About us 📥 Training **Q**Search 🖶 EMBL-EBI 🕅 Research Services Training Train at EMBL-EBI Train outside EMBL-EBI Webinars Overview Train online Also in this section About Structural bioinformatics (Virtual) E 7 Date: Monday 23 - Friday 27 November 2020  $\times$ ĿЧ Virtual St Mary and <u>St. John</u> FMBL-EBI, Hinxton, Venue: Virtual - EMBL-EBI, Hinxton, CB10 1SD, United Kingdom Church, Hin CB10 1SD, United Application opens: Monday 13 July 2020 Kingdom Application deadline: Friday 02 October 2020 (https://www.google.co /maps?g=Virtual+EMB Participation: Open application with selection EBI, +Hinxton, +CB10+ Contact: Meredith Willmott (mailto:meredith@ebi.ac.uk) Registration fee: £200.00 **Registration closed** Wellcome

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Dates additional information: Please note this course will take place virtually.

# **Overview**

Structural biology, determining the three-dimensional shapes of biomacromolecules and their complexes, can tell us a lot about how these molecules function and the roles they play within a cell. Data derived from



structure determination experiments enables life-science researchers to address a wide variety of questions.

This course explores bioinformatics data resources and tools for the investigation, analysis, and interpretation of biomacromolecular structures. It will focus on how best to analyse and interpret available structural data to gain useful information given specific research contexts. The course content will also cover predicting protein structure and function, and exploring interactions with other macromolecules as well as with low-MW compounds.

This course will be a virtual event delivered via a mixture of live-streamed sessions, pre-recorded lectures, and tutorials with live support. We will be using <u>Zoom (https://zoom.us/)</u> to run the live stream sessions (all fully password protected) with support provided by <u>Slack (https://slack.com/intl/en-gb/)</u>. In order to make the most out of the course, you should make sure to have a stable internet connection throughout the week. There will also be networking and short social activities throughout the course.

Selected participants will be sent materials prior to the course. These might include pre-recorded talks and required reading or online training that will be essential to fully understand the course.

### Audience

This course is aimed at wet-lab scientists generating structural data or scientists utilising structural data in their analysis and/or interpretation. No previous experience in the field of structural bioinformatics is required, however a basic knowledge of protein structure would be of benefit.

#### Prerequisites

A working knowledge of the Linux operating system and ability to use the command line would be a benefit but is not mandatory.

### Syllabus, tools and resources

During this course you will learn about:

 Public repositories of structural data: Protein Data Bank (PDB) and Electron Microscopy Data Bank (EMDB), and tools to search and analyse information in these repositories from <u>PDBe (Protein Data Bank</u> <u>in Europe) (//www.ebi.ac.uk/pdbe/)</u> including <u>PDBe-KB (//www.ebi.ac.uk/pdbe/pdbe-kb)</u>

# How to apply

Please read our page on <u>application advice</u> (//www.ebi.ac.uk/training/handson /<u>application</u>) before starting your application. In order to be considered for a place on this course, you must do the following:

- Complete the online application form providing answers as directed
- Ensure you add relevant information to the "Application submission" section where you are asked to provide three 100-word paragraphs that cover your:
  - scientific biography
  - work history
  - current research interests
- Upload a letter of support from your supervisor or a senior colleague detailing reasons why you should be selected for the course

Please submit all documents during the application process by midnight on Friday 02nd October 2020.

Incomplete applications will not be considered.

All applicants will be informed of the status of their application (successful, waiting list, rejected) by Friday 16th October 2020. If you have any questions regarding the application process please contact Meredith Willmott (<u>Meredith@ebi.ac.uk</u> European Bioinformatics Institute

- UniProt (https://www.uniprot.org/) and basic Sequence alignment tools (//www.ebi.ac.uk/Tools/msa/)
- Protein structure analysis and classification: <u>HMMER (//www.ebi.ac.uk/Tools/hmmer/)</u>, <u>InterPro</u> (//www.ebi.ac.uk/interpro/), <u>Pfam (https://pfam.xfam.org/)</u>, <u>CATH (http://www.cathdb.info/)</u>, <u>PDBeFold (//www.ebi.ac.uk/msd-srv/ssm/)</u>, <u>PDBePISA (//www.ebi.ac.uk/msd-srv/prot\_int/pistart.html)</u>
- Protein structure prediction and docking: <u>PHYRE2 (http://www.sbg.bio.ic.ac.uk/~phyre2</u> /<u>html/page.cgi?id=index</u>) and <u>HADDOCK (https://haddock.science.uu.nl/services/HADDOCK2.2/)</u>
- Structure validation and assessment tools and strategies
- Tools and resources for drug discovery: ChEMBL (//www.ebi.ac.uk/chembl/)

# Outcomes

After this course you should be able to:

- Access and browse a range of structural data repositories
- Determine whether appropriate structural information exists about a given small molecule, macromolecule or complex, applying available structure-quality information
- Build a structural model for a protein which has a structurally characterised relative and evaluate its quality
- Predict the function of a protein based on sequence and structure data
- Explore protein-complex modeling approaches

# Additional information

All participants are expected to virtually present a poster during the course. We expect the posters to provide other delegates and trainers with information on your research and will act as a talking point. They should give an idea of the work you are engaged in, what you are planning to do next, and anything of interest that might be useful for sharing. When preparing the poster keep in mind that other participants will view it on a computer screen. make it concise, clear, and avoid small images. Further information regarding poster presentations will be provided after the deadline.

# Programme

This course will be delivered as a mixture of live-streamed sessions, pre recorded lectures, and practicals, which you will work through at your pace with live trainer support. The format will provide you with some

https://www.ebi.ac.uk/training/events/2020/structural-bioinformatics-virtual

(mailto:Meredith@ebi.ac.uk))

#### Application deadline

02 October 2020

Registration closed

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### Organisers

Piraveen Gopalasingam - EMBL-EBI, UK

David Armstrong - EMBL-EBI

Gerard Kleywegt

Christine Orengo - University College London, UK

# Trainers

David Armstrong - EMBL-EBI, UK

Christine Orengo - University College London, UK

Piraveen Gopalasingam - EMBL-EBI, UK

Gerard Kleywegt - EMBL-EBI, UK

Rossana Zaru - EMBL-EBI, UK

Fabio Madeira - EMBL-EBI, UK

European Bioinformatics Institute

flexibility in each day and you will not be expected to attend a live session for the whole day. However, in order to gain the most from this virtual course, we recommend that you make yourself available for the full course as if you were attending an onsite course. We ask you to be available between the hours of 09:00 - 17:00 GMT (UTC+0) each course day.

- Day 1 Introductory talks and activities
- Day 2 Sequences, folds, and families
- Day 3 Working with existing structural data
- Day 4 Structure prediction and docking
- Day 5 Aggregated and small molecule data

#### EMBL-EBI Training is part of the ELIXIR infrastructure

The EMBL-EBI Training Programme contributes to the ELIXIR Training Platform. Learn more > (https://www.elixir-europe.org/platforms/training)

https://www.ebi.ac.uk/training/events/2020/structural-bioinformatics-virtual

Alexandre Bonvin - Utrecht University

Lawrence Kelley - Imperial College London

Michael Sternberg - Imperial College London, UK

Anna Gaulton - EMBL-EBI, UK

Typhaine Paysan-Lafosse - EMBL-EBI, UK

Osman Salih - EMBL-EBI, UK

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