Elettra
Sincrotrone
Trieste

IDEAS for collaborative research exploiting the colours of synchrotron light at Elettra

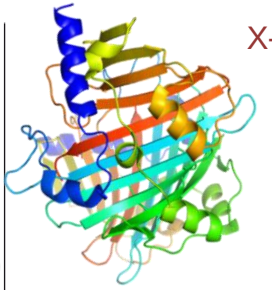
Lisa Vaccari

Elettra Sincrotrone Trieste

IDEAS
Imaging Diffraction Emission Absorption and Scattering

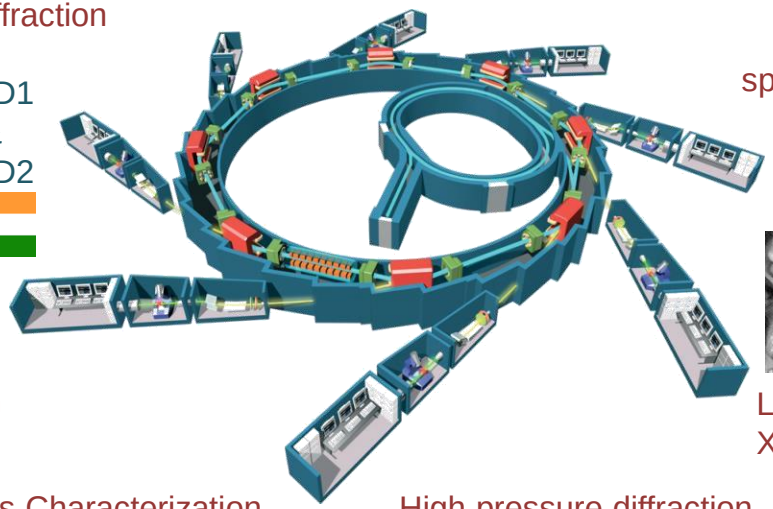
Elettra Sincrotrone Trieste

TwinMic
XRF
SYRMEP
IUVS
SISSI
Nano Innovation
Structural Biology
XRD1
XRD2
MCX
Xpress
XAFS

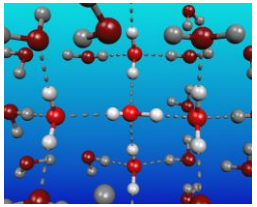


X-ray Diffraction

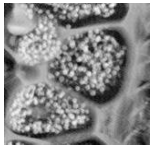
XRD1 & XRD2



IR and Raman spectro-microscopies

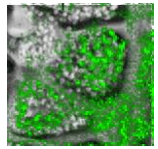


IUVS and SISSI



X-ray Microscopy

TwinMic

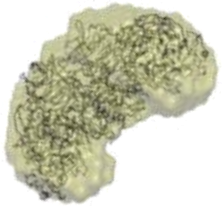


Low Energy X-ray Fluorescence

Small angle X-ray Scattering

SAXS

TU Graz



Materials Characterization by X-ray

High pressure diffraction

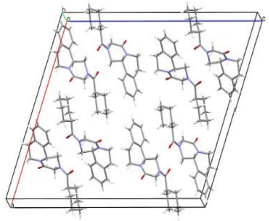
X-ray μ-CT

X-ray Fluorescence

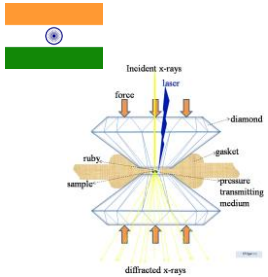
XRF

IAEA

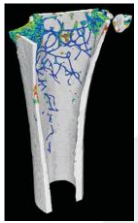
MCX

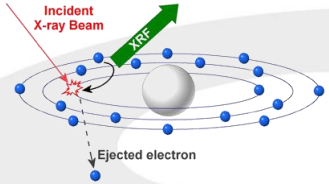


Xpress

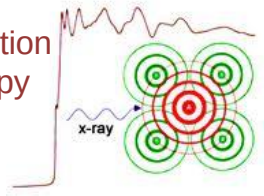


SYRMEP





X-ray Absorption Spectroscopy



XAFS

Environmental Sciences at TwinMic beamline

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TwinMic

XRF

SYRMEP

IUVS

Nano Innovation

Structural Biology

XRD1

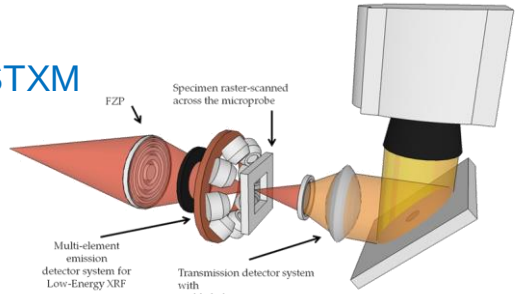
XRD2

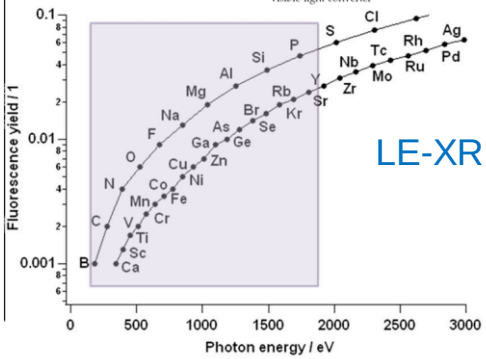
MCX

Xpress

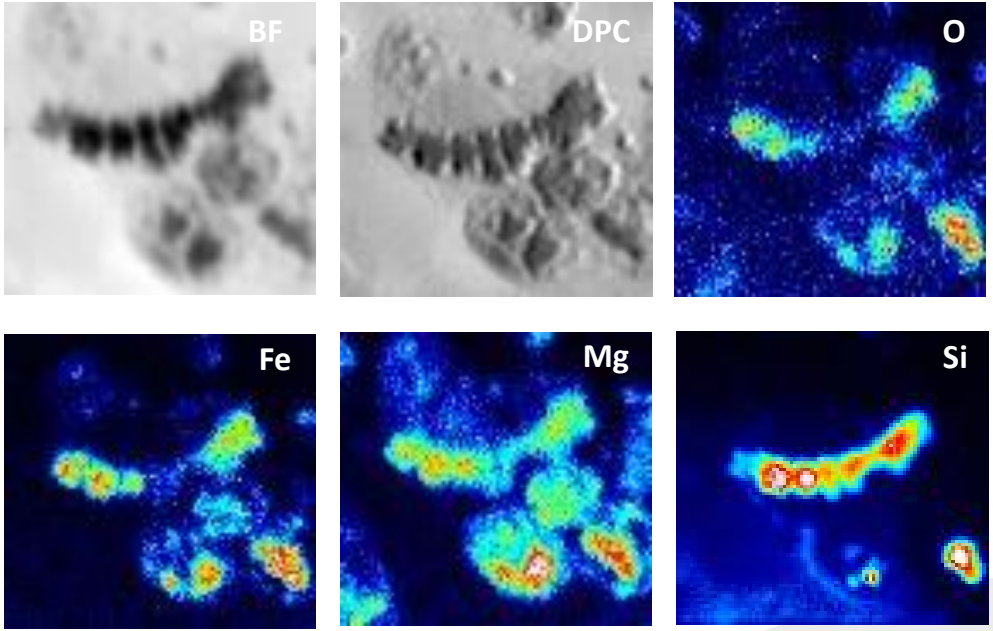
XAFS

Absorption and Phase contrast X-ray images with sub-micron resolution coupled with elemental mapping (low energy X-ray Fluorescence)





Novel features of asbestos body morphology and composition in human lung tissues



E=2019 eV, 50µm x 50 µm, 100 x 100 pixels, 15s/pixel LEXRF, 4 SDDs

L. Pascolo, et al. Particle and Fibre Toxicology 2011, 8:7
L. Pascolo, et al. Scientific Reports 2013, 3.

Life Sciences at TwinMic beamline

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SISSI
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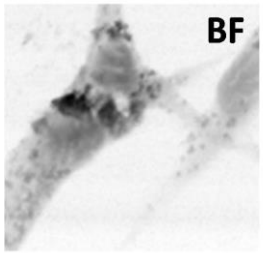
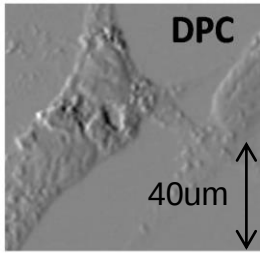
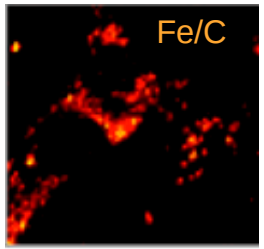
Nanotoxicology

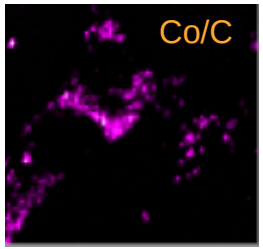
Assessment of toxic effects of nanomaterials at subcellular level in cells and tissues

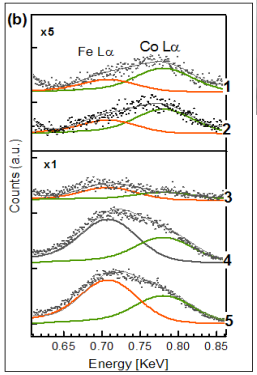
Effect and distribution of $CoFe_2O_4$ NPs in fibroblast cells

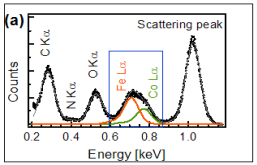


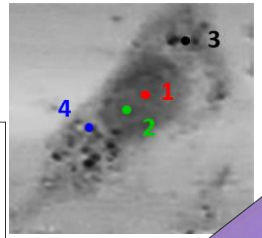


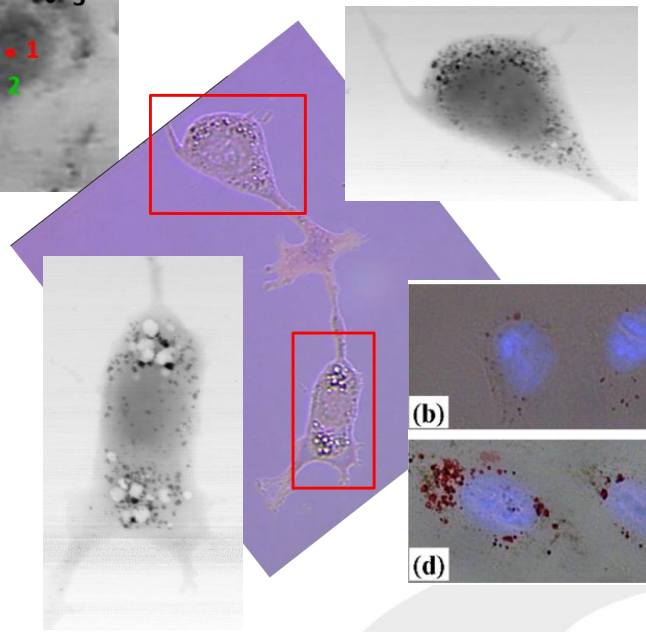












P. Marmorato, et al., *Cellular distribution and degradation of Cobalt Ferrite Nanoparticles in Balb/3T3 Fibroblasts*, Toxicology Letters, 2011, 207 - 2, 128.

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IAEA International Atomic Energy Agency *Atoms for Peace*

Extending the energy range: XRF beamline

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MCX
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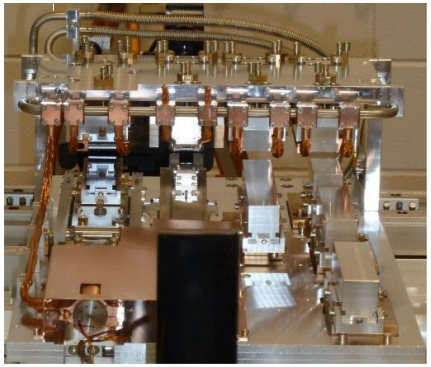
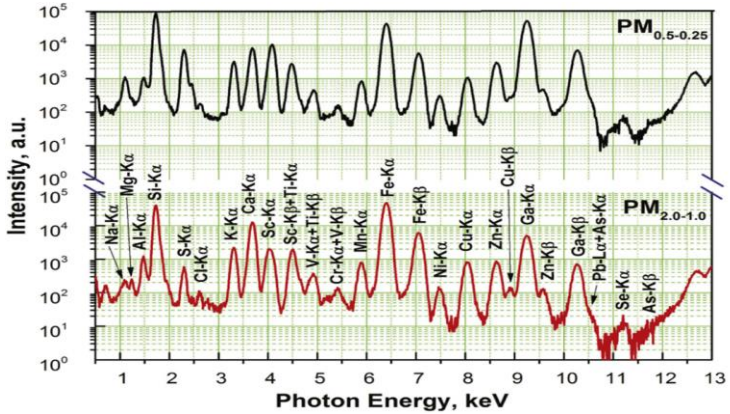
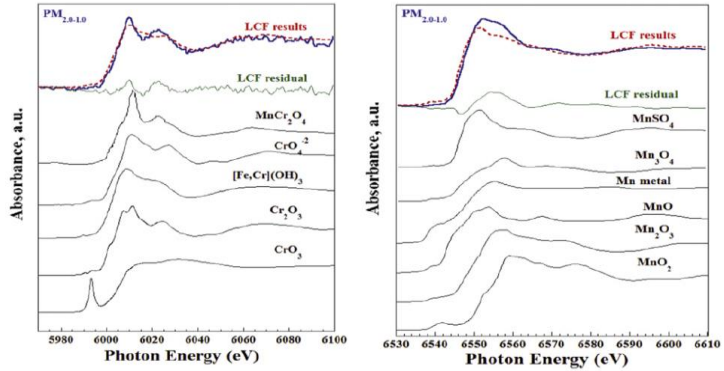
XAFS

SR-TXRF and XANES of air particulates from Jeddah, Saudi Arabia



Operated in partnership with the International Atomic Energy Agency (IAEA), X-Ray Fluorescence is a highly versatile beamline that covers the energy range 1KeV-14KeV





Element and its spectral line
Na-Kα
Mg-Kα
Al-Kα
S-Kα
Cl-Kα
K-Kα
Ca-Kα
Sc-Kα
Ti-Kα
V-Kα
Cr-Kα
Mn-Kα
Fe-Kα
Ni-Kα
Cu-Kα
Zn-Kα
As-Kβ
Se-Kα
Br-Kα
Pb-Lα

Soil

Fuel Combustion

Coal Powdered Stations

Abdallah A.Shaltout et al., Synchrotron radiation total reflection X-ray fluorescence (SR-TXRF) and X-ray absorption near edge structure (XANES) of fractionated air particulates collected from Jeddah, Saudi Arabia, Microchemical Journal 137, 2018, Pages 78-84

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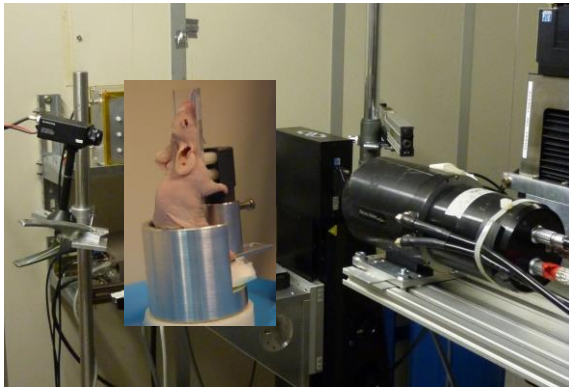
X-ray micro-computed tomography
From 2D to 3D at SYRMEP

Cell tracking studies for imaging brain tumors in rats



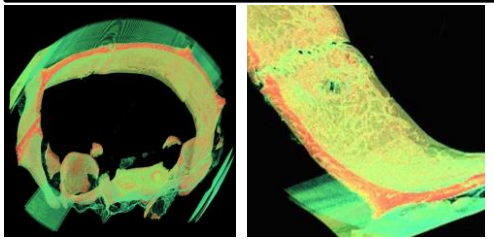
Glioblastoma multiforme (GBM) is the most common and aggressive primary brain tumor in humans. Glioma cells exposed to colloidal Gold Nano Particles (GNP) were implanted into the brain of adult male Wistar rats under general anesthesia.

Aim of the cell tracking

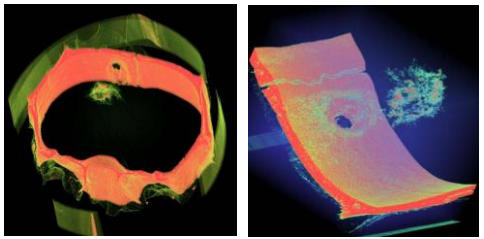
monitor the dynamic of tumour growth
follow the migration of tumour cells
understand the dynamic of metastasis spread

The SYRMEP (SYnchrotron Radiation for MEdical Physics) beamline has been designed for μ-CT in the 8-35 keV range.
Research in medical diagnostic radiology, material science and life science applications.

A. Astolfo et al., Nanomedicine: Nanotech., Biology and Medicine, Vol. 9, Issue,2013



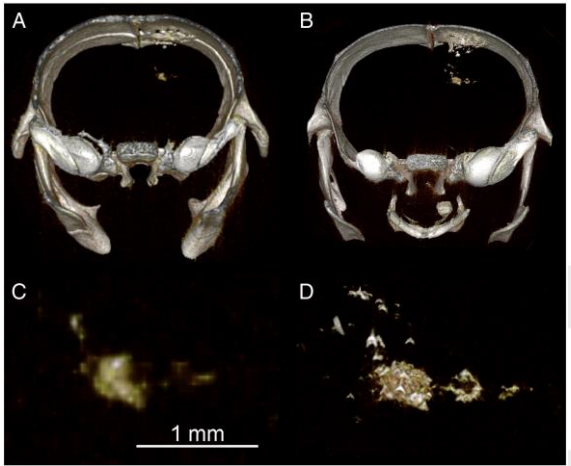
Control



Animal injected with marked cells

Low dose *in vivo* data

High dose *ex vivo* data



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Clinical studies at SYRMEP

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Nano Innovation
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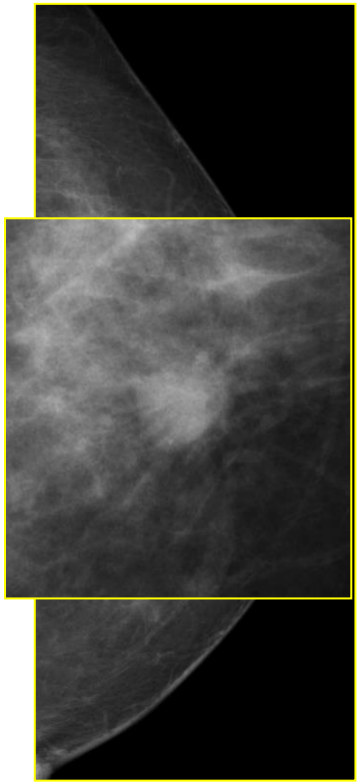
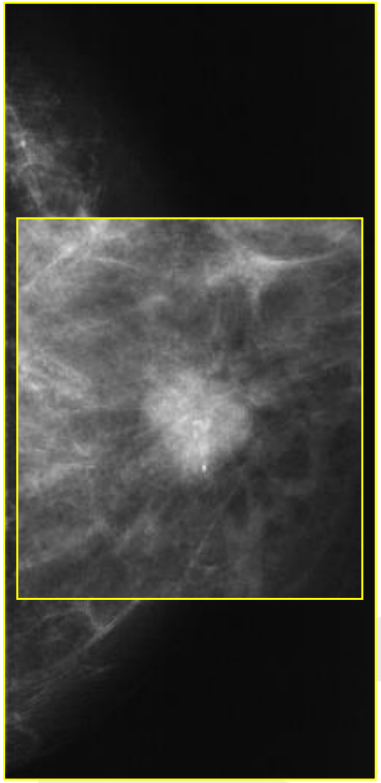
XRD2
MCX
Xpress
XAFS

Clinical Mammography

CONVENTIONAL unit



Synchrotron Radiation



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Vibrations to reveal chemistry
IUVS beamline

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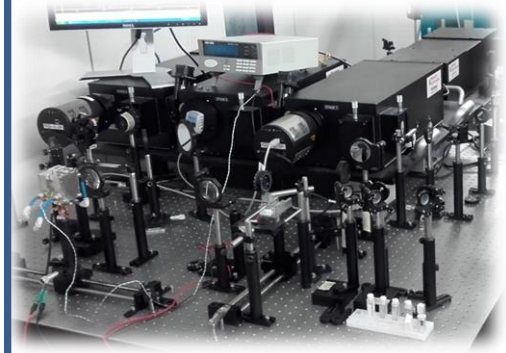
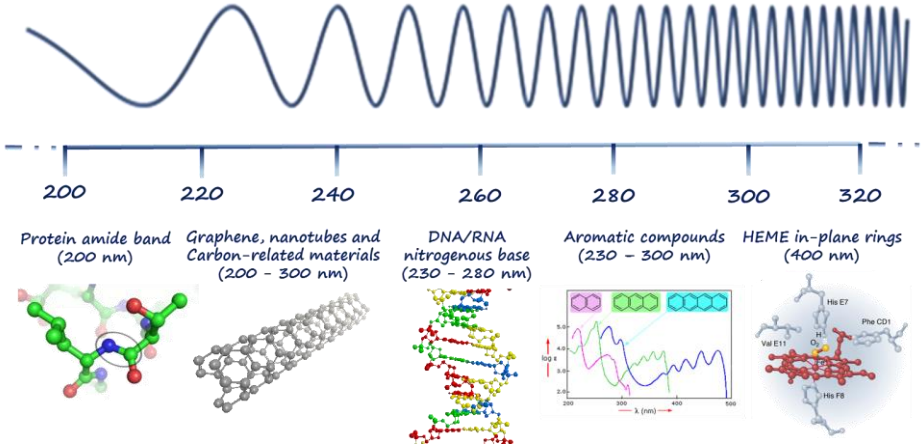
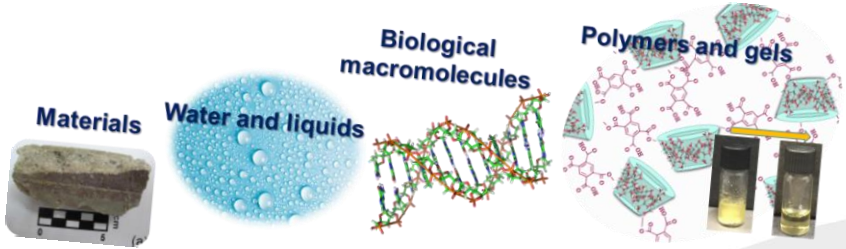
IUVS
SISSI
Nano Innovation
Structural Biology
XRD1
XRD2
MCX
Xpress
XAFS

From macro to micro capability



Sensitive and selective UV-Raman spectra at micrometric lateral resolution





B. Rossi et al, Synchrotron based UV Resonant Raman scattering for material science, in Molecular and Laser Spectroscopy, Volume 2 (eds V. P. Gupta, Y. Ozaki), Publisher: Elsevier 2020 in press.

Vibrations to reveal chemistry at IUVS

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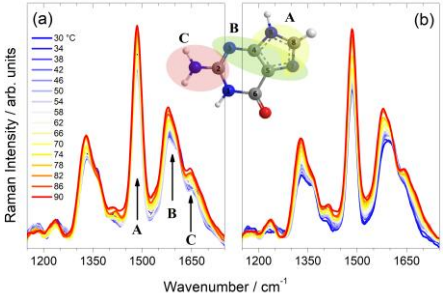
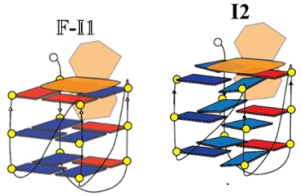
Non-invasive characterization of **STRUCTURE** and **DYNAMICS** of biological systems under ***physiological conditions***

-> *DNA and THEIR ASSEMBLIES*

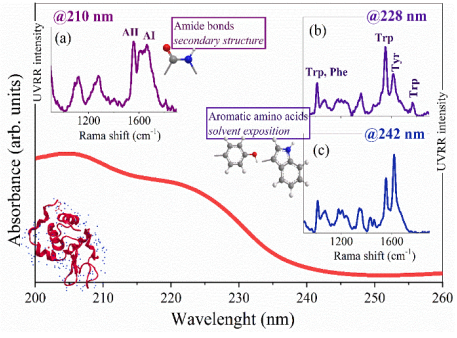


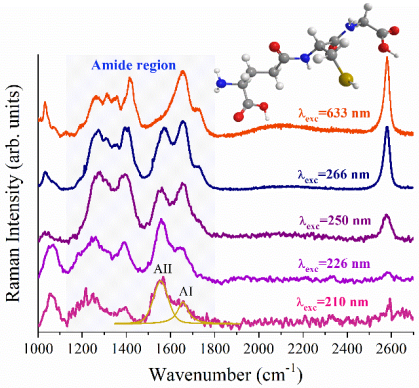


Structure of human telomere G-quadruplex in the presence of a model drug along the thermal unfolding pathway
Bianchi F. et al, *Nucleic Acids Research, Vol. 46 - 22, pp. 11927-11938 (2018)*

Conformational stability of DNA in hydrated ionic liquid by synchrotron-based UV resonance raman
Bottari C. et al. Proceedings of SPIE - The International Society for Optical Engineering, Vol. 11086 - 110860Q, pp. 1-8 (2019)

-> *PEPTIDES AND PROTEINS*





Aqueous solvation of glutathione probed by UV resonance Raman spectroscopy
Catalini S. et al. Journal of Molecular Liquids, Vol. 283, pp. 537-547 (2019)

Frontiers of UV resonant raman spectroscopy by using synchrotron radiation: the case of aqueous solvation of model peptides
Rossi B. et al., Proceedings of SPIE - The International Society for Optical Engineering, Vol. 11086 - 110860N, pp. 1-10 (2019)

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Life Sciences at SISSI-Bio – the microscale

TwinMic
XRF
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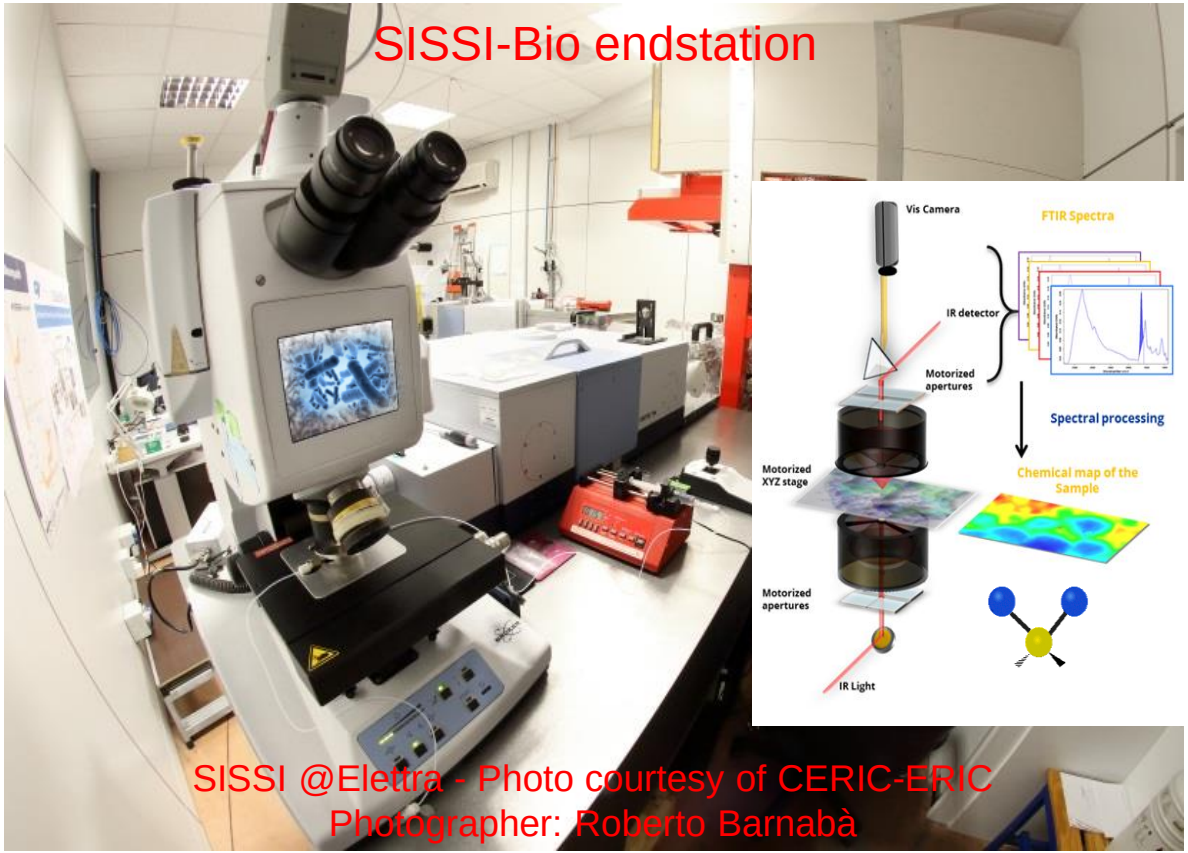
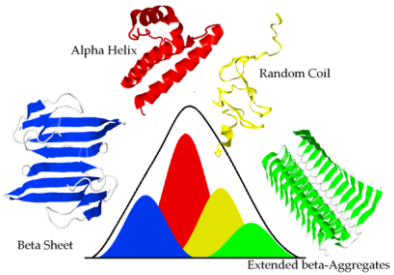
XAFS

SISSI-Bio endstation



SISSI @Elettra - Photo courtesy of CERIC-ERIC
Photographer: Roberto Barnabà

Synchrotron Radiation FTIR microscopy provides biochemical information on bio-samples, with micrometric lateral resolution



Far–filed microscopy

Lateral resolution is diffraction limited

$\delta \approx \lambda$

Life Sciences at SISSI-Bio – the microscale

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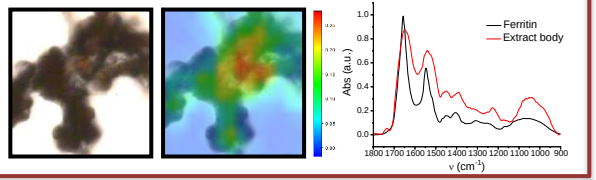
Tissue Analysis

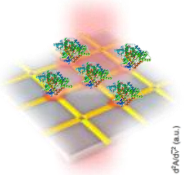
Label-free morpho-chemical analysis
A quantitative alternative to traditional histology

Key studies
- Cancer diagnosis and treatment
- Neurodegeenrative disorders
- Vibrational characterization of male and female gametes
- Nanotoxicology
- Rare diseases

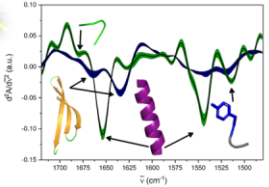
Differential protein folding in lung tissues exposed to asbestos



Plasmonic devices for protein conformational studies



An ultrasensitive plasmonic platform for protein-binding studies.



Bridging CD and structural studies (XRD, SAXS, NMR, cryo-EM)

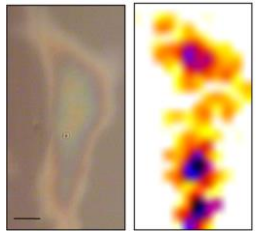
Structural Biology Lab
NanoInnovation Lab

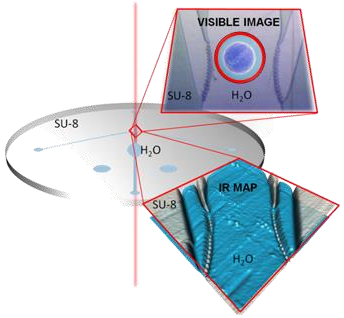
Cellular and sub cellular studies

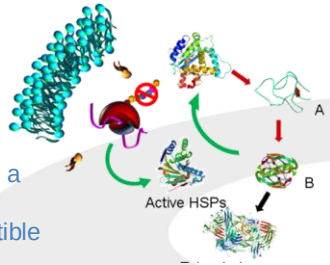
Label-free cellular biology
A complement to traditional cell-based assyas

Key studies
- Cell death, cytotoxicity and viability assays
  - Cellular response to chemicals and exogenous stresses
  - Possibility for dynamic studies on live cells
- In-situ cell sorting in accordance with the cell-cycle stage
- Microbiology

Prion infection in GT1 cell model







Protein misfolding and aggregation as a consequence of heat shock.
Dynamic live cell studies in biocompatible fluidic devices

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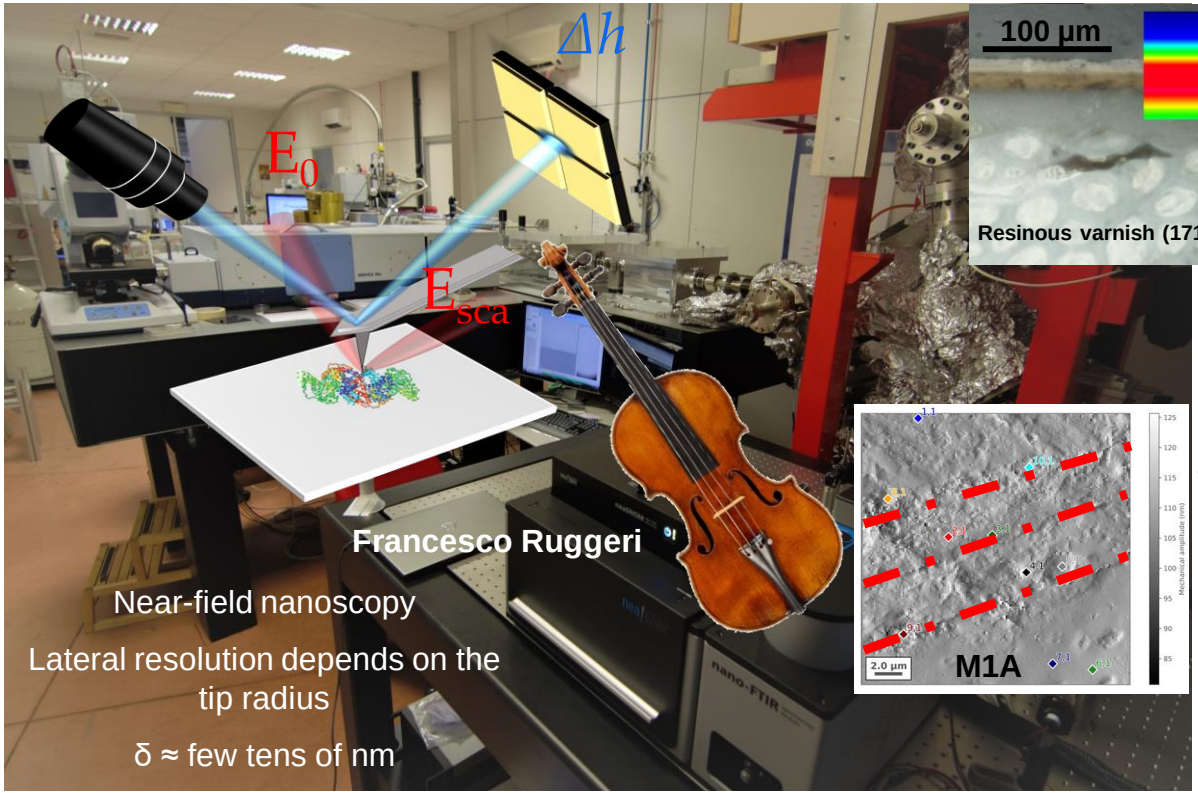
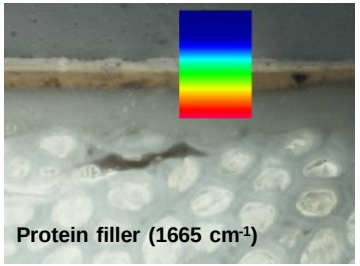
SISSI-Bio
The Nanoscopy endstation

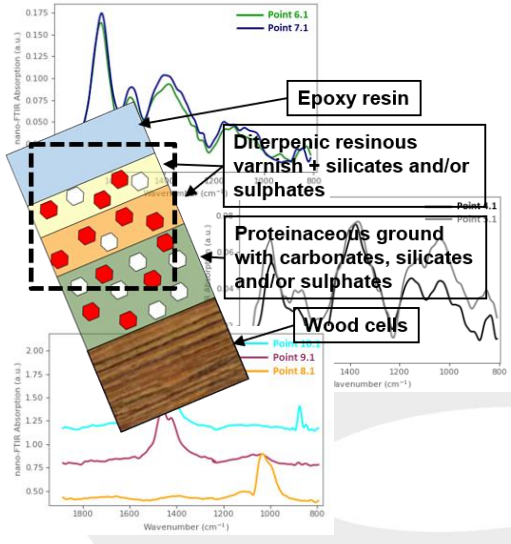
Elettra Sincrotrone Trieste
TwinMic
XRF
SYRMEP
IUVS
SISSI
Nano Innovation
Structural Biology
XRD1
XRD2
MCX
Xpress
XAFS



From micro



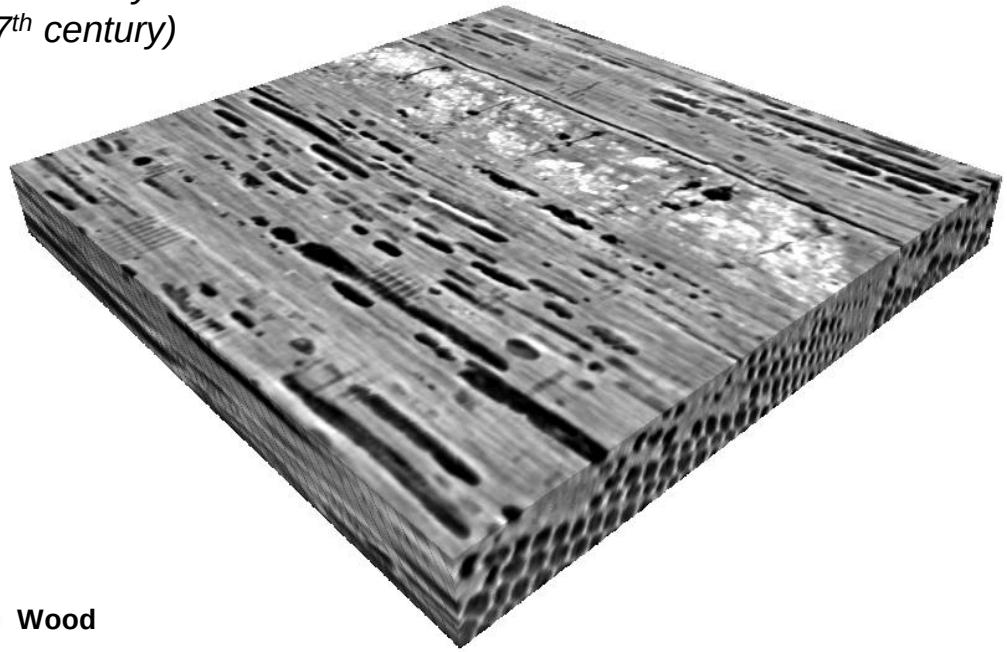
To nano



Bridging Nano-chemistry and 3D morphology

3D RECONSTRUCTION at SYRMEP

Fragment of cello made by Andrea Guarneri (17th century)



Wood

G. Fiocco et al., "Synchrotron radiation micro-computed tomography for the investigation of finishing treatments in historical bowed string instruments: issues and perspectives", European Physical Journal Plus. **133**, 525-34 (2018)

G. Fiocco et al., "A Micro-Tomographic Insight into the Coating Systems of Historical Bowed String Instruments", Coatings, **9**, 81 (2019)

Bridging Nano-chemistry and 3D morphology

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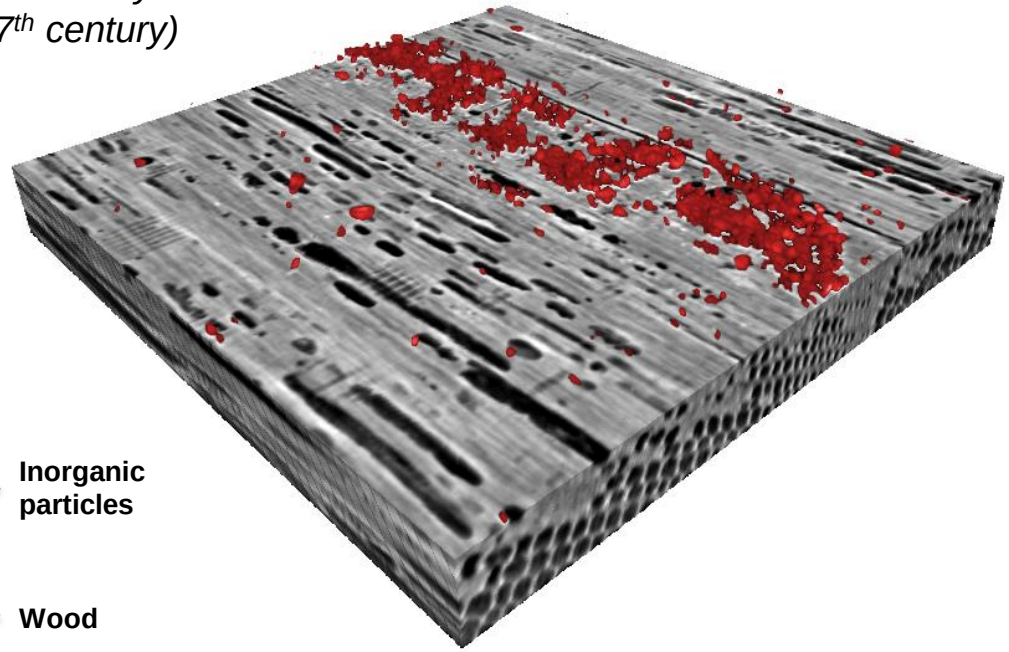

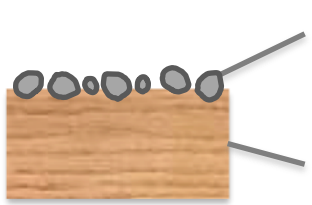

G. Fiocco et al., "Synchrotron radiation micro-computed tomography for the investigation of finishing treatments in historical bowed string instruments: issues and perspectives", European Physical Journal Plus. **133**, 525-34 (2018)
G. Fiocco et al., "A Micro-Tomographic Insight into the Coating Systems of Historical Bowed String Instruments", Coatings, **9**, 81 (2019)

X-ray micro-computed tomography From 2D to 3D at SYRMEP

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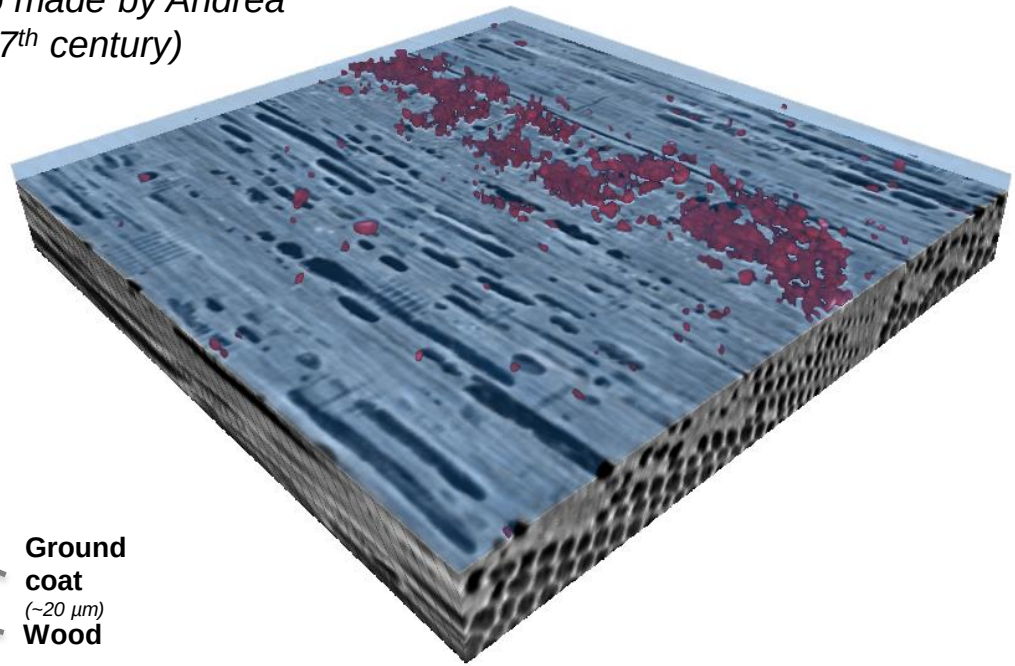
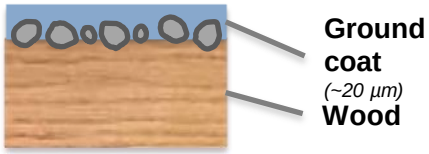
3D RECONSTRUCTION at SYRMEP

Fragment of cello made by Andrea Guarneri (17th century)





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Bridging Nano-chemistry and 3D morphology

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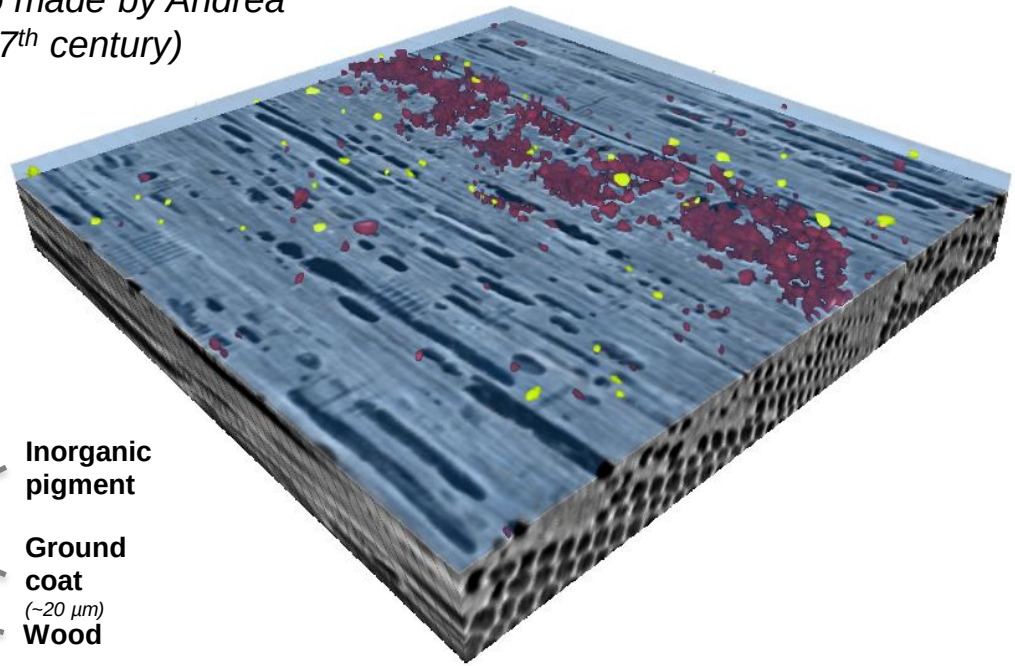

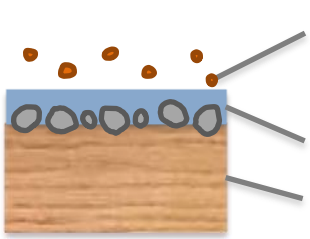

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Bridging Nano-chemistry and 3D morphology

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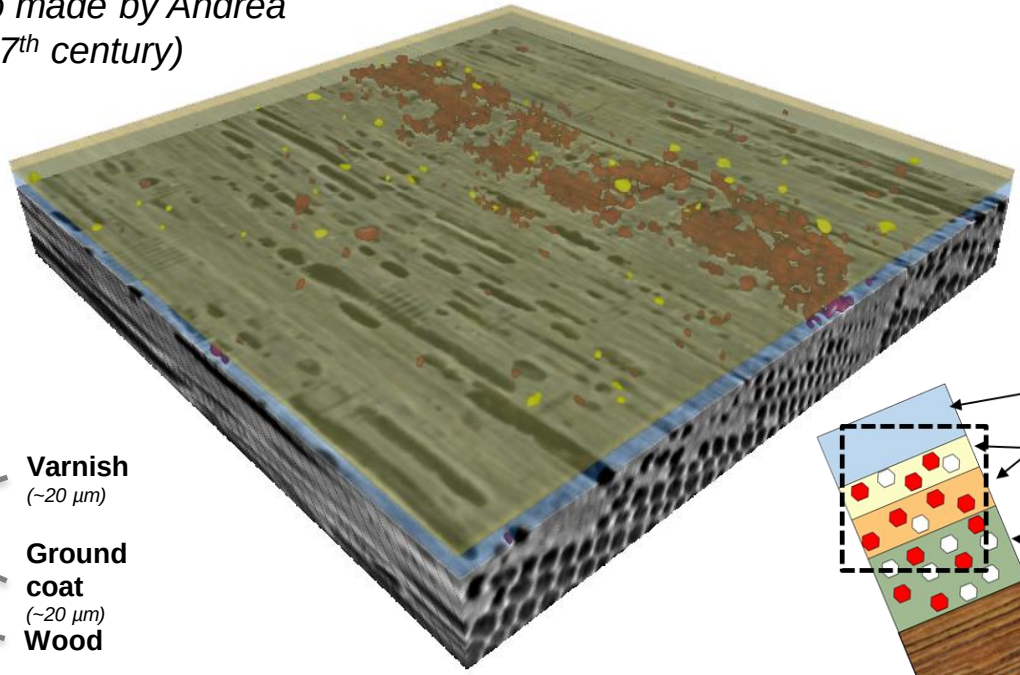

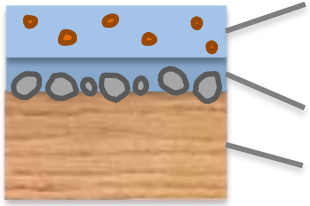

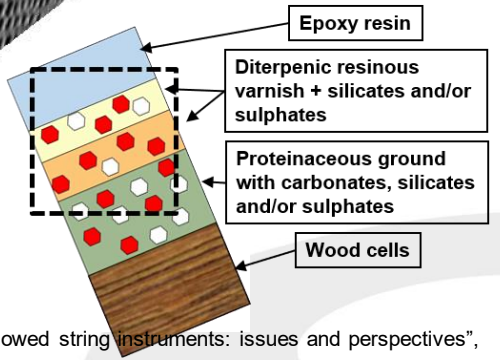

G. Fiocco et al., "Synchrotron radiation micro-computed tomography for the investigation of finishing treatments in historical bowed string instruments: issues and perspectives", European Physical Journal Plus. **133**, 525-34 (2018)

G. Fiocco et al., "A Micro-Tomographic Insight into the Coating Systems of Historical Bowed String Instruments", Coatings, **9**, 81 (2019)

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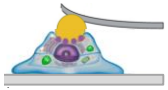
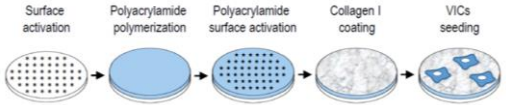
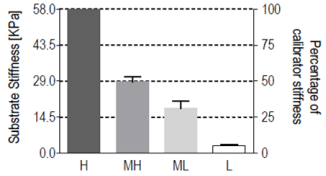
Bridging Nano-chemistry and Mechanobiology: NanoInnovation Lab

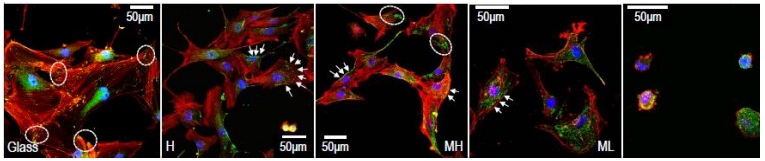




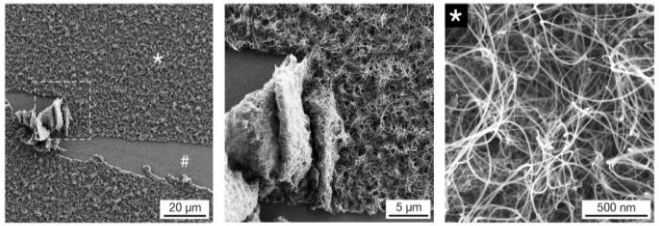


CELL MECHANOSENSING

Polymeric and carbon-based biocompatible materials are used as tunable scaffold for cell growth to study **cell mechanosensing and mechanotransduction** in the context of diverse diseases (aortic valve (AV) interstitial cells in AV calcific disease; breast cancer cells



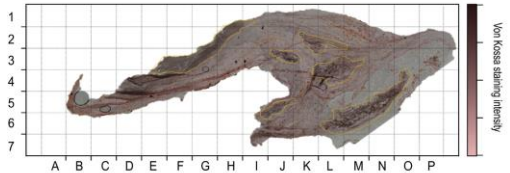
Biomaterials 2018, 181

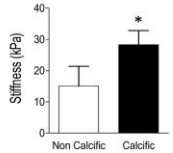


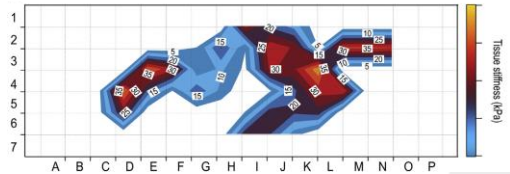
Advanced Biosystems 2019, 3

NANOINDENTATION HISTOLOGY

Mechanical compliance of **human aortic valve leaflets measured via AFM** (isobar-like layout) to complement classical histological staining







Biomaterials 2018, 181

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Pharma at Elettra

Elettra Sincrotrone Trieste

TwinMic

XRF

SYRMEP

IUVS

SISSI

Nano Innovation

Structural Biology

XRD1

XRD2

MCX

Xpress

XAFS

Structural Biology Laboratory

XRD1 XRD2 MCX beamlines

Drug (API molecule) target-based drug design

Drug (API molecule) characterization

Drug (solid state – powder) p*re-formulation and formulation:* Definition of processes and quality control methods, stability and compatibility, scale up, regulatory and legal documents

Drug (solid state – powder) *manufacturing*: From incoming goods quality to end-product quality.

Structural Biology Lab

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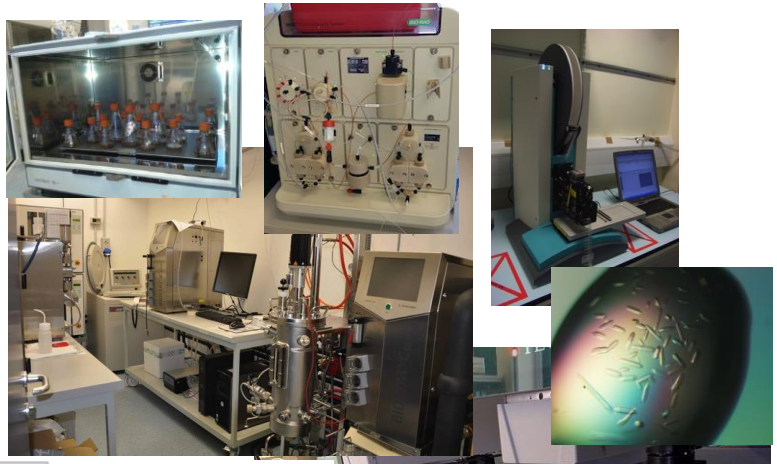
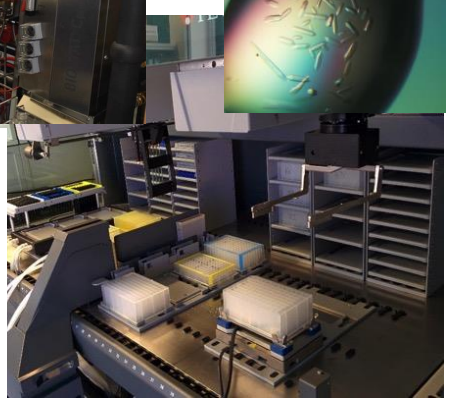
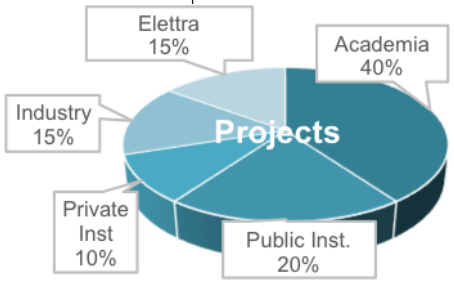
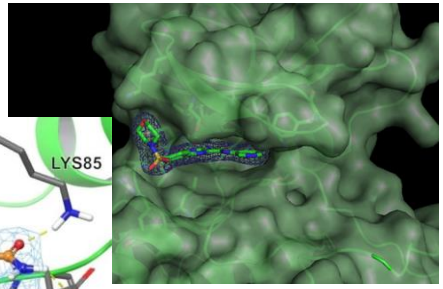
TwinMic
XRF
SYRMEP
IUVS
SISSI
Nano Innovation
Structural Biology

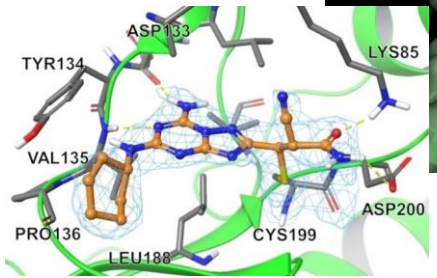
Construct Design → HT Cloning → Expression → Purification → Scale-up → QC







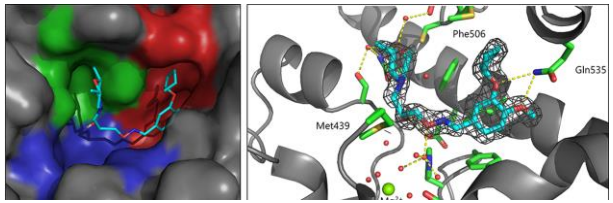




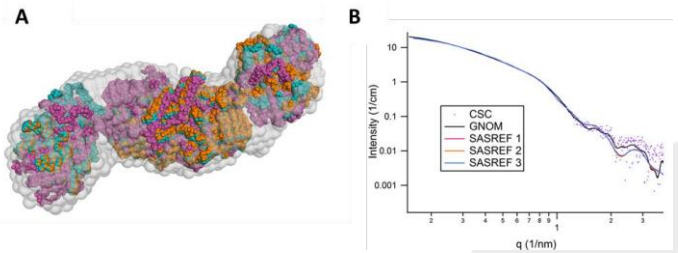
X-ray structure of kinase GSK-3β with inhibitor covalently bound in ATP pocket

S. Redenti *et al., ChemMedChem.* (2018)

Anti-Alzheimer drugs to selectively target PDE4 isoforms without side effects



T. Prosdocimi et al., Biochemistry(2018)



Cystein Synthase SAXS architecture for new antibiotics design

B. Rosa et al., Int.J.Mol.Sci. (2019)

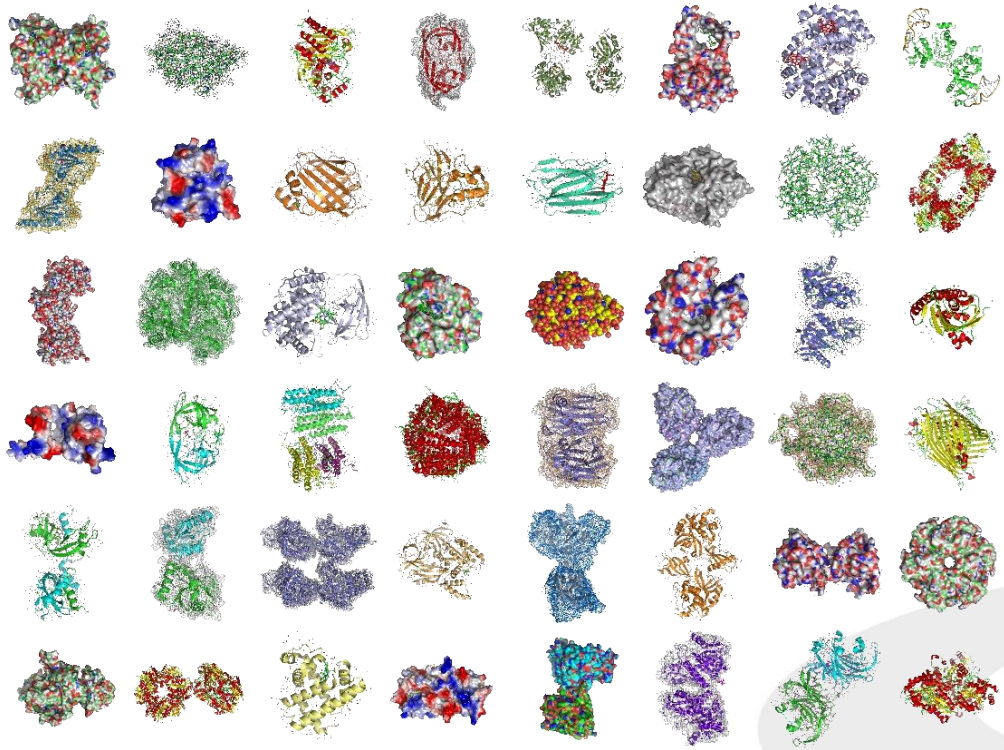
XRD2 beamline

Source
SCW
[fulfills the needs of
both Xpress and XRD2]

Energy range
8-25 keV

Indian Institute of Science
Bangalore

Drug (API molecule) target-based drug design



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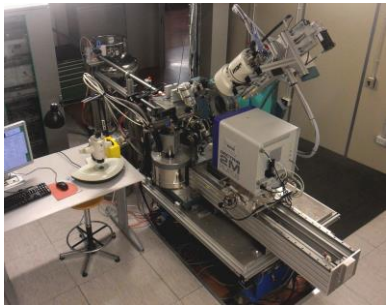
XRD1 beamline

Elettra Sincrotrone Trieste
TwinMic
XRF
SYRMEP
IUVS
SISSI
Nano Innovation
Structural Biology
XRD1
XRD2
MCX
Xpress
XAFS

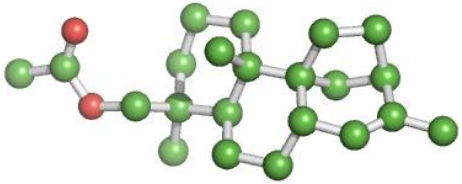


Source wiggler

Energy range 4-21,5 keV

Drug (API molecule) characterization

Phytoalexins produced in plants act as toxins to the attacking organism.
When a plant cell recognizes a pathogen, a *short-term* response and a delayed *long-term* specific response are launched.
Long-term resistance, involves communication pathways that in turn involve plant hormones such as jasmonic acid, ethylene, abscisic acid or salicylic acid.
The reception of the signal leads to global changes within the plant, which induce genes that protect from further pathogen intrusion, including enzymes involved in the production of phytoalexins.

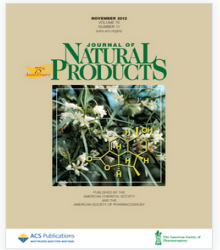


RETURN TO ISSUE | < PREV **ARTICLE** NEXT >

Regio- and Diastereoselective Synthesis and X-ray Structure Determination of (+)-2-Deoxyoryzalexin S from (+)-Podocarpic Acid. Structural Nonidentity with Its Nominal Natural Isolated Enantiomer

Francesca Leonelli[*†], Valentina Latini[†], Andrea Trombetta[†], Gabriele Bartoli[†], Francesca Ceccacci[†], Angela La Bella[†], Alessio Sferrazza[†], Doriano Lamba[‡], Luisa M. Migneco[†] and Rinaldo Marini Bettolo[*†]

View Author Information



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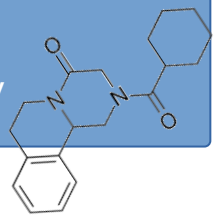
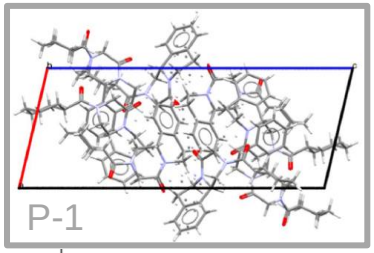
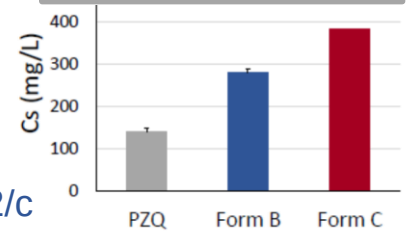
MCX beamline

X-rays at sample
Energy range
6-22 keV
Photon flux
10^{11} photons/sec
Beam size at sample
10x1 mm^2 - 0.3x0.3 mm^2
Energy resolution
$\Delta E/E$ $2x10^{-4}$

Drug (solid state – powder) *manufacturing*:
From incoming goods quality to end-product quality

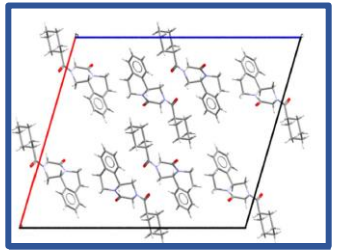




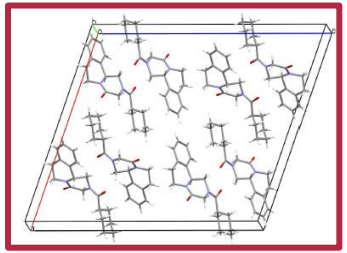


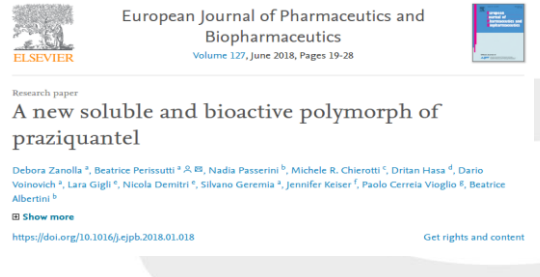
BACKGROUND:
PZQ (Praziquantel) is the only available drug to treat Schistosomiasis, a recurrent disease in developing countries caused by water contaminated with parasitic worms (Schistosomes).
Praziquantel utilization is limited by the **high therapeutic dose needed**, resulting in large tablets and capsules difficult to be swallowed.
STUDY: Find a new soluble form (crystalline polymorph) of Praziquantel with different physical properties

C2/c



C-I2/c





European Journal of Pharmaceutics and Biopharmaceutics
Volume 127, June 2018, Pages 19-28

Research paper

A new soluble and bioactive polymorph of praziquantel

Debora Zanolla [a], Beatrice Perissutti [a, 2, 8], Nadia Passerini [b], Michele R. Chierotti [c], Dritan Hasa [d], Dario Voinovich [a], Lara Gigli [e], Nicola Demitri [e], Silvano Geremia [a], Jennifer Keiser [f], Paolo Cerreia Vioglio [g], Beatrice Albertini [b]

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https://doi.org/10.1016/j.ejpb.2018.01.018

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Xpress – high pressure diffraction beamline

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IUVS
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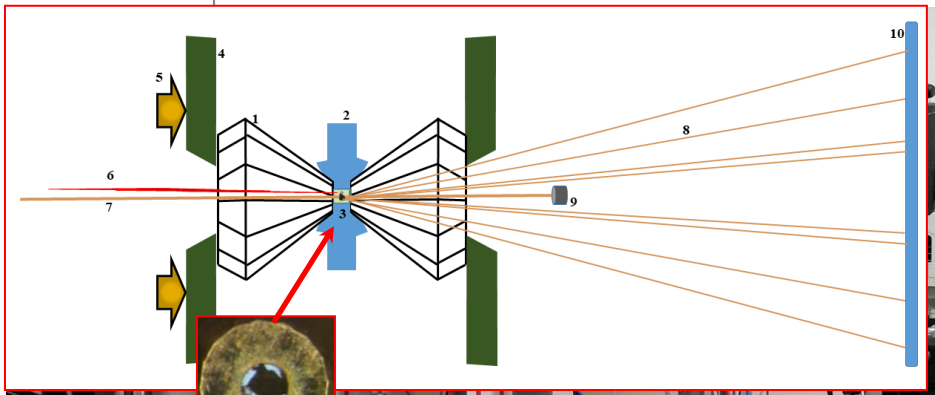
Nano Innovation
Structural Biology
XRD1
XRD2
MCX
Xpress
XAFS



Hard x-ray diffraction beamline with monochromatic energy 25 keV (fixed). In-situ high pressure measurements (50 GPa) using diamond anvil cells. Ruby fluorescence for in-situ pressure monitorning.

Routinely used for powder diffraction, recently single crystal high pressure diffraction capablilities are shown (P. Lotti et al., J. Synchrotron Rad (2020)).

Will be soon upgraded with a Pilatus6M detector (2021).

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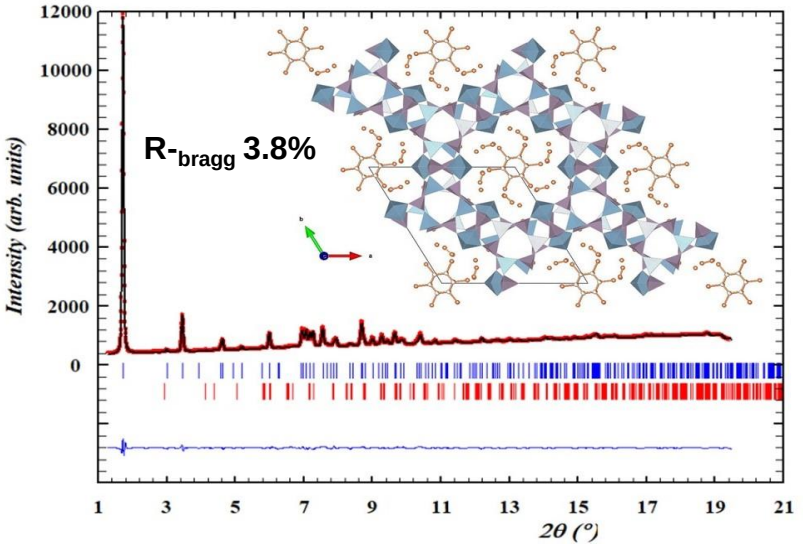
Xpress – high pressure diffraction beamline

Most users are from condensed matter physics background.
Investigations are on pressure induced structural phase transitions, metallization, isostructural transitions/novel electronic states etc, but also on creating novel materials.

Recently there is an increasing activity on porous materials.

- Stability under pressure
- Guest – host interaction : how pores can host the guest molecules under pressure and thus modify the properties.
- Pressure-induced intercalated molecoles undergo further reactions (bonding to host, polymerization) under varying conditions (laser irradiation, pressure cycling, heating etc) to yield unique novel material with nanochannels inside!



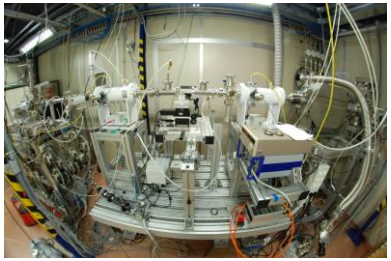
Polymerizion of C_8H_6 in the 12 Å channels of the large-pore aluminosphoshate VF-zeolite under high temperature-high pressure conditions of about 0.8 GPa and 140 °C.

The resulting conductive polymer/insulating host composite consists of disordered predominantly trans-polyphenylacetylene chains in the pores of the host structure.

in-situ and *operando* measurements at XAFS

Elettra Sincrotrone Trieste

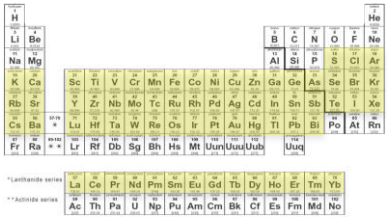
TwinMic
XRF
SYRMEP
IUVS
SISSI
Nano Innovation
Structural Biology
XRD1
XRD2
MCX
Xpress
XAFS



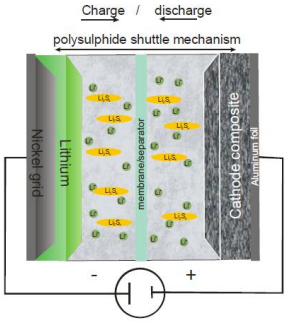
Source
Bending Magnet

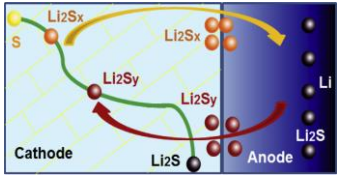
Energy range
2.4-27 keV

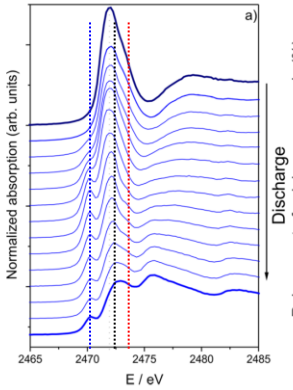
K edges: S - Ag
L edges: Y - Bi

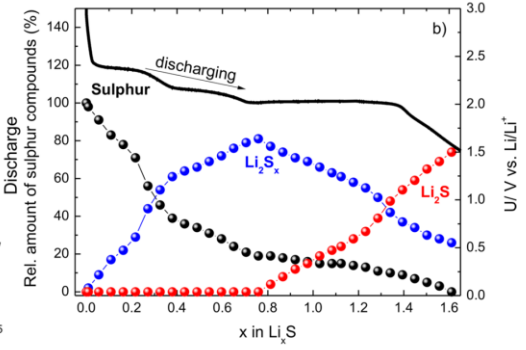


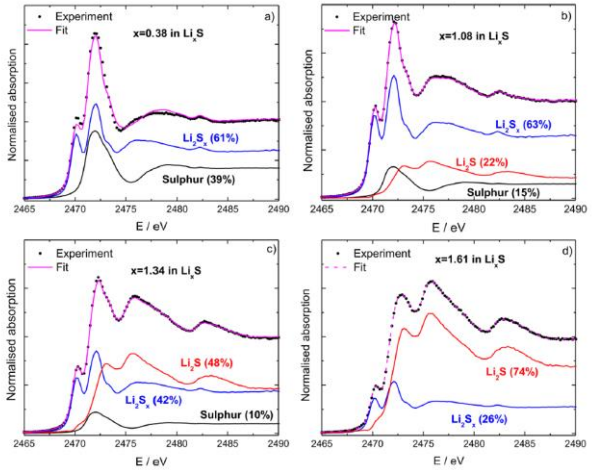
Analytical Detection of Polysulfides in the Presence of Adsorption Additives by Operando X-ray Absorption Spectroscopy











R. Dominko et al., *Phys. Chem C* **119**, 19001 (2015)

Elettra Sincrotrone Trieste

IDEAS
Imaging Diffraction Emission Absorption and Scattering

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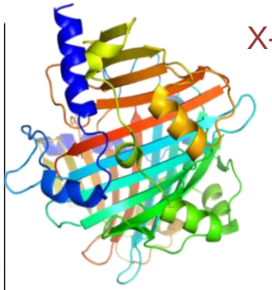
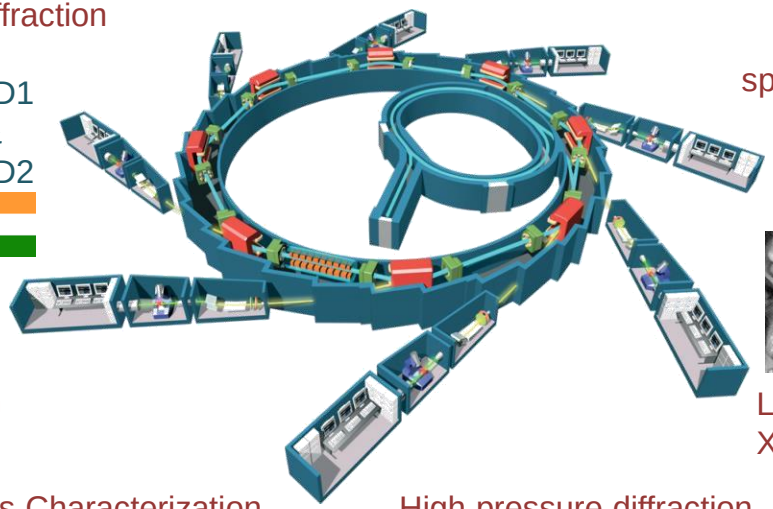
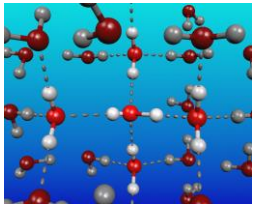


X-ray Diffraction

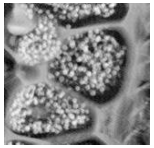
XRD1 & XRD2



IR and Raman spectro-microscopies

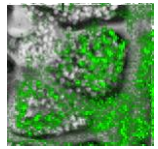


IUVS and SISSI



X-ray Microscopy

TwinMic

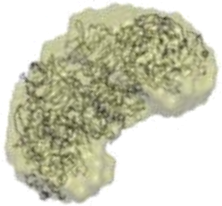


Low Energy X-ray Fluorescence

Small angle X-ray Scattering

SAXS

TU Graz



Materials Characterization by X-ray

High pressure diffraction

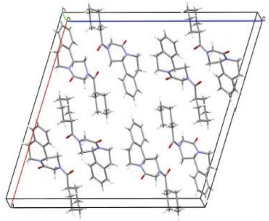
X-ray μ-CT

X-ray Fluorescence

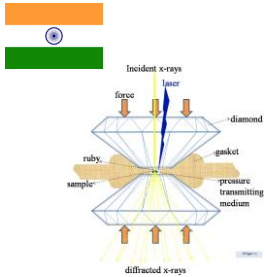
XRF

IAEA

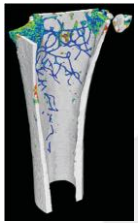
MCX

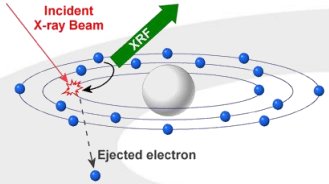


Xpress

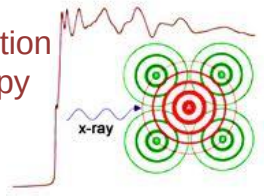


SYRMEP





X-ray Absorption Spectroscopy



XAFS

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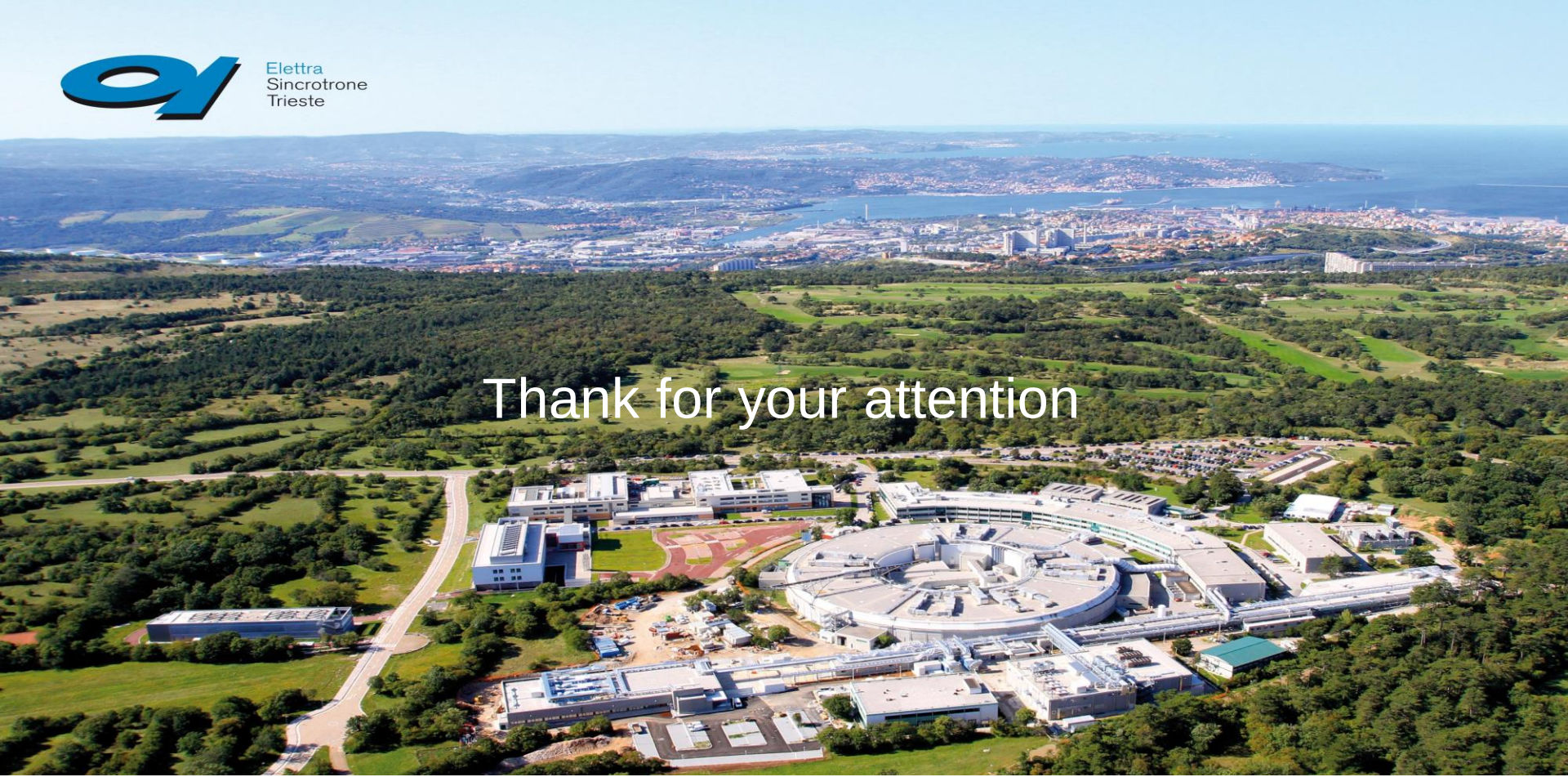
Sincrotrone
Trieste



Thank for your attention

lisa.vaccari@elettra.eu