









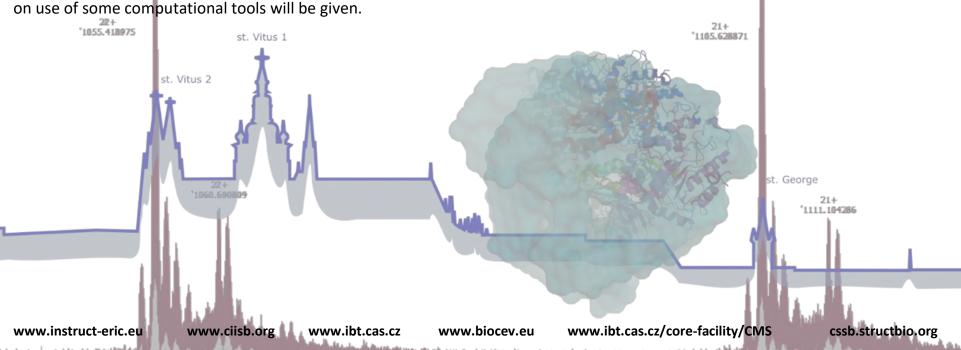
# Instruct-ERIC workshop

# **Computational Approaches in Integration of Structural Biology Techniques**

**Dates:** October 8 – 10, 2019

Venue: Institute of Biotechnology of the Czech Academy of Sciences, Research centre Biocev, Prumyslova 595, 25250 Vestec near Prague, Czech Republic

Aim: The course will be focused on the growing need to combine computational tools in structural biology projects. The main aims are in providing deeper insights in the computational approaches for selected techniques and then to build on the good foundations and cover also integration of data coming from various structural approaches, e.g. mass spec, NMR and other restraints used in structural analysis, together with SAXS envelopes and cryoEM maps applied in and with crystallographic analysis, use of biophysics to enhance/help in structure analysis, etc. Practical experience with selected structural biology techniques will be provided and tutorials













## **Preliminary programme:**

### October 8

Morning: Overview of selected structural biology techniques, covering SAXS, SANS, diffraction, structural mass spec, CryoEM, macromolecular docking, computational tools for integration of structural data and some biophysical techniques.

Afternoon: Tutorials at instruments in IBT CMS – SAXS, diffraction, biophysics, structural mass spec.

### October 9

Morning: Lectures on data integration, examples, user cases - lessons and know how to learn.

Afternoon: 3 workshops on data processing and interpretation, cross-techniques, combinations of information from individual techniques (participants' laptops, a few computers will be provided by the organizers)

#### October 10

Morning: Lectures on bioinformatics, validation and data presentation.

Afternoon: Computational workshops on macromolecular docking (HADDOCK/DisVis), Integrative structural determination (IMP) and other.

## **Confirmed speakers/tutors:**

Haydyn Mertens (EMBL Hamburg); Daniel Nemecek (Thermofisher Scientific); Jorge Roel (Bonvin lab, Utrecht University); Ignacia Echeverria (Sali lab, UCSF); Pavel Plevka (CEITEC Masaryk University, Brno); Stuart McNicholas (University of York), Nikolay V. Dokholyan (Penn State College of Medicine), Charlotte Uetrecht (Leibniz Institute for Experimental Virology, Hamburg).

Costs: The workshop programme, accommodation (4 nights maximum, 7-11 October) and meals during the workshop are covered by Instruct-ERIC and IBT for all selected and registered participants. Workshop participants are asked to arrange and pay for their own travel and also for subsistence before and after the workshop. The program schedule will start in the morning of October 8 and the close of the workshop is planned on October 10, around 4 p.m. A special workshop dinner is planned on October 9 in Villa Lanna in Prague.

To apply: Contact Jan Dohnálek (jan.dohnalek@ibt.cas.cz) or Magdalena Schneiderová (magdalena.schneiderova@ibt.cas.cz) with a brief professional CV (maximum 2 pages), a motivation letter, and one letter of recommendation from a supervisor or a senior scientist.

**Application deadline:** July 12, 2019

For more information see ibt.cas.cz

cssb.structbio.org www.ibt.cas.cz/core-facility/CMS www.instruct-eric.eu www.ciisb.org www.ibt.cas.cz www.biocev.eu