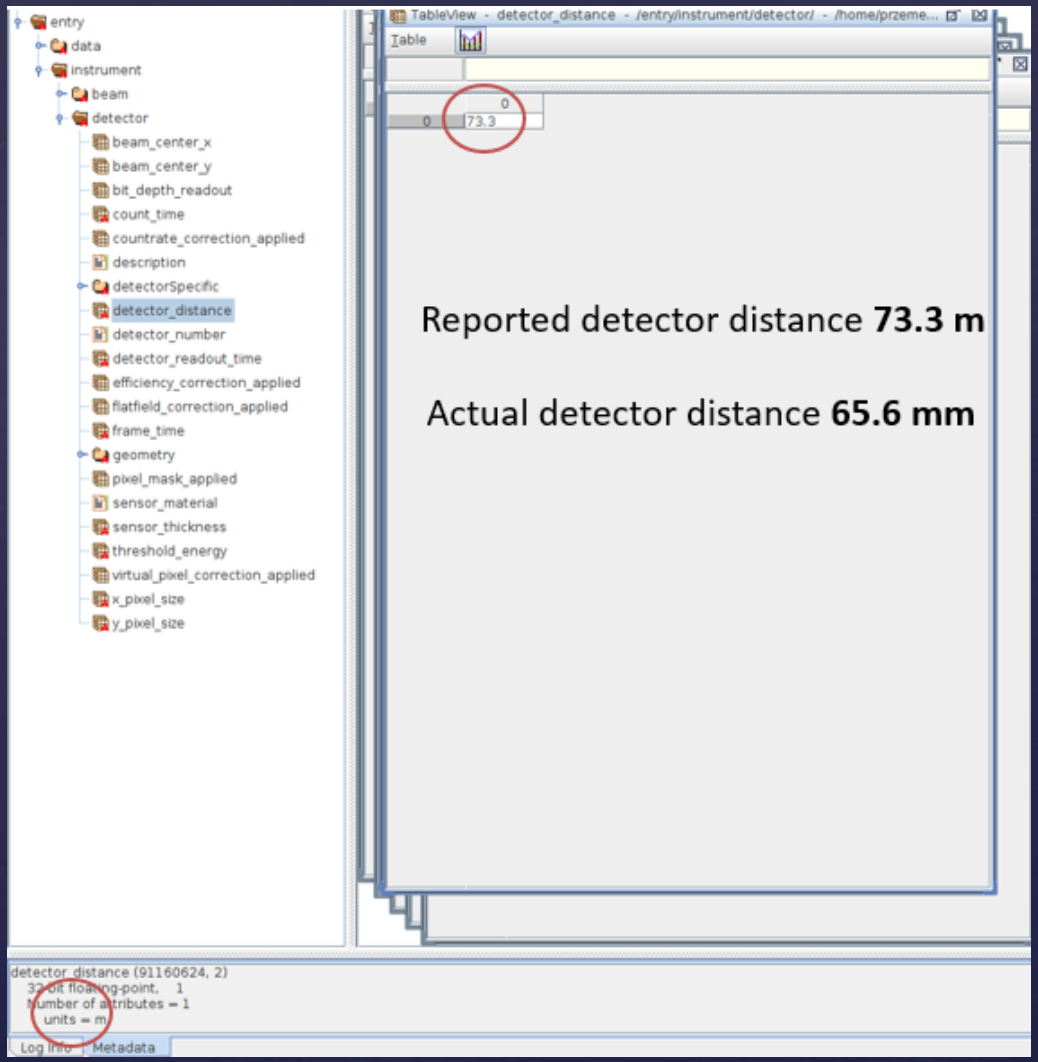
Last month (25 Mar 2015 - 24 Apr 2015)

HDF5 vs CBF
Structural Biologist Perspective

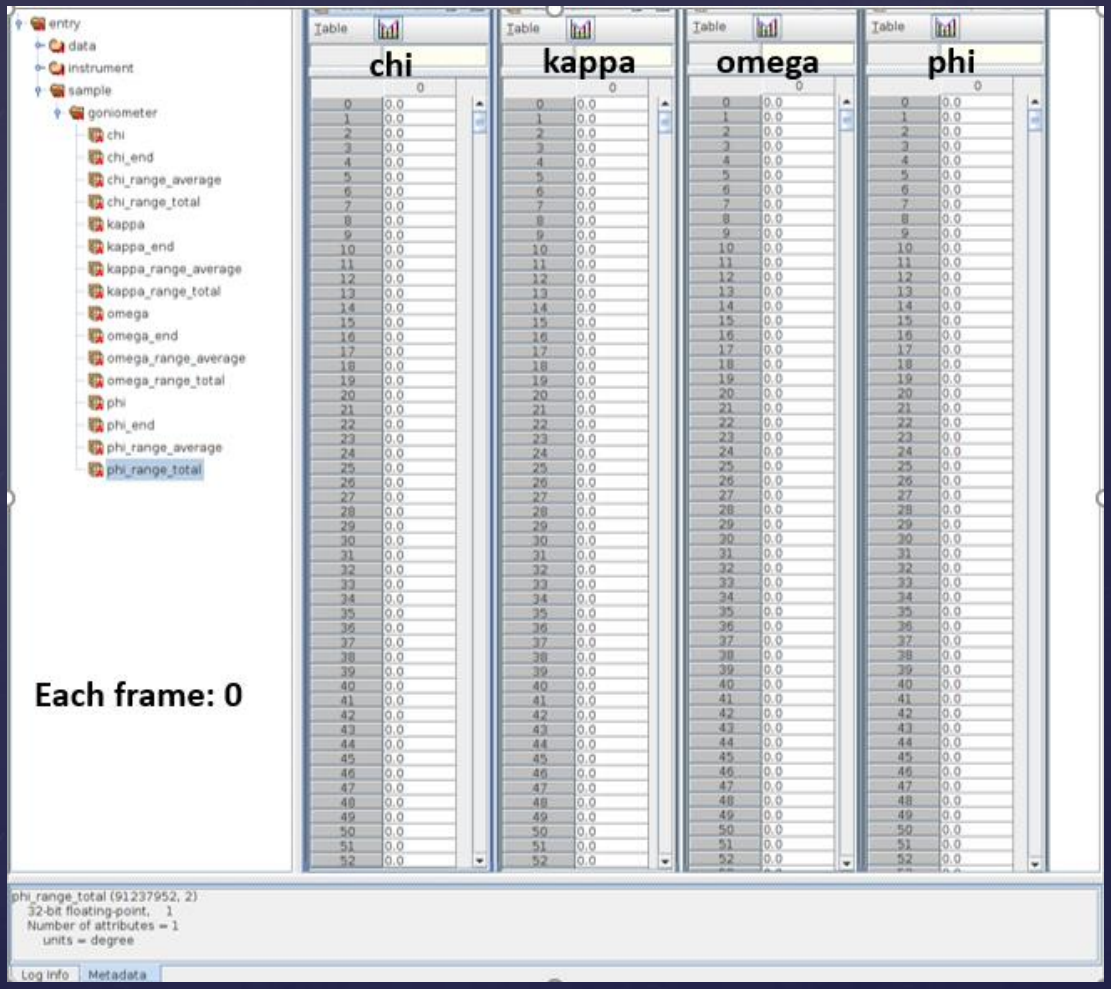
	Size	Processing time	Rmerge/Rmeas/Rpim
HDF5	3GB	21 min	0.054/0.057/0.018
CBF	3GB	21 min	0.054/0.057/0.017

Changing compiler suite **GCC** -> **Intel**
processing time **21 min** -> **4 min**

HDF5 vs CBF
Structural Biologist Perspective



HDF5 vs CBF
Structural Biologist Perspective



HDF5 *vs* CBF *vs* 321 other formats
Structural Biologist Perspective

New format new trivial inconveniences:

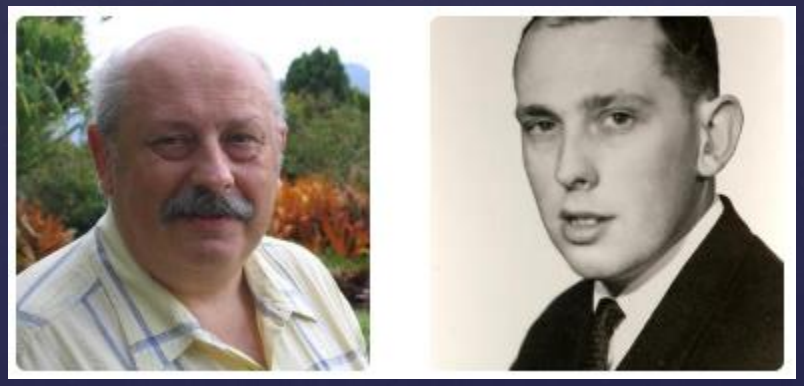
- File renaming
  - need to modify links in HDF5 master file
- New libraries and plugins
  - LZ4 compression plugin compatible only with newer versions of HDF5 library

What is special in Eiger and HD5 ?

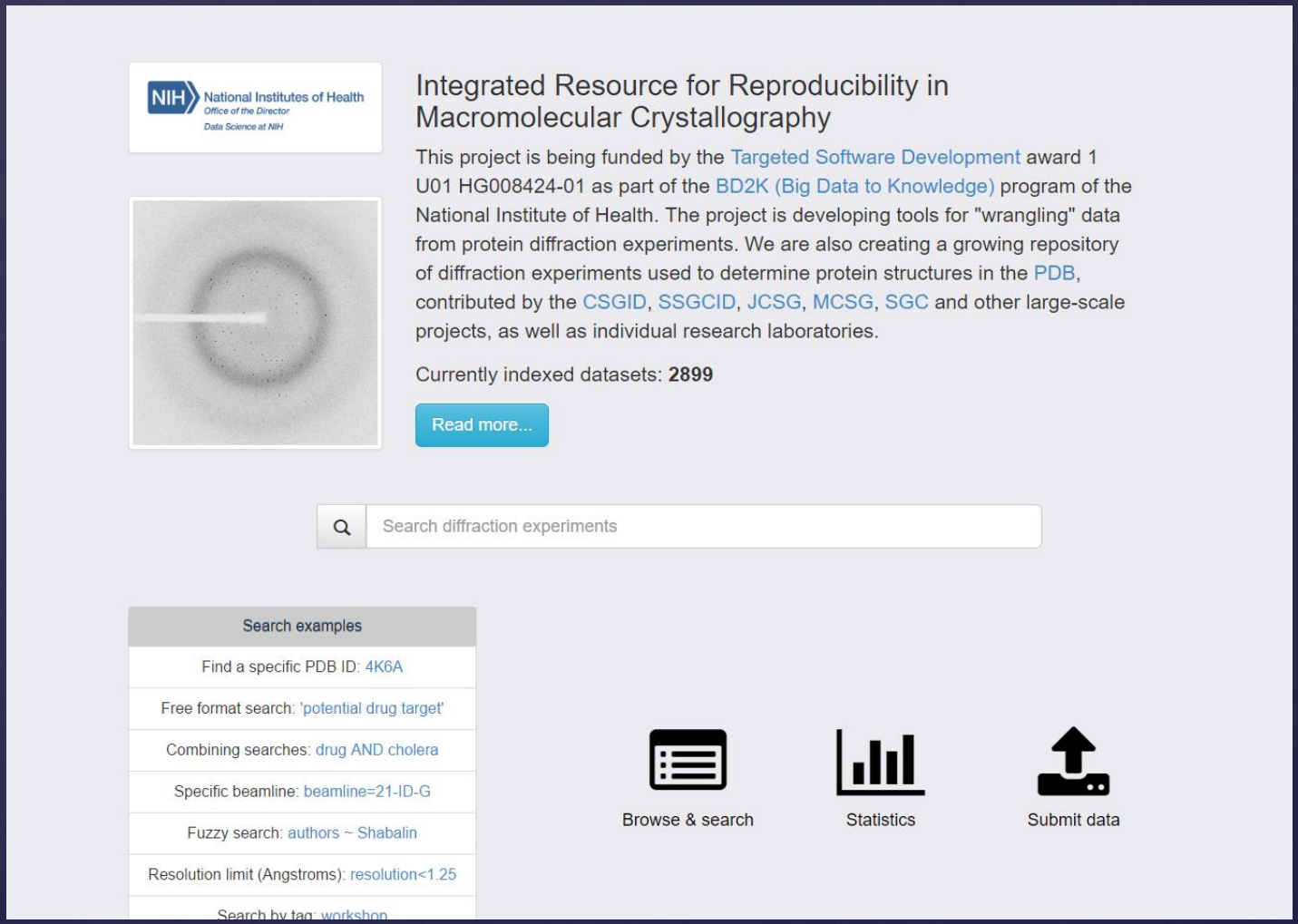
CBF – MAF
HDF5 – MAF

What is special in Eiger and HD5 ?

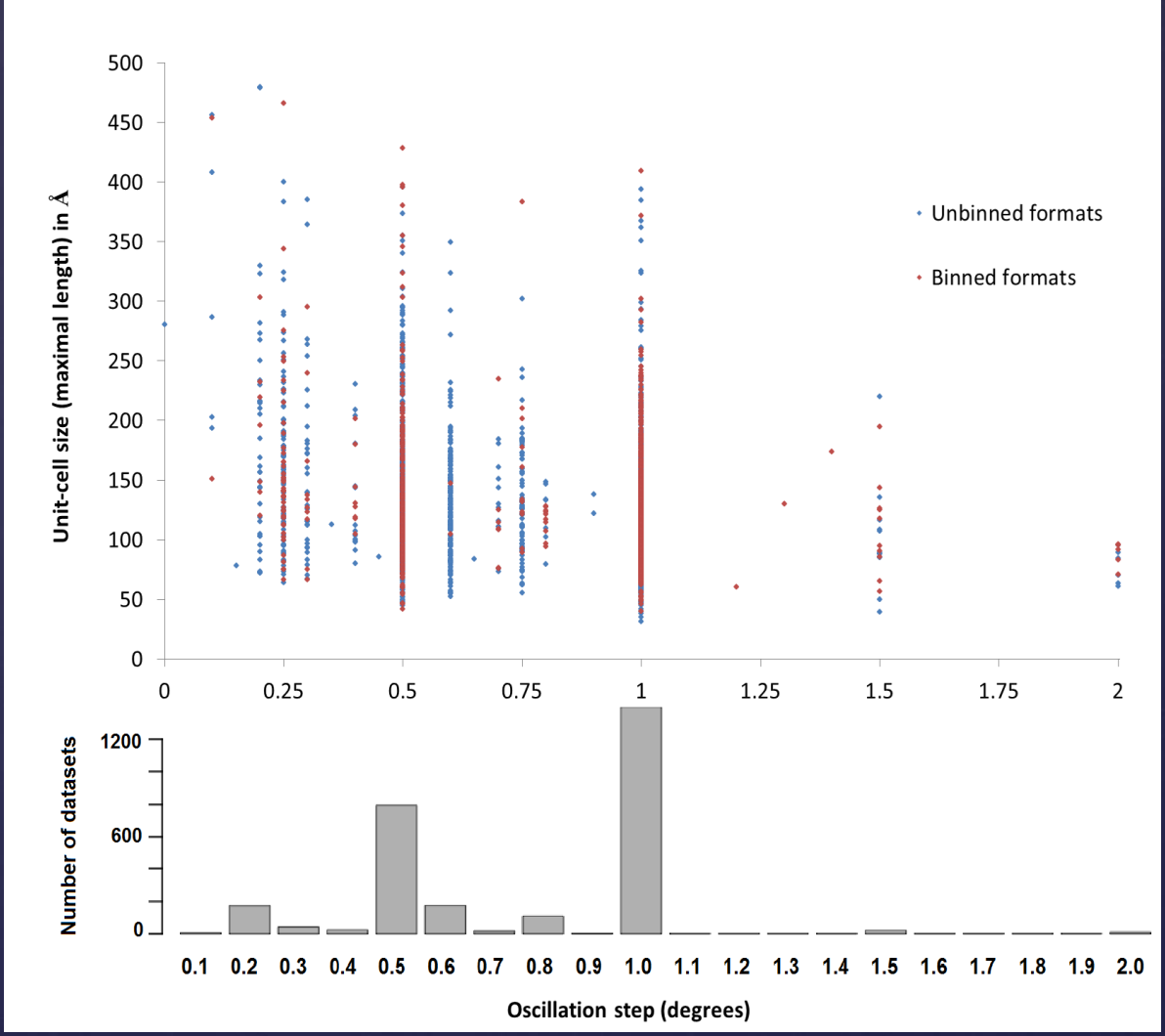
……. - MAH
CBF – MAF
HDF5 – MAF



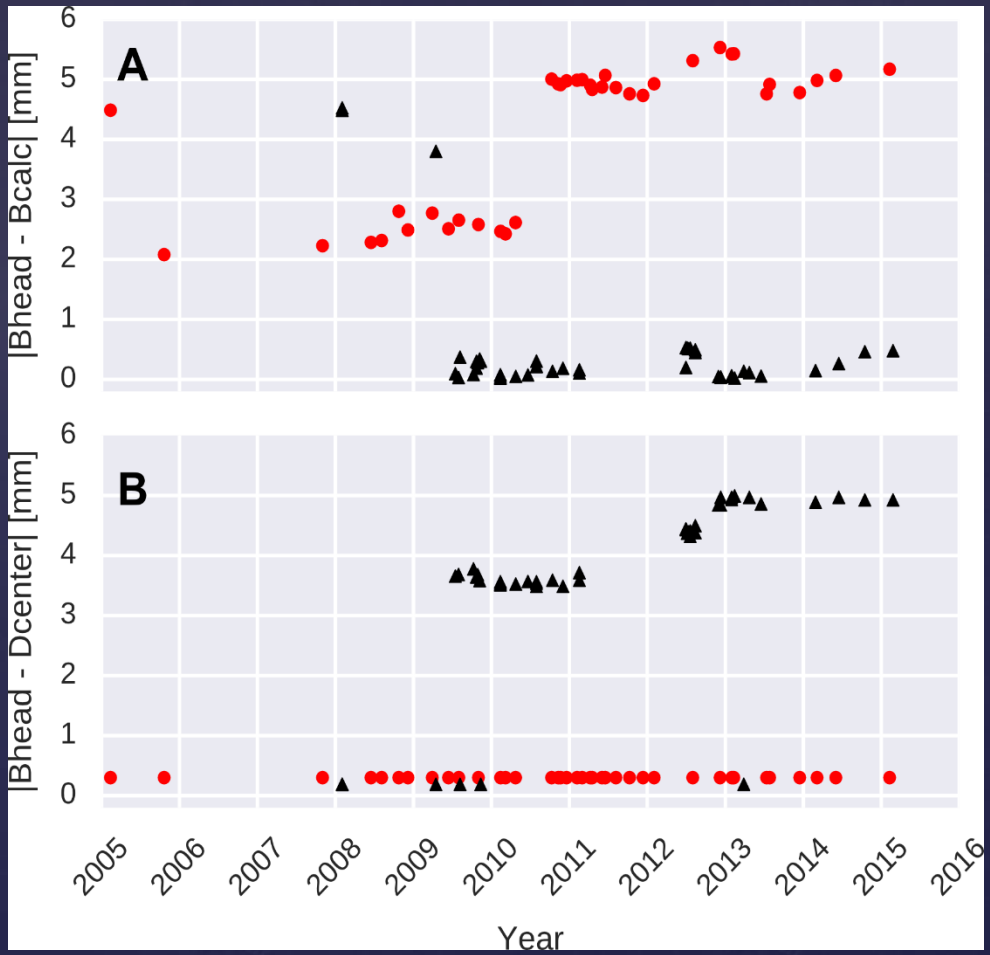
http://www.proteindiffraction.org



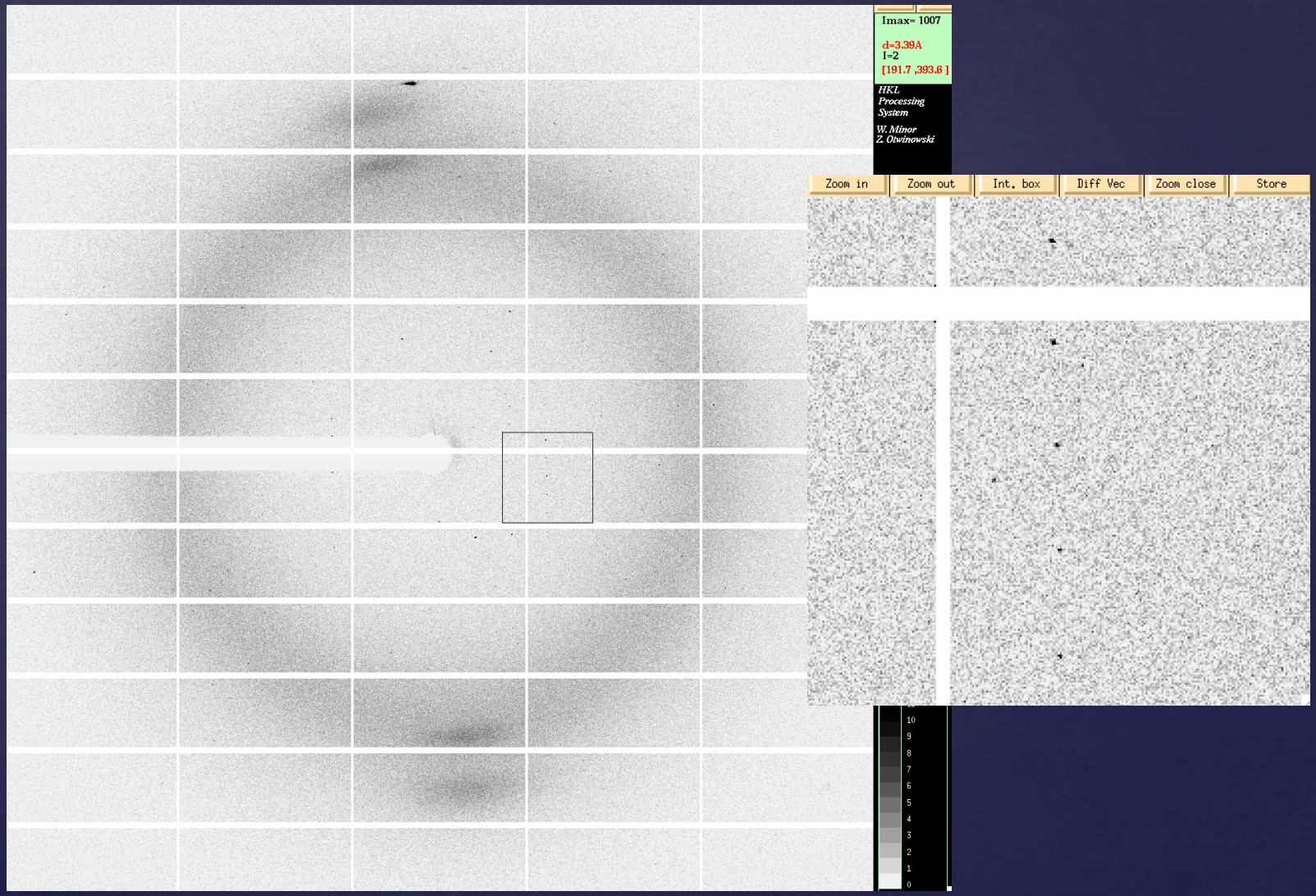
http://www.proteindiffraction.org



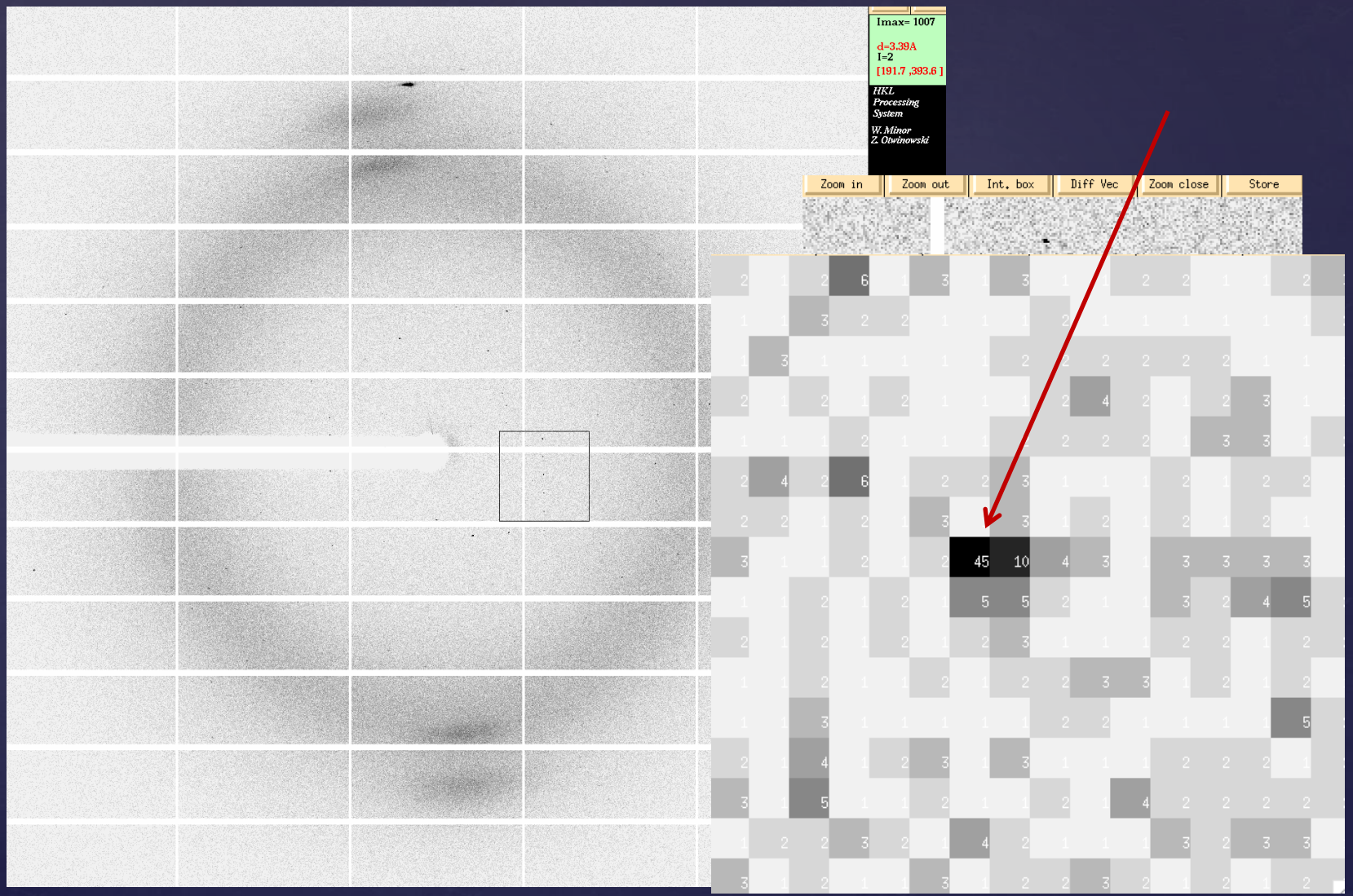
Beam position
Structural Biologist Perspective



Optimal data collection ?



Optimal data collection ?



Header – is CBF header a MAH ?

```
# 2015/May/06 10:30:40
# Pixel_size 172e-6 m x 172e-6 m
# Silicon sensor, thickness 0.001 m
# Oscillation_axis omega
# Excluded_pixels:  badpix_mask.tif
# Chi 0.0000 deg.
# Angle_increment 0.1000 deg.
# Polarization 0.99
# file_comments
# N_oscillations 2500
# Beam_xy (1223.03, 1256.56) pixels
# Exposure_time 0.020000 s
# Phi 0.0020 deg.
# Energy_range (0, 0) eV
# Start_angle 160.6000 deg.
# Detector_distance 0.617619 m
# Detector_Voffset 0.0000 m
# Alpha 0.0000 deg.
# Flat_field: (nil)
# Threshold_setting 7619 eV
# Exposure_period 0.020950 s
# N_excluded_pixels: = 321
# Kappa 0.0020 deg.
# Tau = 0 s
```

Do you like this image?

Do you like this image ?

How expensive is bright lens ?

See more choices

Canon EF 85mm f1.2L II USM Lens for Canon DSLR Cameras - Fixed
by Canon

$1,999.00 Prime
Get it by **Monday, Aug 24**

More Buying Choices
$1,999.00 new (22 offers)
$1,499.99 used (24 offers)

Trade-in eligible for an Amazon gift card

★★★★★ ▾ 159

See Style Options

Canon EF 85mm f/1.8 USM Medium Telephoto Lens for Canon SLR Cameras - Fixed
by Canon

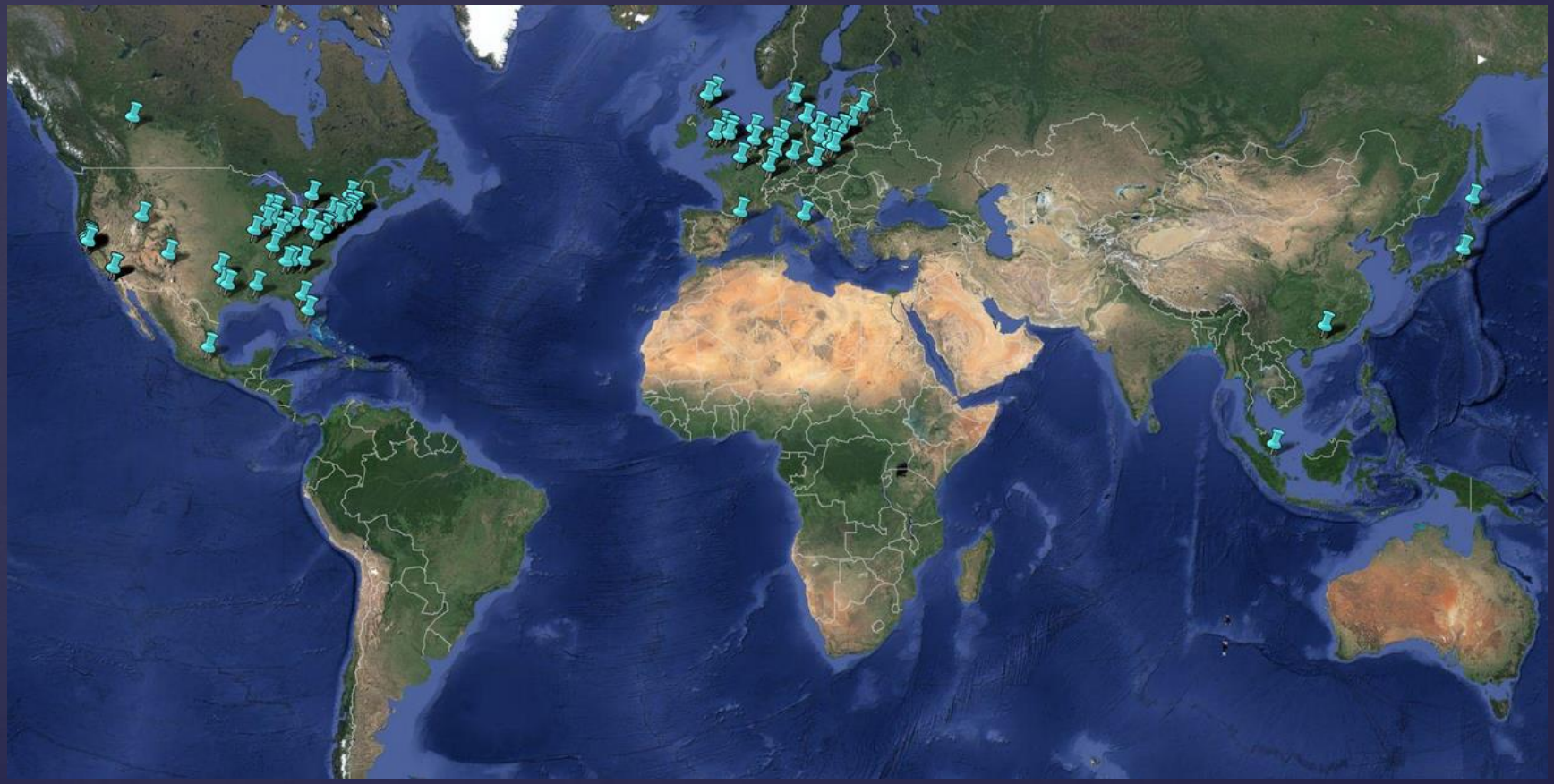
$369.00 Prime
Get it by **Monday, Aug 24**

More Buying Choices
$369.00 new (27 offers)
$298.00 used (26 offers)

Trade-in eligible for an Amazon gift card

★★★★★ ▾ 770

Collaborations documented by at least one paper



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