Structural bioinformatics is shaping its community

We present an initiative to form an ELIXIR community of structural bioinformaticians in Europe, named 3D-BioInfo, and invite you to participate in the launch meeting on 19 October 2018, where we will start to draft the goals of the community.

Relevance of structural informatics

Structural bioinformatics has a broad impact across the life sciences and provides tools to archive, visualise, analyse, annotate, and predict the structure of biological macromolecules. Furthermore, the science of structural bioinformatics is traditionally very strong in Europe offering many software tools, methodologies, and databases, as well as community-wide prediction challenges. Its applications cover research activities from structural biology to drug discovery and personalized medicine. We envision that establishing an ELIXIR Community will facilitate deeper integration of our broad range of tools and services.

The leading research groups and activities in structural bioinformatics in Europe are already well represented within the ELIXIR nodes (*e.g.* SWISS-MODEL). Several ELIXIR core data resources belong to this field, some of them, such as PDBe and CATH are of fundamental importance. Some of the highly cited ELIXIR tools also belong to the field of structural bioinformatics. The 3D-BioInfo Community is building on this strength and links to several other infrastructures and EC projects. Tools and resources established by the 3D-BioInfo Community have users in the field of structural biology (Instruct, iNEXT), cheminformatics (OpenScreen), system biology (ISBE), and molecular simulations (BioExcel), and these will benefit from collaborative projects with 3D-BioInfo. The 3D-BioInfo initiative will undoubtedly broaden this scope.

ELIXIR and Instruct-ERIC

Instruct-ERIC is a very important collaborator and the 3D-BioInfo Community will coordinate closely with experimental structural biologists. We expect our collaborative projects to help link structural bioinformatic tools with emerging structural techniques, to help relate function to structure. This will attract new users and support the recognition of both ELIXIR and instruct-ERIC services. We expect potential collaborations to involve all five ELIXIR platforms (interoperability, data, tools, compute, training).

Goals of the community

The long term goals of the community include: improving integration of structural information with data on protein function, genomic variants, disease links, and drug action; developing platforms for sharing, and benchmarking software for protein structure prediction, modeling protein assemblies and complexes with various ligands; integrating resources and tools for protein structural and evolutionary analyses; development and integration of various structural biology enabling tools, in close collaboration with Instruct-ERIC.

How to join

If you are interested in participating, come to the launch meeting in Basel, 19 October 2018, to find out more. You will have the opportunity to present a poster and give a flash talk presenting your tools and suggesting how you might contribute to community activities. This meeting will be critical for collecting ideas for community activities, which will be the basis for a formal application to the ELIXIR Heads of Nodes to become an approved community in ELIXIR.

If you would like to give a flash talk (one slide) to advertise a poster at the meeting on a proposed ELIXIR activity (involving collaborations across two or more groups within an ELIXIR node and preferably involving two or more nodes) please send a summary (maximum one page) to c.orengo@ucl.ac.uk outlining the groups and ELIXIR nodes involved and the ELIXIR platforms this activity would relate to i.e. interoperability, data, tools, compute or training. The proposed activity can involve multiple platforms.

Registration site: https://swissmodel.expasy.org/25years/

For information on the timelines for forming an ELIXIR Community in Structural Bioinformatics please see:

https://drive.google.com/file/d/10a5PTWA8b00i7jYeuyOQQ0OXdn-EUoUI/view?usp=sharing

For information on suggested major themes and activities of the 3D-BioInfo Community – please see link below. You are welcome to add comments on additional activities.

https://drive.google.com/file/d/10DYf1uMg9jaHFOGX7gvKsHIAVRRwqyx1/view?usp=sharing