3D Bio Info

Community Annual Meeting

Tuesday 24th, Wednesday 25th, Thursday 26th, November 2020
Venue: Online

The meeting will start at 1200 (GMT) on Tuesday 24th and end at 1600 (GMT) on Thursday 26th.

WEB LINK

ELIXIR Community in Structural Bioinformatics – 3DBioInfo

ELIXIR Communities enable the participation of communities of practice in different areas of the life sciences in the activities of ELIXIR, which underpin the evolution of a data, tools, interoperability, compute and training infrastructure for European life science informatics (see www.elixir-europe.org/use-cases).

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

The meeting will be virtual this year due to the COVID-19 pandemic.
Submission of abstracts for posters is encouraged, as researchers with accepted posters will be offered the opportunity to pre-record short talks for their poster. Authors of selected poster talks will be invited to give longer talks during the main meeting sessions.

To find out more about the 3D-BioInfo Community, please go to the website:

- www.elixir-europe.org/communities/3d-bioinfo

Overview of Programme

The meeting will start with a brief overview of the aims of the 3DBioInfo Community. This will be followed by **Breakout sessions** for each of the major 3D-BioInfo Activities described below. These breakout sessions will be held sequentially, allowing participants to attend any number of sessions they want. Next will come a **Plenary session**, at which coordinators of the different **Activities** will present their reports.

All the sessions and talks will be recorded, with the recordings made available at later dates.

Call for Abstracts

- 500 words maximum – for short talks relating to Activities 1–5.
- Please specify which activity you want the abstract considered for in the Subject Line of the email.
- **Oct 1 deadline for abstracts.**
  Please send to Christine Orengo at c.orengo@ucl.ac.uk

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Programme

Activity I

FAIR access to experimental and predicted 3D models and associated structural and functional annotations

Coordinator: Sameer Velankar

1. Update on PDBe-KB – new resources/infrastructure/plans.
2. Report from the survey on existing visualisations used to display annotations and structures.
3. 3D-Beacons – use cases and prototype implementation.
4. 3D-Beacons – structure quality and future plans.
5. Discussion on 3D-Beacons.
6. New data resource presentations who want to contribute to PDBe-KB – based on abstract.

Activity 2

Open resources for sharing, integrating and benchmarking software tools for modelling the proteome in 3D

Coordinator: Shoshana Wodak

- Introduction: Activity 2 implementation study, current status.

1. The benchmark dataset
   - Presentations on the first version of benchmark dataset of predicted *'physiological and non-physiological'* protein assemblies.
   - Discussion on the Benchmark dataset.
2. The benchmarked tools and analysis
   - Presentations of tools for evaluating and predicting interfaces of biological assemblies.
   - New tools of groups interested in participating, based on Abstracts.
   - Discussion on how to analyse and compare results from different methods.

Activity3

Protein-ligand interactions

Coordinator: Vincent Zoete

1. Identify, review and evaluate tools, resources and databases available for curation of a large-scale fundamental-research centric benchmark set of ligand-biomacromolecule complexes, along with ligand and protein annotations.
2. Discuss strategies for creating the benchmark, as well as organise, store and distribute the data, and a plan to achieve this with limited resources.

Activity 4

Tools to Describe, Analyse, Annotate, and Predict Nucleic Acid (NA) Structures

Coordinator: Bohdan Schneider

1. RNA structure predictions: tools for NA structure determination and annotation.
2. Reporting the results of the taskforce reviewing the NA valence geometry dictionaries and their implementation.
3. Selected talks from submitted abstracts.

Activity 5

Protein Engineering

Coordinator: Lynne Regan

1. Discussion of scope of the Protein Engineering Activity.
2. Discussion of resources currently available.
3. Discussion of the new Protein Engineering and Design section of BioStudies.
4. Short presentations by individuals interested in contributing to the Protein Engineering and Design activity (in any way) – selected based on abstracts.
5. Wrap up discussions and plans going forward.