



MEMORANDUM OF UNDERSTANDING

between

ELIXIR

and

Instruct-ERIC

FY 2024-2029

Preamble

ELIXIR Europe (hereinafter "ELIXIR") is an intergovernmental organisation that as of **October** 2024, brings together life science resources from across its 21 Member States and EMBL and three Observer countries. Legally established as an international organisation, its headquarters are in Hinxton, UK, and Nodes in each participating country. It connects over 200 national institutes that provide a wide range of services to users. These include databases, tools and workflows, registries, interoperability resources, compute, training, and data management support. ELIXIR Europe is represented by its Director Prof. Tim Hubbard.

Instruct-ERIC (hereinafter "Instruct") is a European Research Infrastructure Consortium, a specific legal form that facilitates the establishment and operation of Research Infrastructures with European interest, on a not-for-profit basis. Instruct has 17 Members as of **November** 2024 and is governed by Member representatives in accordance with the ERIC regulation.

Instruct has its statutory seat and Hub located in Oxford, UK. It is represented by its Director Prof. Harald Schwalbe.

Instruct provides open access to cutting-edge structural biology, specifically supporting research that uses integrated approaches and technologies. It prioritises scientific excellence in its services and ensures transparency, equality, and legality in its operations and the research it supports.

Instruct has established a distributed pan-European infrastructure of high-end technologies for integrated structural biology. This recognises the need to set molecular structure in the biological context. Its scope thus includes the traditional techniques of crystallography, NMR, and electron microscopy, but it aims to encourage the integration



of these and other technologies, extending to techniques including cryo-electron tomography, X-ray microscopy, and correlative microscopy. Instruct, through different national Centres, offers access to its infrastructure for academic and industrial researchers and supports this with training programmes and other networking events.

ELIXIR and Instruct are hereinafter jointly referred to as “The Partners” and agree:

- Taking into consideration the importance of ensuring cooperation between European Research Infrastructures, to deepen links between bioinformatics and structural biology research;
- As of October 2024, recognising the joint membership of 13 Member States and EMBL in both organisations, the strengthening of links will support the alignment of activities in areas of mutual scientific and technical interest across Members of both research infrastructures;
- Noting the enormous benefits of emerging applications of Artificial Intelligence (AI) on scientific research, to work together to facilitate access to well curated and structured biological data;
- Given the geographical proximity of both organisations' headquarters, collaboration will be enabled through meetings and information sharing on operational and other matters necessary for the implementation of world class research infrastructures.

Principles

This Memorandum stipulates mutually beneficial areas of collaboration between Instruct and ELIXIR in the areas of bioinformatics and structural biology for the benefit of advancing life science research in Europe.

Scope of collaboration

The Partners identify the following principal areas of shared interest to strengthen joint activities for mutually beneficial cooperation.

1. Increase sustainability and openness of data by collaborating to facilitate easier data deposition and collaboration between Instruct data resources, ELIXIR Core Data Resources, and external data resources of mutual interest, such as EMDB, MPIAR, PRIDE, PDBe, BMRB, SASBDB, CryoET Data Portal and ModelArchive.



Increased FAIRification by linking deposition in these resources to data and metadata available at Instruct research facilities

2. Enhance interoperability and data sharing in structural biology research through the development and promotion of standards for storing and sharing diverse types of data among the research community, especially in areas lacking such resources, such as FRET or circular dichroism,
3. Foster collaboration on AI research, development, and application in structural biology by providing access to analysis services, including the use of AI, for researchers, joint training opportunities, research collaborations, and validation of AI models using Instruct's expertise in experimental methods for structure elucidation by NMR, cryo-EM, crystallography and related biophysical approaches, and ELIXIR's expertise on AI standards and quality reporting such as the Data, Optimization, Model and Evaluation in Machine Learning (DOME-ML).
4. Fostering development of AI ready data repositories in emerging areas like Fragment screening and structure-based drug design.
5. Recognizing the strong emphasis on training within both organisations, the Partners will explore opportunities to develop and share information on joint training initiatives, assessments, and capacity-building activities.
6. Interactions with European Union (EU) initiatives in areas relevant to the Partners, e.g. European Open Science Cloud (EOSC) Nodes, including sharing of information on plans and proposed engagement.
7. To encourage collaborations between the respective ELIXIR and Instruct national nodes where these don't already overlap and where there is a natural complementarity in experimental and data expertise.
8. Information sharing regarding international collaboration, engagement in EU projects, and scientific and socio-economic impact assessment.
9. Collaborate on future joint EU-funded projects to address emerging challenges,, while also ensuring visibility for relevant nationally and internationally-funded joint activities in the areas of proposed collaboration.

Financial Responsibilities

For implementing activities in the proposed areas of mutual interest, ELIXIR and Instruct will, unless otherwise specified, bear any costs of participation of their representatives from their own resources.



Intellectual Property Rights and Confidentiality

Should any intellectual property arise from any collaboration activities, the Partners will deal with this in a separate agreement. The Partners will treat any information that is labelled as such during collaborative activities as confidential.

General terms

In the event that questions arise concerning the interpretation of this Memorandum, the Partners shall consult with each other and find a mutually acceptable consensus.

Each Partner may suggest at any time written modifications to this Memorandum. The Memorandum shall enter into force when it has been signed by both Partners and shall remain valid for five years, i.e. until November 2029.

This Memorandum of Understanding is not a legally binding document and is not intended to constitute, and shall not be construed to create a legally binding agreement between the Partners.

A handwritten signature in black ink, appearing to read "H. Schwalbe", written above a horizontal line.

Signed for Instruct-ERIC: Prof. Harald Schwalbe, Director

Date: November, 2024

A handwritten signature in black ink, appearing to read "T. Hubbard", written above a horizontal line.

Signed for ELIXIR: Prof. Tim Hubbard, Director

Date: November, 2024