**First Meeting of the 3D-BioInfo ELIXIR Community in Structural Bioinformatics**

**Organising Committee:** Christine Orengo, Bohdan Schneider, Torsten Schwede, Joel Sussman, Janet Thornton, Sameer Velanakar, Shoshana Wodak.

The Steering Committee of 3D-BioInfo, comprising representatives from 15 European ELIXIR node countries will also be discussing ideas for this meeting and proposing speakers and activities.

**Background**

Structural Bioinformatics has a broad impact across the life sciences and provides tools to archive, visualise, analyse, annotate, and predict molecular structures. 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.

The aim of this meeting is to launch an ELIXIR endorsed 3D-BioInfo Community in Structural Bioinformatics which will form an indispensable interface between the researchers producing the structural data and users of these data. This community will play a valuable role in further improving the validation procedures and interpretation of derived structural data.

Structural bioinformatics impacts a broad range of fields from nanotechnologies studying molecular machines to pharmacology. The impact of these fields depends on reusability and interoperability of the structural data. The tools and services offered by the 3D-BioInfo Community have already many users (millions/year) and the 3D-BioInfo initiative will undoubtedly broaden this scope.

The structural bioinformatics community in Europe includes world leading research groups in the field and activities of structural bioinformatics, which are well represented within the ELIXIR nodes (e.g SWISS-MODEL, SWISS-DOCK). Several ELIXIR **Core Data Resources** belong to this field, some of them, such as PDBe and CATH are of fundamental importance. Some of the most cited ELIXIR tools belong to the field of structural bioinformatics. The 3D-BioInfo Community will bring together leading figures in the field of structural bioinformatics across Europe.

Furthermore, the 3D-BioInfo Community bridges several infrastructures, their providers as well as users, namely the structural biology initiative instruct-ERIC, cheminformatics (OpenScreen), system biology (ISBE), and molecular simulations (BioExcel) as well as the EC project iNEXT. 3DBioInfo community has a tight relation especially to the instruct-ERIC infrastructure.

This meeting is an important step in establishing the 3D-BioInfo ELIXIR Community within ELIXIR as its participants will formulate the purpose of the Community and set its goals and plans for the future. Formal establishment of a Community will allow enable collaborative projects and promote integration of structural bioinformatics data, tools and resources across Europe. We believe that the 3D-BioInfo community will become an important component of European scientific networks.

The launch meeting for the community on **Friday 19th October, in Basel**. This meeting will be critical for collecting ideas for activities, to write a formal application the ELIXIR Heads of nodes to become an approved community in ELIXIR.

**Preliminary Schedule**

***Session times may vary from those shown here, but start and end times of the meeting are fixed.***

***10:00 – 11:10 Session 1: 3D-BioInfo themes and synergies with EU initiatives***

* 10.00 – 10.30: Introduction to ELIXIR Communities and 3D-BioInfo (30 minutes); Brief overview of ELIXIR Communities, and presentation of themes and aims of the 3D-BioInfo Community.
* 10.30 – 10.50: *Invited Speaker (TBA*): Representative from the instruct-ERIC European ESFRI on Structural Biology, highlighting synergies between instruct-ERIC activities and 3D-BioInfo.
* 10.50 – 11.10: *Invited Speaker (TBA)*: Representative from BioExcel, highlighting synergies between BioExcel activities and 3D-BioInfo.

***11.10 – 11.40 Coffee break and posters***

***11.40 – 1.10 Session 2:******Flash talks on suggested 3D-BioInfo activities (Speakers TBA):***

Series of flash talks to present ideas for activities within the 4 major themes of the 3D-BioInfo community. Talks will be organised according to these themes.

***1.10 – 2.15 Lunch and posters***

***2.15 – 3.00 Session 3: 3D-Bioinfo potential Synergies with ELIXIR communities***

Speakers (TBA) from ELIXIR Communities that 3D-BioInfo would seek collaborations with i.e. Communities involved in activities that would benefit from structural data.

**3*.00 – 3.30 Coffee break and posters (30 minutes)***

***3.30 – 5.00 Session 4: 3D-BioInfo activities related to ELIXIR platforms.***

* **Data and Interoperability:** *Dr Sameer Velankar, European Bioinformatics Institute*: Developing common ontologies to increase links and promote interoperability between related structural bioinformatics resources across Europe
* **Tools and compute**: *Speaker TBA*
* **Benchmarking:** *Professor Shoshana Wodak, VIB, Belgium*: Promoting joint initiatives for benchmarking tools and methods for modeling protein 3D structures, protein interactions and conformational ensembles
* **Training platform,** *Speaker TBA*: Training workflows for efficient utilization of offered tools and services.

***5.00-5.30 Wrap up and Discussion of future activities (30 mins)***

* Presentation and discussion of a preliminary draft of the 3D-BioInfo Community whitepaper.