

National infrastructures in EOISC

Events



National perspective on “horizontal” services, software, and tools developed in Universities, e-infrastructures for the benefits of other communities and larger-scale collaboration

The Structural Biology NRI

Evangelia D. Chrysina

Senior Researcher, Institute of Chemical Biology, National Hellenic Research Foundation

Docent in Medical Science-Biomedicine, Örebro University, Sweden

echrysina@eie.gr

inspired RIs

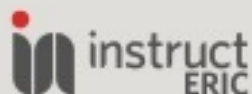
The National Research Infrastructures
on Integrated Structural Biology,
Drug Screening Efforts &
Drug target functional characterization

INSPIRED – MIS 5002550

www.inspired-ris.gr



Affiliated with the pan-European
Research Infrastructure Consortium on
«Integrated Structural Biology, Instruct-ERIC».



inspired RIs



- Supported by:
- 13 Greek Industries, Companies, SMEs, Clusters
 - 4 Large International Companies
 - 10 Greek Academic - Research - Public Organisations
 - 10 European Academic - Research organizations
 - 2 International Academic - Research Organizations
 - 1 ESFRI Research Infrastructures
 - 4 National Research Infrastructures affiliated with ESFRI RIs
 - 4 Regions in Greece

 info@inspired-ris.gr
www.inspired-ris.gr | inspired-ris.catalogue.athenarc.gr

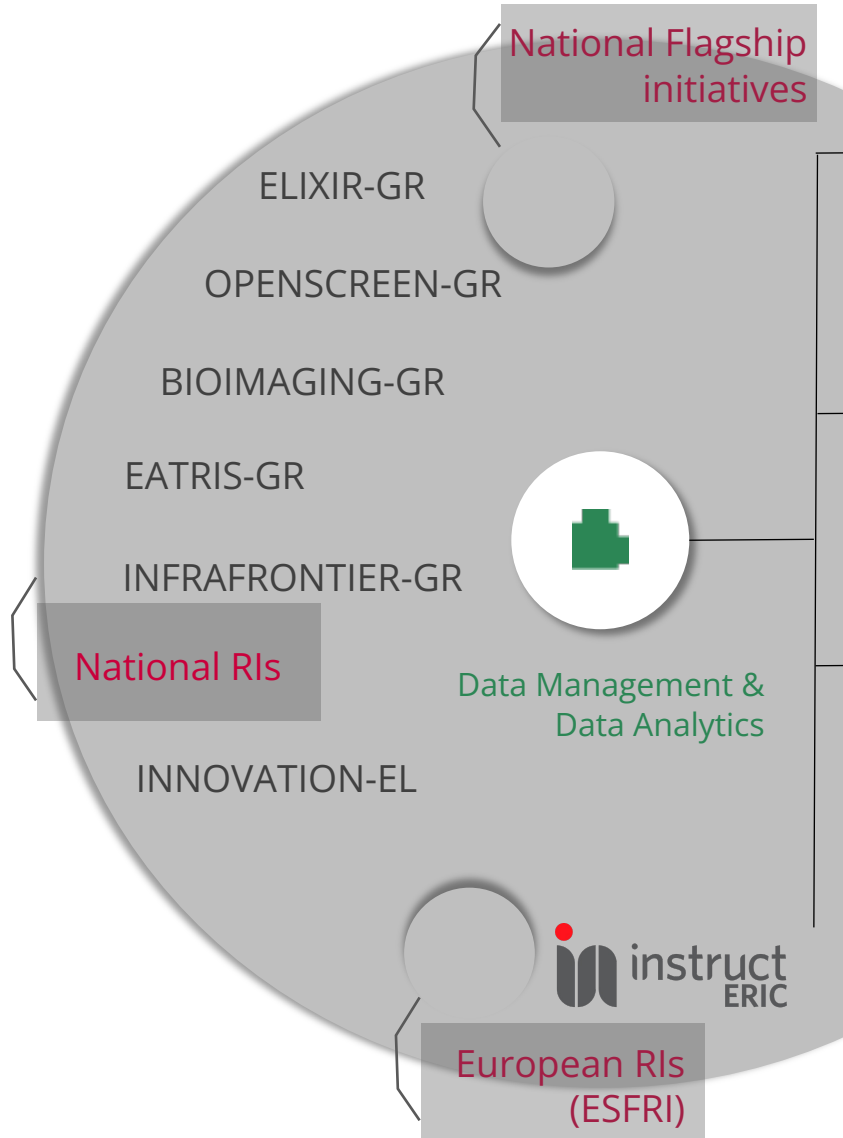








EPA nEK 2014-2020
OPERATIONAL PROGRAMME
COMPETITIVENESS, ENTREPRENEURSHIP, INNOVATION



Co-financed by Greece and the European Union

 Services



-  Protein sample preparation
-  Biophysical studies of macromolecules
-  Structural studies using X-rays (protein crystallography, powder diffraction)
 Structural characterization of pharmaceutical targets using NMR
-  Functional characterization with toxicological / pharmacological studies
 Biomarkers, Pharmacogenomics & Personalized Medicine

- Expertise
- Specialized equipment
- Methods development
- Access to new markets

Targeted Users

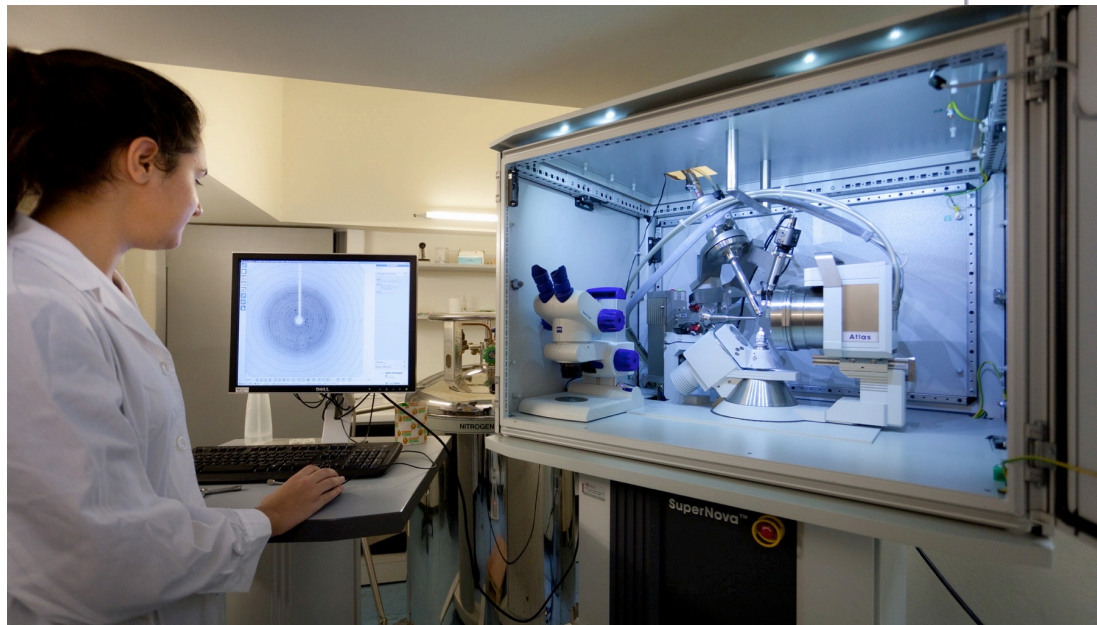
- Industries / Private sector**
 - Pharma Companies
 - SMEs
 - Microbiology Laboratories
- Public Sector**
 - Hospitals
 - Academic Organizations
 - Research Centers
- Young Scientists**
- Interdisciplinary Applications**
 - (Bio)Materials
 - Environmental Sciences
 - Digital Sciences



Proteins in 3D

X-ray sources

In house X-ray protein crystallography facility
"Nikos Oikonomakos" @ NHRF
Instruct-EL hub

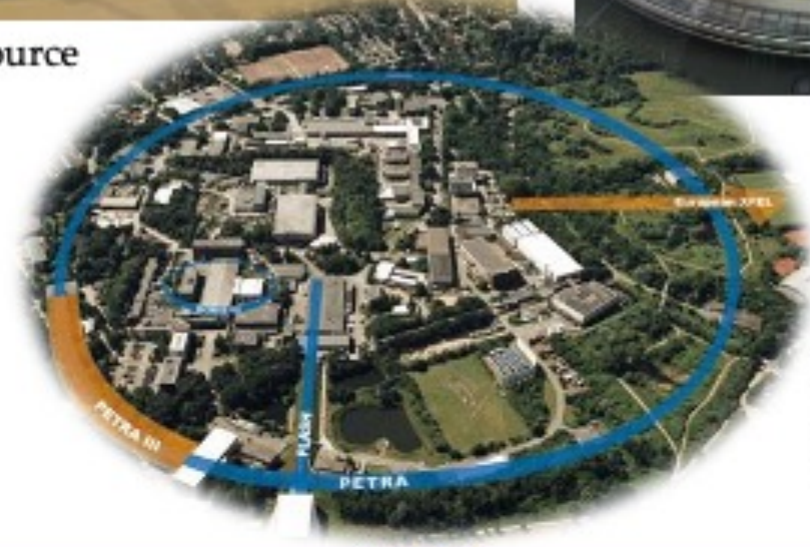


ED Chrysiná - 11.10.2022

Synchrotron Radiation Sources



Diamond Light Source
Oxford, UK



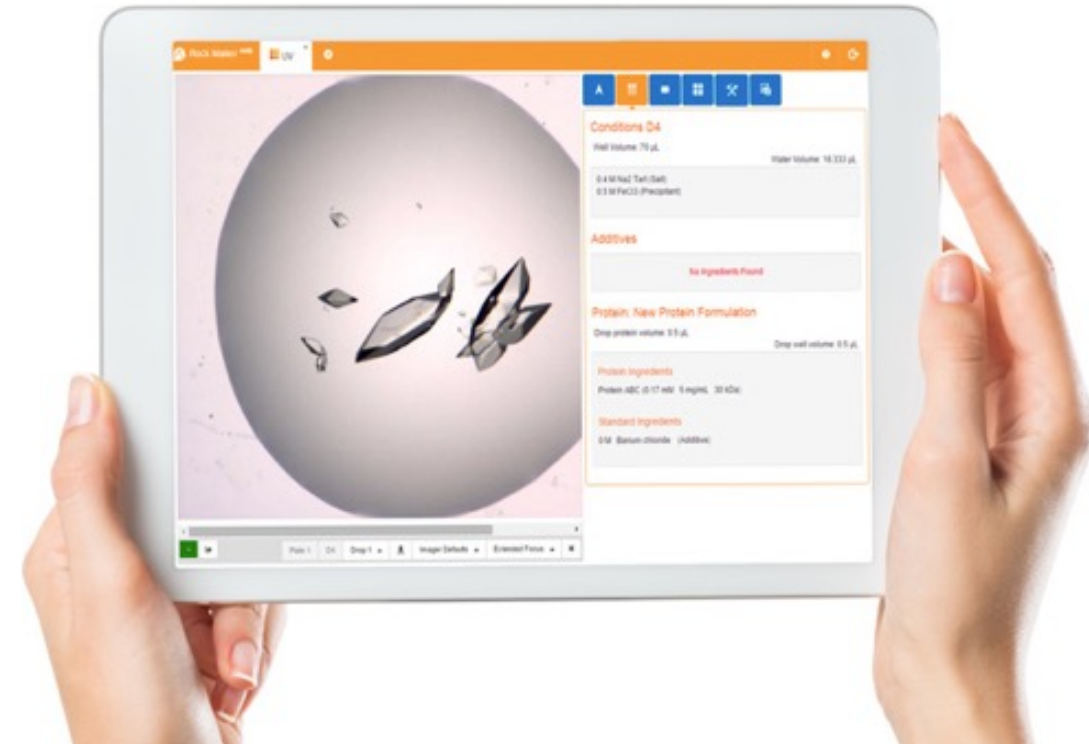
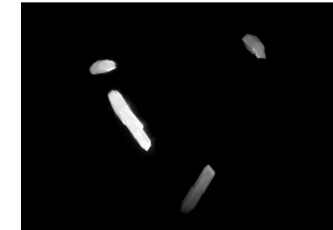
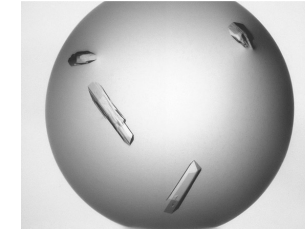
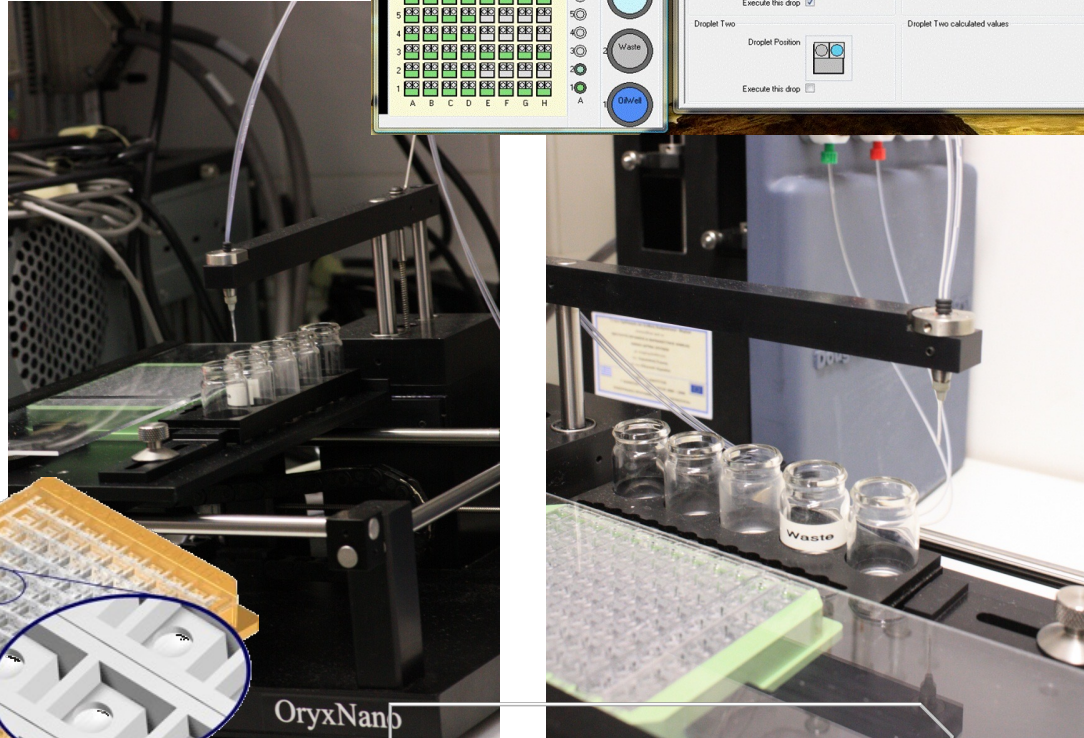
PETRA III
EMBL-Hamburg Uni
Hamburg, Germany

X-ray generator: Oxford Diffraction
Cu K α radiation, $\lambda=1.54 \text{ \AA}$,
Microfocus sealed tube; CCD detector 135 mm;
Cryogenic system with liquid N $_2$

Automated approaches → Numerous DATA

Protein crystallization

High-throughput protein crystallisation robot 3rd generation OryxNano Douglas Instr. Ltd. equipped with stereoscope 160 x Leica MZ16



Our Structural Biology RI



EOSC Future Goals



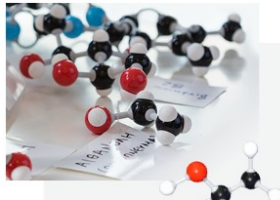
Sample preparation



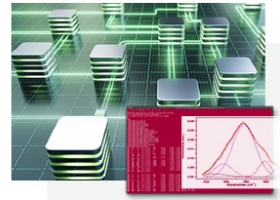
Biophysical characterization



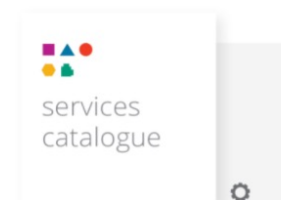
Structural studies



Functional Characterization



Data management & Data analytics



services catalogue

providers

1

Delivering and operating the EOSC-Core, developing and operating key components of the platform and integrating them with a growing set of services to realise EOSC-Exchange

Define

- type of resources
- type of data
- Extent of interoperability required within datasets in the same field and crossdisciplinary

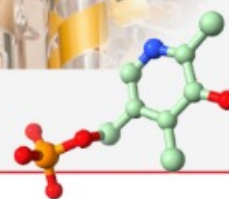


Set the requirements for FAIR infrastructure for 3D data

EOSC core technologies to develop services catalogues



● Structural analysis



Electron Microscopy

Apply

Light microscopy

Apply

In silico structural studies and analyses

Apply

Native Mass Spectrometry

Apply

Small Angle X-ray Scattering (SAXS)

Apply

Solution NMR

Apply

X-ray Diffraction

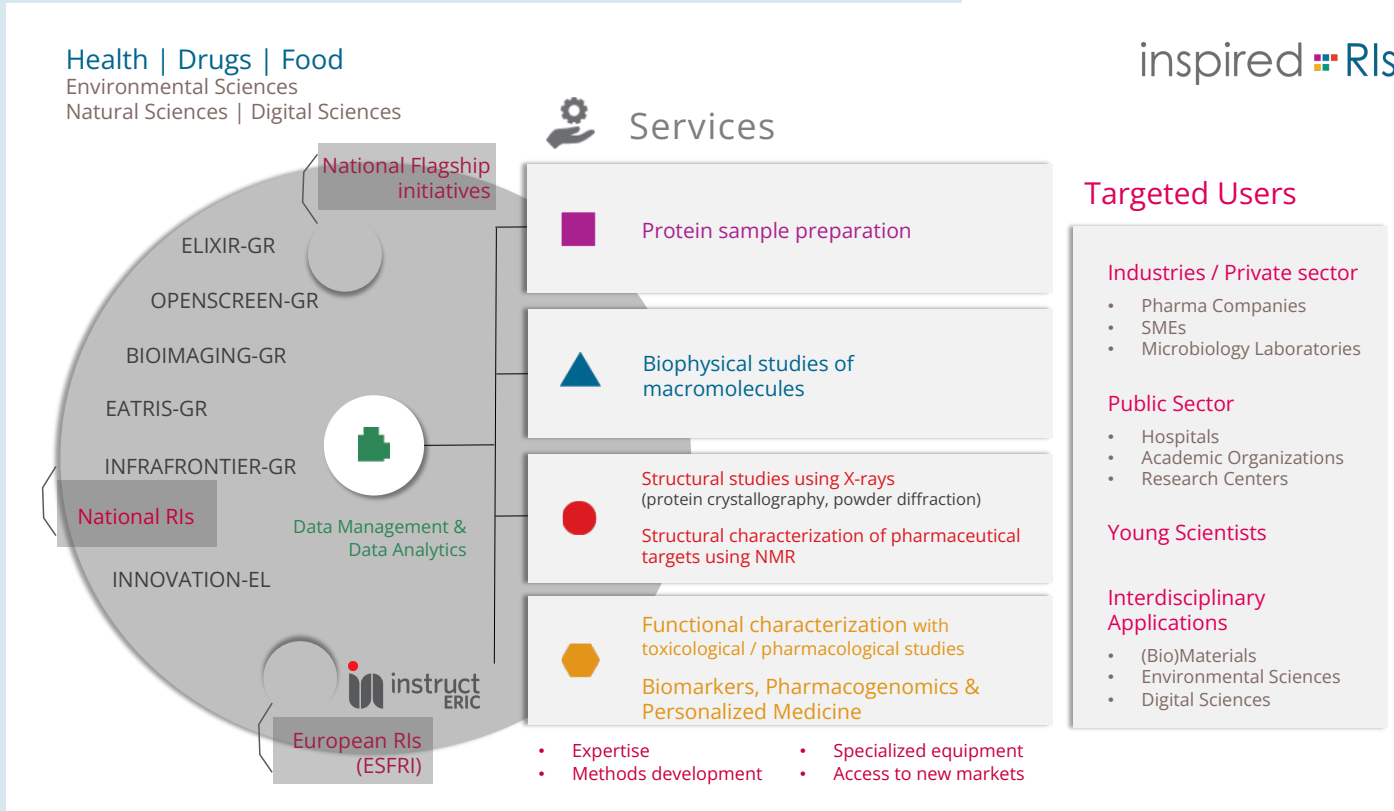
Apply

Use the model of the CatRIs to design and implement the catalogue of services, equipment and expertise for Inspired-RIs.

Our Structural Biology RI



EOSC Future Goals



2

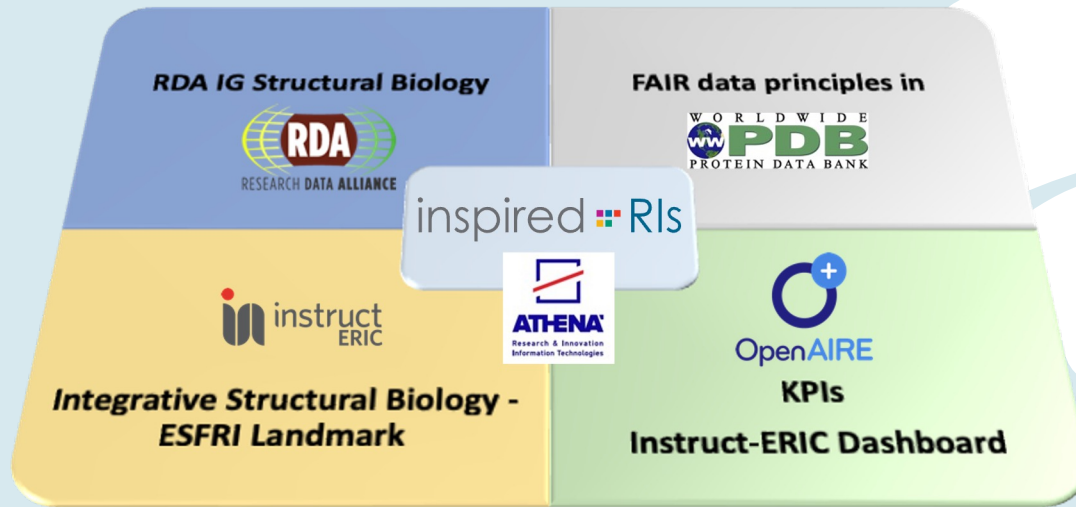
Expanding EOSC-Exchange with resources from across scientific disciplines, delivering common services for scientific workflows and integrating resources from national and pan-European e-infrastructures and research infrastructures

Need to foster cross fertilization between disciplines and the research conducted in RIs



e-Infrastructures already available may develop a cross talk with ESFRI projects

Our Structural Biology RI

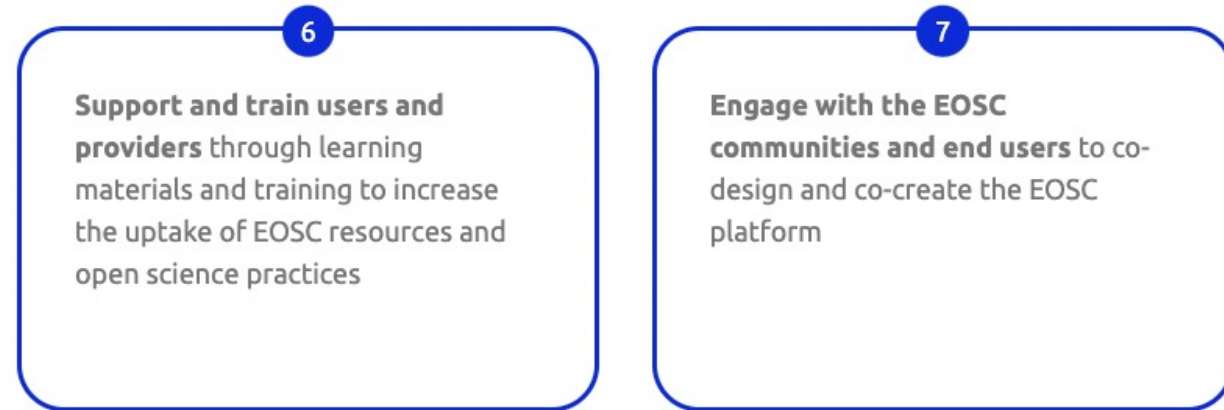


Engagement of our community through :

- open databases for 3D protein structures
- open access publications
- Universal data format
e.g. Crystallographic Information File (CIF) is the standard format for storing crystallographic structural data.
- Structure-based vs EOSC requirements



EOSC Future Goals



- Develop a "vocabulary" for 3D Communities
i.e. work with communities in Structural Bioinformatics (INSTRUCT + ELIXIR)
- Perform a SWOT analysis and inform keystone stakeholders on
 - What has been achieved
 - What are the challenges
 - What does EOSC want to know from RIs and user communities



A dashboard for Inspired-RIs has been prepared.

All research products related to the NRI including

- Publications
- Data
- PDBs
- Other research products

A screenshot of the Inspired RIs dashboard. The top navigation bar includes links for Home, Deposit, Link, Search, About, Develop, and Manage, along with an EU flag. The main heading is "INSPIRED RIs". Below this is a search bar with a "Type" dropdown set to "Research products" and a "Scholarly works" dropdown set to "Search in OpenAIRE". On the right side, there are buttons for "Member" and "Invite users". The main content area shows a "Summary" tab selected, with sub-tabs for "Publications (63)" and "Research data (30)". The text describes INSPIRED as a national research infrastructure in Structural Biology, focusing on bioactive molecules, diagnostics, and pharmacology. It also lists the curators as Thanasis Vergoulis and Evangelia D. Chrysina, and notes it was created on 26-May-2021 with 3 members.



will provide training to Inspired-RIs Partners and Users through

- OpenAIRE National Open Access Desk (NOAD)
- Tools like ARGOS for data management, data infrastructure design

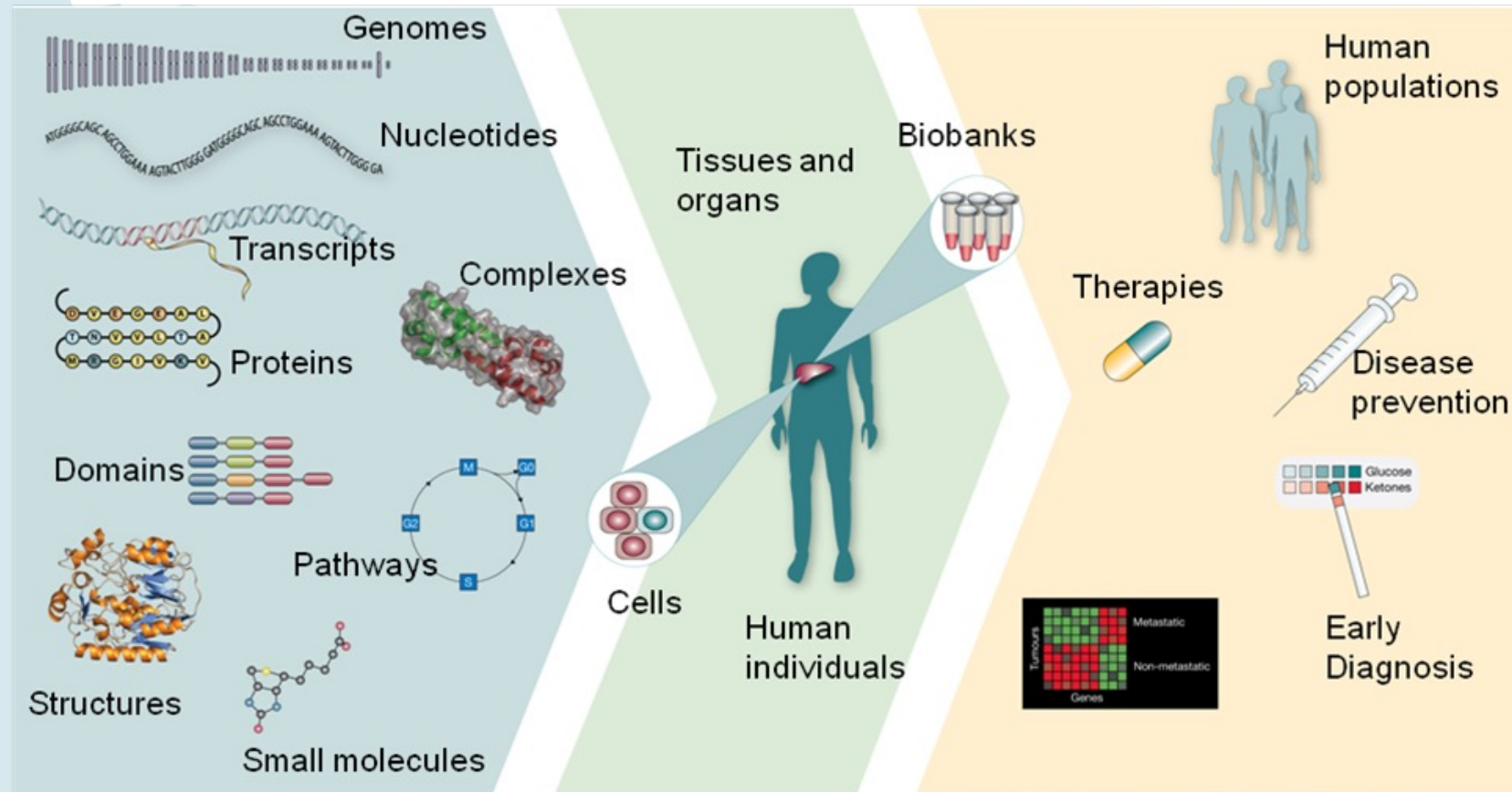
From molecules to medicine

The BMS Research Infrastructures constitute a well coordinated series of facility providing technologies and expertise relevant in the biological, medical, translational and clinical domains."

Molecular components

Integration

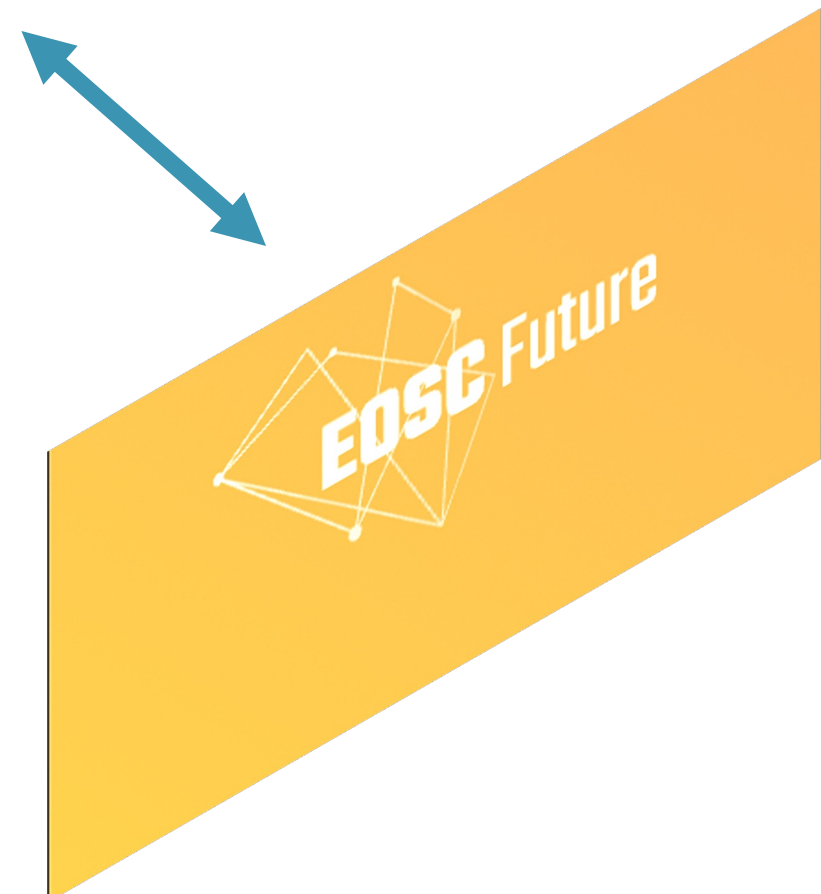
Translation



Committed to
our cause :

Bring structural biology at the forefront of research

Help all people recognize the role it plays in
understanding the mechanisms of life



inspired  RIs

INSTRUCT-EL hub |



ΕΘΝΙΚΟ ΙΔΡΥΜΑ ΕΡΕΥΝΩΝ
National Hellenic Research Foundation

E.D. Chrysinia
Senior Researcher at ICB-NHRF
Docent at Orebro Univ. Sweden
echrysinia@eie.gr