INFRAIA H2020

iNEXT

integrated
NMR
EM
X-rays
Translational research

The Call

- **Research Infrastructures for translating research on biological structures into innovation in biomedicine.** This activity should expand the availability of structural biology services (such as X-ray and neutron scattering, advanced NMR and advanced imaging technologies) to **new communities of users**, and in particular to **scientists with backgrounds other than structural biology**, including from SMEs, to **benefit translational research** in drugs discovery, informed drugs and vaccine design and other fields like biotechnology and biomaterials. Synergies with relevant ESFRI Infrastructures, such as **INSTRUCT**, **EUROBIOIMAGING**, EU-OPENSCREEN, and EATRIS, should be duly exploited.

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The Partnership

- 23 Partners from 14 Countries

- NMR centres
  - Berlin, Brno, Florence, Frankfurt, Lyon, **Utrecht (coordinator)**
- Six synchrotron sites
  - Diamond, EMBL-HH, EMBL-GR, ESRF, MAX IV, Soleil
- Five EM facilities
  - Brno, Diamond, EMBL-HD, Leiden, Madrid
- Protein interactions *in vivo* and *in vitro*
  - **Amsterdam (deputy coordinator)**, EMBL-HD
- Training centres
  - Brno, Budapest, Lisboa, Oulou, Patras, Rehovot
- Research Partners
  - Aarhus, Lund (ESS)

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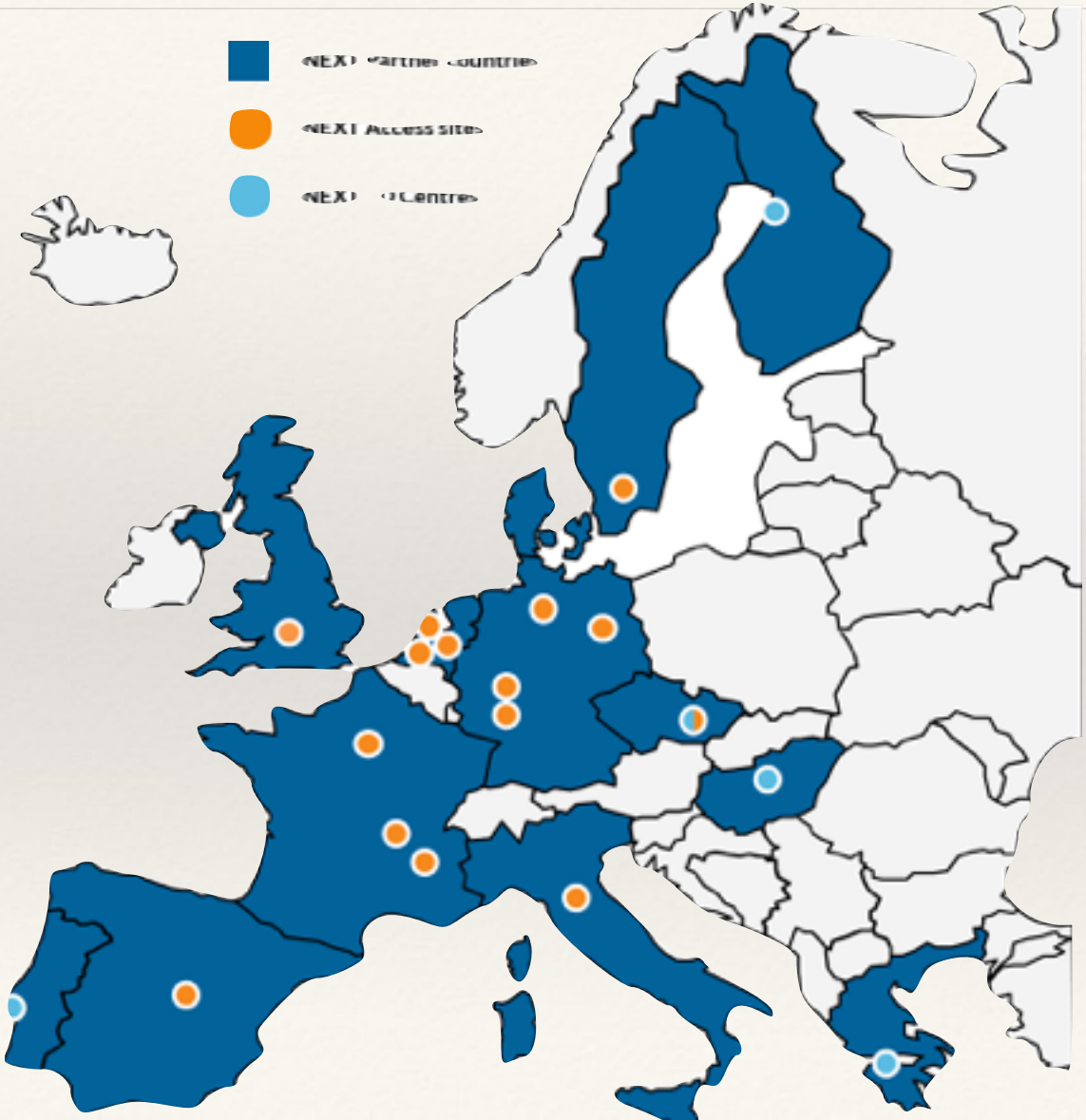
Geographic spread



Aims

- User access to macromolecular X-ray crystallography, solution scattering, NMR, EM and advanced light microscopy.
- Show the possibilities offered by the ESS
- Linking in vitro studies to in-cell interaction studies
- Reach out to industry by collaborative research, networking, trainings and showcasing of new opportunities.

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Three Themes of Access

1. Structural Audit
2. Enhanced Support
3. High-End Data Collection

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Structural Audit

- A sample of a macromolecule (or complex) is evaluated for
  - Purity
  - Stability and aggregation in different buffer formulations
  - Multimeric state by MALLS
  - SAXS data collection for low resolution shape determination
  - Crystallisation
  - NMR HSQC (if labeled)
  - Utility for EM (if >200kD)
- Results are combined in a Structural Audit Report

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Enhanced Support

- Guided access involves training and active participation of guests
- Structure determination by X-ray crystallography, EM, SAXS or NMR
- Ligand and fragment screening
- Study of in vitro or in-cell macromolecular interactions

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High-END: "Traditional" Access

- Synchrotron Data Collection
  - Applications for single translation research theme
  - One or more group leaders under a common team
  - No Biostruct-type BAGS, but research-theme based
- High-field NMR data collection
  - HSQC characterisation required
- Advanced cryo-EM data collection
  - Only if initial data are available to establish grid quality

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Enhanced Support Modalities

- X-ray structural analysis (EMBL-GR/ESRF, EMBL-HH)
- NMR Structure analysis (UU, Florence, Frankfurt)
- EM sample optimisation (EMBL-HD)
- Ligands and Fragment Screening (EMBL-GR, Diamond)
- Macromolecular Interactions Platform (NKI)
- Advanced Light Imaging (EMBL-HD)

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Training

- Integrating X-ray techniques and EM
- Combining X-Rays and Neutrons for Crystallography and Scattering
- Combining solution methods: NMR - SAXS - Biophysics
- Structural biology for drug development
- The toolkit to study macromolecular interactions
- Integrated methodologies and approaches for Structural Biology
- Training centra in Brno, Budapest, Lisboa, Oulou, Patras, Rehovot

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Joint Research Applications

1. Structure-based small molecule inhibitor discovery (ligand screening)
2. Integrated study of membrane proteins.
3. Study of macromolecules and their complexes in cells.

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Networking

- Involving and training new scientific communities and the general public.
- Gateways to industry.
- Strengthening the iNEXT community.
- Data Management and links with e-Infrastructures.

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Website: www.inext-eu.org

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