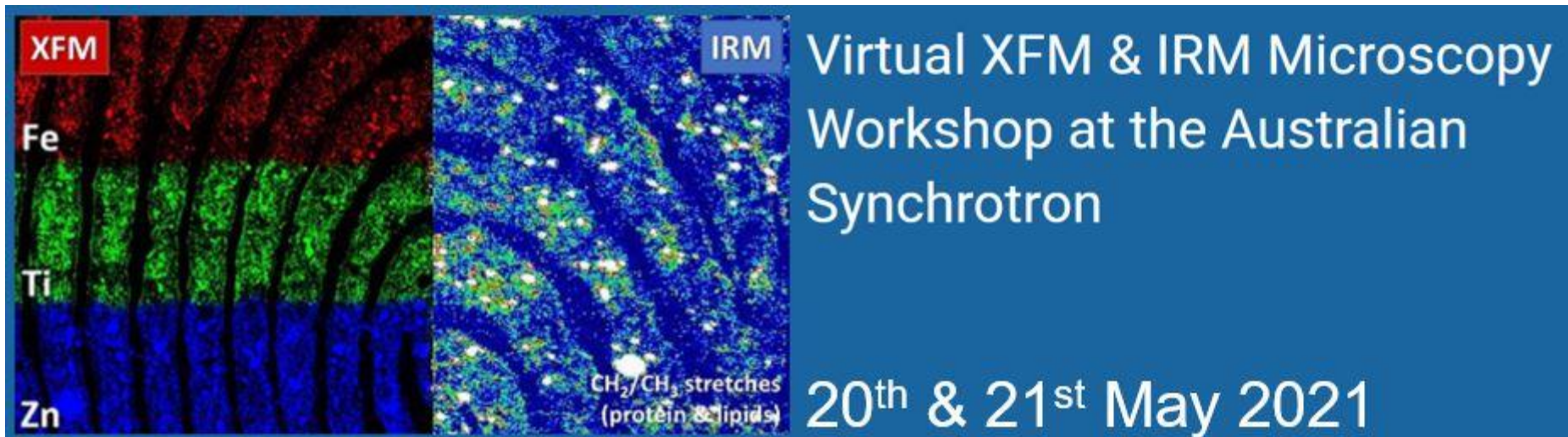


XFM capabilities

mail-in & remote access
data analysis GeoPIXE on ASCI

David Paterson



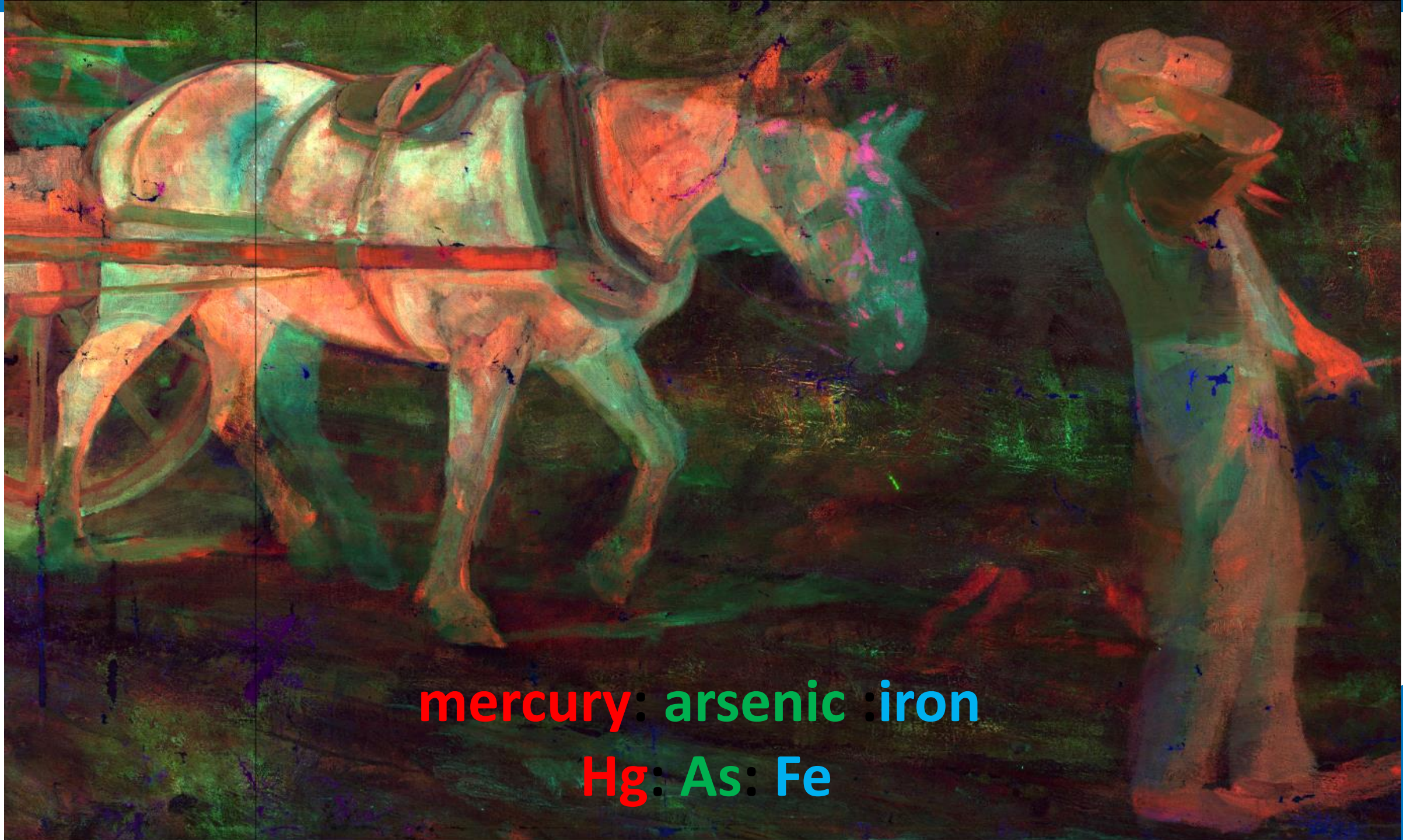
The banner features two side-by-side microscopy images. The left image is an XFM map showing Fe (red), Ti (green), and Zn (blue) distribution. The right image is an IRM map showing CH₂/CH₃ stretches (protein & lipids) in white/yellow against a blue background. Text on the right side of the banner includes the workshop title, location, and dates.

XFM
Fe
Ti
Zn

IRM
CH₂/CH₃ stretches
(protein & lipids)

Virtual XFM & IRM Microscopy
Workshop at the Australian
Synchrotron

20th & 21st May 2021



mercury: arsenic :iron

Hg: As: Fe

Outline

XFM capabilities

- X-ray Fluorescence Microscopy
- Milliprobe and High-energy capabilities (Daryl)
- Ptychography (Cameron)

Beyond 2D Time resolved

- XRF Tomography
- Chemical Speciation Imaging XANES imaging
- Real time imaging, time resolved studies

Remote access Data analysis

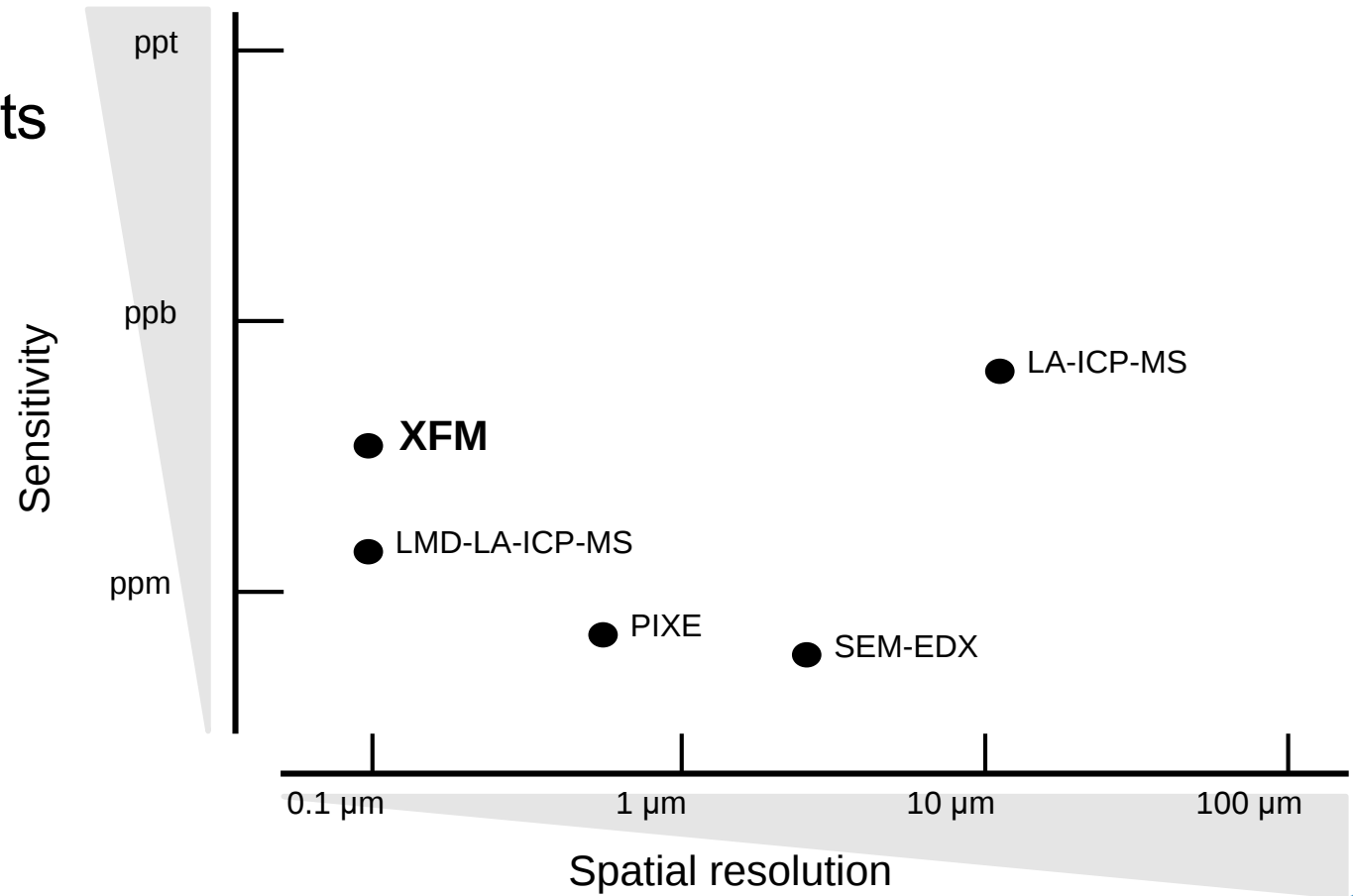
- Mail-in capabilities
- GeoPIXE data analysis in ASCL environment

Future

- DMM => higher flux at higher energies
- Higher spatial resolution => 600 nm
- Nanoprobe beamline (Cameron)

X-ray Fluorescence Microscopy (XFM)

- Simultaneous access to 10+ elements
- No contrast agents required
- Quantitative
- High signal-to-noise ratio
 - ppb sensitivity, improving with Z
- Little sample damage
- Extended penetration depth
 - Study “intact” specimens
- Sensitive to chemical bonding
 - XANES mapping



X-ray Fluorescence Microscopy

www.ansto.gov.au/user-access/instruments/australian-synchrotron-beamlines

Periodic table of elements showing atomic numbers, symbols, names, and atomic weights. The table is color-coded by groups: IA (Hydrogen), IIA (Alkali Earths), IIIA-IVIA (Main Group Metals), VIIA (Halogens), VIIIA (Noble Gases), IB-IIB (Transition Metals), and VIII (Iron Group).

Legend:

- Alkali Earth
- Alkaline Earth
- Rare Earth
- Other Metals
- Non-Metals
- Halogens
- Transition Metals
- Metalloids
- Noble Gases

Key elements and their atomic weights:

- Hydrogen (H): 1.008
- Helium (He): 4.003
- Lithium (Li): 6.941
- Beryllium (Be): 9.012
- Sodium (Na): 22.990
- Magnesium (Mg): 24.305
- Potassium (K): 39.098
- Calcium (Ca): 40.08
- Scandium (Sc): 44.956
- Titanium (Ti): 47.88
- Vanadium (V): 50.942
- Chromium (Cr): 51.996
- Manganese (Mn): 54.938
- Iron (Fe): 55.847
- Cobalt (Co): 58.933
- Nickel (Ni): 58.70
- Copper (Cu): 63.546
- Zinc (Zn): 65.39
- Gallium (Ga): 69.72
- Germanium (Ge): 72.61
- Arsenic (As): 74.922
- Selenium (Se): 78.96
- Bromine (Br): 79.904
- Krypton (Kr): 83.80
- Rubidium (Rb): 85.468
- Strontium (Sr): 87.62
- Yttrium (Y): 88.906
- Zirconium (Zr): 91.22
- Niobium (Nb): 92.906
- Molybdenum (Mo): 95.94
- Technetium (Tc): (98)
- Ruthenium (Ru): 101.07
- Rhodium (Rh): 102.906
- Palladium (Pd): 106.42
- Silver (Ag): 107.868
- Cadmium (Cd): 112.41
- Indium (In): 114.82
- Tin (Sn): 118.71
- Antimony (Sb): 121.76
- Tellurium (Te): 127.60
- Iodine (I): 126.905
- Xenon (Xe): 131.29
- Cesium (Cs): 132.905
- Barium (Ba): 137.33
- Lanthanum (La): 138.906
- Hafnium (Hf): 178.49
- Tantalum (Ta): 180.948
- Tungsten (W): 183.85
- Rhenium (Re): 186.207
- Osmium (Os): 190.2
- Iridium (Ir): 192.22
- Platinum (Pt): 195.08
- Gold (Au): 196.967
- Mercury (Hg): 200.59
- Thallium (Tl): 204.38
- Lead (Pb): 207.2
- Bismuth (Bi): 208.980
- Polonium (Po): (209)
- Astatine (At): (210)
- Radon (Rn): (222)
- Francium (Fr): (223)
- Radium (Ra): 226.025
- Actinium (Ac): 227.028
- Cerium (Ce): 140.12
- Praseodymium (Pr): 140.908
- Neodymium (Nd): 144.24
- Promethium (Pm): (145)
- Samarium (Sm): 150.36
- Europium (Eu): 151.97
- Gadolinium (Gd): 157.25
- Terbium (Tb): 158.925
- Dysprosium (Dy): 162.50
- Holmium (Ho): 164.930
- Erbium (Er): 167.26
- Thulium (Tm): 168.934
- Ytterbium (Yb): 173.04
- Lutetium (Lu): 174.967
- Thorium (Th): 232.038
- Protactinium (Pa): 231.036
- Uranium (U): 238.029
- Neptunium (Np): 237.048
- Plutonium (Pu): (244)
- Americium (Am): (243)
- Curium (Cm): (247)
- Berkelium (Bk): (247)
- Californium (Cf): (251)
- Einsteinium (Es): (252)
- Fermium (Fm): (257)
- Mendelevium (Md): (258)
- Nobelium (No): (259)
- Lawrencium (Lr): (260)

<https://asuserwiki.atlassian.net/wiki/spaces/UO/pages/22609927/XFM+Beamline>

X-ray Fluorescence Microscopy

Energy range: 4 to 25+ keV

- Hard x-ray microprobe $\Delta E/E \sim 10^{-4}$
- X-ray fluorescence mapping (μ -XRF)
- X-ray fluorescence μ -XANES $\Rightarrow$ XANES imaging
- X-ray fluorescence tomography
- Scanning X-ray Diffraction Microscopy, Ptychography

Australasia's only hard X-ray microprobe, but Nanoprobe coming very soon!

XFM team

David Paterson

- Environmental and geological science

Daryl Howard

- Cultural heritage, forensic and mm-scale investigations

3rd Scientist recruiting now!

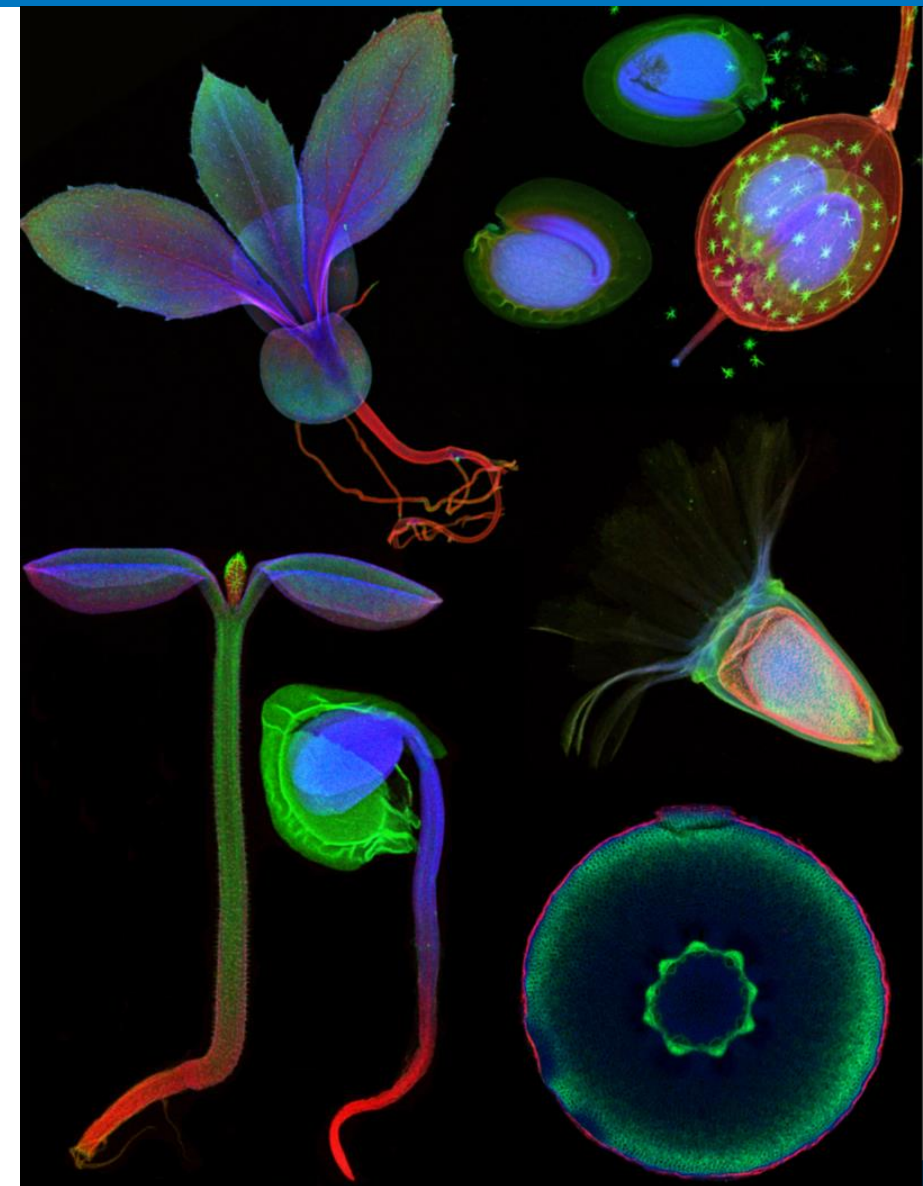
Past XFM scientists

Cameron Kewish Nanoprobe scientist

- SXDM, Ptychography analysis pipeline + EIGER detector experiments

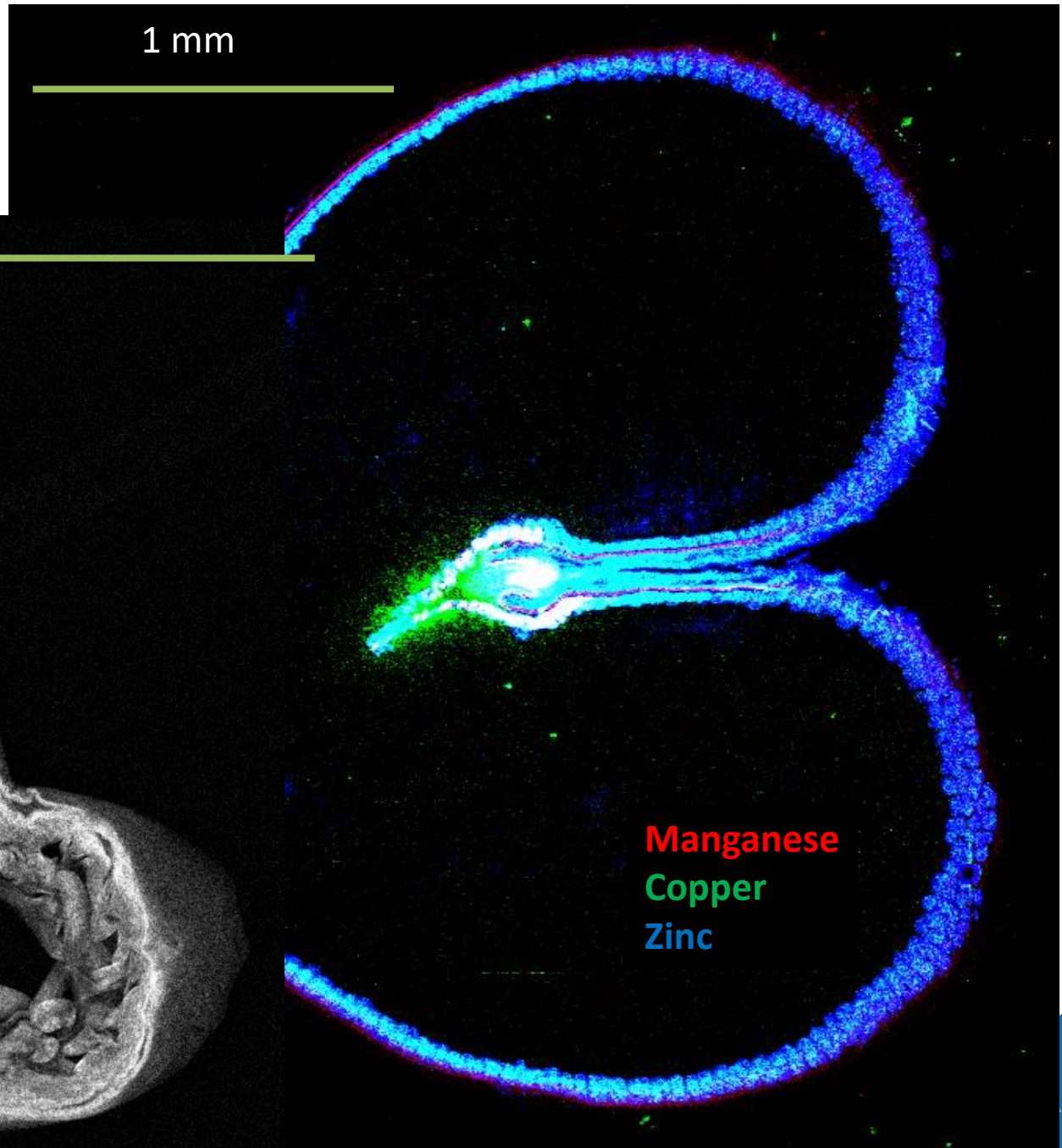
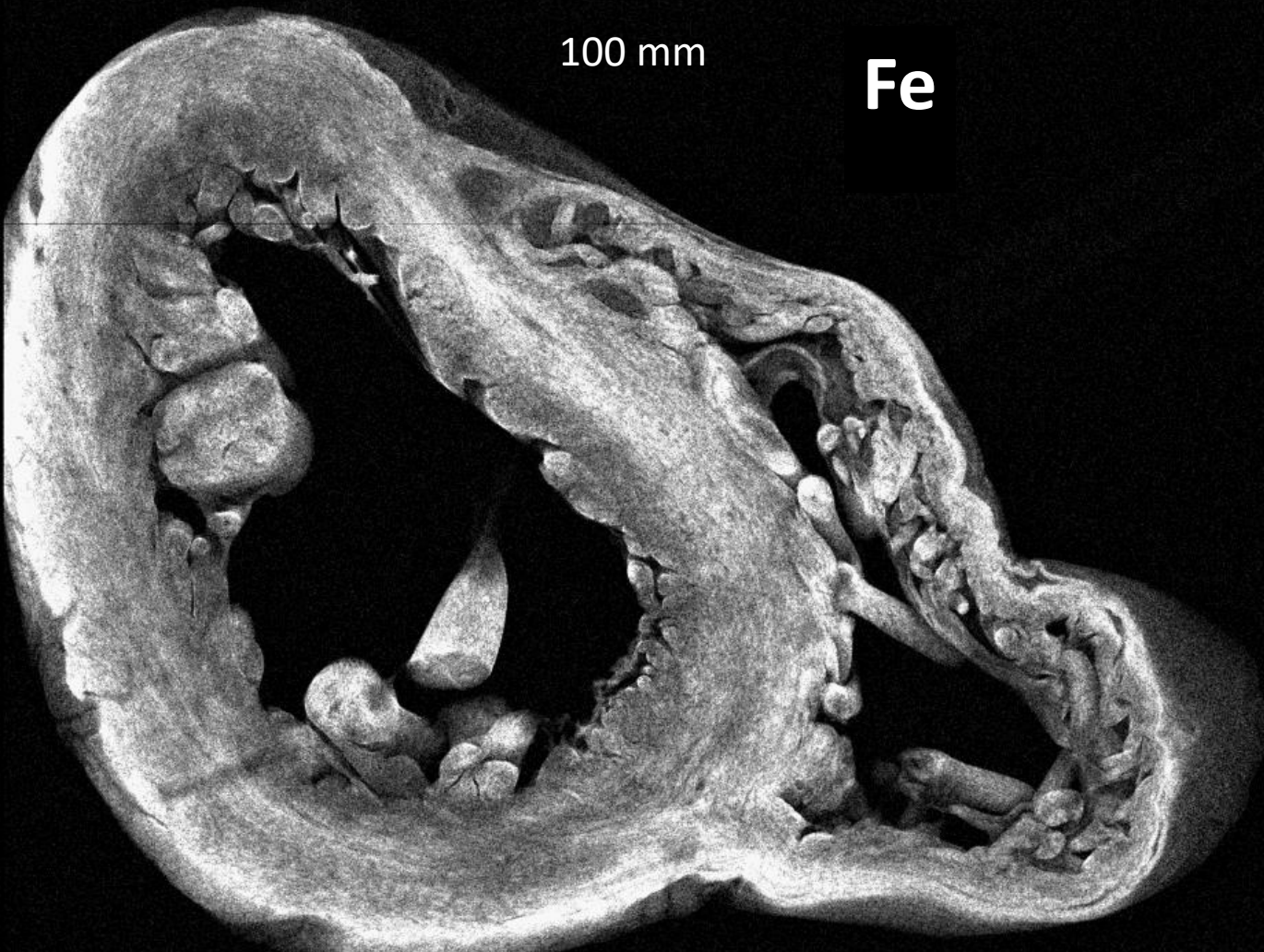
Martin de Jonge Nanoprobe lead scientist

- biological, biomedical and life science, tomography



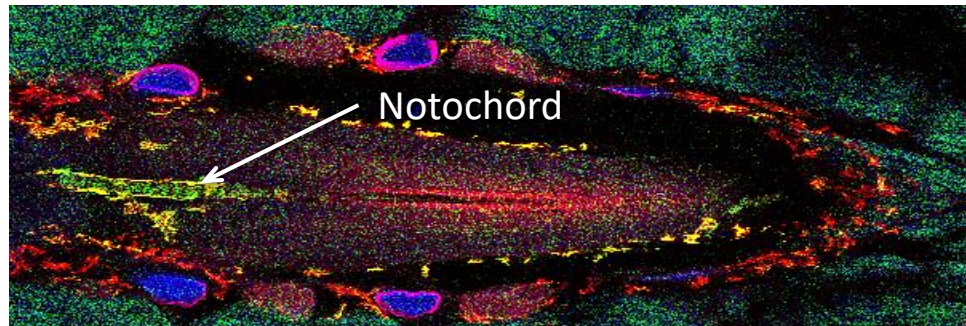
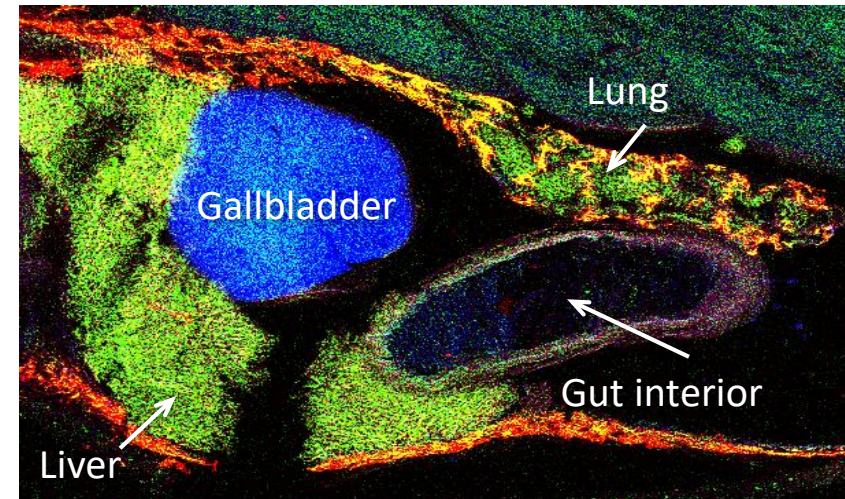
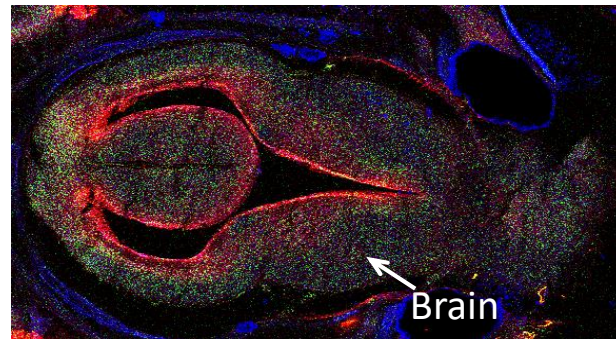
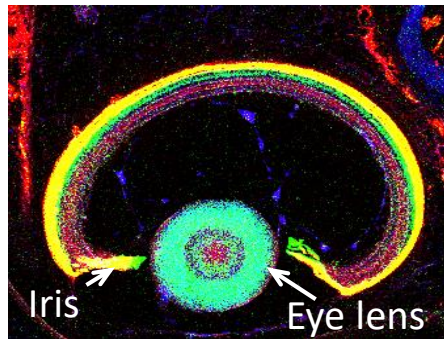
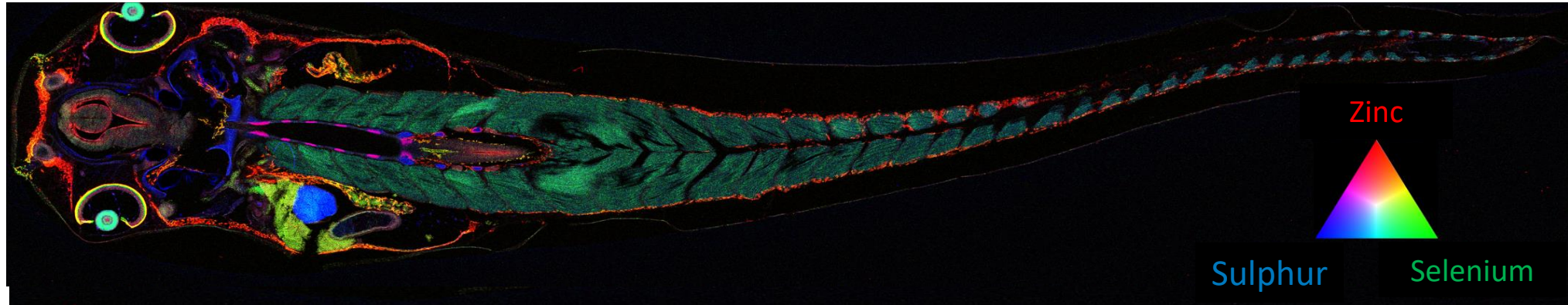
Probe	Resolution	Field of View H X V
KB Microprobe	1 μm	140 X 100 mm
Milliprobe	50 μm	600 X 1200 mm

Imaging across multiple length scales



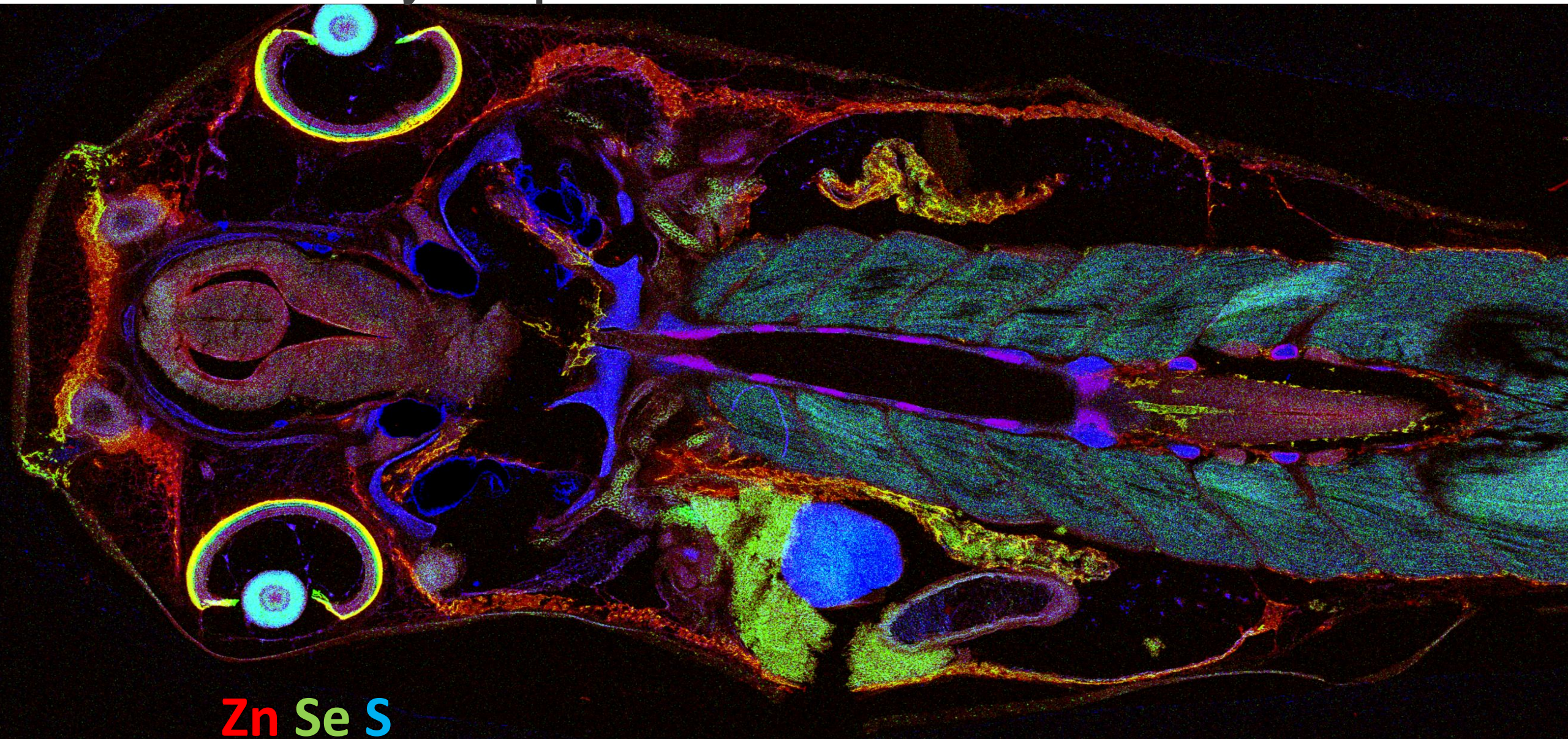
Bioaccumulation on the micron scale

Tadpole exposed to SeIV (30 µg/L) for 7 days



Chantal Lancôt (Griffith University),
Tom Cresswell (Environmental Research
ANSTO) *et al.*

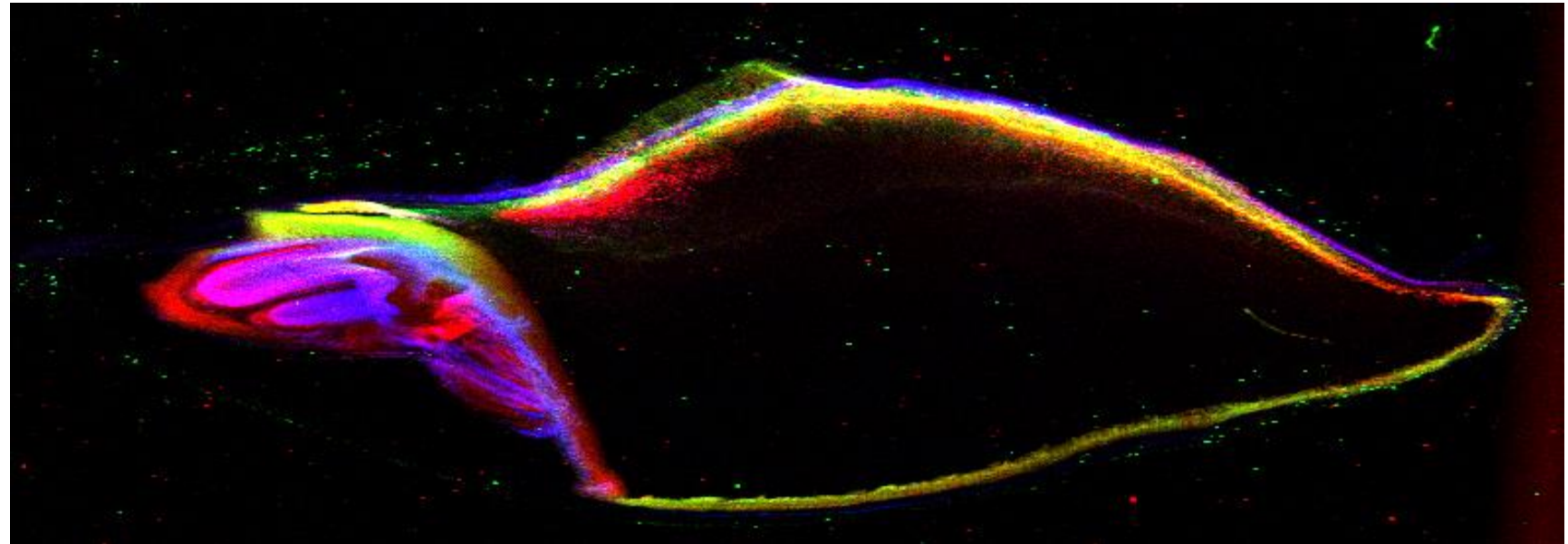
Selenium toxicity in aquatic environments



Megapixels/hour: bio-fortification of cereal grains

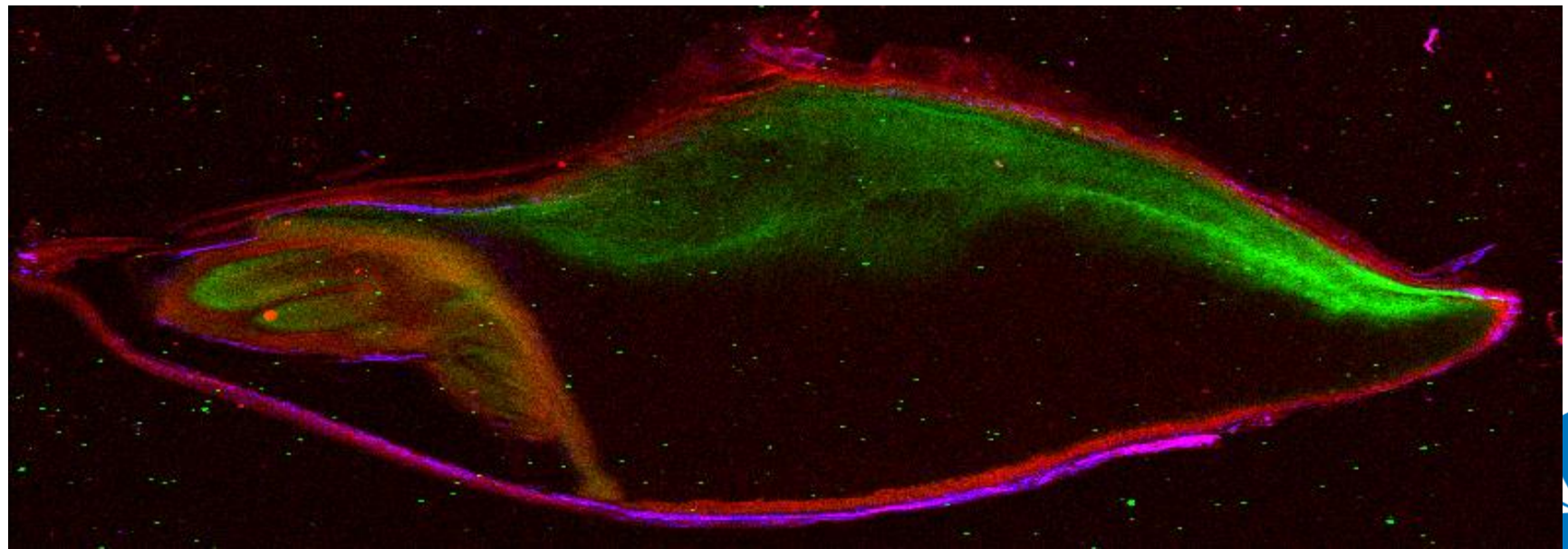
10 keV
incident

Potassium
Copper
Calcium

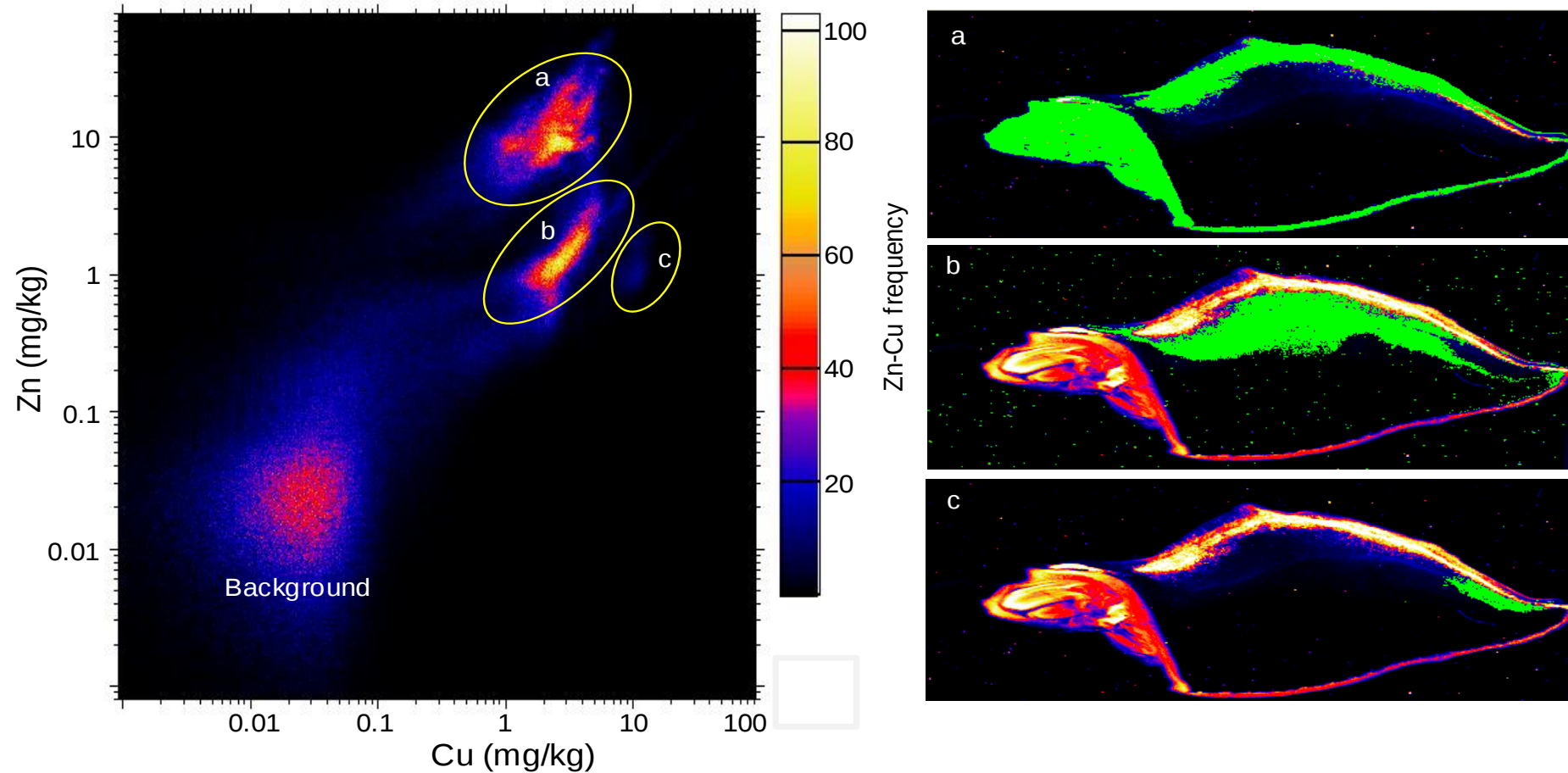


Lombi *et al.*
J. Exp. Botany
62, 273 (2011).

Zinc
Iron
Manganese

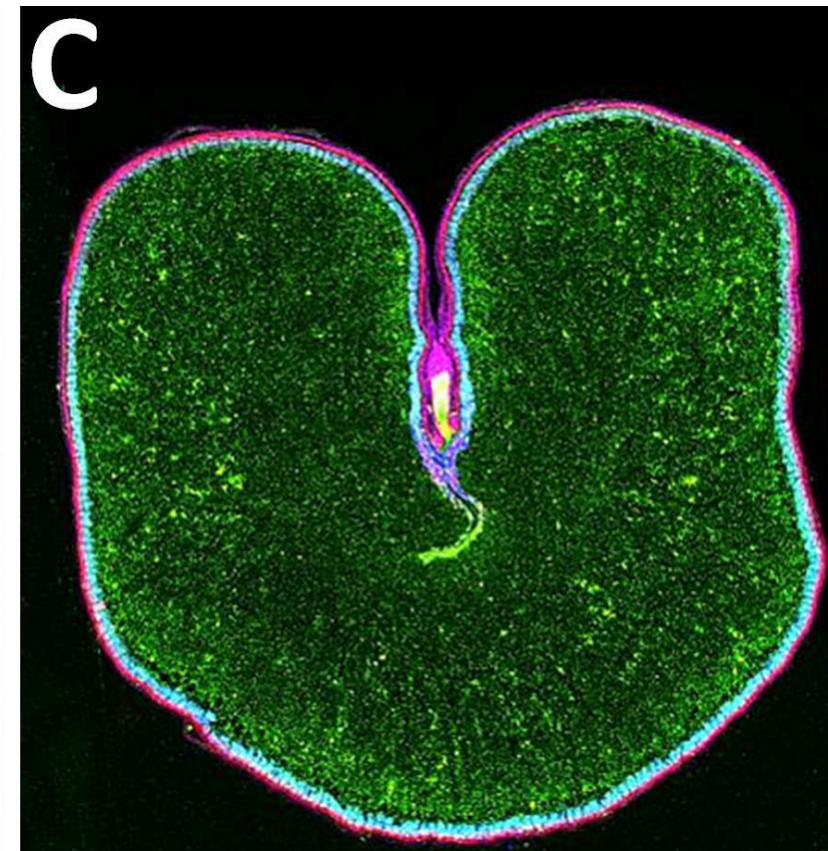
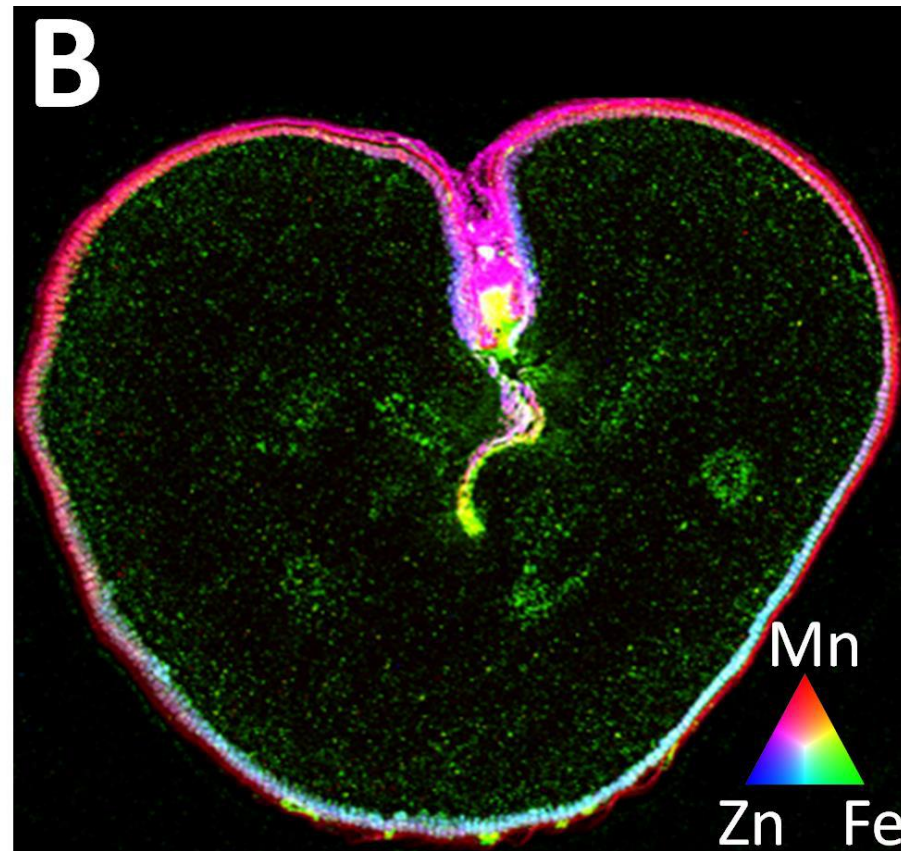
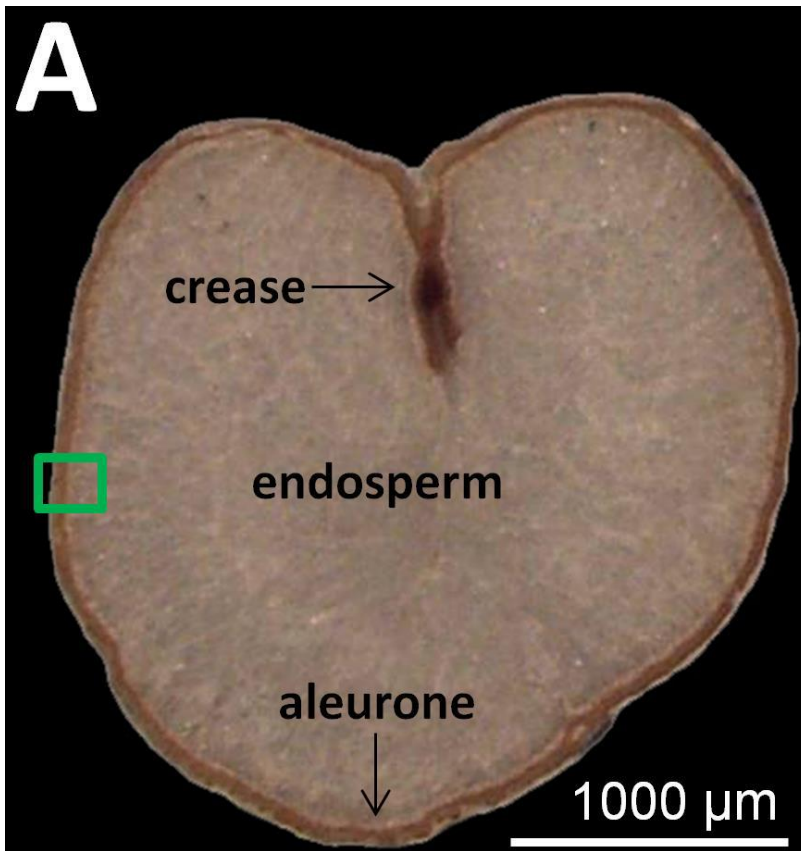


High definition analysis of elemental correlations



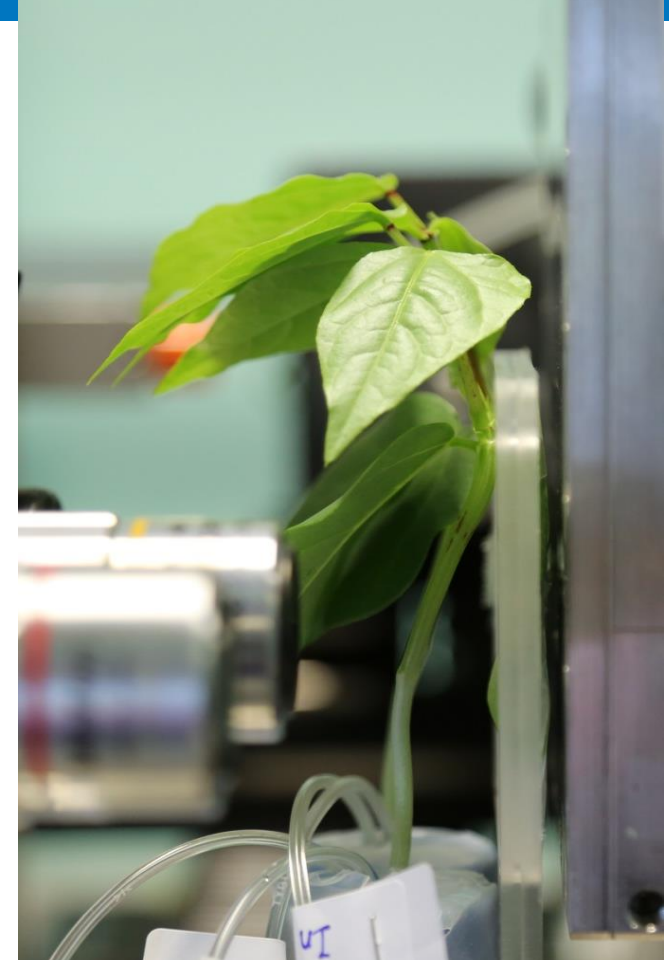
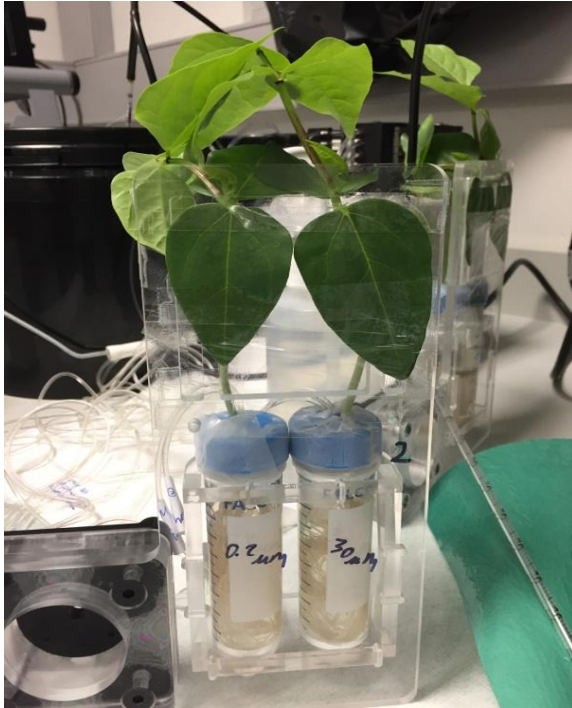
Enzo Lombi, *et al.* Journal of Experimental Botany **62**, 273 (2011).
“Megapixel imaging of micronutrients in mature barley grains.”

Nutrition: iron biofortification in rice and wheat

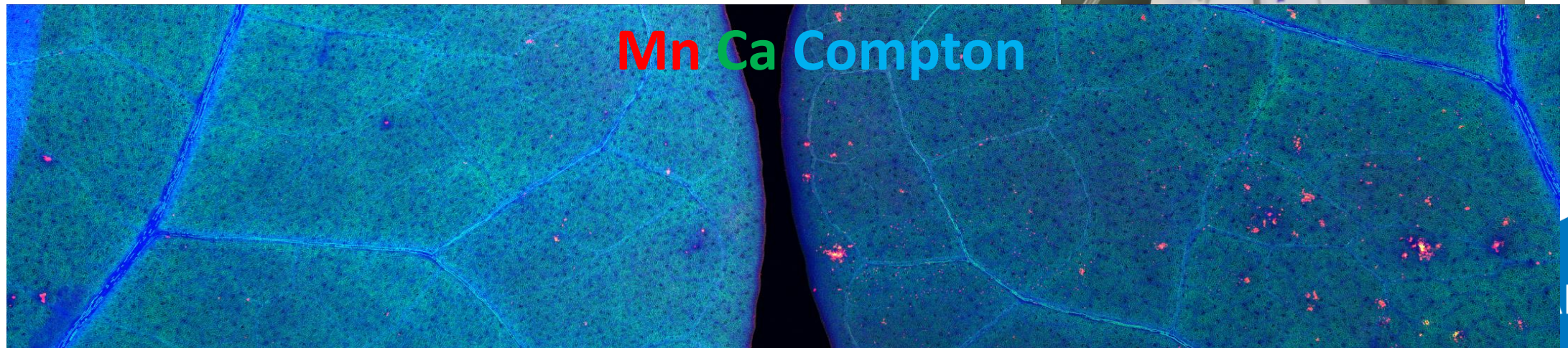


Trijatmiko *et al.*, *Biofortified indica rice attains iron and zinc nutrition dietary targets in the field*, Scientific Reports 6 19792 (2016).

In situ and time-based studies



Blamey *et al.* Environmental & Experimental Botany **156**, 151 (2018)

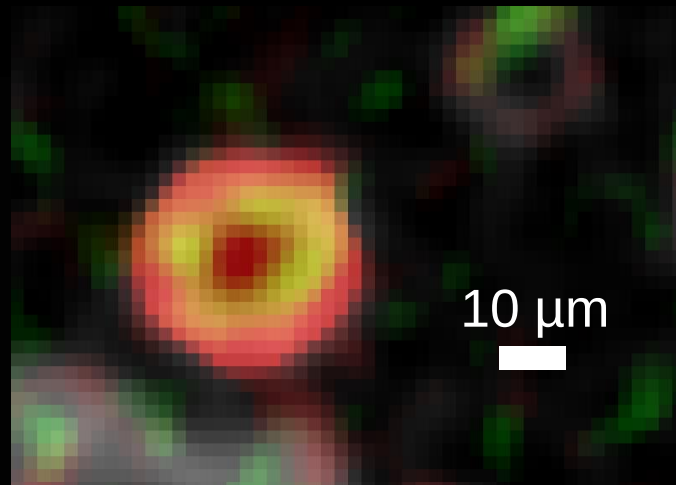


High-definition fast fluorescence tomography

Compton

Ge

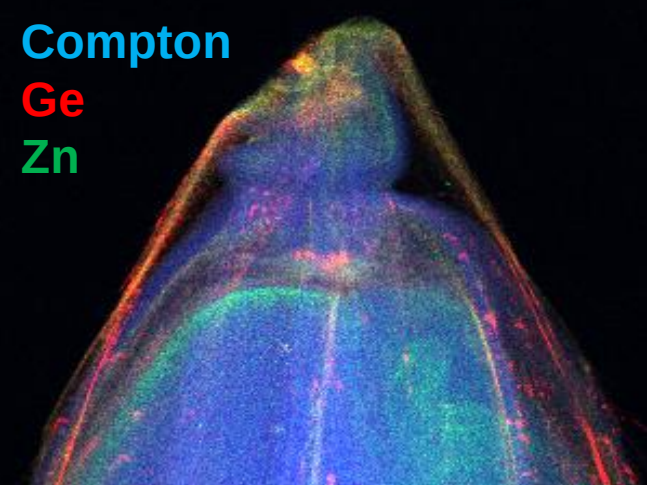
Zn



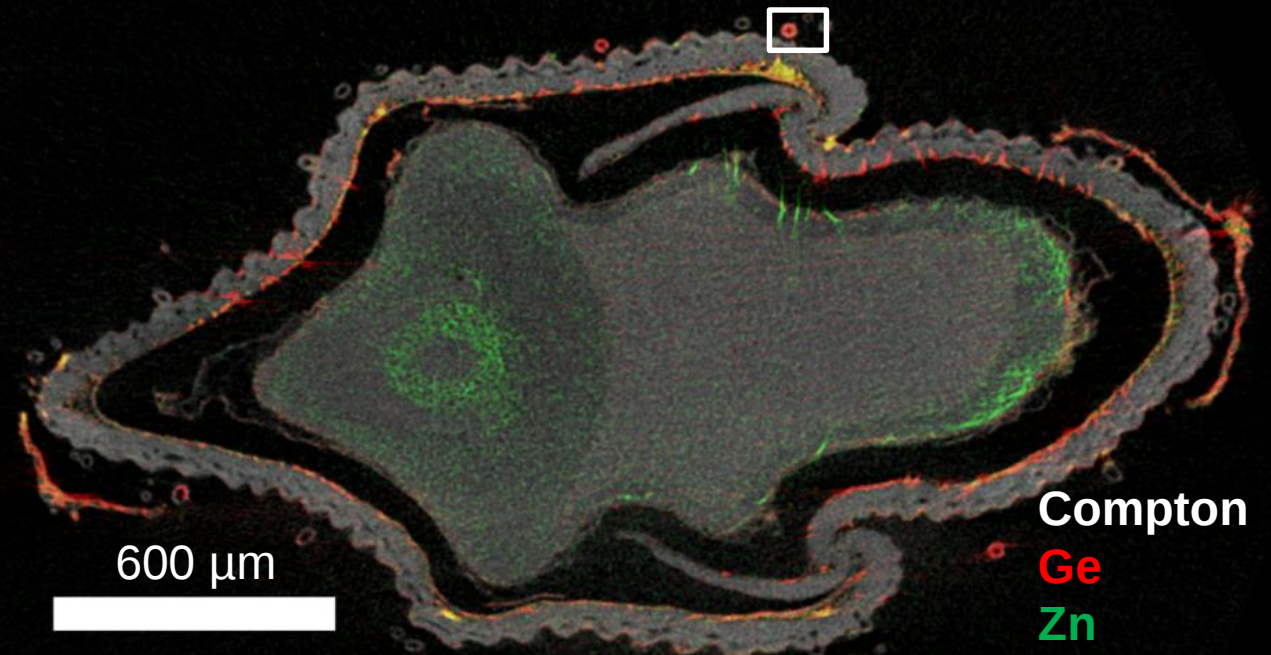
Compton

Ge

Zn



$\Delta = 2 \mu\text{m}$, $\tau = 2 \text{ ms}$
2291 pixels, 2001 projections (4.6 Mpix).
3 hrs measurement time
Rice grain with husk,

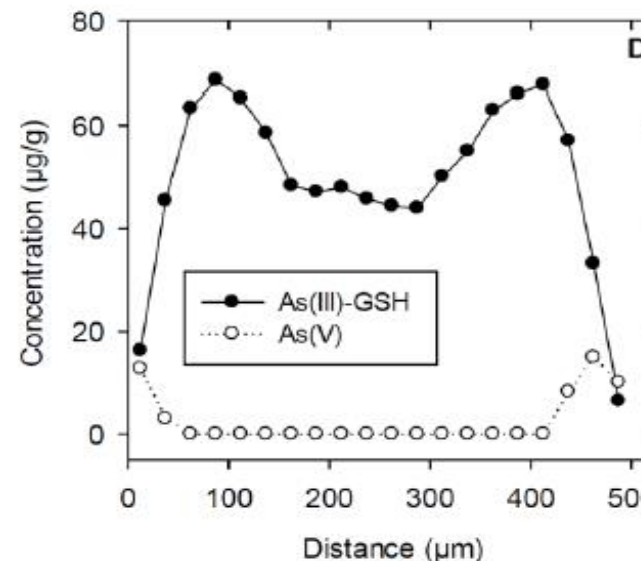
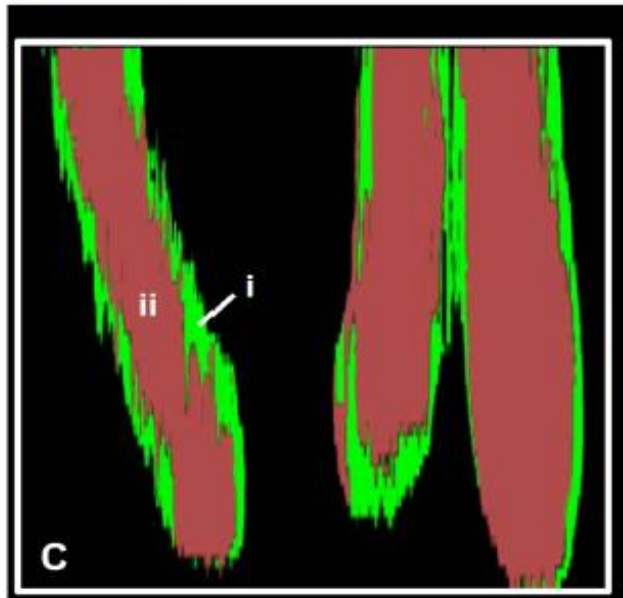
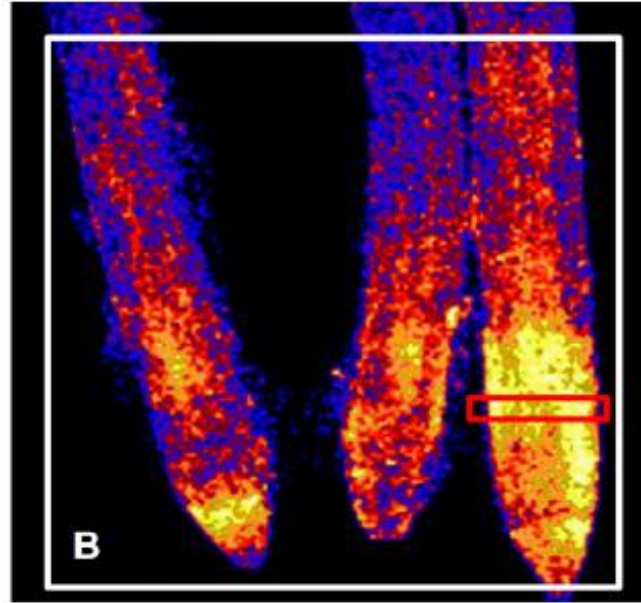
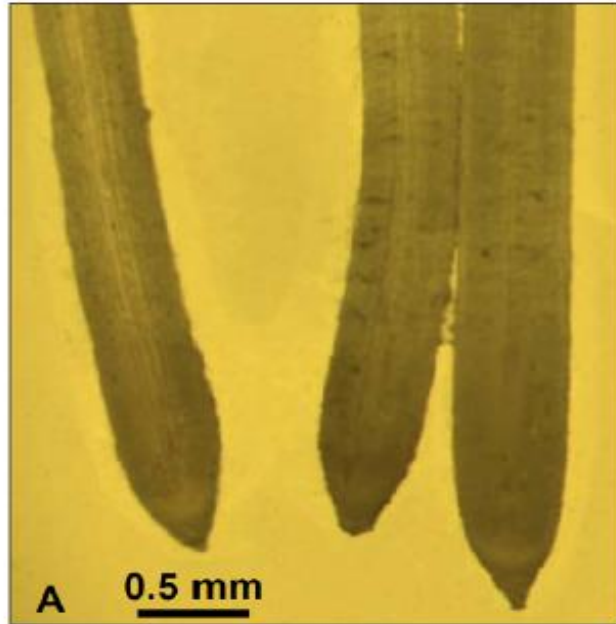


Compton

Ge

Zn

Detailed XANES analysis in hydrated roots



Wheat roots exposed 2 μM As(V) ca. 24 hr

- A. Light micrograph taken after completion of the XANES imaging
- B. Elemental map showing total As distribution after the XANES imaging.
- C. Spatial distribution of pixel-populations identified by comparing energy intensities.
- D. Concentrations of uncomplexed As(V) and As(III)-thiol complexes in the transect = red rectangle in B.

Kopittke *et al.* **New Phytologist** **201**, 1251-1262 (2014).

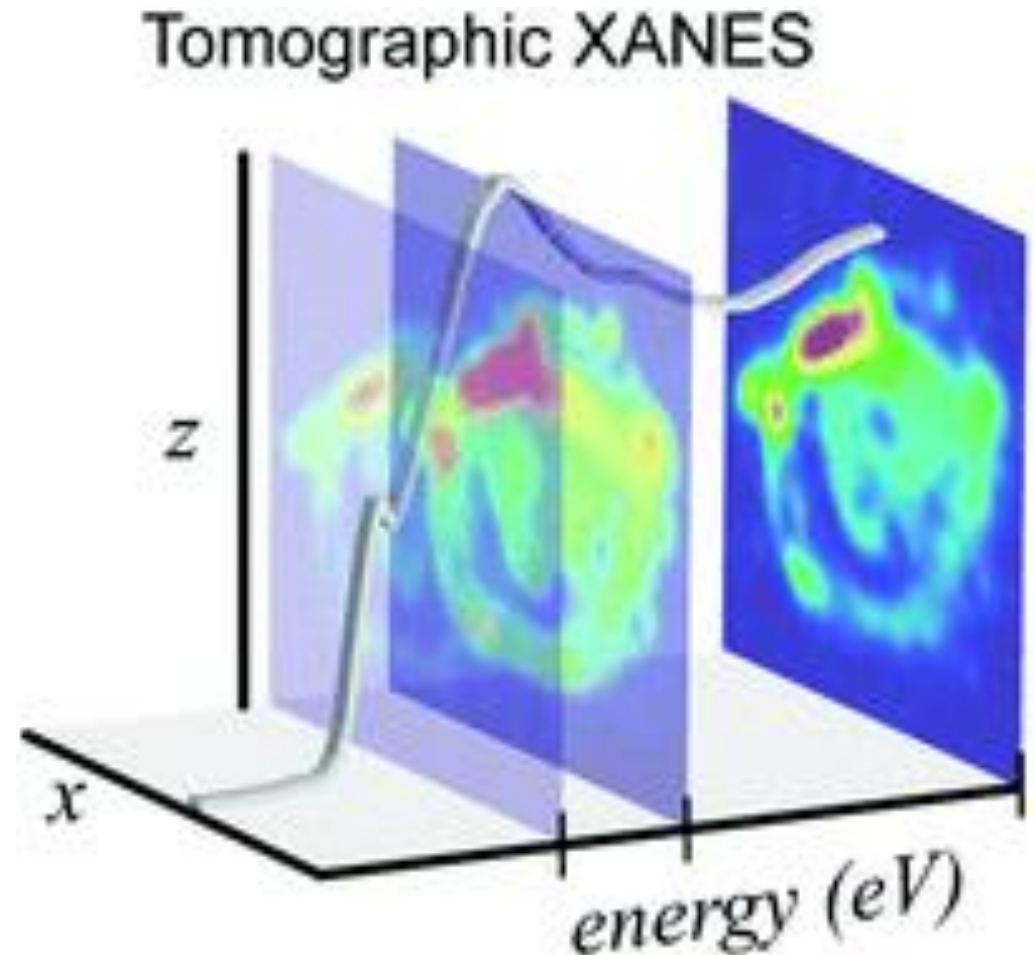
Tomographic XANES

- Fluorescence X-ray absorption near-edge structure tomography
- Study the spatial arrangement of biological coordination chemistry within intact organisms
- Demonstrated by mapping the distribution of cuprous and cupric complexes within *Drosophila melanogaster*.

S. A. James, et al.

Visualising Coordination Chemistry:

Fluorescence X-ray Absorption Near Edge Structure Tomography,
Chem. Comm. **52**, 11834–11837 (2016).



Mail-in and remote access and guidance

- XFM conducted 90% of experiments fully remotely during COVID restrictions
- Ideal Mail-in samples:
 - robust
 - transportable
 - do not require complicated on-site preparation and mounting
 - E.g. petrographic sections
- ASCI is powerful environment for data analysis and real time experiment guidance
 - Overview scan of entire platen
 - Selecting ROIs for detailed analysis



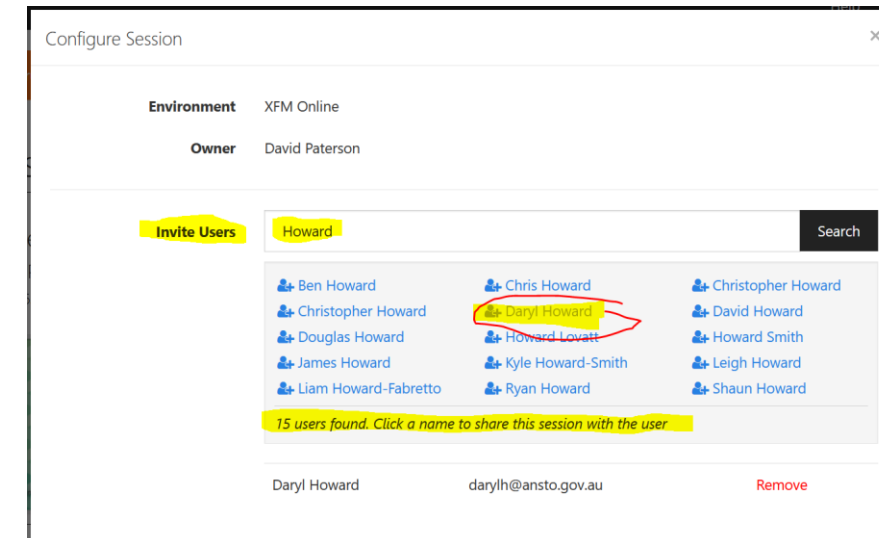
Data analysis: GeoPIXE within ASCI sessions

- Ideal environment to
 - Share data
 - Remote and on-site
 - Train new collaborators
 - Collaborate on
- data analysis & synthesis
 - During (XFM on-line) and
 - After (XFM Offline) your experiment

XFM



Sessions



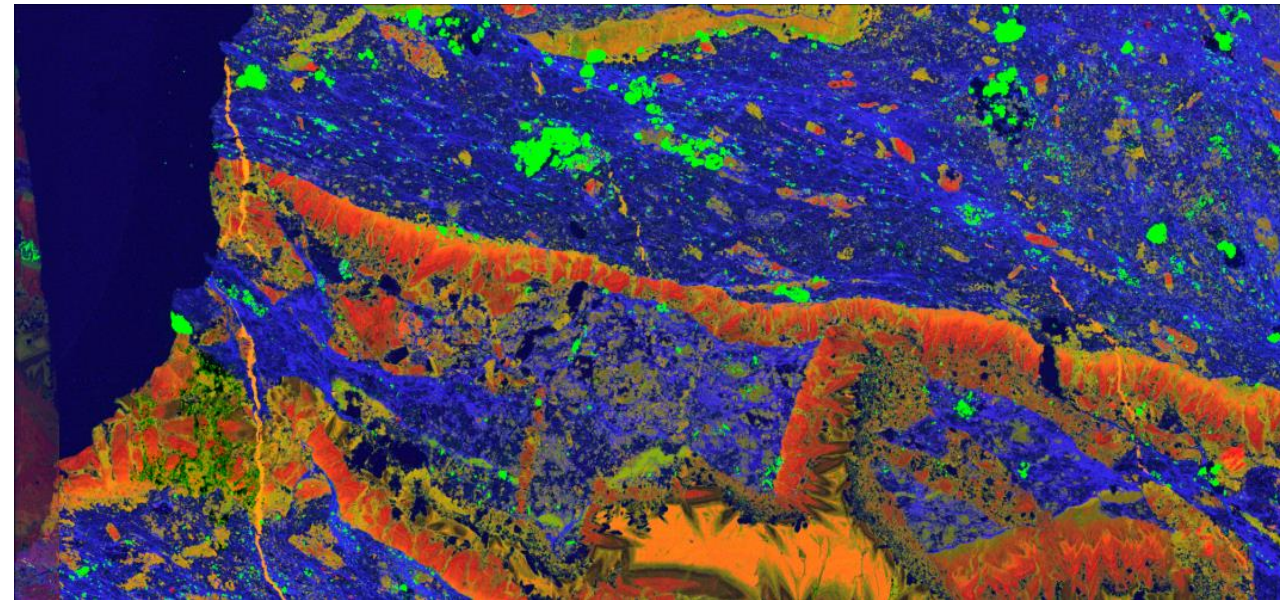
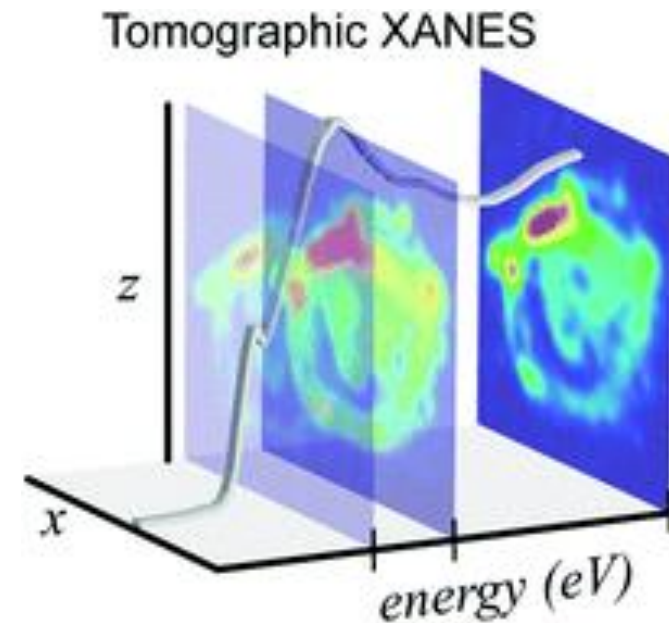
Summary and outlook

XFM

- Fast efficient mapping
- Fluorescence tomography
- Chemical XANES imaging
- ❑ Correlated ptychography
- ❑ 4D studies
 - › Time resolved
 - › XANES 3D tomography

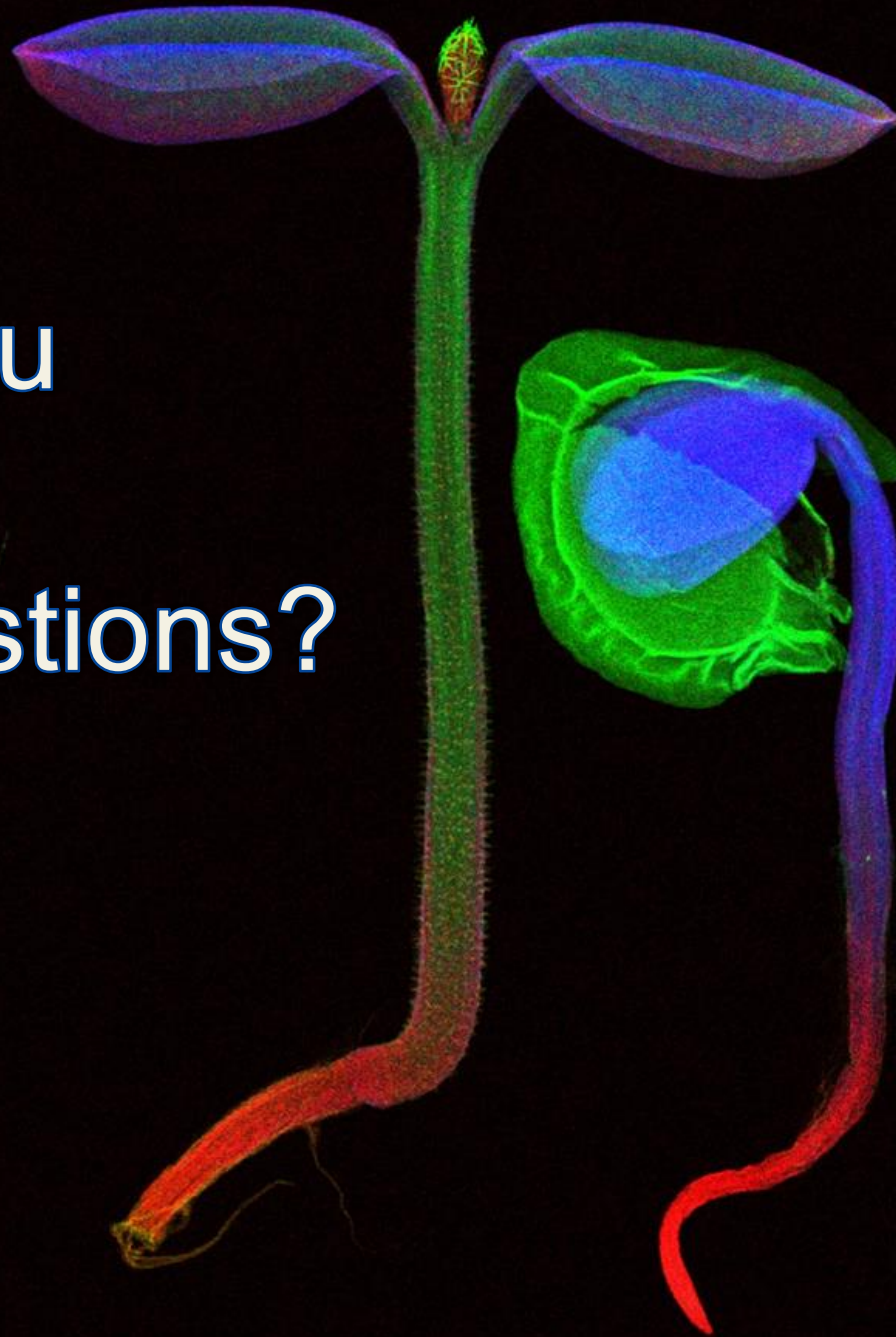
Future

- Higher energy (20 - 30 keV)
- Higher flux (DMM)
- Remote Access enhancements



Thank you

Any Questions?



Acknowledgements

XFM Daryl Howard, Martin de Jonge, Juliane Reinhardt, Cameron Kewish, Michael Jones, Simon James, ...

ANSTO Nader Afshar, Andy Starritt, Adam Walsh, Noel Basten, Nicole Cain, ...

CSIRO Chris Ryan, Robin Kirkham, Murray Jensen, D...

Collaborators / material contributed

University of South Australia: Enzo Lombi, Erica Donner, ...

University of Melbourne: Alex Johnson, ...

University of Queensland: Peter Kopittke, Peng Wang, ...

The Florey Institute: Gaiwan McColl, ...

Queensland University of Technology: Michael Jones, ..