

Instruct-ERIC workshop

Talks, 8th October 2019 (Tuesday morning)

- ~ 8:30 Arrival, coffee, instructions, meeting others
- 9:00-9:10 **Welcome, Overview of structural biology techniques and opportunities in Biocev**
Jan Dohnalek, IBT Biocev
- 9:10-9:30 **3D-Bioinfo: ELIXIR initiative in structural bioinformatics and its integration into structural biology**
Bohdan Schneider, IBT Biocev
- 9:30-9:50 **Diffraction techniques - focus on data processing and computational aspects**
Jan Stransky, IBT Biocev
- 9:50-10:20 **Constraint-driven protein structure modelling**
Nikolay V. Dokholyan, Penn State College of Medicine
- 10:20-10:40 **Biophysical techniques for the structural and functional biomolecules characterisation**
Tatsiana Charnavets, IBT Biocev
- 10:40-11:00 Coffee break w. snack
- 11:00-11:30 **CryoEM - update and focus on computational approaches**
Daniel Nemecek, Thermofisher
- 11:30-12:00 **CryoEM model building and other tools in Phenix**
Dorothee Liebschner, LBNL Berkeley
- 12:00-12:30 **Macromolecular docking, HADDOCK and related, applications**
Jorge Roel, Bonvin lab, Utrecht University
- 12:30-13:00 **Computational tools for integration of structural data**
Ignacia Echeverria, Sali lab, UCSF San Francisco

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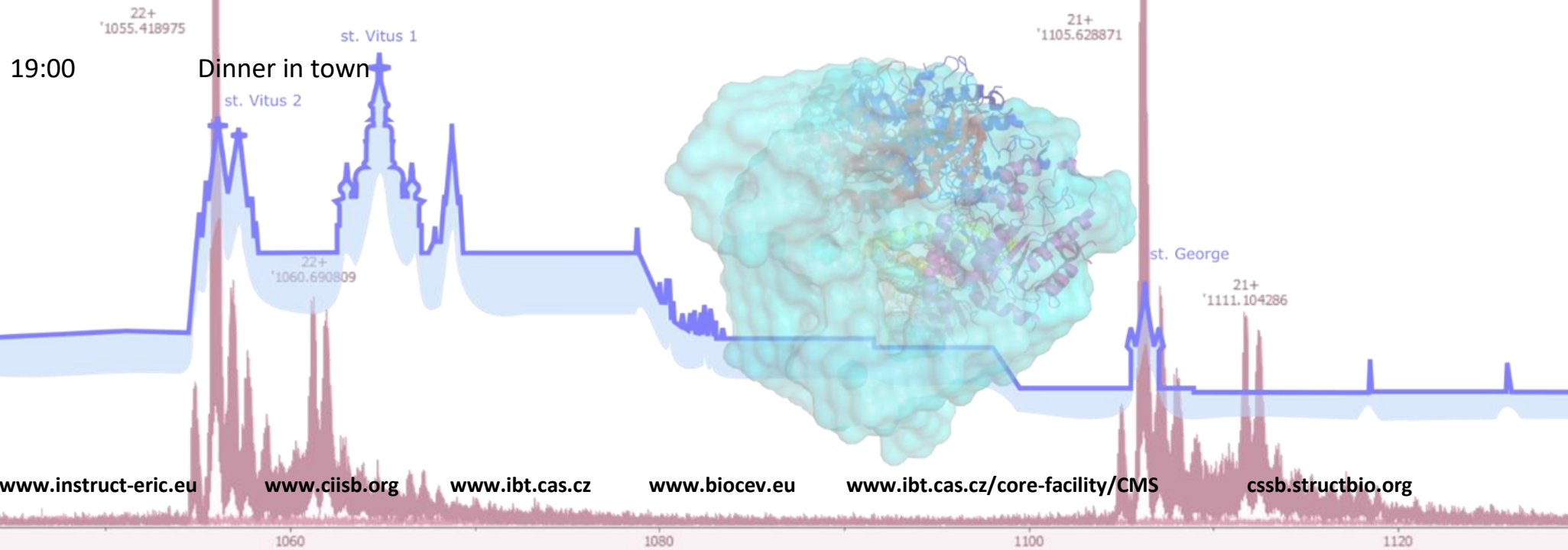


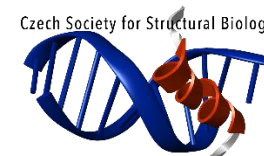
13:00-14:00 Lunch (local canteen)

Introduction to experimental techniques 8th October (Tuesday afternoon)

14:00-14:45	Group 1 Mass spectrometry	Group 2 Biophysics	Group 3 X-ray diffraction	Group 4 Small Angle X-ray Scattering
14:45-15:30	Biophysics	X-ray diffraction	Small Angle X-ray Scattering	Mass spectrometry
15:30-16:00	Coffee break w. snack			
16:00-16:45	X-ray diffraction	Small Angle X-ray Scattering	Mass spectrometry	Biophysics
16:45-17:30	Small Angle X-ray Scattering	Mass spectrometry	Biophysics	X-ray diffraction

Tutorials on individual techniques at instruments (CMS Biocev). Participants divided into 4 groups





Instruct-ERIC workshop

Talks, 9th October 2019 (Wednesday morning)

- ~ 8:30 Arrival, coffee
- 9:00-10:00 **Structure and mechanism of DNA delivery of gene transfer agent studied by cryo-EM**
Pavel Plevka, CEITEC MU
- 10:00-10:30 **Integrative approach for structural analysis of flexible protein complexes**
Evzen Boura, IOCB Prague
- 10:30-10:50 **A glimpse into the structure-function relationship of the mysterious RNA polymerase effector – HelD**
Tomas Koval, IBT Biocev

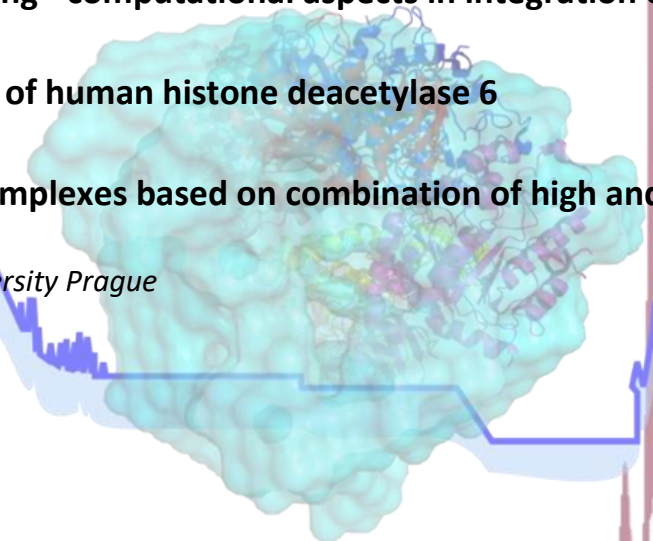
10:50-11:10 Coffee break w. snack

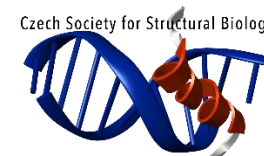
11:10-11:40 **Small angle X-ray and neutron scattering - computational aspects in integration of structural data**
Haydyn Mertens, EMBL Hamburg

11:40-12:10 **Integrative structural characterization of human histone deacetylase 6**
Cyril Barinka, IBT Biocev

12:10-12:40 **Structural biology of 14-3-3 protein complexes based on combination of high and low resolution approaches**
Tomas Obsil, Faculty of Science, Charles University Prague

12:40-13:30 Lunch





Computational workshops
9th October (Wednesday afternoon)

13:30-14:45 **Data processing and interpretation: X-ray – CryoEM**

Dorothee Lieschner, LBNL Berkley

14:45-15:00 Coffee break

15:00-16:15 **Data processing and interpretation: SAXS - X-ray - CryoEM**

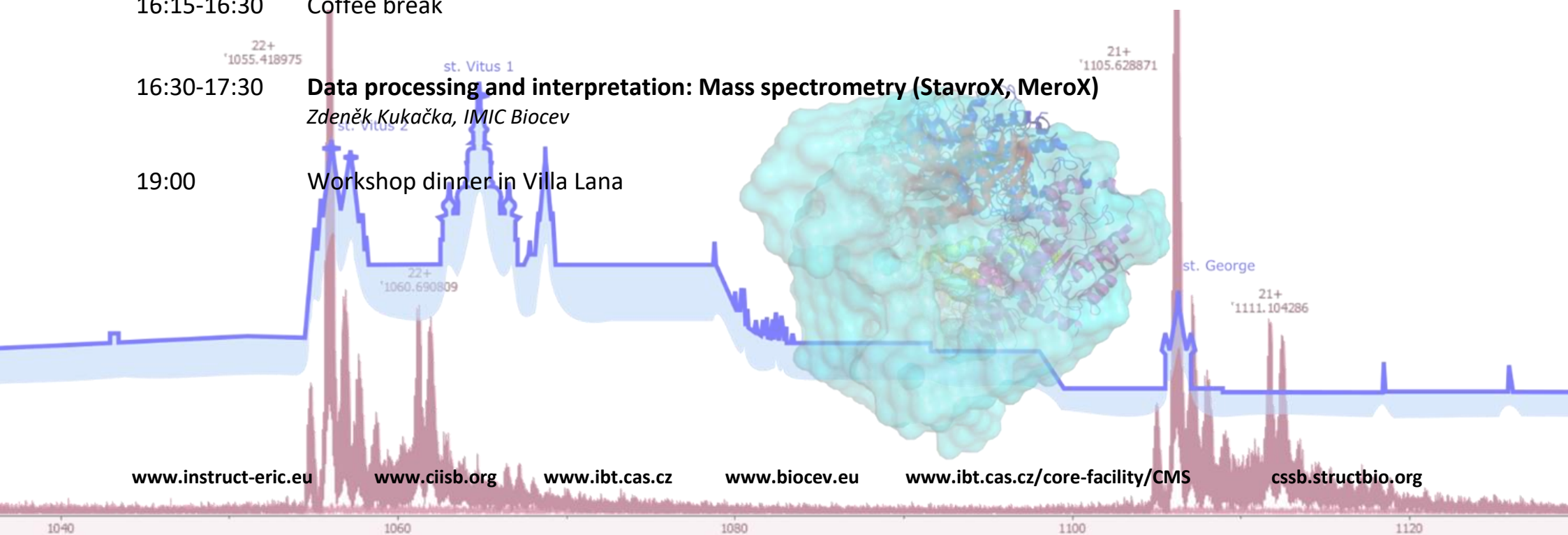
Haydyn Mertens, EMBL Hamburg

16:15-16:30 Coffee break

16:30-17:30 **Data processing and interpretation: Mass spectrometry (StavroX, MeroX)**

Zdeněk Kučačka, IMIC Biocev

19:00 Workshop dinner in Villa Lana

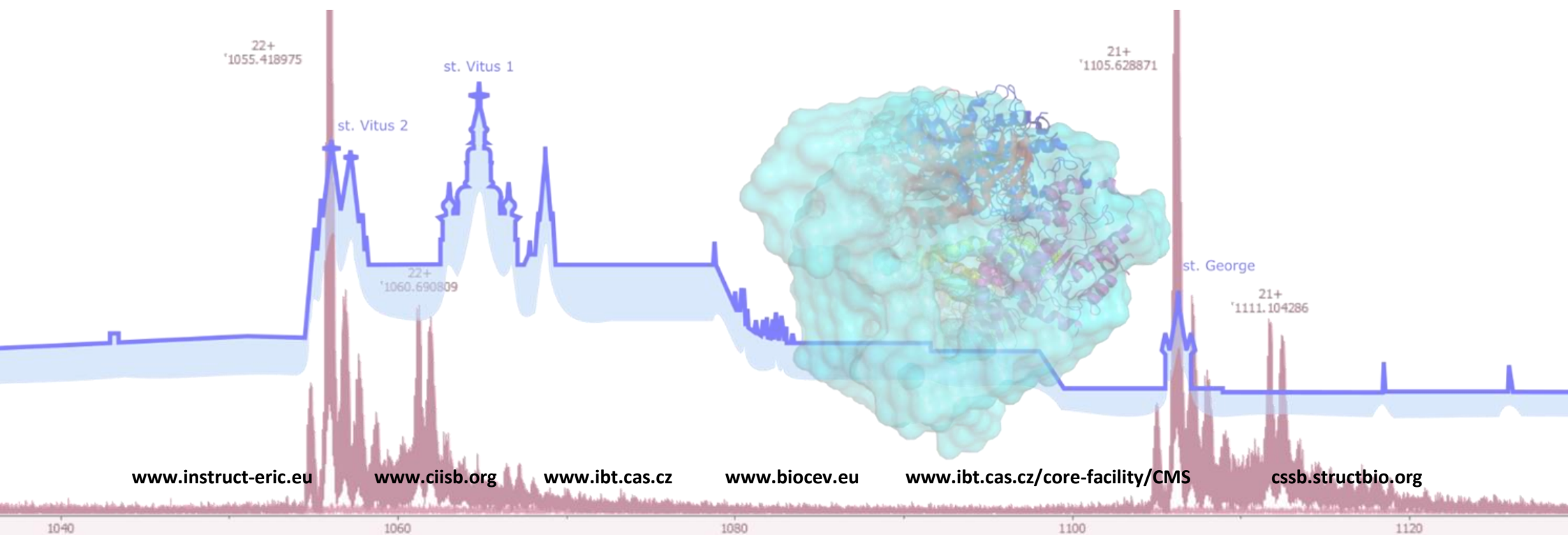




Instruct-ERIC workshop

Talks, 10th October 2019 (Thursday morning)

- ~ 9:00 Arrival, coffee
- 9:15-10:00 **Native MS in biophysical and structural characterization of protein complex**
Charlotte Uetrecht, Leibniz Institute for Experimental Virology, Hamburg
- 10:00-10:30 **CCP4MG for analysis and presentation of structural results**
Stuart McNicholas, University of York
- 10:30-11:00 Coffee break



Computational workshops
10th October (Thursday)

11:00-12:30 **HADDOCK/DISVIS tutorial**
Jorge Roel, Bonvin lab, Utrecht University

12:30-14:00 Lunch, coffee and goodies

14:00-15:30 *Parallel workshops*

A. CCP4MG for analysis and presentation of structural results

Stuart McNicholas, University of York

B. Integrative structural determination using IMP: Applications and examples

Ignacia Echeverria, Sali lab, UCSF

C. Rapid tutorial on calculation of molecular envelopes from SAXS data

(Users will learn basic principles of molecular envelope calculation using ATSAS package, and how to make it faster)

Jan Stransky, CMS, IBT Biocev

15:30-15:40 Workshop Close

