Coordination of structural bioinformatics activities across Europe

Motivation & General Goals
- Structural bioinformatics has a broad impact across the life sciences and provides tools to archive, visualise, analyse, annotate, and predict molecular structures.
- 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 personalised medicine that are all well represented within the national ELIXIR nodes.
- We believe that working together to coordinate the many concurrent activities will help to leverage the vast structural bioinformatics expertise in Europe and thus maximize the impact of structural bioinformatics to the benefit of all researchers in the field and the scientific community at large.
- We therefore propose to establish an ELIXIR Community in Structural Bioinformatics (3DBioInfo) to represent the broad group of activities in this field.

As Interim Executive Committee we are establishing an Interim Steering Committee with a structural bioinformatics representative from each ELIXIR node to capture the interests and activities in each country.

The Steering Committee as well as participants of the kick-off workshop will formulate the goals of the 3DBioInfo Community to form the basis of a formal application to the ELIXIR Heads of Nodes.

A selection of suggested activities

Data and Interoperability
- Develop common ontologies to enable seamless links and promote interoperability between major structural bioinformatics resources across Europe.
- Establish networks of groups predicting, annotating and visualising protein structures and their functions to promote integration of the data.

Tools and Benchmarking
- Establish open platforms for sharing, integrating and benchmarking software tools for modeling protein assemblies and complexes with various ligands (small molecules, nucleic acids, sugars, lipids, and peptides and other proteins).
- Establish open platforms for sharing, integrating and benchmarking software tools for inferring functional sites on proteins.
- Establish open platforms for sharing integrating and benchmarking software tools for inferring impacts of genetic variations on protein structure and function.
- Promote community-wide initiatives for the development of user-friendly bioinformatics and computational tools for modeling conformational flexibility of proteins and nucleic acids.
- Promote community-wide initiatives for the development of user-friendly bioinformatics and computational tools for integrative modelling and for the sharing and deposition of the related data and models, i.e. to communicate better the structure/function relationship of biomacromolecules.
- Develop and integrate tools for statistical analysis, visualization and validation of 3D structures of nucleic acids, sugars and lipids and interface these tools with macromolecular structure refinement and visualization packages.

Training
- Organise workshops concentrating on efficient utilization of offered tools and services.
- Build web based training workflows in the ELIXIR TESS portal for a range of structural bioinformatics activities eg how to obtain predicted structural data for a query protein.
- Organize workshops and hands-on sessions on applications of various Machine Learning and AI tools for the prediction of protein 3D structures, their interactions and functions.

Timeline to form 3DBioInfo
- Fall 2017: first initiative to form the community.
- March 2018: formation of the Interim Executive Committee.
- Establishment of an Interim Steering Committee with a structural bioinformatics representative from each ELIXIR node: – May 2018: email to the ELIXIR Heads of Nodes to nominate representatives.
- End of May 2018: formation of the Interim Steering Committee.
- End of August: Gather ideas from the Interim Steering Committee.
- Summer 2018: Posters at important conferences (ECB 18 Athens, ECM-31 Oviedo), to propagate the idea.
- 19 October 2018: A kick-off workshop for this Community in Basel, Switzerland.
- By the end of 2018: application to the ELIXIR Board to recognize the 3DBioInfo community.
- Beginning of 2019: 3DBioInfo as the official ELIXIR Community. First application for ELIXIR funding.

Interim Executive Committee

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Links with other communities

We plan to link our activities to:
- INSTRUCT - Structural Biology Infrastructure
- ELIXIR Community on proteomics
- ELIXIR Community on Protein Disorder
- ELIXIR Community on Metagenomics
- ELIXIR Community on Bioimaging
- CAPRI, Community-wide challenge / Critical Assessment of Predicted Interactions

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