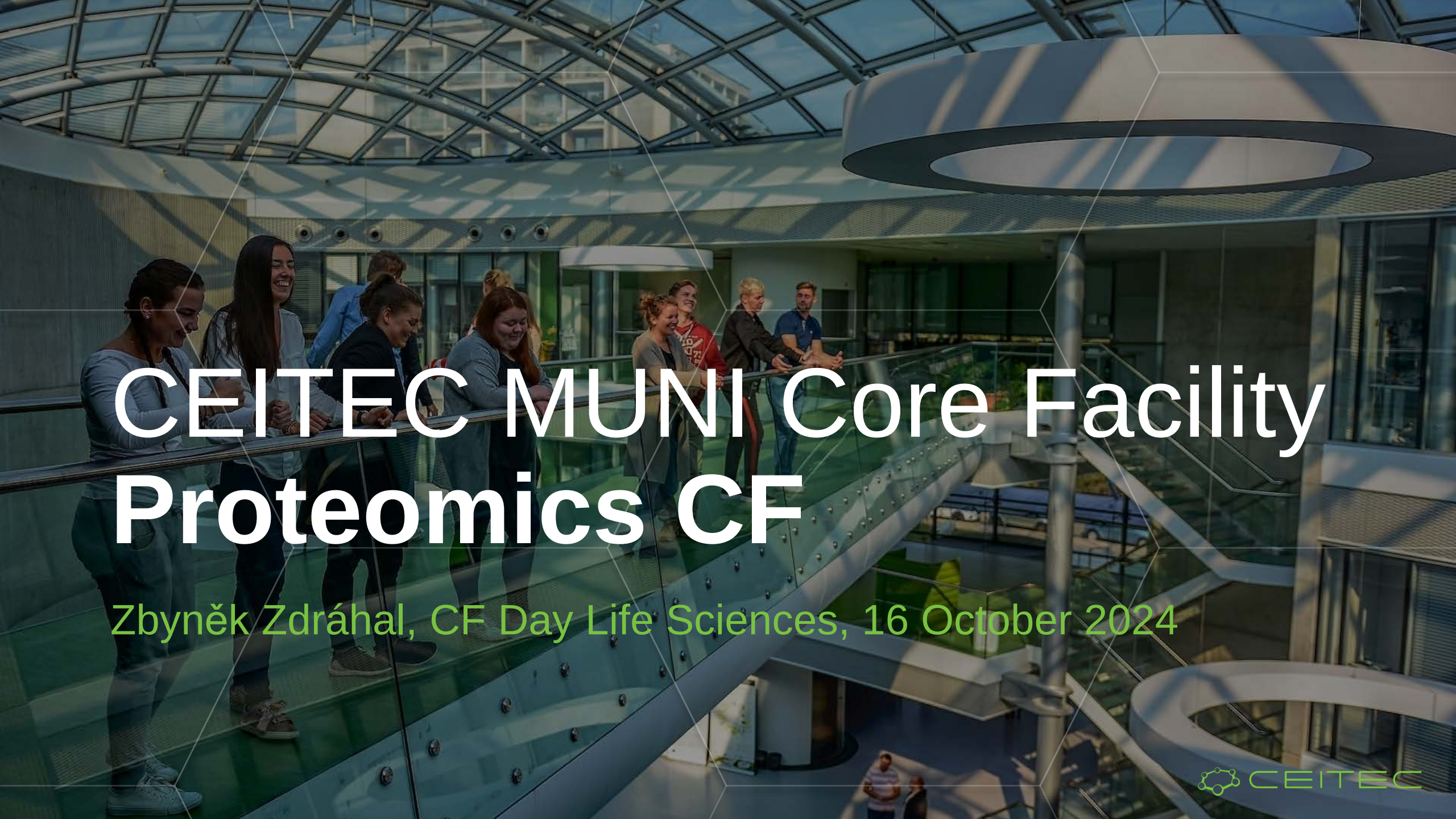
MUNI | CEITEC MUNI ICS MUNI MED MUNI PHARM MUNI SCI MUNI SPORT

Core Facility Day 2024
Life Sciences

16 OCTOBER, 2024
CEITEC, E35/211+ATRIUM

Curious about what expert services are available to researchers on campus? What instruments can you use in shared mode and under what conditions? Do you want to see everything for yourself?

Register at: muni.cz/go/fba265



CEITEC MUNI Core Facility
Proteomics CF

Zbyněk Zdráhal, CF Day Life Sciences, 16 October 2024

CEITEC

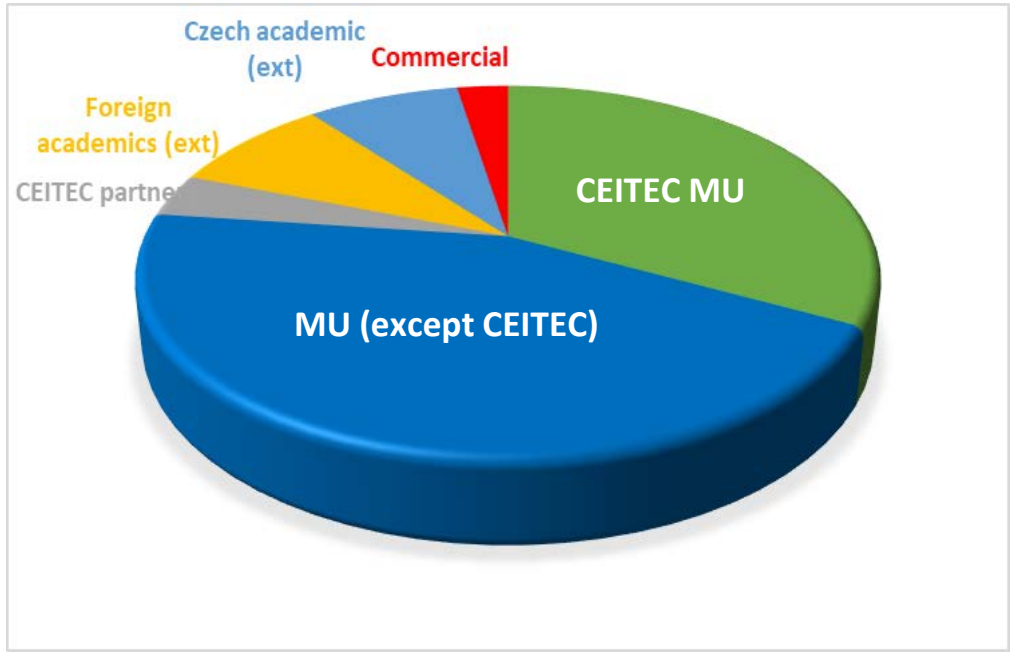
Content

- CF overview
- Services
- Access rules
- News
- New instrumentation
- Acknowledgment
- Result example

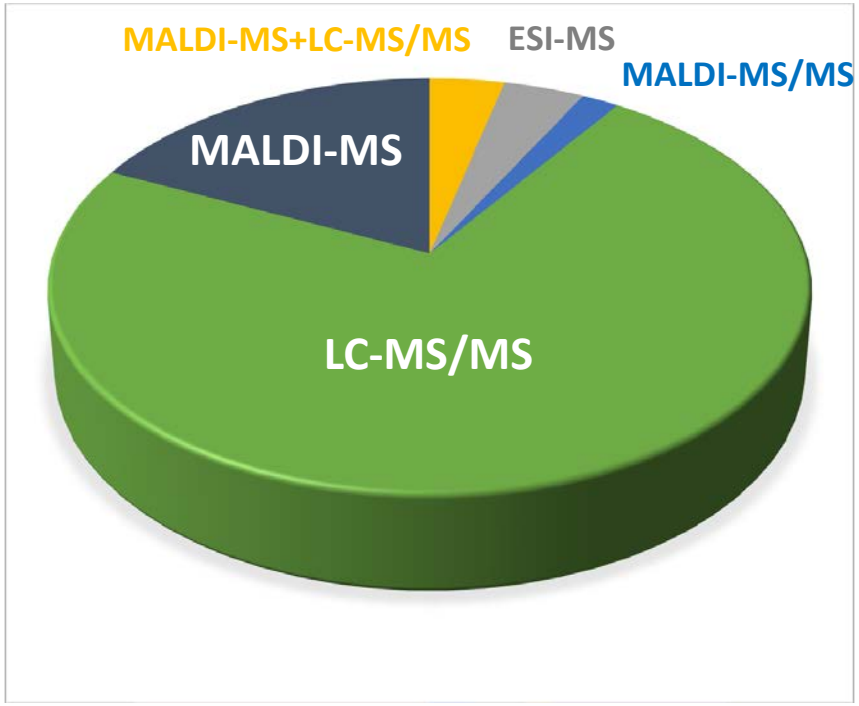
CF overview 2023

187 users (78 students) ● **472 orders** ● **5040 samples** ● ~ 25 000 hrs

User community distribution

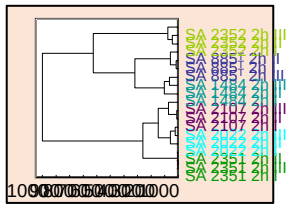


Distribution of samples according to analysis type



- **33 clear acknowledgements to our CF** (~ 30 % of CIISB)

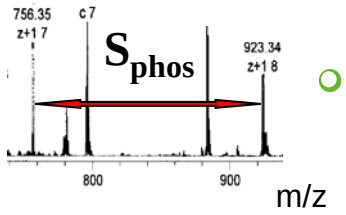
Services



- ***Intact mass measurement***
  (MW, MALDI-MS profiling)

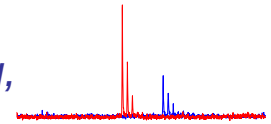
- ***protein identification***
  (de novo sequencing)

- ***protein complexes analysis***
  (-protein, -RNA, -DNA)



- ***characterization of protein modifications***
  *(**phosphorylation**,acetylation, methylation etc.)*

- ***quantification of complex protein mixtures***
  (relative and absolute quantitation, isotopic labeling, label-free)



Overview of our services is available at
https://www.ceitec.eu/proteomics-core-facility/cf95

Access rules

Full service mode

Register • Order • Bring sample • Pick-up report

https://www.ceitec.cz/centralni-laborator-proteomika/cf95

please talk to us:

prior you start a proteomic experiment in your lab

Personal discussion is highly recommended.

Selection of optimal design of the whole experiment (**also on your side**) enables to maximize obtained information, **saves a lot of your** (and our) **time and work.**

News

Prices - 2025

- As usual, **the pricelist will be updated** for 2025 in the beginning of the year, **slight changes are expected**
- Payment at quarterly basis
- Prepayments should be spent ideally during the following year
- The CIISB discount **will stay on 85 % of full costs**

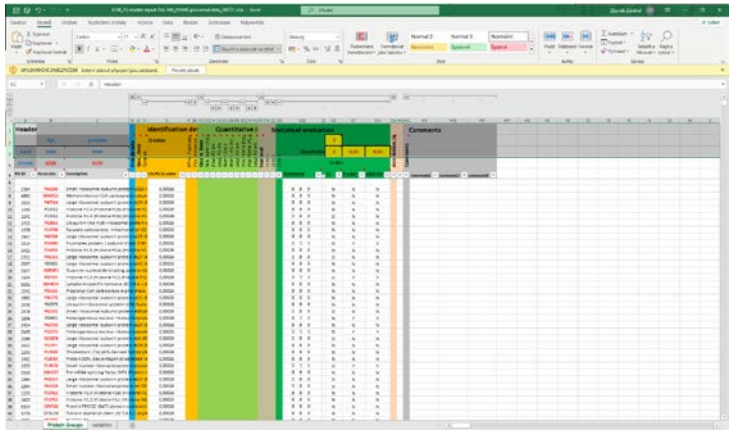
15 % to pay

News

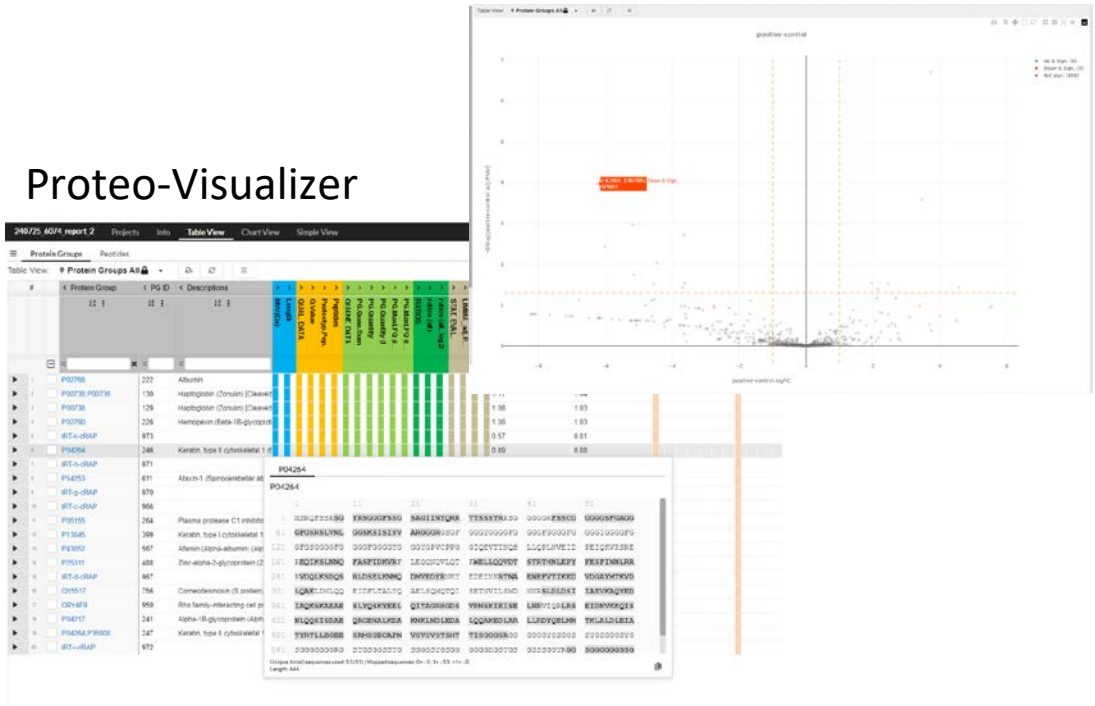
- **New format of our reports**

  stand-alone, portable, offline

Excel



Proteo-Visualizer



- basic training in January/February 2025
- user manual is under progress

New Instrumentation

timsTOF Pro 2

spring 2025

timsTOF HT

- **Deeper proteome coverage**

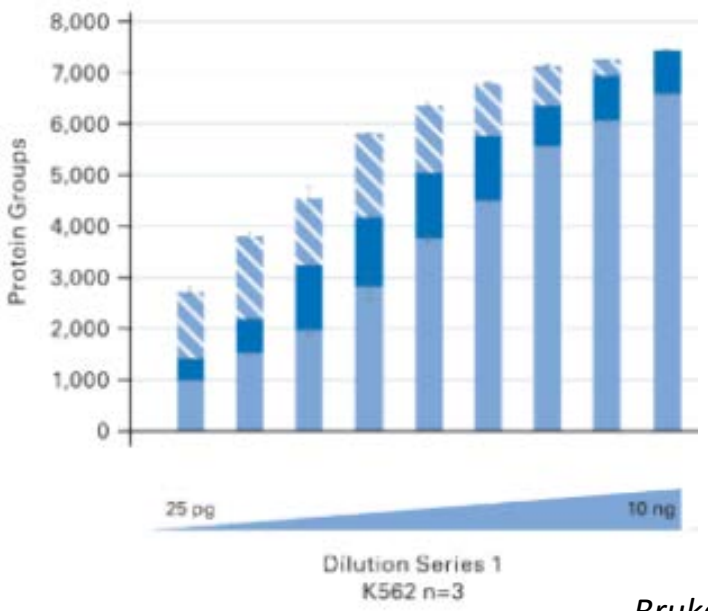
Max. injection amount:	250 ng	→	2 000 ng
Scan rate:	100 Hz	→	300 Hz

New Instrumentation

timsTOF Ultra 2

spring 2025

- Ultimate sensitivity
- Scan rate - 300 Hz



Bruker.com

- **Spatial proteomics**
- **Single cell proteomics**

Sample preparation protocols should be established

Acknowledgment

- **Preferred version:** *„CIISB, Instruct-CZ Centre of Instruct-ERIC EU consortium, funded by MEYS CR infrastructure project LM2023042, is gratefully acknowledged for the financial support of the measurements at the CEITEC Proteomics Core Facility.“*

  Computational resources were provided by the e-INFRA CZ project (ID:90254), supported by the Ministry of Education, Youth and Sports of the Czech Republic

- **Short version:** *„We acknowledge CEITEC Proteomics Core Facility of CIISB, Instruct-CZ Centre, supported by MEYS CR (LM2023042).“*

Current version at: https://www.ceitec.eu/proteomics-core-facility/cf95/tab?tabId=132

Result example

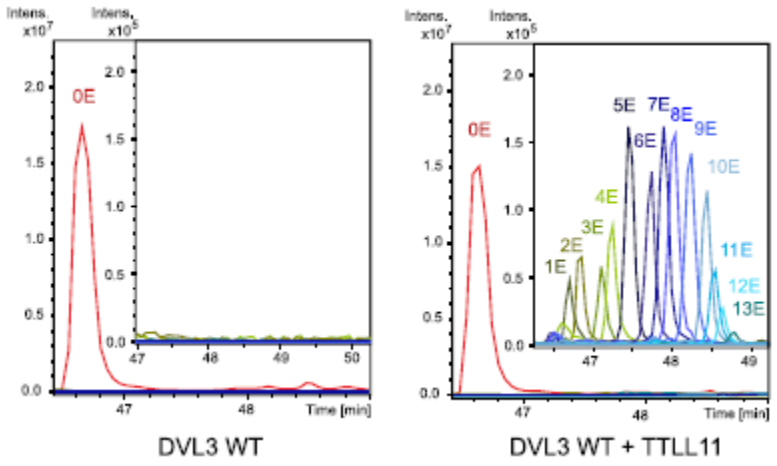
THE EMBO JOURNAL

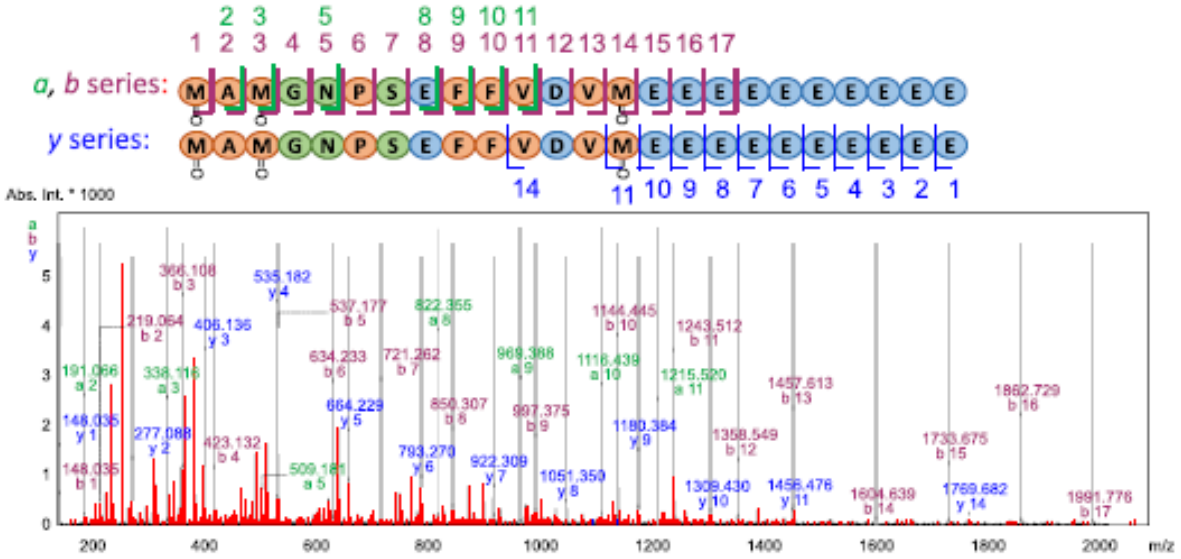
CIISB
Czech Infrastructure for Integrative Structural Biology

Vita Bryja's lab

Kravec M. *et al.*
Carboxy-terminal polyglutamylation regulates signaling and phase separation of the Dishevelled protein

- new type of PTM





https://doi.org/10.1038/s44318-024-00254-7

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Central European
Institute of Technology
Thank you for your attention!
Questions?
core.facility@ceitec.muni.cz
ceitec.eu/core-facilities/
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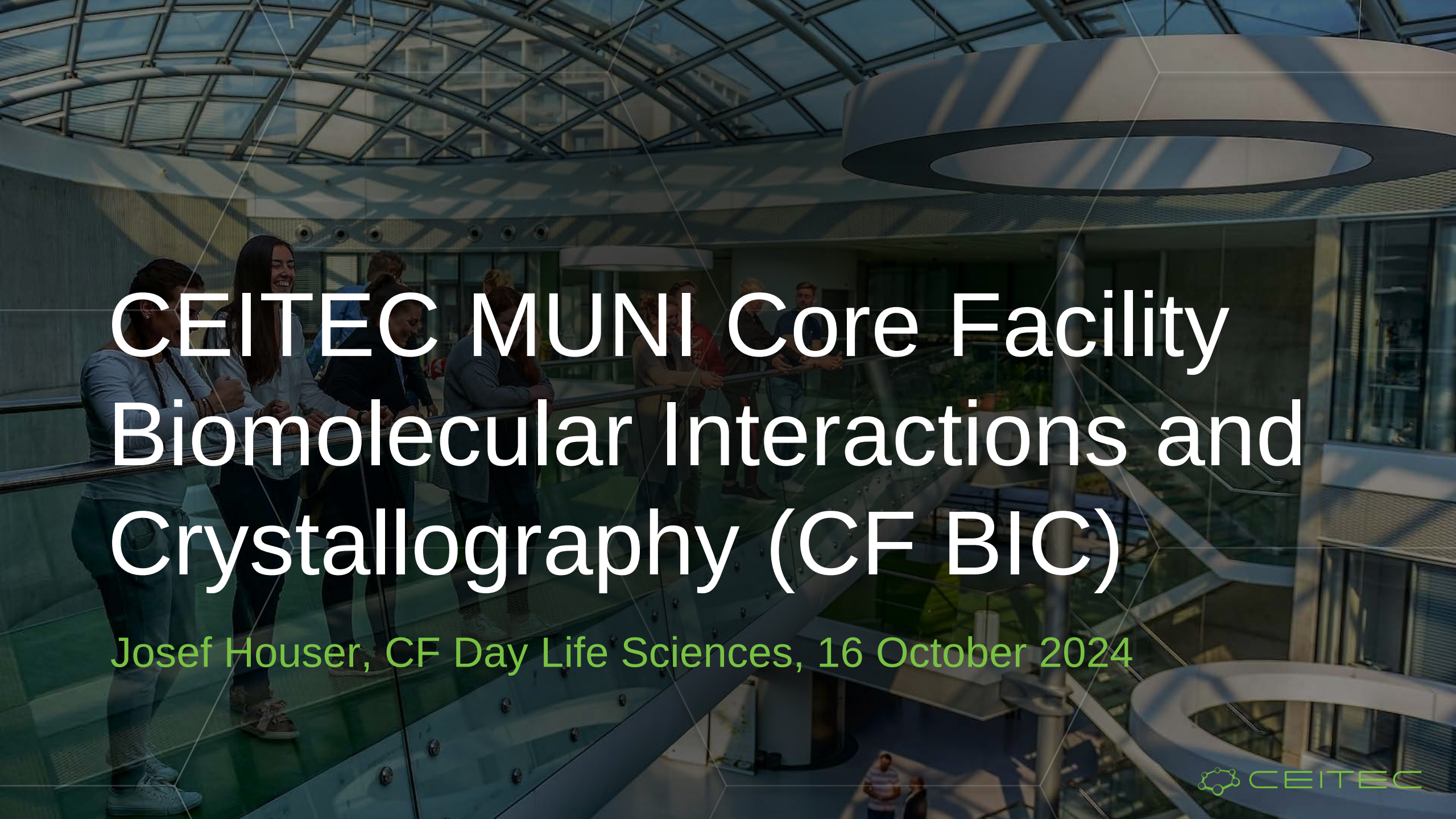


CEITEC MUNI Core Facility Biomolecular Interactions and Crystallography (CF BIC)

Josef Houser, CF Day Life Sciences, 16 October 2024

CEITEC

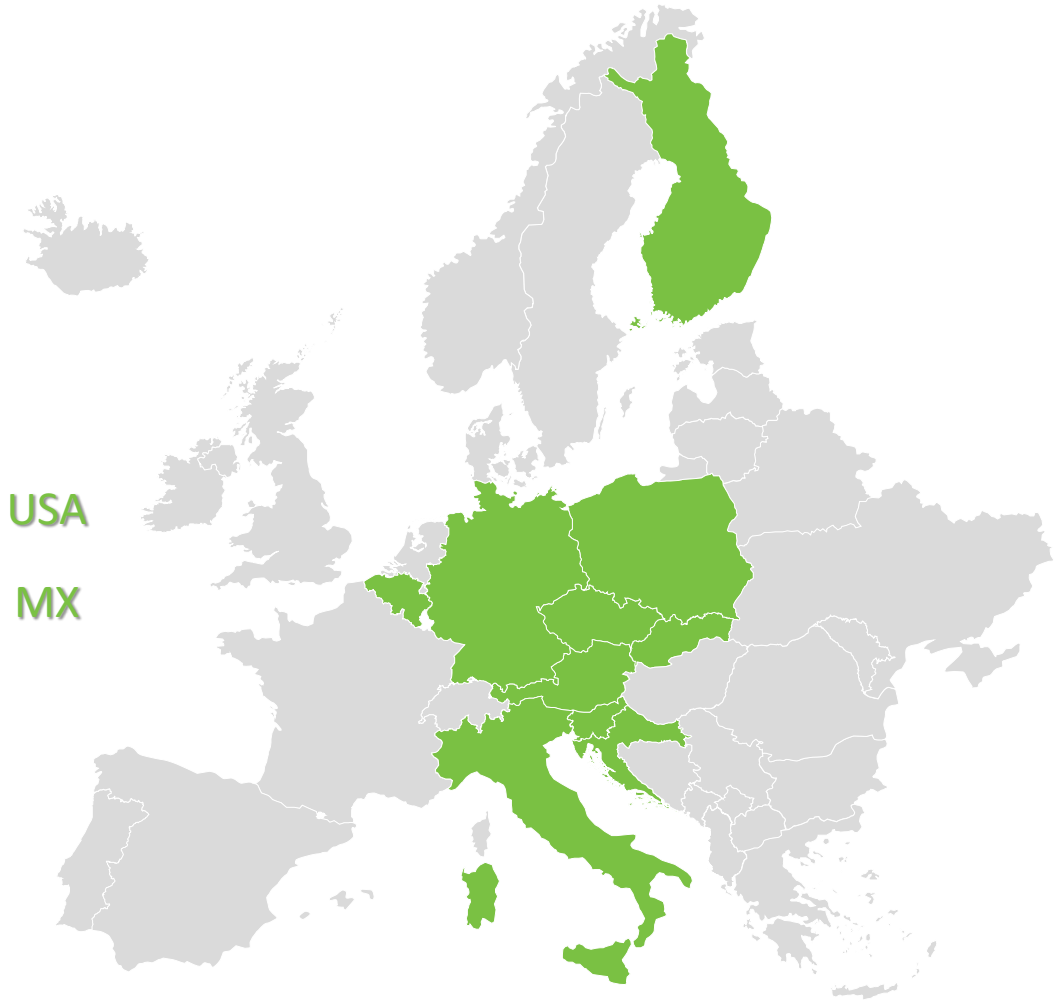
Expertise

20 techniques with 30 instruments

- Studies of physical properties of the molecules,
  e.g. size distribution, homogeneity, stability, structural content
- Characterization of (bio)molecular interactions including thermodynamics and/or kinetics parameters
- High-throughput crystallization screening and optimization of conditions for a crystal growth
- X-ray diffraction and 3D structure solving

International network

Users



Projects

CIISB
Czech Infrastructure for Integrative Structural Biology

instruct ERIC

InnoCore

ISIDORe

Collaboration

ARBRE
Association of Resources for Biophysical Research in Europe

Vienna BioCenter
CORE FACILITIES

BOKU
CORE FACILITY
Biomolecular & Cellular Analysis

ISTA
Institute of Science and Technology Austria

MBS

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Biophysical characterization

- Homogeneity
  - Molecular mass
  - Oligomeric state
  - Aggregation
- Stability
  - Temperature
  - Buffer composition
- Folding
  - Secondary structure
  - Shape

- Analytical ultracentrifugation (AUC)
- Size exclusion chromatography (SEC-LS)
- Dynamic light scattering (DLS)
- Differential scanning fluorimetry (DSF)
- Differential scanning calorimetry (DSC)
- Circular dichroism spectroscopy (CD)
- Small-angle X-ray scattering (SAXS)
- Mass photometry (MP)
- UV/VIS spectroscopy

Optima AUC

ProteomeLab XL-I

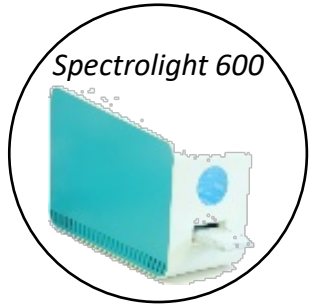
Chirascan V100

Auto PEAQ-DSC

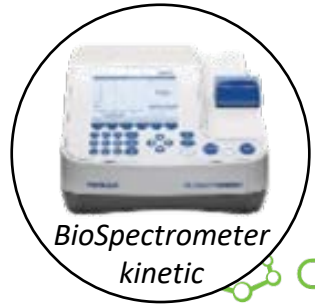
DelsaMAX

Prometheus NT.48

TwoMP


Spectrolight 600

OmniSEC


BioSpectrometer kinetic

BioSAXS 2000

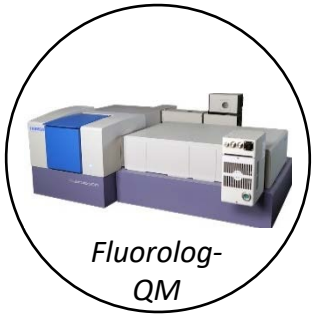
Biomolecular interactions

- Various principles
  - In solution
  - On surface
  - Cell-based
- Parameters
  - Affinity
  - Thermodynamics
  - Kinetics
- Types of molecules
  - Proteins, nucleic acids, small molecules

- Isothermal titration calorimetry (ITC)
- Micro-scale thermophoresis (MST)
- Bio-layer interferometry (BLI)
- Surface plasmon resonance (SPR)
- Analytical ultracentrifugation (AUC)
- Fluorescence anisotropy (FA)
- Cell sorting (FACS)

Optima AUC

ProteomeLab XL-I


Fluorolog-QM

Monolith NT.117

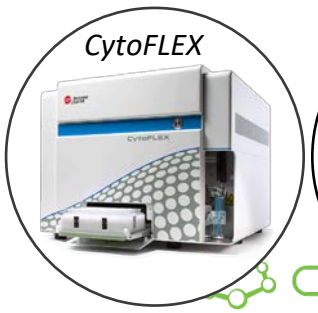
Auto PEAQ-ITC

Biacore S200

Octet RED96e

VP-ITC

Monolith NT.117 Pico


CytoFLEX

SPR imaging

Crystallography

- Complete instrumentation for crystallization screening
- Optimization of crystallization
- Diffraction data collection
- 3D structure determination

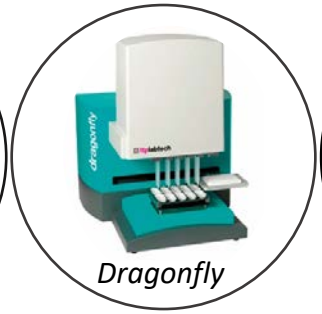
- Crystallization plates set-up robotics
- Plates storage and imaging
- Crystallization temperature optimization
- Optical microscopes
- X-ray diffraction
- Accessories for cryo-crystallography

XtaLAB Synergy

Actor

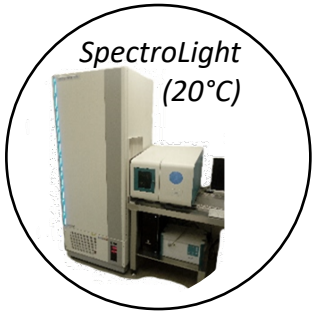
UniPucks

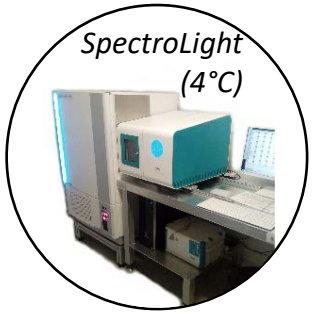
Phoenix


Dragonfly

Mosquito

epMotion


SpectroLight (20°C)


SpectroLight (4°C)

TG40

SMZ800

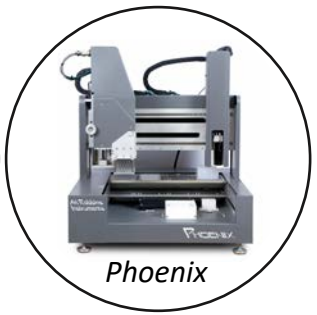
High throughput

- Robotization and automation for HTS
- Pipetting from 500 pl to 1 ml
- Microarrays
- 96 and 384-well plates handling
  - Aliquoting
  - Gradient preparation

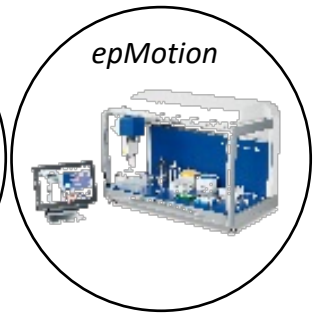
- Parallelization
  - In plates – DLS, BLI, crystallization
  - In capillaries – DSF
- Autosamplers
  - Walk-away operation, 24/7
  - SPR, ITC, DSC, SEC-LS
- Pipetting robotics
  - SBS plate preparation
  - Microarrays

sciFLEXARRAYER

Odyssey M


Phoenix

Mosquito


epMotion

Auto PEAQ-DSC

Auto PEAQ-ITC

Biacore S200

CEITEC

Equipment news

- Fluorimeter – Fluorolog QM
  - **Fluorescence anisotropy**
  - Time resolved single-photon count
  - Temperature controlled

- CD spectrometer – Chirascan V100
  - **Secondary structure** analysis
  - High stability, sensitivity and precision
  - Temperature control (4-100 °C)

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Equipment news

- Mass photometer – Refeyn MP2
  - Sample **homogeneity** and **mass analysis**
  - Broad concentration range
  - Proteins and their complexes

- Analytical size-exclusion chromatography – fraction collector
  - Collection of separated fractions
  - Pre-step for **MS or EM analysis**

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Case study – 14-3-3ζ protein

- Important **human regulatory protein**
- Various roles in organism
- **Monomer-dimer transition** depending on phosphorylation

Phosphomimicking mutants

ζ_S58E

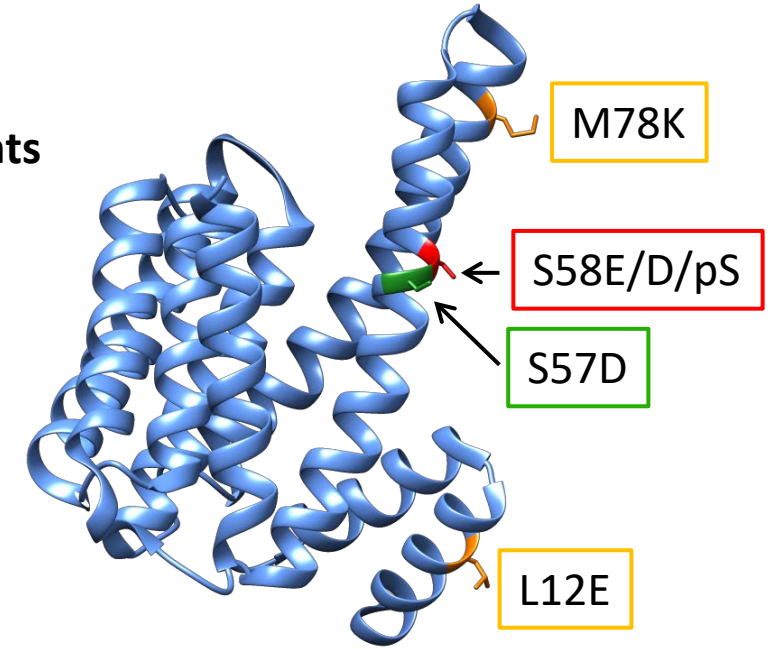
ζ_S58D

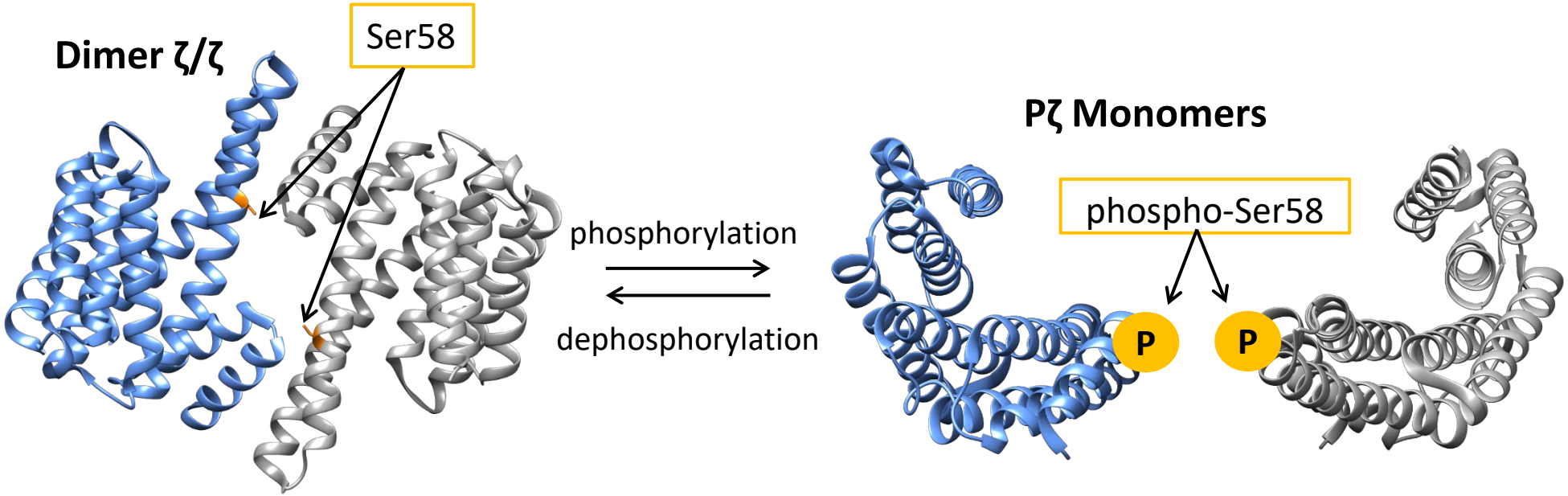
ζ_S57D_S58D

Monomeric mutants

ζ_L12E_M78K = ζm

Phosphorylated ζ_pS58





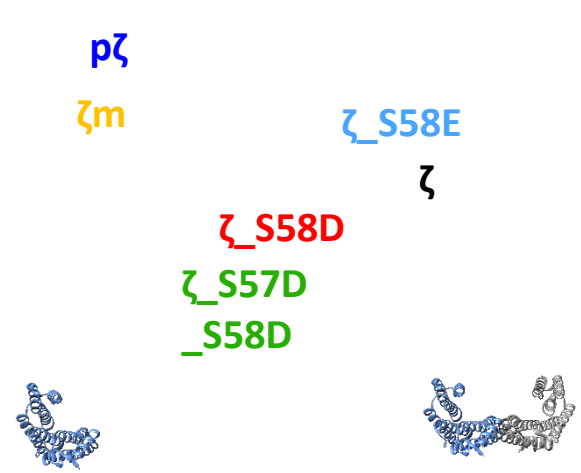
Jozef Hritz

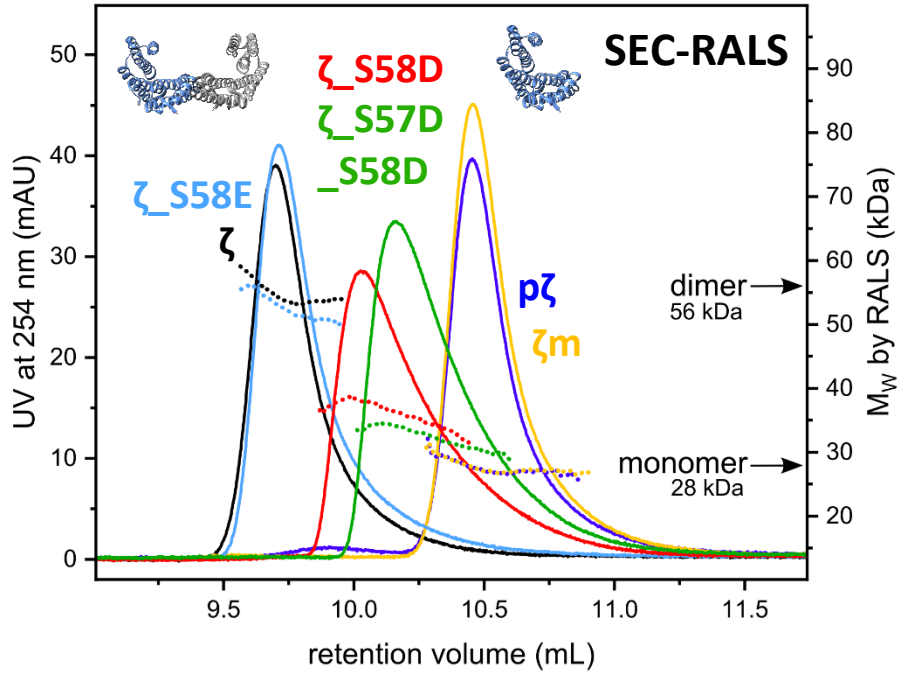
CEITEC

Case study – 14-3-3ζ protein

- Combination of multiple methods
- FRET, MST, AUC, SEC-LS, nanoDSF, DSC
- **High-variability** among "phosphor-mimicking" mutations (K_D varies by 4 orders)

14-3-3 construct	K_D (AUC/SEC)	T_m (nanoDSF) [°C]	T_m (DSC) [°C]
ζ_WT	5.5 ± 0.8 nM	60.35 ± 0.15	60.28 ± 0.01
ζ_S58E	0.35 ± 0.25 µM	58.19 ± 0.09	57.64 ± 0.01
ζ_S58D	132 ± 7 µM	54.21 ± 0.03	53.89 ± 0.01
ζ_S57D_S58D	348 ± 19 µM	53.58 ± 0.10	53.70 ± 0.01
ζm	4.6 ± 0.1 mM	53.04 ± 0.12	53.34 ± 0.02
ζ_pS58	7.6 ± 0.8 mM	50.70 ± 0.11	50.88 ± 0.02





Kozeleková *et al.*, **2022**, *Front Chem*

How to use CF BIC?

- CF BIC is **opened to everyone**
- Majority of users from CEITEC and Masaryk University

Modes of access

- Service mode
- User mode

Pricing

- Full prices – based on cost matrix
- **Reduced fee** – national/international projects
- Collaboration – specific cases

- Compliance with CF BIC rules required

- Acknowledgement obligatory

Workshops in 2025

- Methods for Characterization of Biomolecular Interactions
  - Lectures on various biophysical techniques
  - Available to students as subject S2004/S2005

27 – 31 Jan 2025

- Bio-SAXS practical course
  - Annual event co-organized with CMS at Biocev
  - Lectures and practicals on SAXS applications

Sep 2025

- Potential workshops
  - inQuiQ (Delta LS) – instrument demo
  - Mass photometry
  - ...

To be announced...

Check **bic.ceitec.cz** and **CEITEC newsletters** for more information

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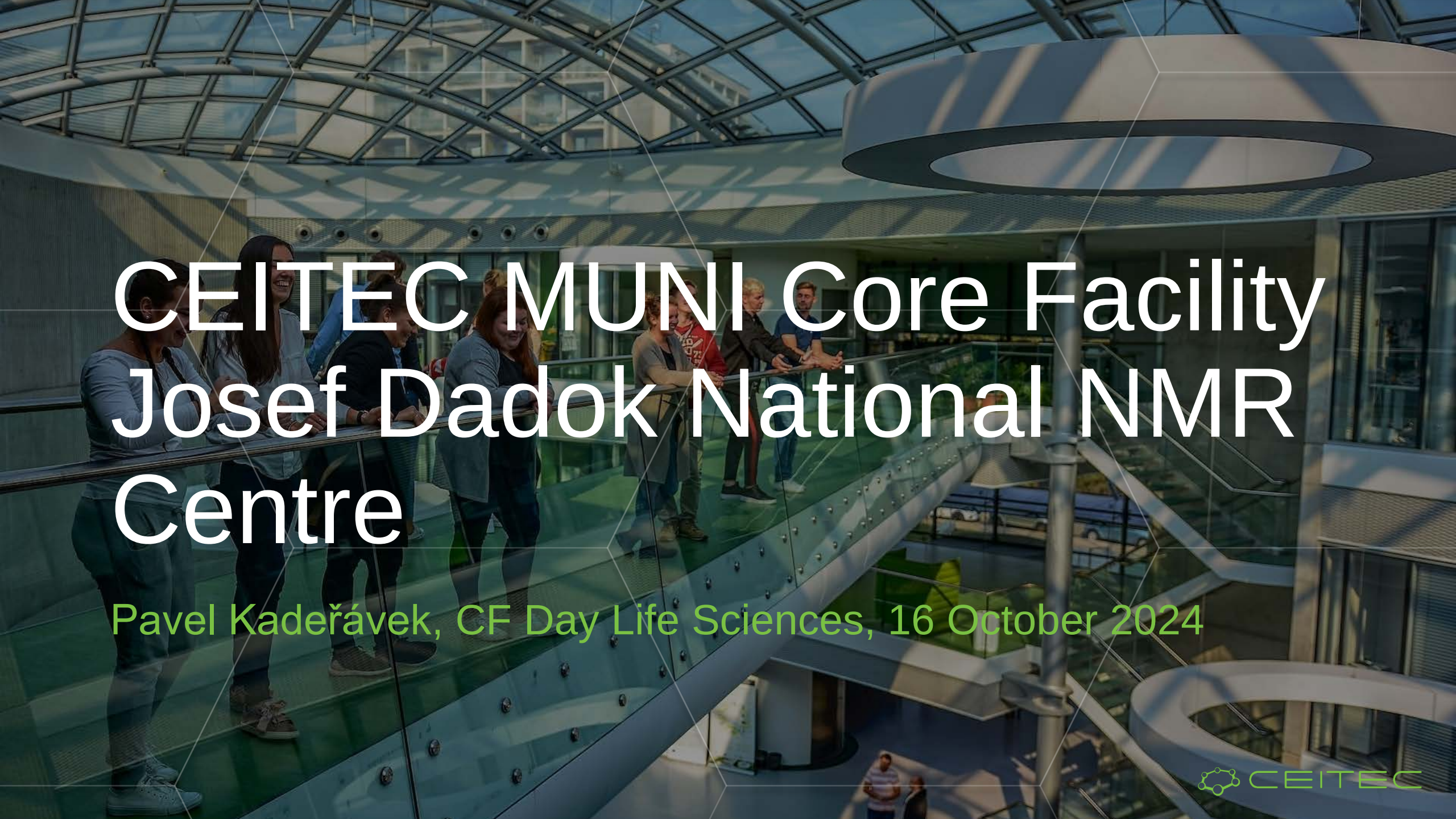

CEITEC MUNI Core Facility Josef Dadok National NMR Centre

Pavel Kadeřávek, CF Day Life Sciences, 16 October 2024

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Content

- **CF overview**
  - Who is Josef Dadok
  - What is NMR good for
  - What you need to use our services
- **Equipment**
- **Users and applications**
- **Access, Training, Data policy**
- **People**
- **Financial support and acknowledgments**
- **Selected publications**

Josef Dadok

- * 28. 2. 1926
- Pioneer of nuclear magnetic resonance spectroscopy in Czechoslovakia
- Important figure in the NMR instrumentation and methodology worldwide.
- Developed instruments for high resolution NMR spectroscopy later produced by Tesla Brno (3rd country in the world, after USA and Japan)
- Since late 1960s lived and worked in USA – Carnegie Melon Univ., Pittsburgh
- First 600 MHz (14.1 T) magnet suitable for high resolution NMR spectroscopy in 1970s.
- Doctor honoris causa of Masaryk University (2013).

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NMR Spectroscopy

Strengths:

- Atomic resolution – detailed information
- Applicable both in solution and solid state
- Good for compound identification, quality control, structure determination
- Can study dynamics & interactions
- Gentle to the sample

Weaknesses:

- Low sensitivity
- Needs lot of sample, measurements long, often needs isotope enrichment
- Data interpretation laborious
- Expensive equipment

CEITEC

What you need to use our CF

Sample:

- Liquid or solid
- **Quantity**
- 0.1 to 30 mg for liquids, depending on nucleus and MW
- dissolved in 600 µl to 180 µl, ~ 10 mg for solids
- **Solubility**
- water, chloroform, benzene, DMSO, DMF (deuterated)
- **Stability**
- at least minutes
- **Temperature (liquid)**
- 0ºC to 80ºC normal, -80ºC to 150ºC extended

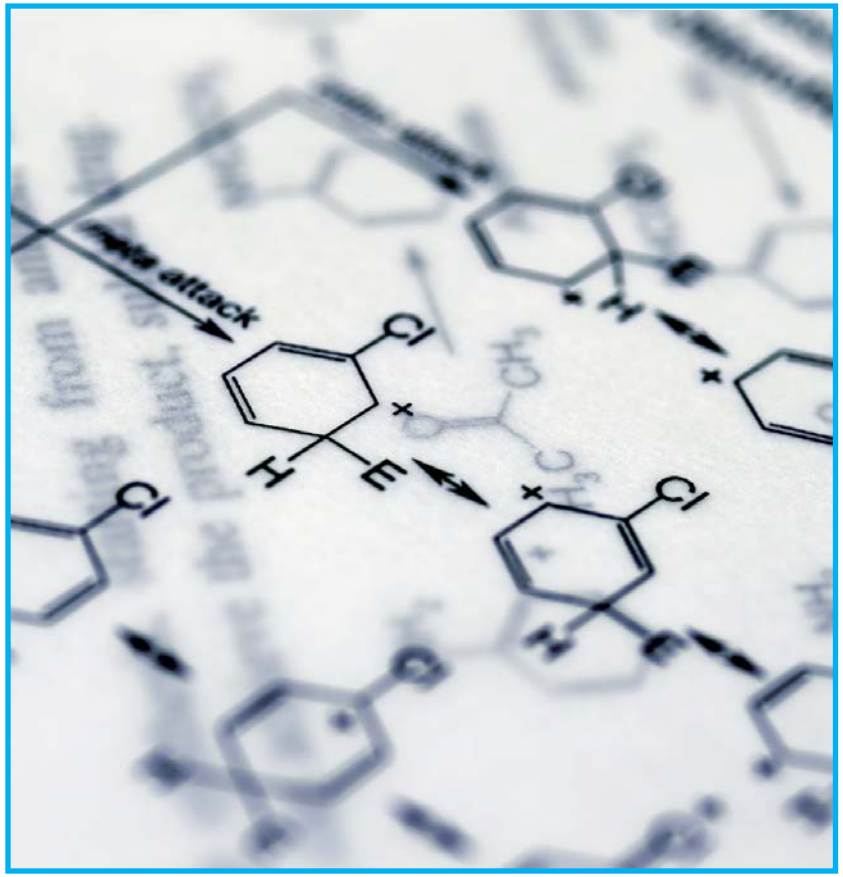
- **Know what are you trying to find out**
- *Send the publication that inspired you!*
- Nuclei ^{1}H, ^{13}C, ^{15}N, ^{31}P, ^{19}F routinely, many others possible
- Type of spectra
- 1D, 2D homonuclear, heteronuclear, etc.

Equipment

- **6 NMR spectrometers**
  - 500 MHz, 600 MHz, two 700 MHz, 850 MHz, 950 MHz
  - 5 cryoprobes, solid-state possible at 500 and 700 MHz
  - Simple X-band EPR spectrometer
- **Extensive upgrades in 2020 - 2022**
  - New electronics (Neo generation)
  - LN2 recycling
  - 4 new cryoprobes, ^{19}F possible everywhere
  - extended temperature range <-40°C, +150 °C >
  - Diffusion probe 700 MHz
- **No new equipment in 2024**
  - (planned new probe for industry applications and helium liquefier)
- **Future plans**
  - Combined EPR/NMR system for hyperpolarized NMR experiments (with Neugebauer RG, CEITEC BUT)
  - Sample changer for 600MHz
  - Solid-state MAS probe with fast rotation (better resolution)
  - 700MHz TCI probe

Users and applications

- **CEITEC research groups**
  - Biomolecular applications - Structure, dynamics and interactions of proteins and nucleic acids
- **Other MUNI**
  - Faculty of Science, Medicine, Pharmacy
  - Organic and inorganic compounds, perspective pharmaceuticals
- **Outside academic users**
  - Charles University, UTB Zlín, Institute of Physics of Materials CAS, Cancer Research Institute SAS, Institute of Neuroimmunology SAS, Vienna University, JKU Linz, Universidad Politécnica de Santa Rosa Jáuregui (Mexico)
  - Proteins, DNA, metabolites
- **Industry**
  - PIB, Synthon, Ratiochem, AI|ffinity
  - Quality control



Access, Training, Data policy

- **Access: User or service mode**
- User mode – trained users only
- **Training** - Practical NMR Spectroscopy of Biomolecules (C7995) Non-students/outside users welcome
- Experienced NMR spectroscopist can get certified based on their previous experience/publications.
- **Booking** - CEITEC reservation system
  - https://booking.ceitec.cz/en/planning-board/
- **Monitoring system**
  - https://nmrinfo.ncbr.muni.cz/nmr/monitoring/
- **Data policy**
  - Users shall work under their own logins
  - Users are owners of their data, no permanent storage in the CF (quotas)
  - Data backed up every night

Financial support

CIISB (Czech, world)

https://www.ciisb.org/open-access/proposal-submission

INSTRUCT (EU)

https://instruct-eric.org/submit-proposal

CEITEC

People

- **Pavel Kadeřávek**
  - CF head, teaching and user training, management of CIISB and Instruct projects, methods development (pulse sequence etc.), spectra measurement for outside users – biomolecules.
- **Radovan Fiala**
  - Deputy head, spectra measurement for outside users – biomolecules, teaching and user training.
- **Jaromír Toušek**
  - booking system, NMR monitoring and information system software, spectra measurement for outside users – liquide + solid state, NMR calibration and testing, cryogen refills.
- **Otakar Humpa**
  - spectra measurement for outside users – organic chemistry, gasses and cryogenic liquids logistics, cryogen refills, communication with Campus Facilities.
- **Kateřina Bouzková**
  - spectra measurement for outside users – solid-state and organic chemistry, cryogenic liquids logistics, cryogen refills.
- **Petr Padrta**
  - Maintenance of computers and network, installations and maintenance of NMR software, troubleshooting, accounts for new users.

Acknowledgement text – CIISB

- **Preferred version:** *„CIISB, Instruct-CZ Centre of Instruct-ERIC EU consortium, funded by MEYS CR infrastructure project LM2023042, is gratefully acknowledged for the financial support of the measurements at the CF Josef Dadok National NMR Centre.“*
- **Short version:** *„We acknowledge CF Josef Dadok National NMR Centre of CIISB, Instruct-CZ Centre, supported by MEYS CR (LM2023042).“*

- *Co-authorship (creative input, substantial contribution)*

Selected publications

Notable publications acknowledging CF

Protein-nucleic acid interactions

PAPAGEORGIOU, Anna C.; POSPÍŠILOVÁ, Michaela; CIBULKA, Jakub; ASHRAF, Raghib; WAUDBY, Christopher A. et al. Recognition and coacervation of G-quadruplexes by a multifunctional disordered region in RECQ4 helicase. Online. Nature Communications. 2023, vol. 14 (1) https://doi.org/10.1038/s41467-023-42503-z.

Nucleic acids

LUO, Yu; ŽIVKOVIĆ, Martina Lenarčič; WANG, Jiawei; RYNEŠ, Jan; FOLDYNOVÁ-TRANTÍRKOVÁ, Silvie et al. A sodium/potassium switch for G4-prone G/C-rich sequences. Online. Nucleic Acids Research. 2024, vol 52 (1) 448-461, https://doi.org/10.1093/nar/gkad1073.

Plants

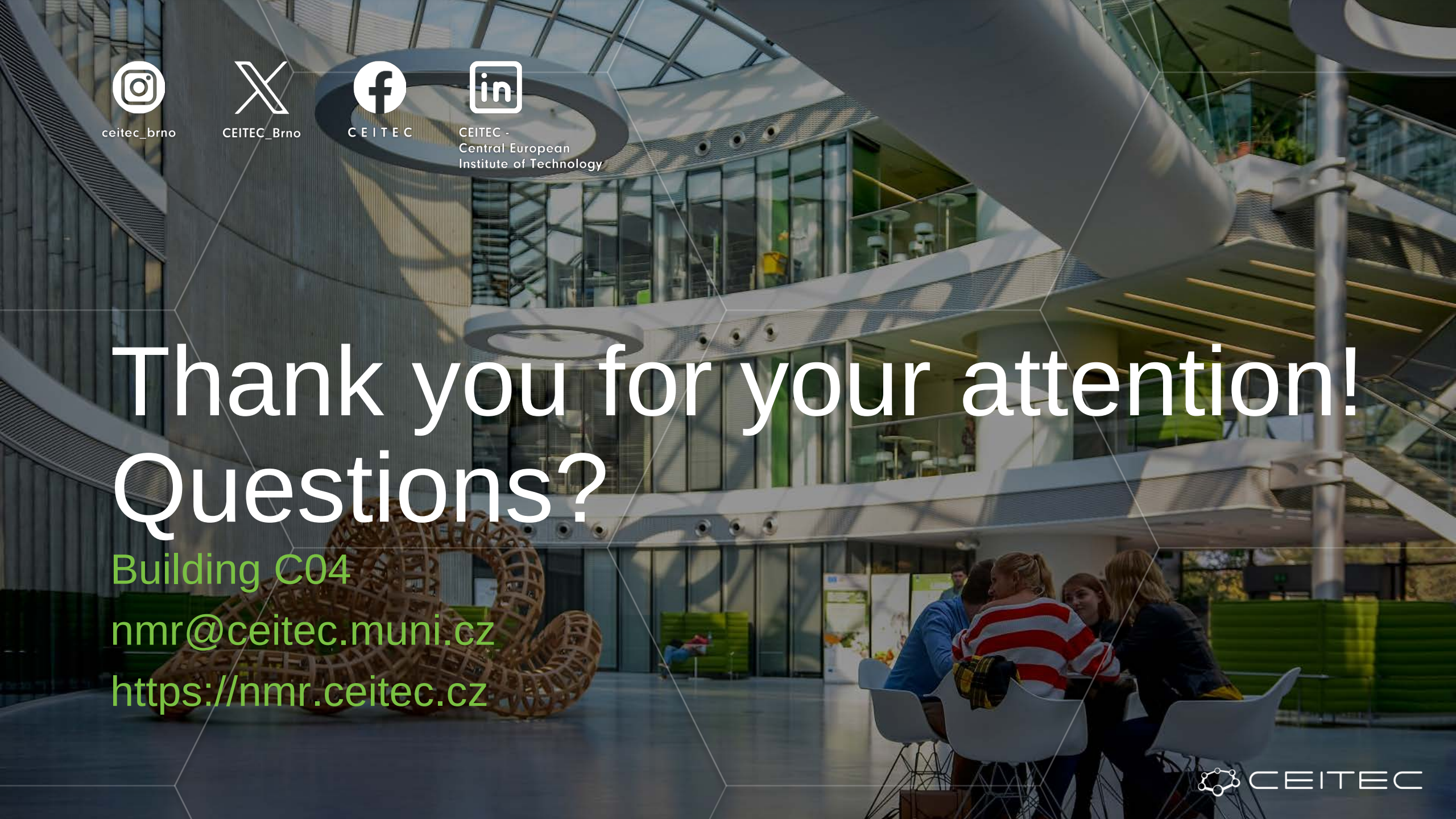
JANKOVSKÁ, Dagmar, JURČOVÁ, Nikol, KUBÍNOVÁ, Renata, VÁCLAVÍK, Jiří, ŠVAJDLENKA, Emil, MASCELLANI, Anna, MARŠÍK, Petr, BOUZKOVÁ Kateřina, MALANÍK MilaN, Anticholinesterase Activity of Methanolic Extract of *Amorpha fruticosa* Flowers and Isolation of Rotenoids and Putrescine and Spermidine Derivatives, Plants, 2024 vol. 13 (9), https://doi.org/10.3390/plants13091181

Material Science

SKODA, David; ZHU, Ran; HANULIKOVA, Barbora; STYSKALIK, Ales; VYKOUKAL, Vit et al. Propylene Metathesis over Molybdenum Silicate Microspheres with Dispersed Active Sites. Online. ACS Catalysis. 2023, vol 13 (19), 12970-12982, https://doi.org/10.1021/acscatal.3c02045.

Small molecules

NOVOTNÝ, Jan, Jan CHYBA, Anna HRUZÍKOVÁ, et al. Flipping hosts in hyperfine fields of paramagnetic guests. Cell Reports Physical Science [online]. 2023, 4(7), doi:10.1016/j.xcrp.2023.101461



Thank you for your attention!

Questions?

Building C04

nmr@ceitec.muni.cz

https://nmr.ceitec.cz

CEITEC

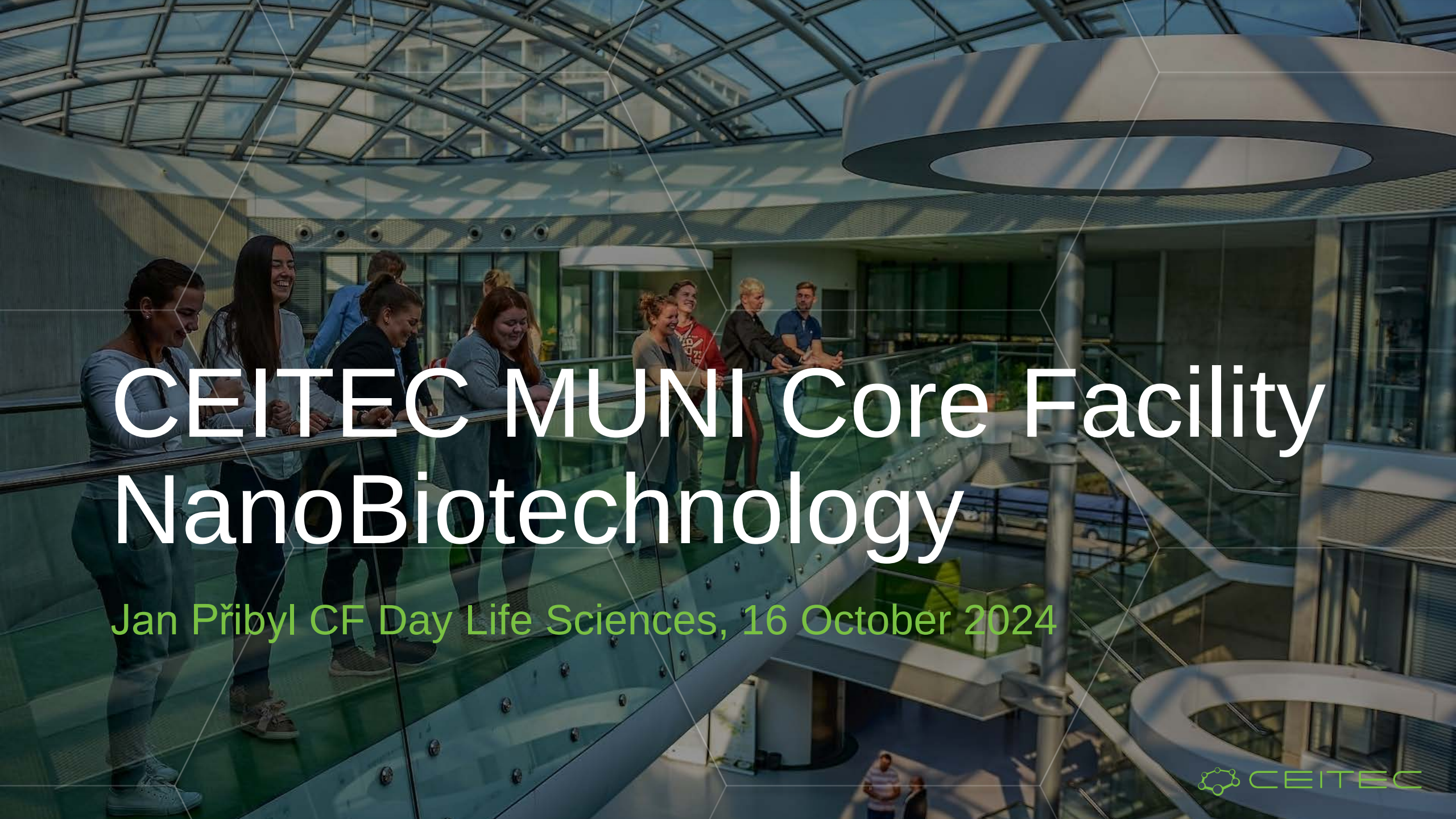
MUNI | CEITEC MUNI ICS MUNI MED MUNI PHARM MUNI SCI MUNI SPORT

Core Facility Day 2024
Life Sciences

16 OCTOBER, 2024
CEITEC, E35/211+ATRIUM

Curious about what expert services are available to researchers on campus? What instruments can you use in shared mode and under what conditions? Do you want to see everything for yourself?

Register at: muni.cz/go/fba265



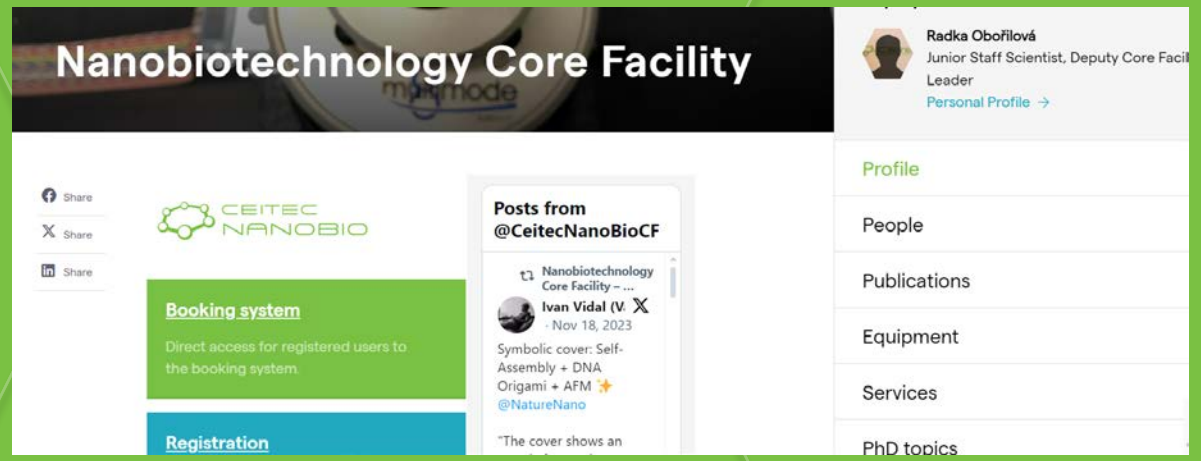
CEITEC MUNI Core Facility NanoBiotechnology

Jan Přibyl CF Day Life Sciences, 16 October 2024

CEITEC

Web page: ***ceitec.eu/nanobio***

- People
- Equipment
- Services
- Access
- Acknowledgement info



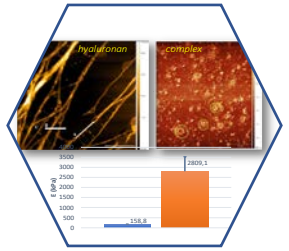
Follow us on X: @**CeitecNanoBioCF**

CEITEC

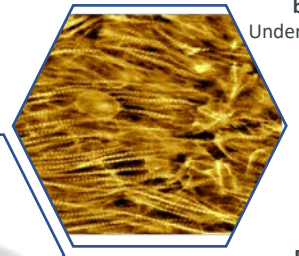
Core Facility Nanobiotechnology

Imaging, mechanical mapping, Raman microscopy

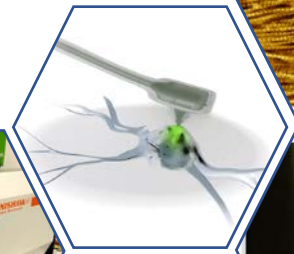
Structure and biomechanics of biomolecules
(AFM imaging and nano-indentation]



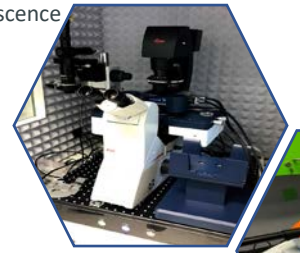
Structure of biomolecules
Under native conditions



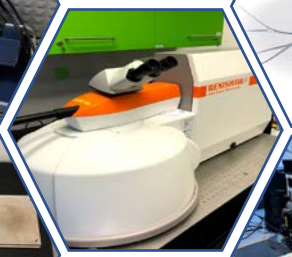
FluidFM
AFM based microfluidics



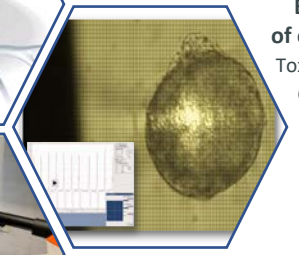
Atomic Force Microscopy of biosamples
Combined with fluorescence microscopy



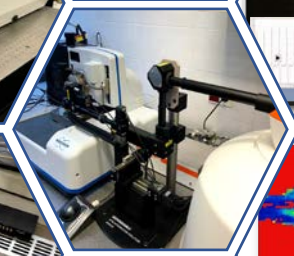
Raman microscopy
Chemical mapping of surface



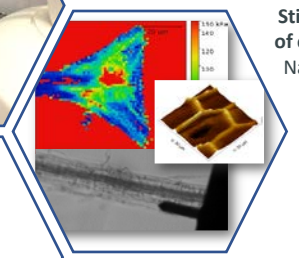
Biomechanics of contractile cells
Toxicology and cell development



Atomic Force Microscopy of biosamples
High-resolution imaging



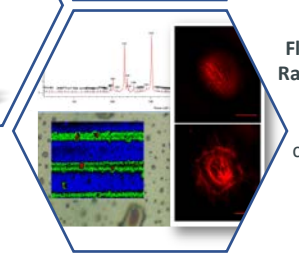
Stiffness mapping of cells and tissues
Nanoindentation under semi-physiology



Multielectrode Array (MEA)
Cellular electrophysiology

NanoIndenter
Indentation of soft samples

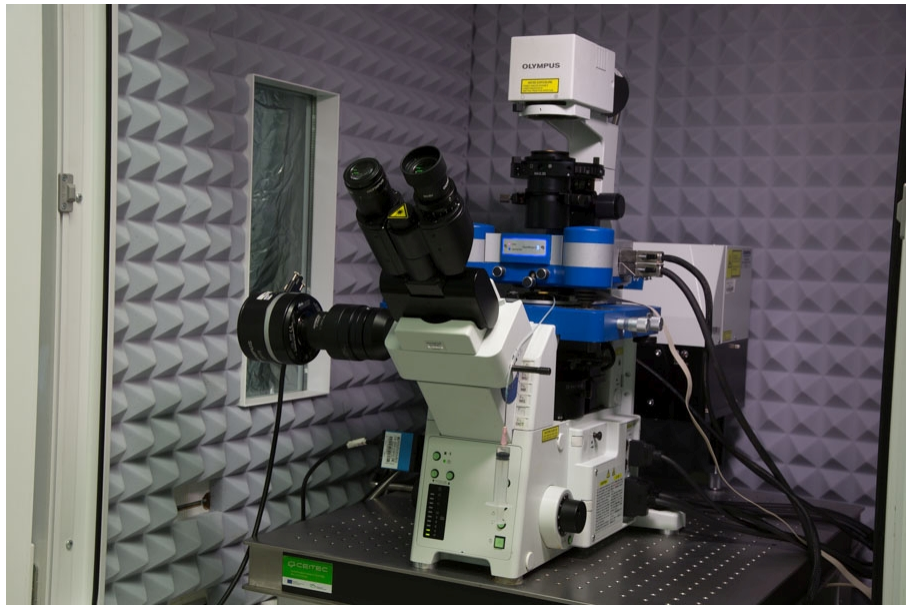
Fluorescence and Raman microscopy
Structural and chemical characterization

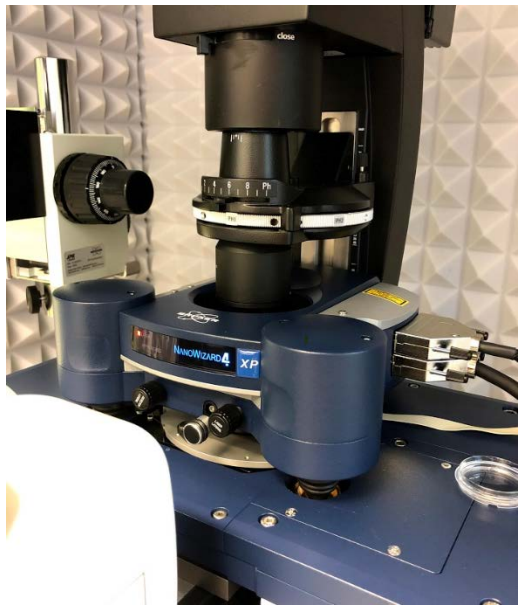


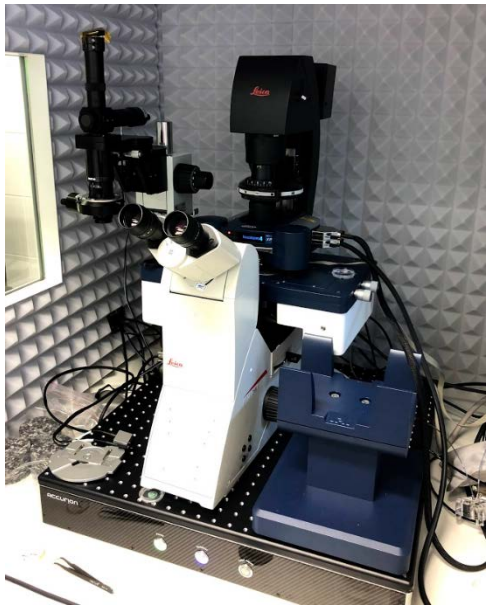
EITEC

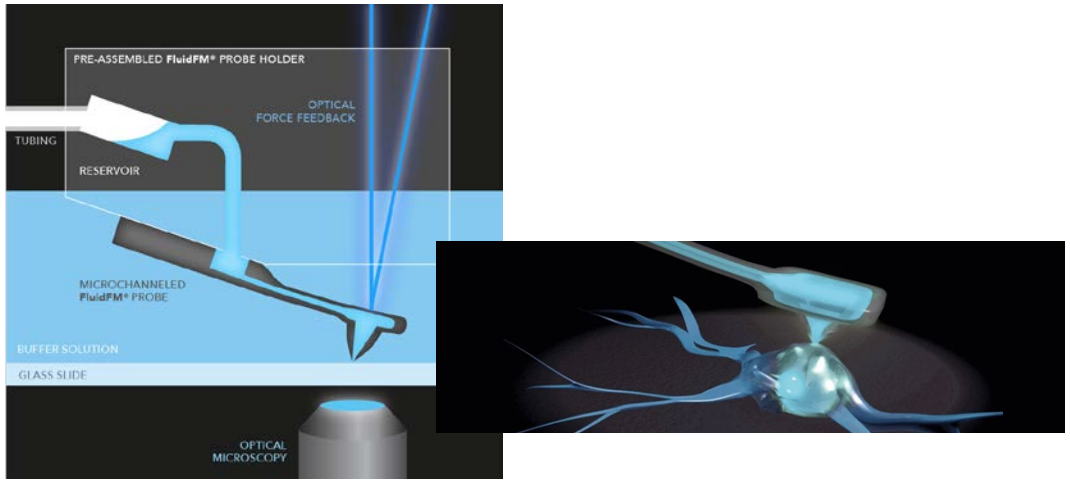
BioAFM – living cells and tissues

JPK NanoWizard 3 and 4 with extended scanning range

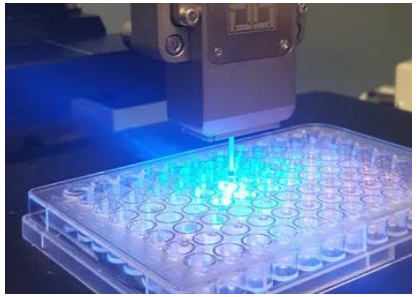








+ CytoSurge FluidFM module



+ Biosoft NanoIndenter

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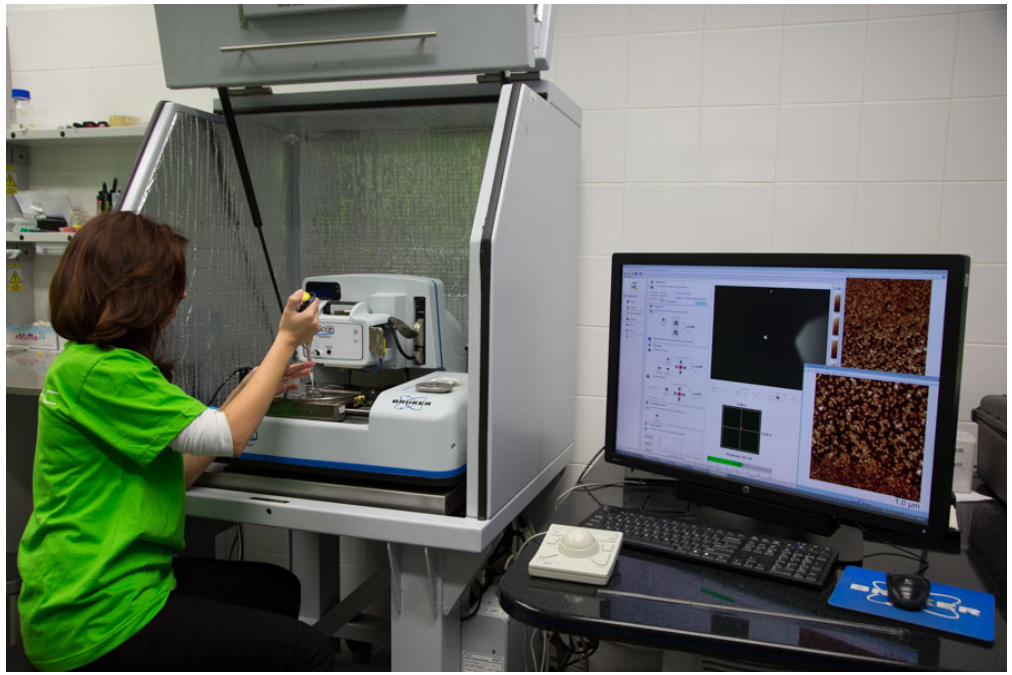
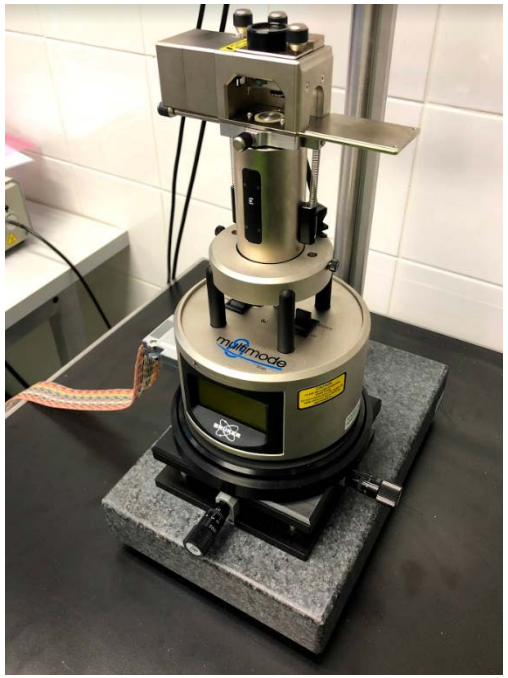
BioAFM – molecules, nanoobjects, molecular complexes





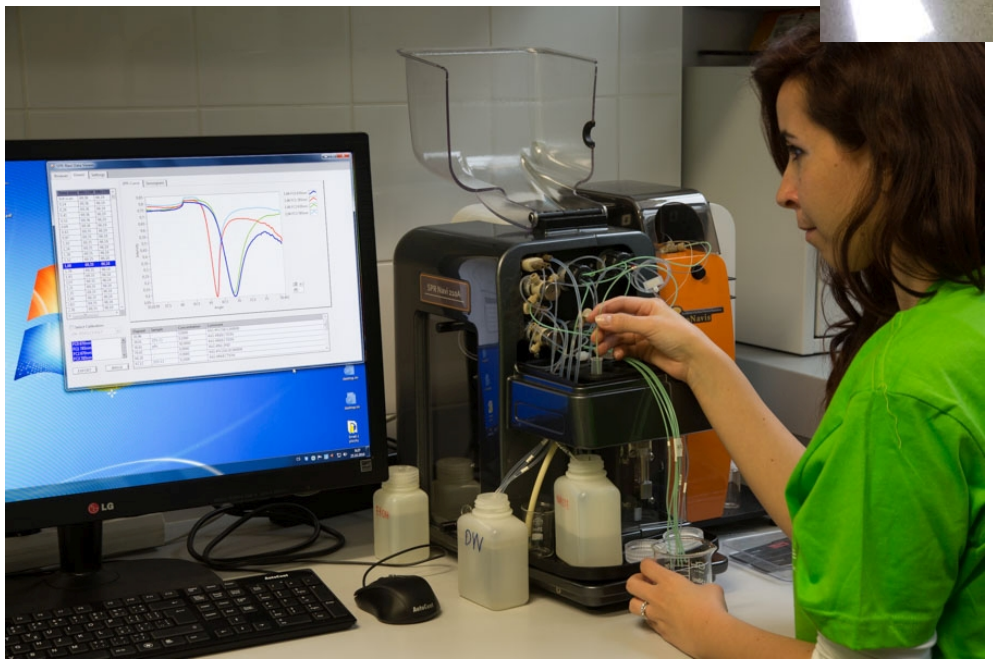
Bruker Dimension Icon FastScan and MultiMode 8HR
NTMDT Ntgra Vita

Raman microscopy, SPR affinity biosensor, Upconverting particles UCNP reader

Renishaw InVia Raman microscope

Bionavis SPR biosensor device

Labrox UPCON reader

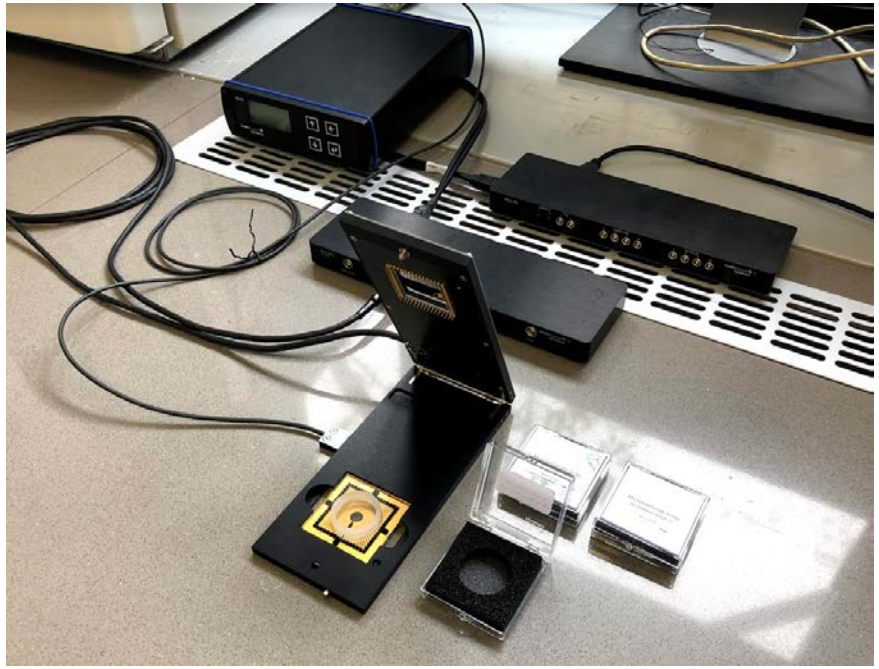


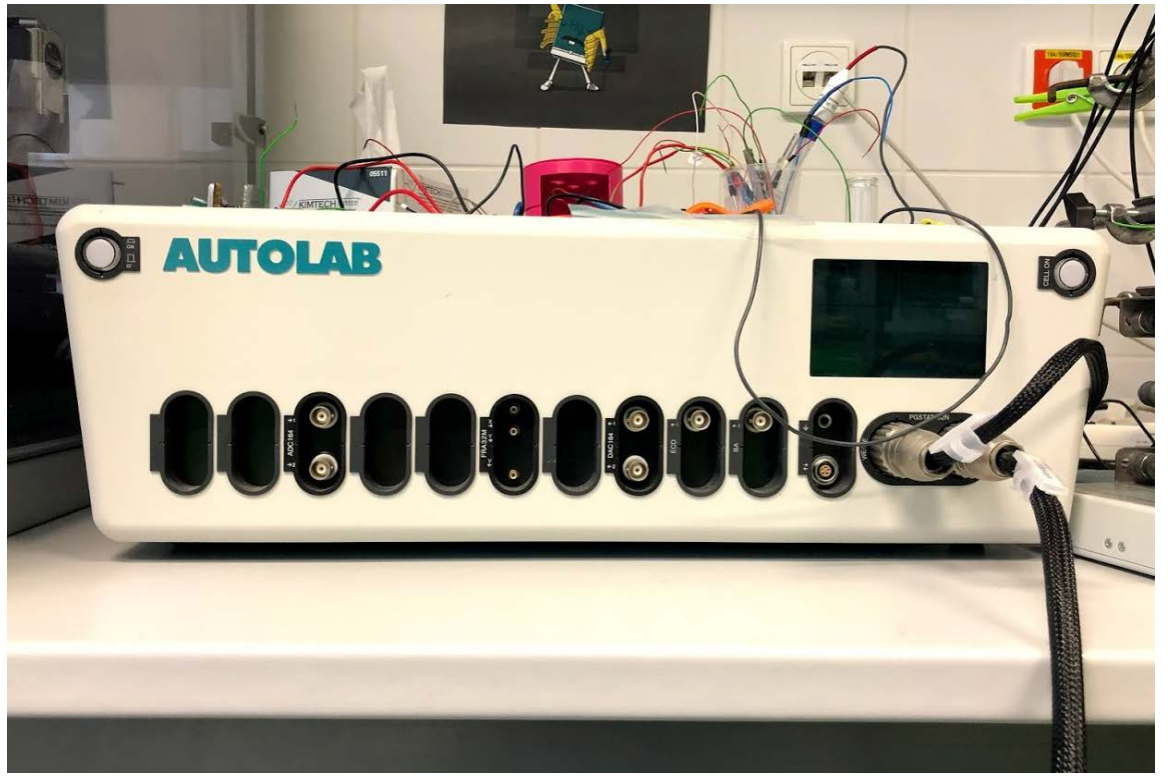
CEITEC

Bioelectrochemistry, Cellular electrophysiology

Autolab Modular potentiostat

MultiChannel MEA2100Lite





CEITEC

Technology and Expertise
List of services

https://www.ceitec.eu/nanobio

1. **Cells – mechanical properties**
2. **Cells - imaging**
3. **Biomolecules - imaging**
4. **Nano-objects imaging**
5. **Raman-AFM combined microscopy**
6. **Raman microscopy**
7. **Electrochemical measurements**
8. **Nanodeposition system**
9. **SPR biosensor**
10. **Scanning of upconversion luminescence**
11. **Multielectrode array recording of cellular potential**

FULL SERVICE / MEASUREMENT only / DATA PROCESSING only

What's new and what's planned?

Upgrades and upgrade plans

OP JAK – infrastructure investments 2023-26

Název infrastruktury	Plánované investiční výdaje 2023–2026 (tis. Kč)[1]	Maximální výše způsobilých výdajů výzvy Výzkumné infrastruktury I OP JAK (tis. Kč)[2]
Czech-BioImaging	1 233 722	493 489
COMPASS	1 050 000	420 000
CzechNanoLab	904 000	361 600
CIISB	720 153	288 061
CZ-OPENSCREEN	377 400	188 700
BBMRI-CZ	369 043	184 522
CCP	357 000	178 500
EATRIS-CZ	281 162	140 581
RECETOX RI	248 600	124 300
METROFOOD-CZ	230 600	115 300
MGML	219 400	109 700
NanoEnviCz	212 720	106 360
CZECRIN	209 682	104 841
ELIXIR-CZ	188 500	94 250
CICRR	159 000	79 500
NCMG	135 300	67 650

40% of the initial plan

CF Nanobio: 16 000 tKč

-15% overhead costs

-29% possible reduction

= 9 000 tKč ~ 380 tEUR

29% over total budget

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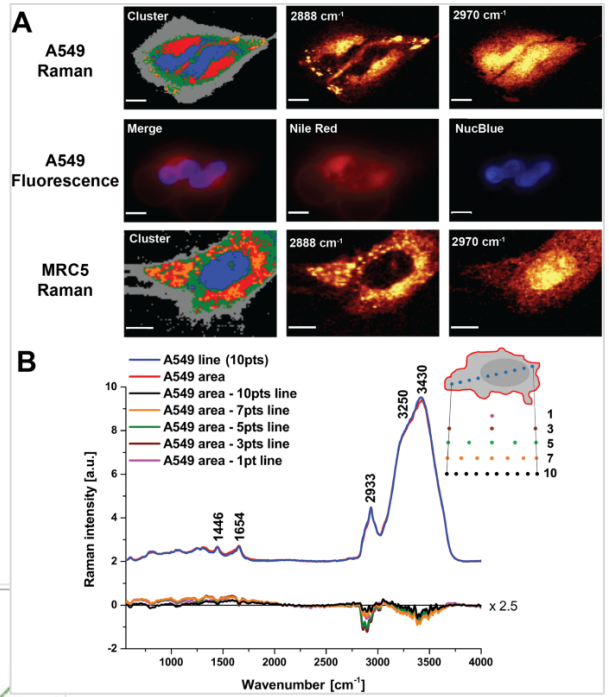
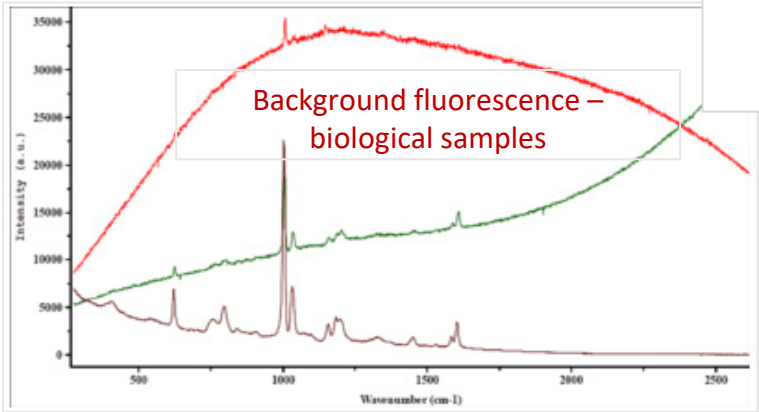
1. Raman microscope upgrade

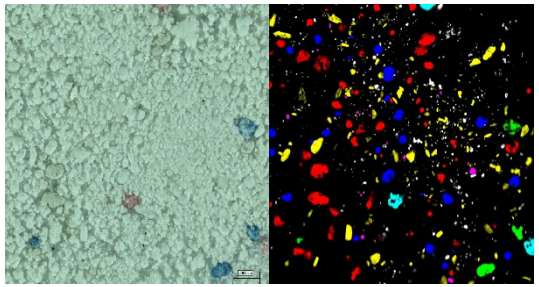
Renishaw InVia confocal Raman microscope



Surmacki, J.M., et al. *Sci Rep* **8**, 12604 (2018).



https://www.azom.com/article.aspx?ArticleID=2950



White light and Raman images of powder

Raman part - upgrade

+ **laser 785 nm**, 100 mW (fluorescence decrease)
+ 1 x 785 nm **polarization**
+ 1 x 633 nm polarization
+ Software upgrade to version **WiRE 5.6**
(incl. **particle analysis** and spectral database modules – **microplastics**)

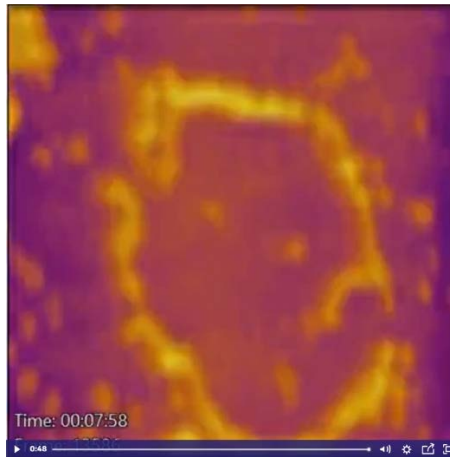
Full integration with AFM

- AFM correlative software
- AFM microscope antivibration solution

Price 140 tEUR

CEITEC

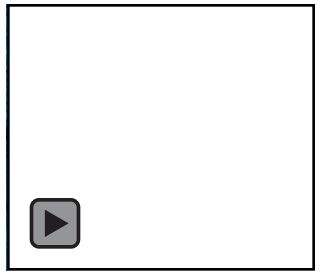
2. High-Speed (Video-Rate) AFM



Size: **425 nm**, line scan rate of **1250 lines/second**
160×32 pixels, (**28 fps**). The playback rate 10×
Source: https://afm.oxinst.com/Video-Rate-AFM-Movies?wvideo=abneb64e3y

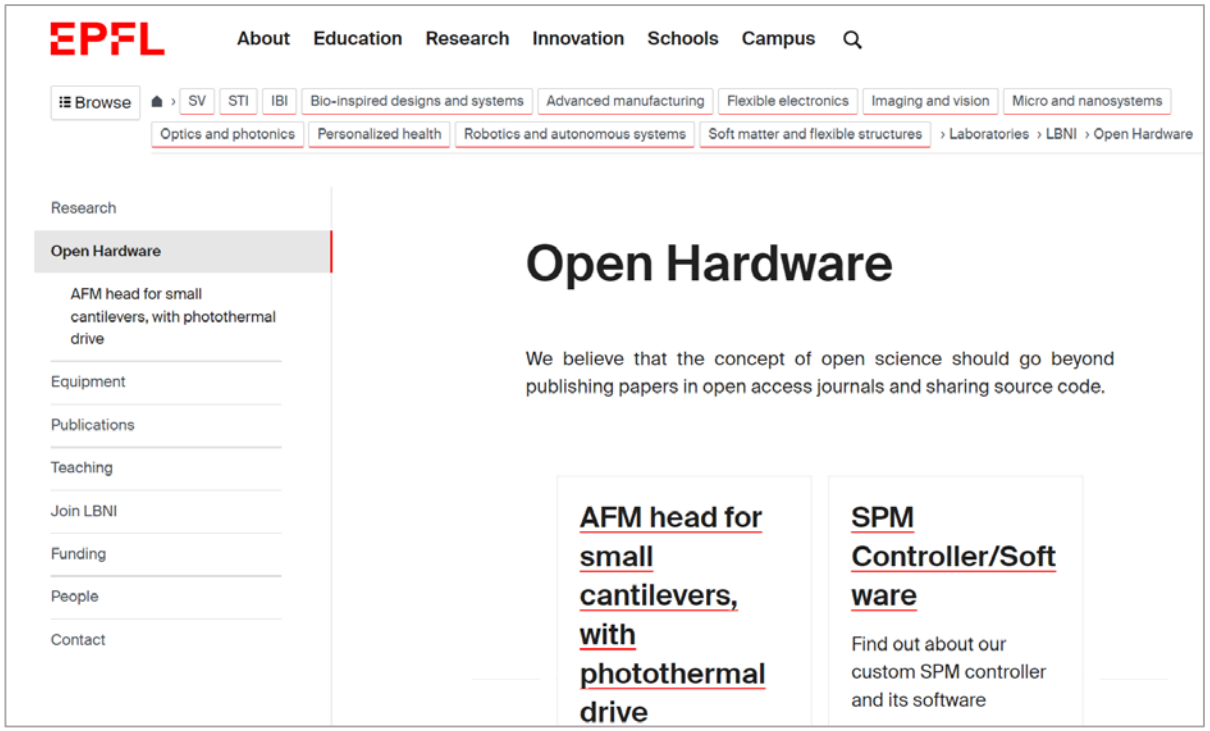
Asylum Cypher VRS1250

Video-Rate High-Speed AFM



Prices from 500 tEUR

Bruker MultiMode 8HR upgrade



https://www.epfl.ch/labs/lbni/openhardware/

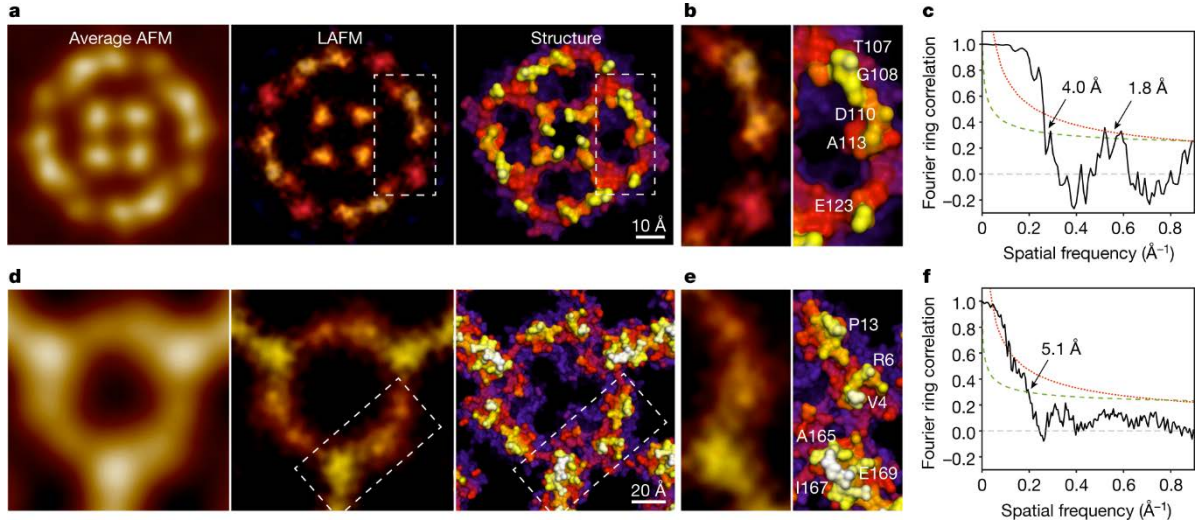
Price 65 tEUR

CEITEC

Advanced data processing

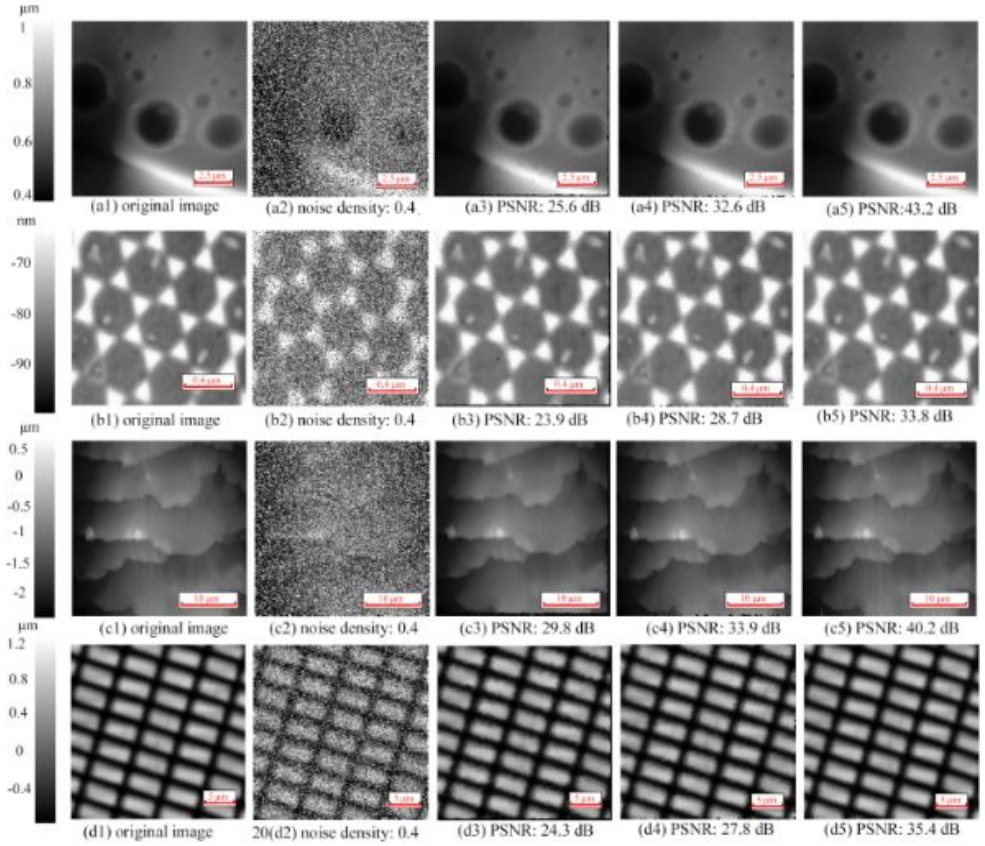
Deconvolution image processing

Deconvolution filters – 50-100 images input (**HS-AFM**):



Heath, G.R., Kots, E., Robertson, J.L. *et al. Nature* **594**, 385–390 (2021).

Denoising with AI:

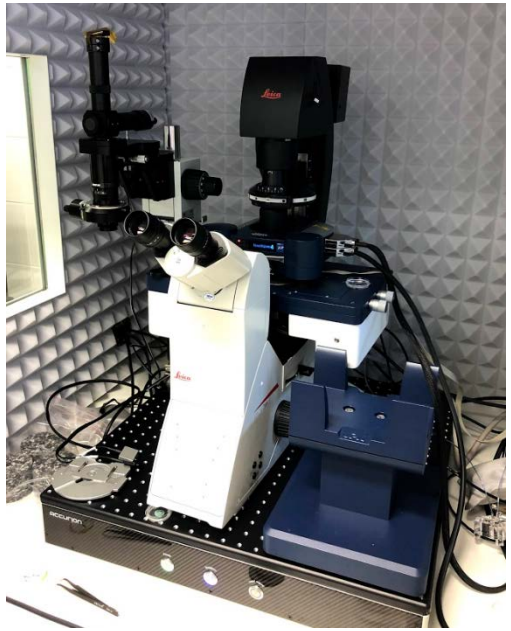


Beilstein J. Nanotechnol. **2019,** *10,* 2346–2356.

Priceless

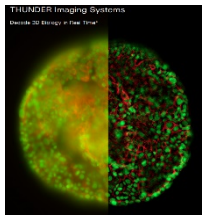
CEITEC

3. Leica Microscope Upgrade



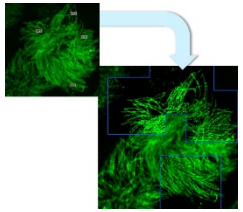
Leica DMi8
*(combined **with JPK NW4XP**)*

+



Leica THUNDER Imaging Systems

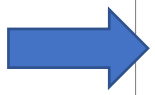
Easily tackle biologically relevant 3D models with THUNDER Imagers.
They bring you high-speed, multicolor imaging of thin and thick samples with increased temporal resolution in the first attempt itself.

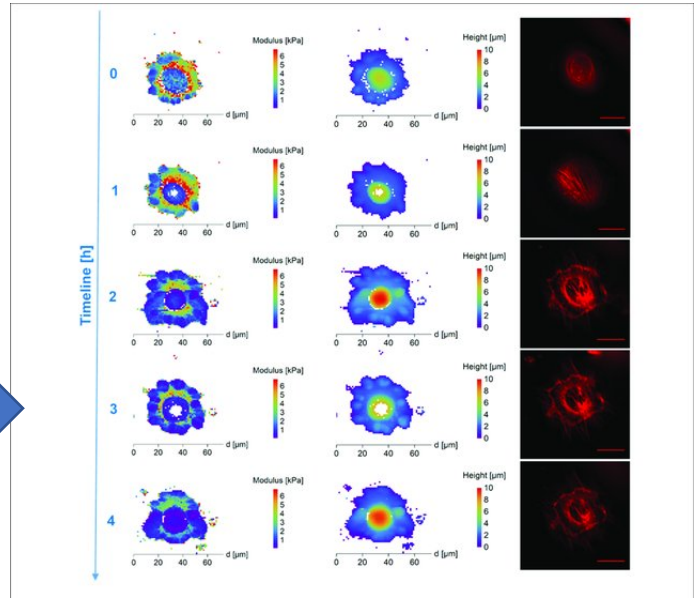


Telight LiveCodim

From conventional to super-resolution microscopy

LiveCodim is a universal, super-resolution imaging platform, designed to interface with any standard fluorescence microscope. It is the solution for live imaging with high resolution and low phototoxicity.



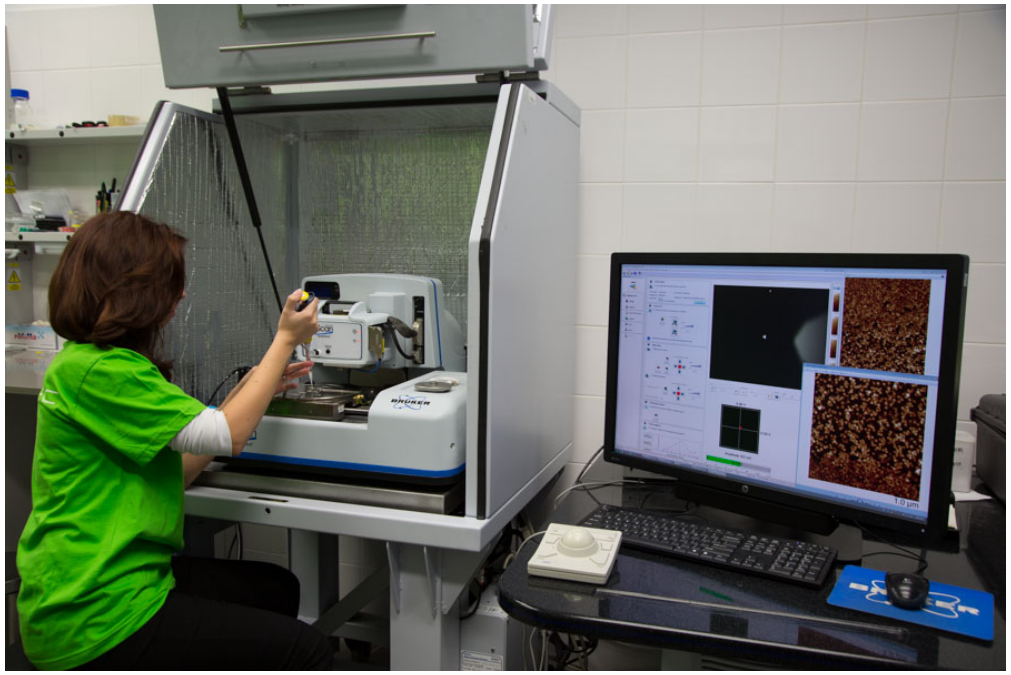


AFM – confocal correlation microscopy

Price 120 tEUR

CEITEC

4. Bruker Dimension FastScan Upgrade



In everyday operation from 2014

AFM controller upgrade:

Price 80 tEUR

CEITEC

CIISB
Czech Infrastructure for Integrative Structural Biology

instruct Integrating Biology

(LM2023042)

EUROPEAN UNION
European Structural and Investment Funds
Operational Programme Research, Development and Education

MINISTRY OF EDUCATION, YOUTH AND SPORTS

OP VVV CZ.02.1.01/0.0/0.0/18_046/0015974

Thank you for your attention!

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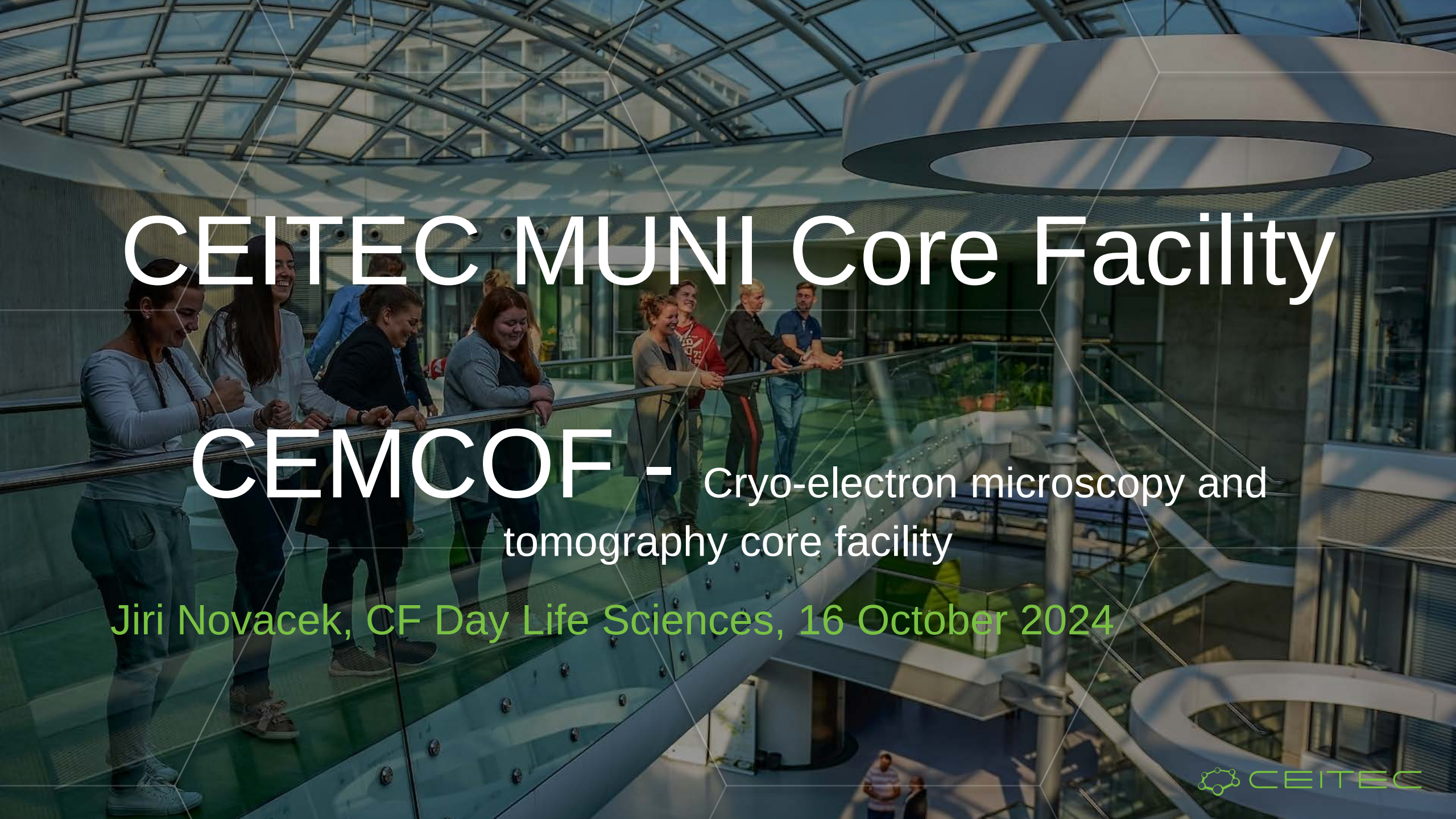
Core Facility Day 2024
Life Sciences

16 OCTOBER, 2024
CEITEC, E35/211+ATRIUM

Curious about what expert services are available to researchers on campus? What instruments can you use in shared mode and under what conditions? Do you want to see everything for yourself?

Register at: muni.cz/go/fba265



CEITEC MUNI Core Facility

CEMCOF - Cryo-electron microscopy and tomography core facility

Jiri Novacek, CF Day Life Sciences, 16 October 2024

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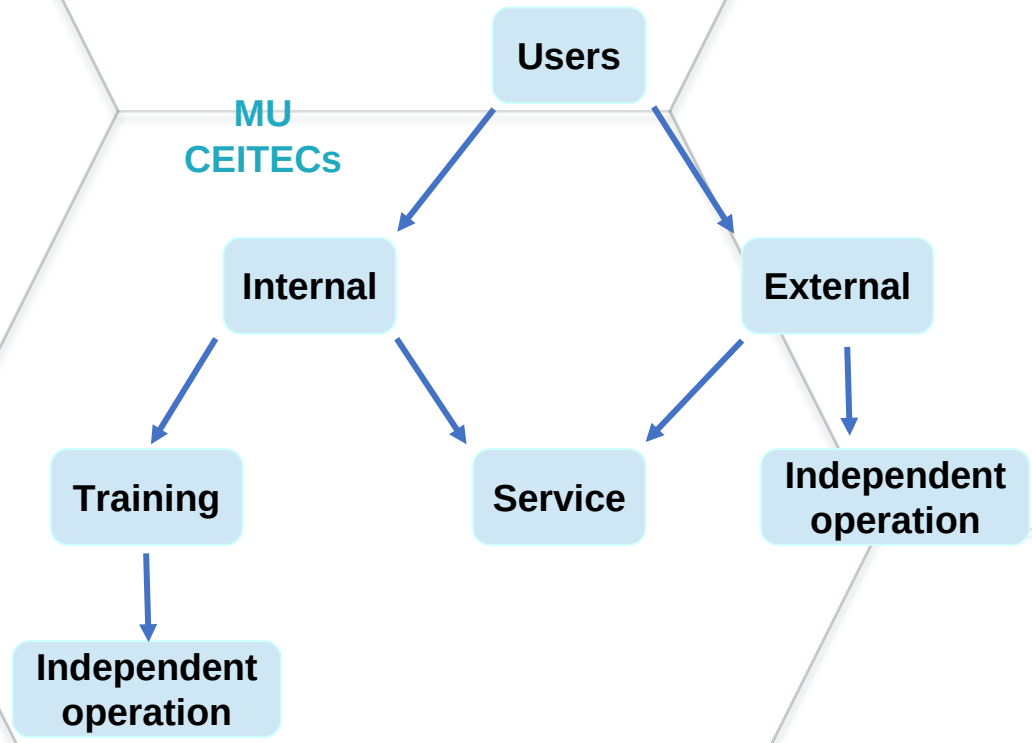
Users & services

- **Services:**
  - TEM/SEM imaging
  - Sample vitrification
  - Resin embedding
  - FIB-SEM tomography
  - Initial structural screening
  - Initial cryo-EM screening
  - Analytical techniques (EDS)
  - Cryo-FIB lamella preparation
  - SPA data collection
  - Cryo-ET data collection
  - Electron diffraction tomography
  - (cryo-)volume EM
  - Data analysis

User mode or service mode available on all instruments



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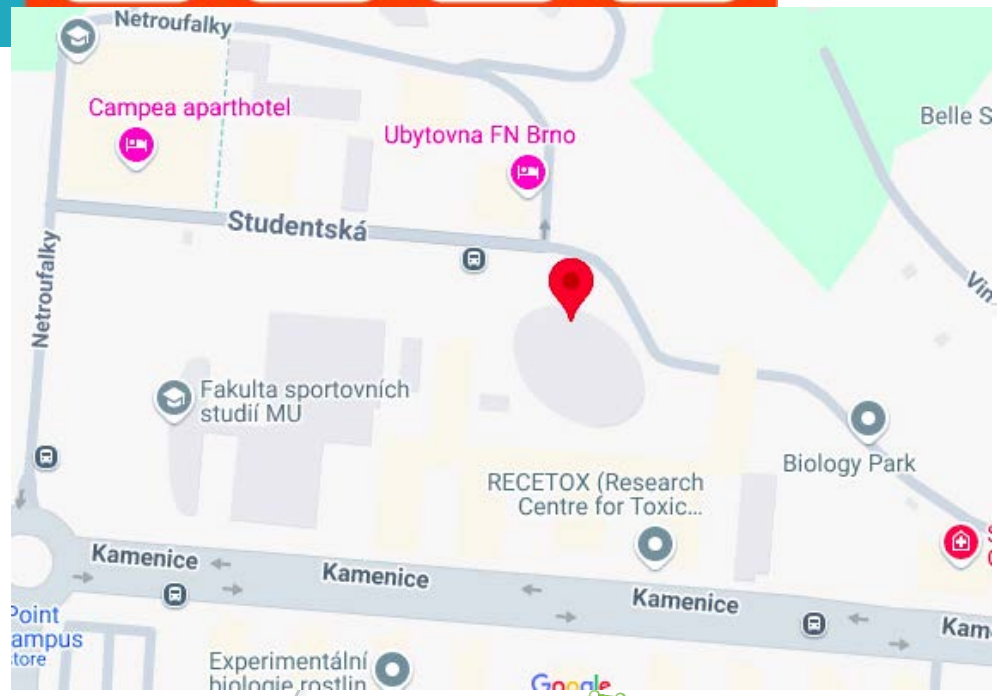
Users & services

- **New users:**
  - select access route
  - Fill in project/application form
  - Arrange service via email
  - Get trained for corresponding instrument

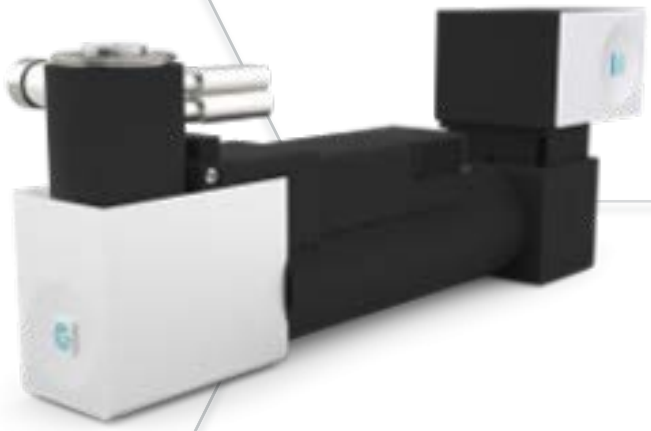
https://cryo.ceitec.cz

- **Active users:**
  - remember to renew your project application – email - single mouse click
  - Instruct – one Visit (access) limited to 2 days of microscope time
  - ask CF staff for help anytime needed
  - report issues

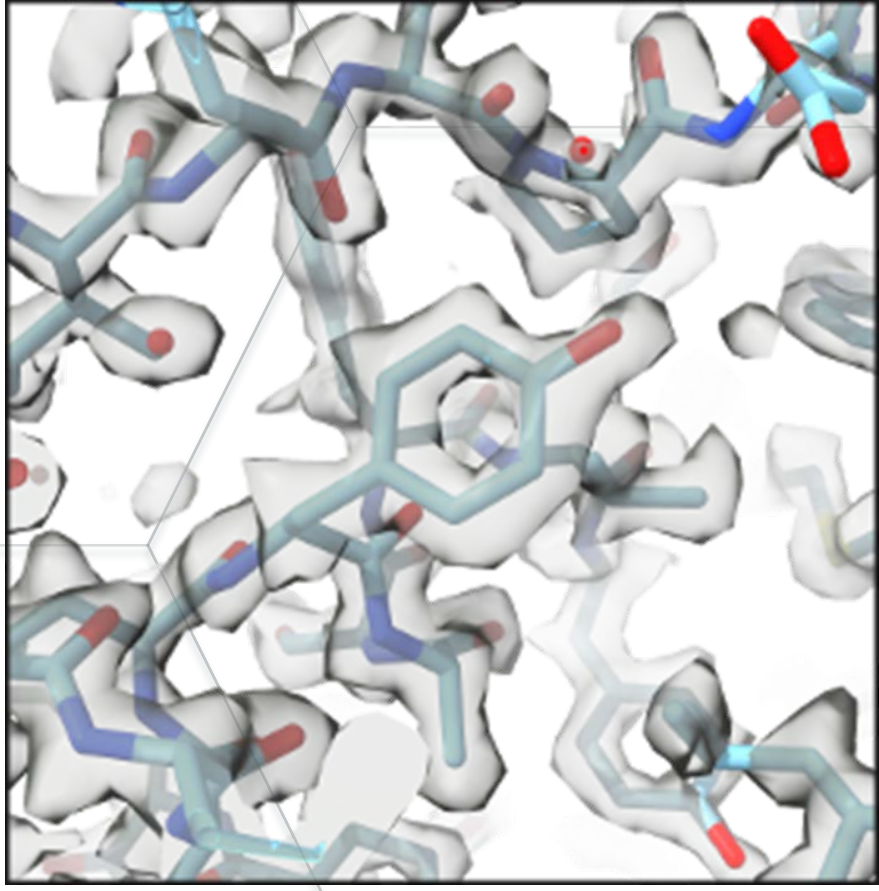


New instrumentation & services

- **Talos Arctica upgrade – Selectris & Falcon4i**
  - Community:
    - Structural Biology



  - Features:
    - high stability
    - simple and robust operation
    - second high-end cryo-TEM (together with Titan Krios)
    - SPA
      - throughtput – 600-900 movies/hour
      - quality – benchmark data on apoferritin < 1.8A
    - cryo-ET
      - tomography on cellular lamellae



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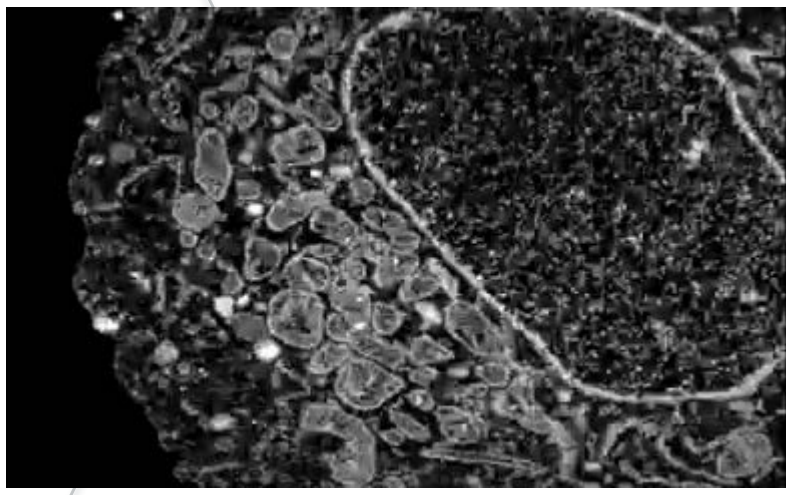
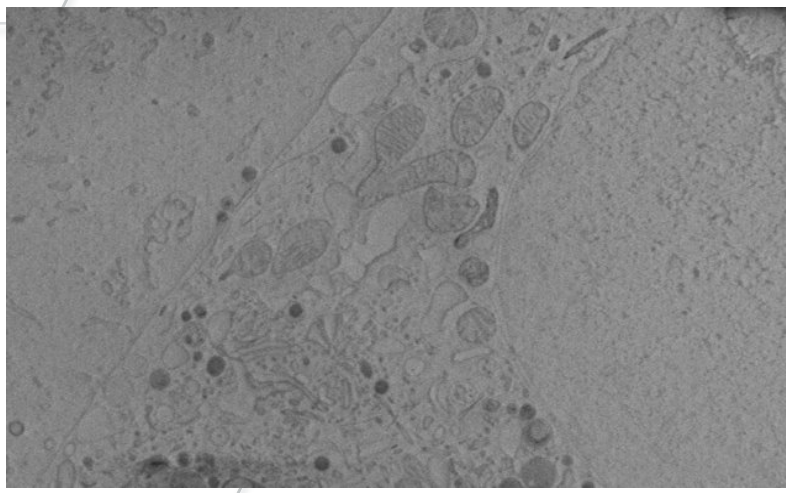
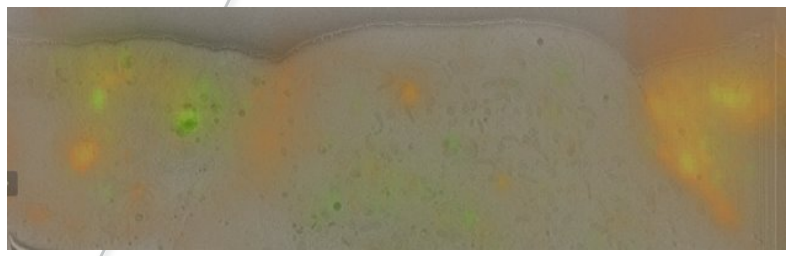
New instrumentation & services

- **pFIB/SEM – Helios Hydra V**
  - Community:
    - Cellular & Structural Biology
  - Features:
    - high-resolution SEM imaging (immersion)
    - cryo-EM & RT applications
      - volume EM of resin samples
      - cryo-volume EM – HPF specimen
    - lamella preparation for cryo-ET
    - correlative volume EM – internal development of on-chamber confocal microscope – Pavel Krepelka
    - development of new techniques on Versa – AFM&SEM







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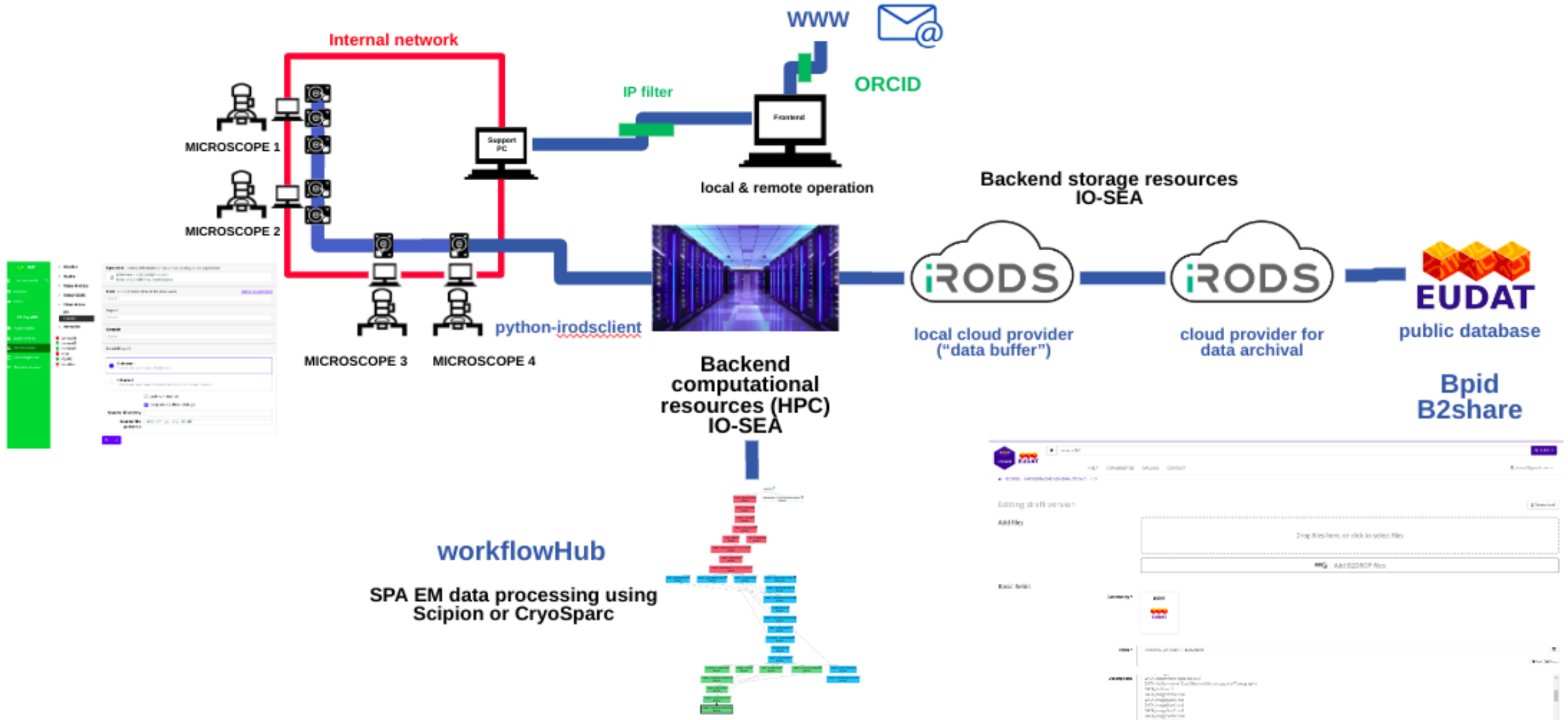
New instrumentation & services

- **Blot free vitrification device – Chameleon**
  - Community:
    - Structural Biology
  - Features:
    - available from December 2024
    - low sample volume (x higher sample concentration)
    - high-level of automation – minimal user interaction (grid handling)
    - Increased reproducibility and repeatebility of sample preparation by freezing sample preparation
    - primarily for SPA

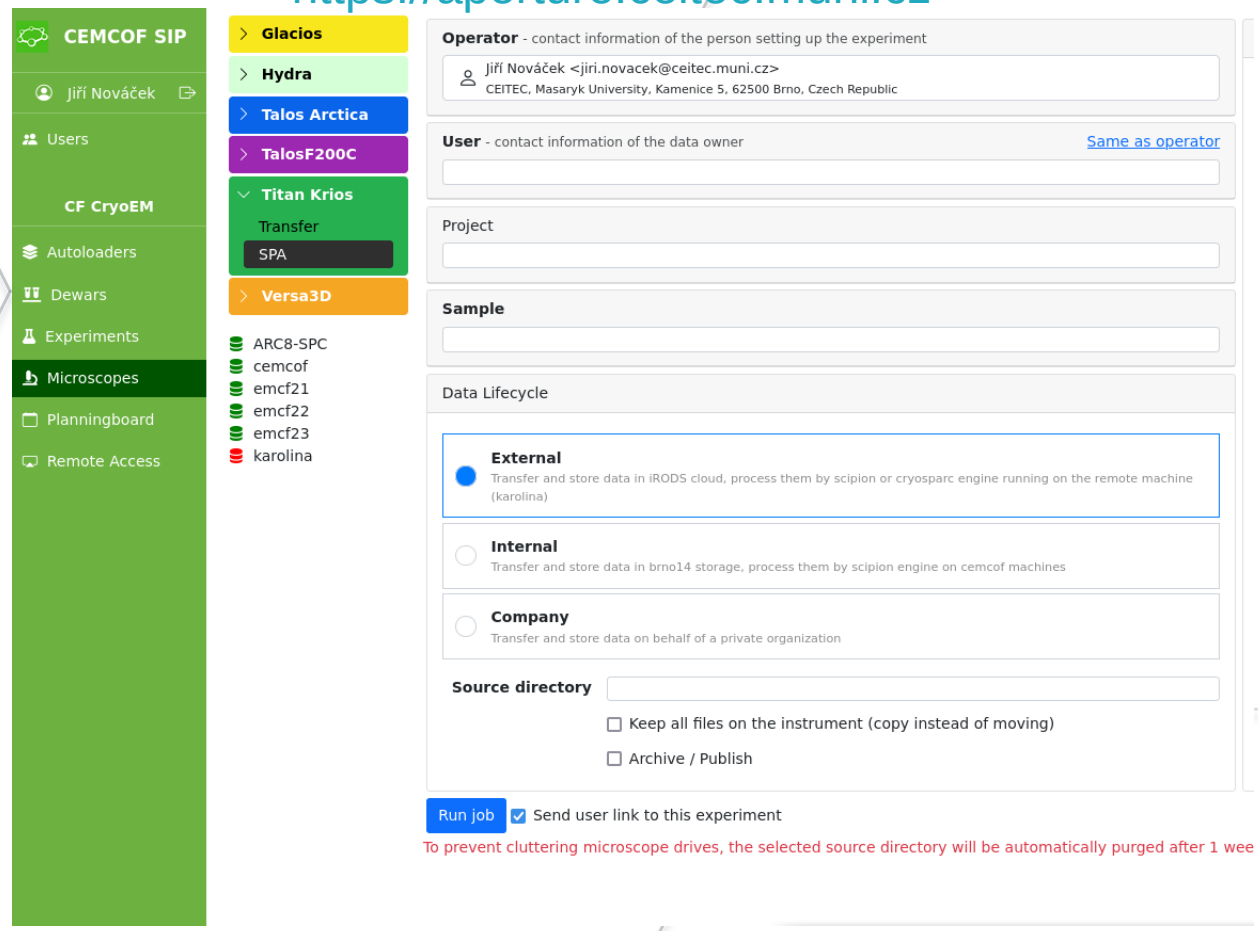
Data management



Data management

- web-browser based operation
- accessible directly from the instrument/microscope
- secure access from outside the microscope network:
  - Google
  - eduID
  - ORCID
- instrument specific setup
- implementation of different data analysis workflows
  - simple data transfer (e.g. cryo-EM screening)
  - single particle analysis
  - cryo-ET
- data-model with four different components:
  - the laboratory (center)
  - the user (data owner)
  - the sample
  - the data
- based on ISPyB data model
- real-time job status
- automated user notification (email)
- local database of the projects

https://aperture.ceitec.muni.cz



Data management

- every experiment has a unique experiment card
  - shared with data owner via email
  - information about experiment (including notes)
  - data acquisition report (quality control)
  - single site for the interaction with data status
  - notification by email before data expiration or publication

- for users: read carefully the data management policy a requested status for particular dataset

- for PIs: each dataset will be assigned with DOI upon publication (after embargo period or upon request) - can be used for raw data publication (currently through EUDAT)

- Future development – implementation of deposition initiation to method-specific database (EMPIAR)

experiment card

241013_IR - Sample test 1

Center	CF CryoEM
Operator	[redacted]
User	
Experiment started	10/14/2024 7:37:15 AM
Instrument	TitanKrios
Experiment technique	EM-SPA
Sample	Sample test 1
Sample keywords	testovaci; test

Data status: Draft creation requested — Do not archive and publish this dataset

Embargo ends: 14.10.2027 (in 2 years, 11 months)

Since this dataset has been marked to be archived, it is expected to be assigned public identifier (DOI) and made publicly available either automatically after embargo period or earlier on your decision.

Request publication now

Data access

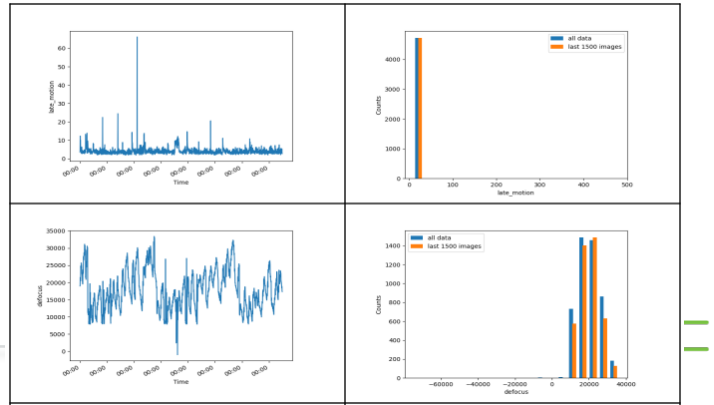
The dataset has been stored at the following location, and you can access it provided that you were given credentials (username/password/ssh key) by the facility:

`storage-brno14-ceitec.metacentrum.cz:/gpfs/vol1/export/nfs4/shared/cemcof/internal/DATA_24/241013_IR`

On Windows, you can use for example WinSCP program to access and copy the data.

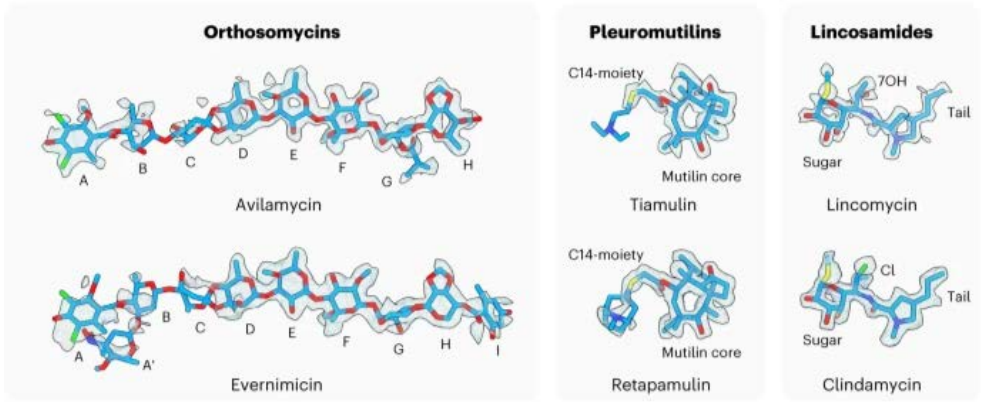
On Linux / macOS, you can use for example the rsync utility:

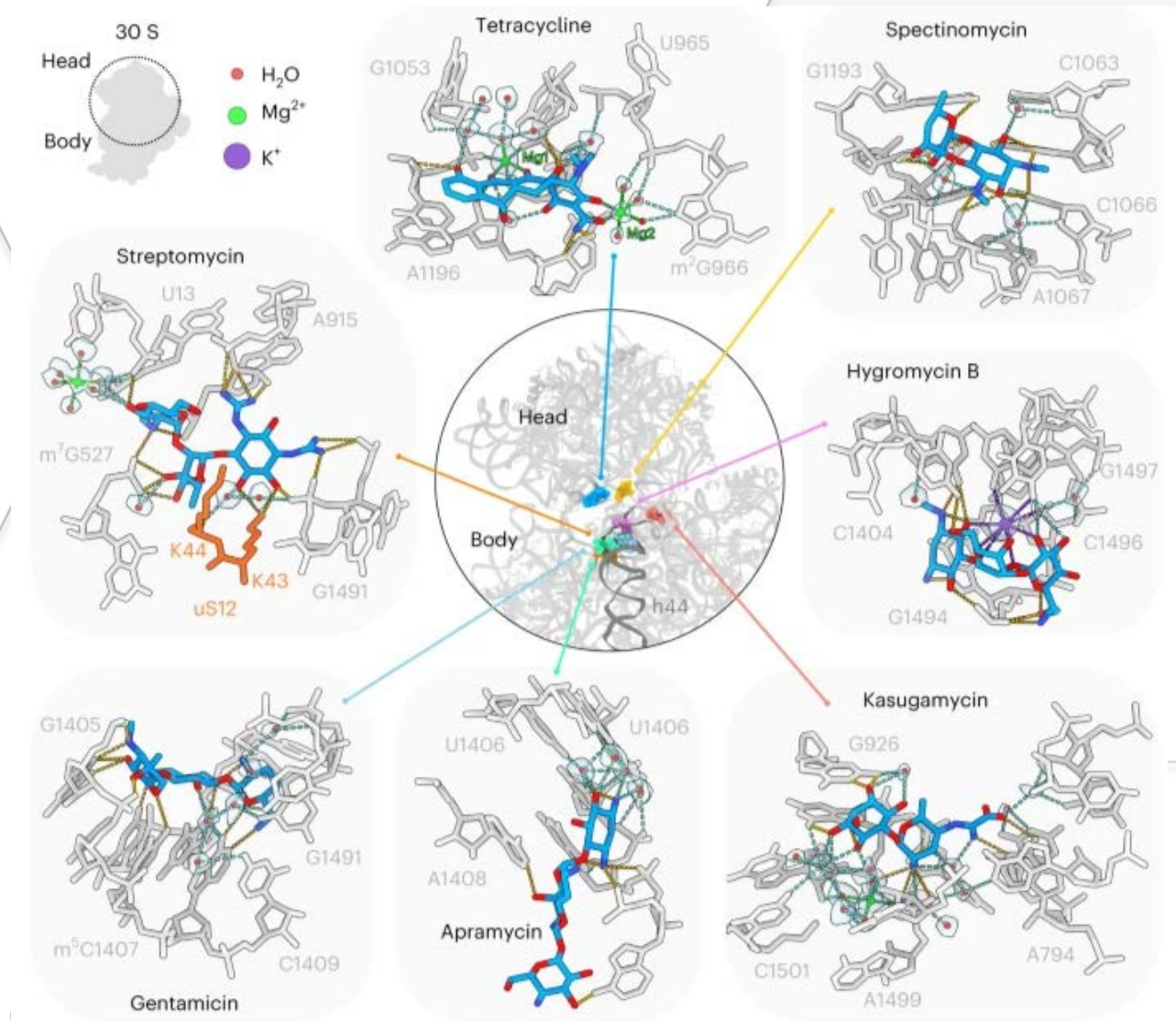
```
rsync -av --progress [username]@storage-brno14-ceitec.metacentrum.cz .
```



User projects/results

- Daniel Wilson group (University of Hamburg)
- sub-2A resolution structures of 17 different antibiotics bound to bacterial ribosome
- antibiotic-RNA interaction network
- conservation of binding mode for antibiotics with the same scaffold
- visualisation of water molecules in the binding site





Patternoga et. al (2023), NSMB, doi.org/10.1038/s41594-023-01047-y

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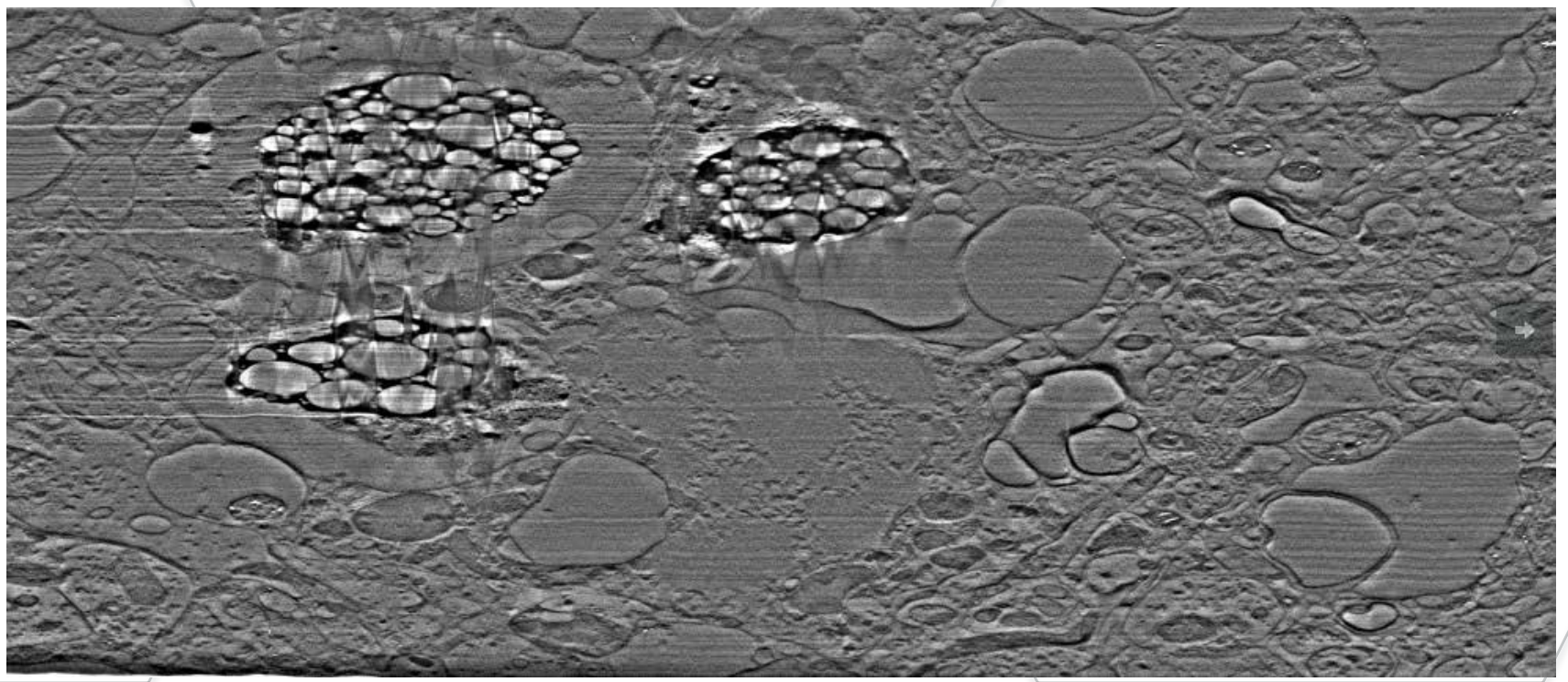
User projects/results

- Hana Nedozralova (Lukas Zidek RG, CEITEC)
- cryo-volume EM of Alzheimer patient's brain
- no heavy metal contrasting -> near-native state (high-pressure frozen)
- volumetric analysis of selected brain tissue regions



Akcnowledgements

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Core Facility Day 2024
Life Sciences

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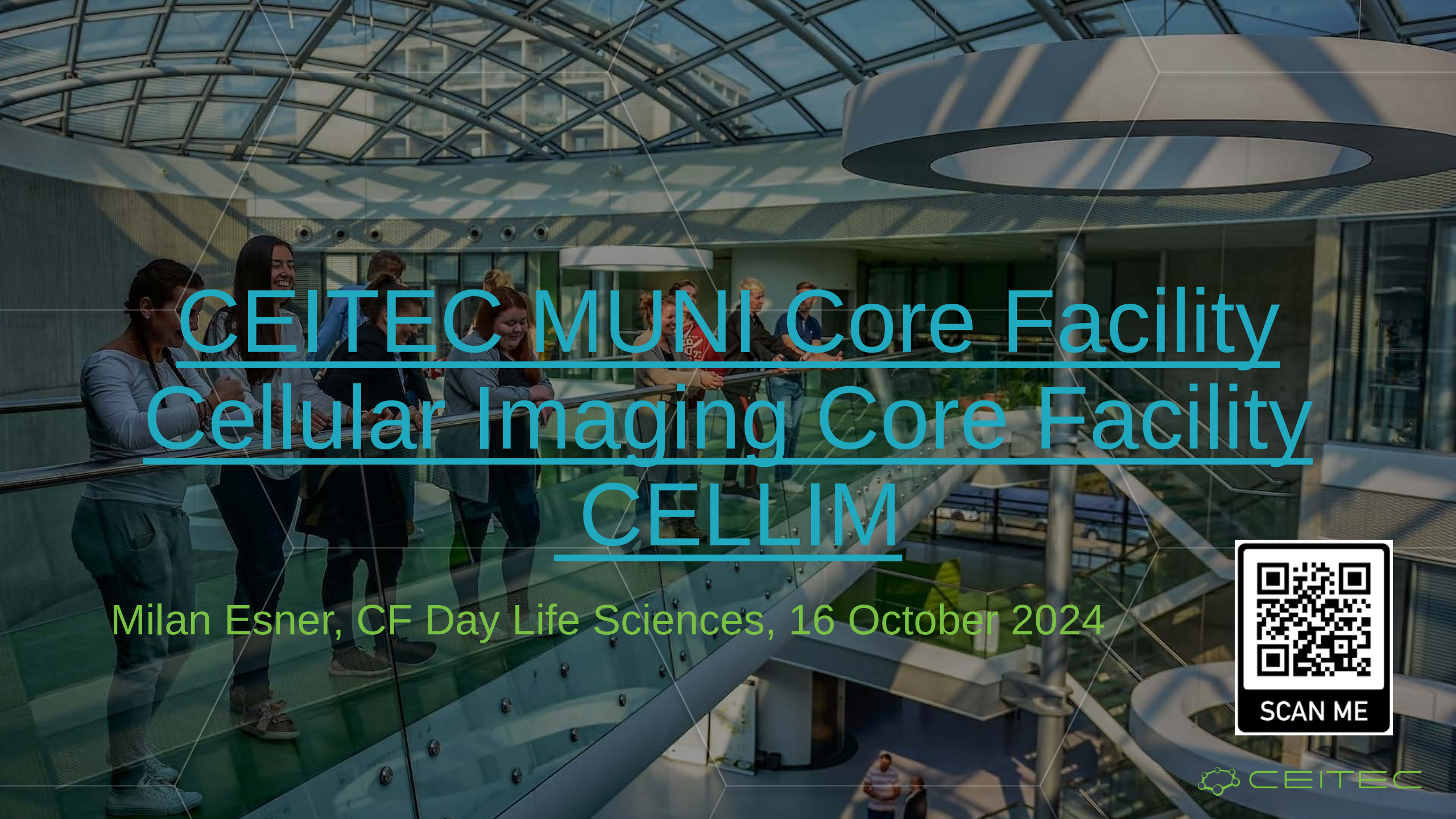

CEITEC MUNI Core Facility Cellular Imaging Core Facility CELLIM

Milan Esner, CF Day Life Sciences, 16 October 2024

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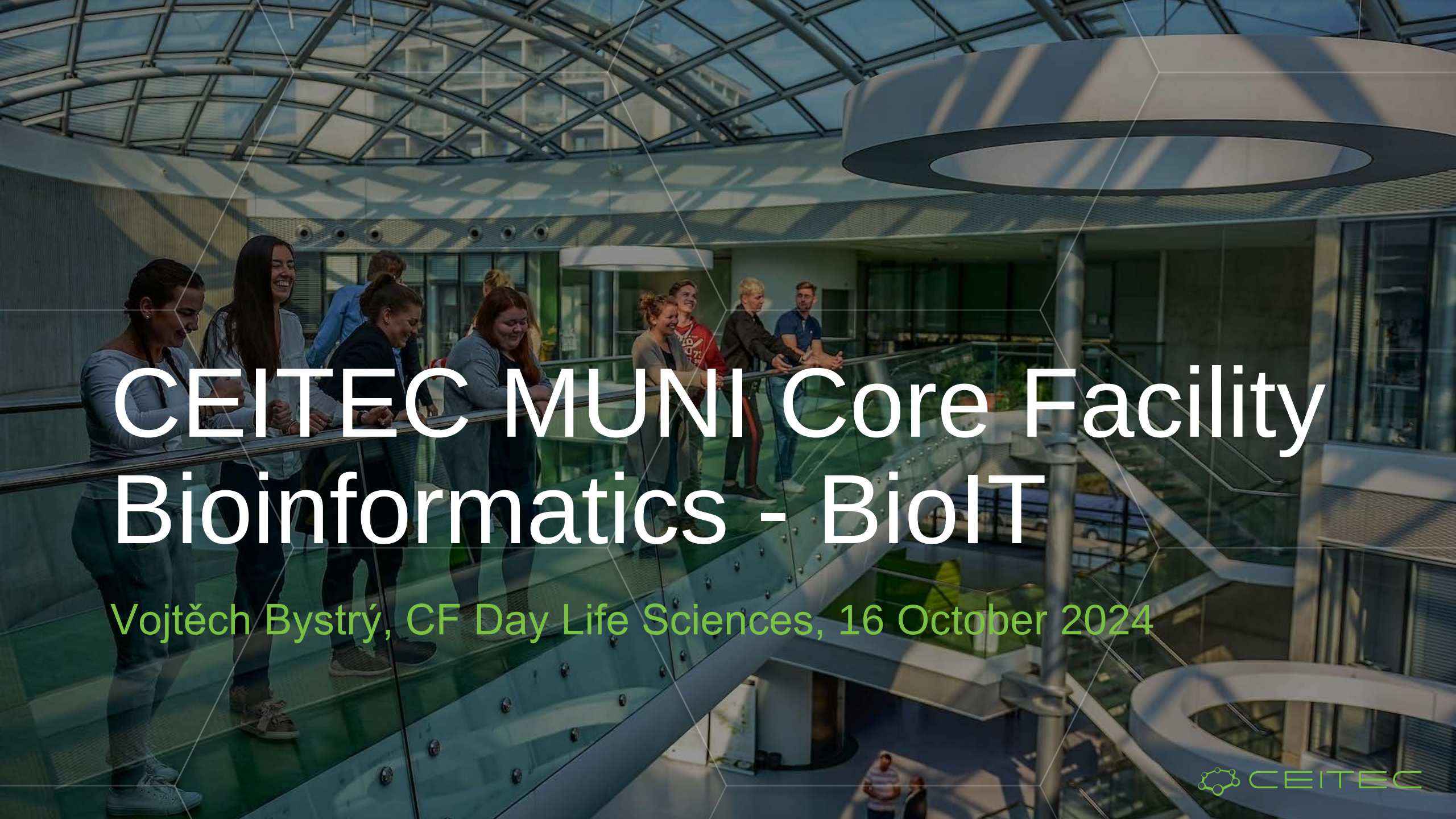

CEITEC MUNI Core Facility Bioinformatics - BioIT

Vojtěch Bystrý, CF Day Life Sciences, 16 October 2024

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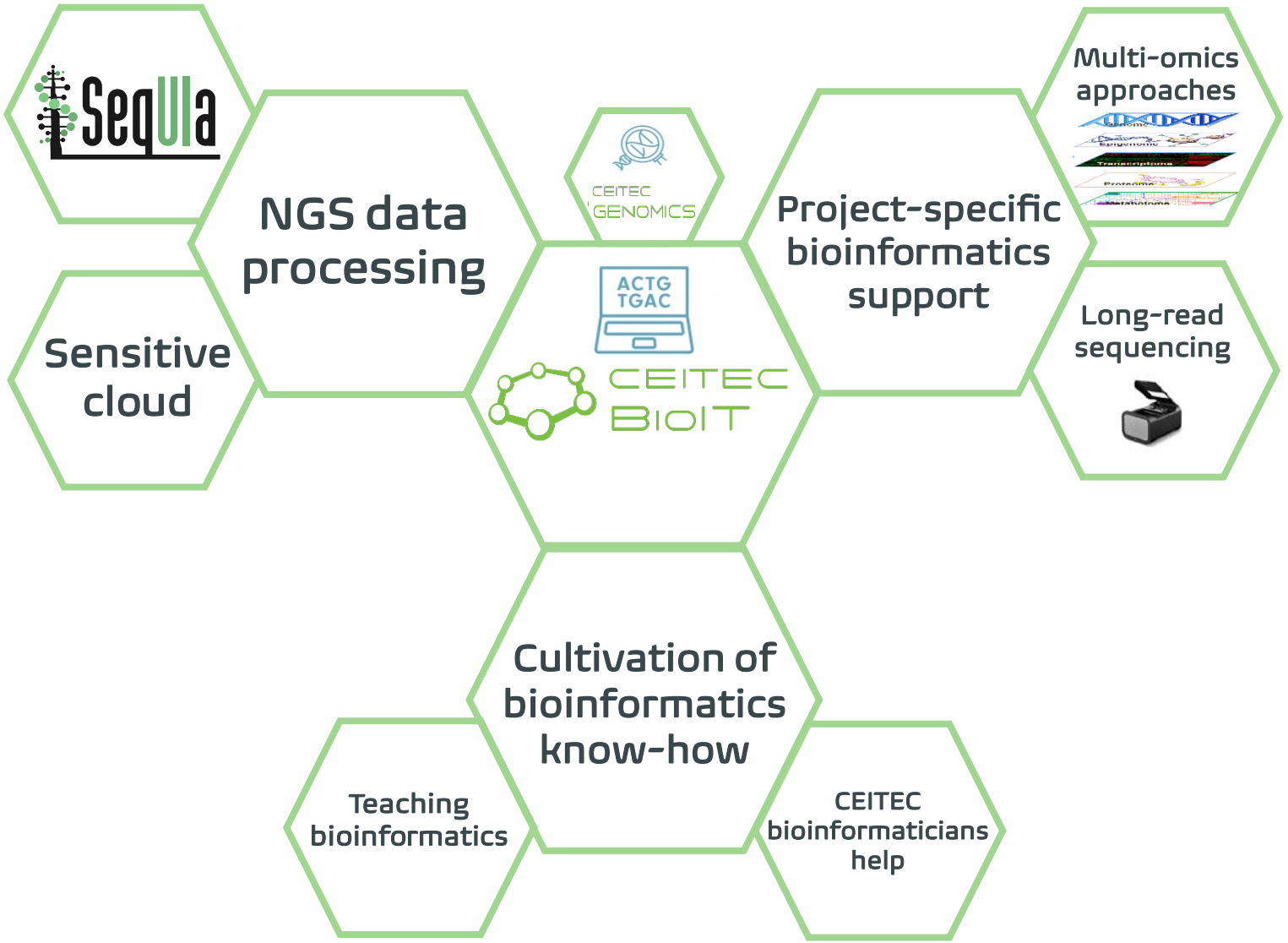
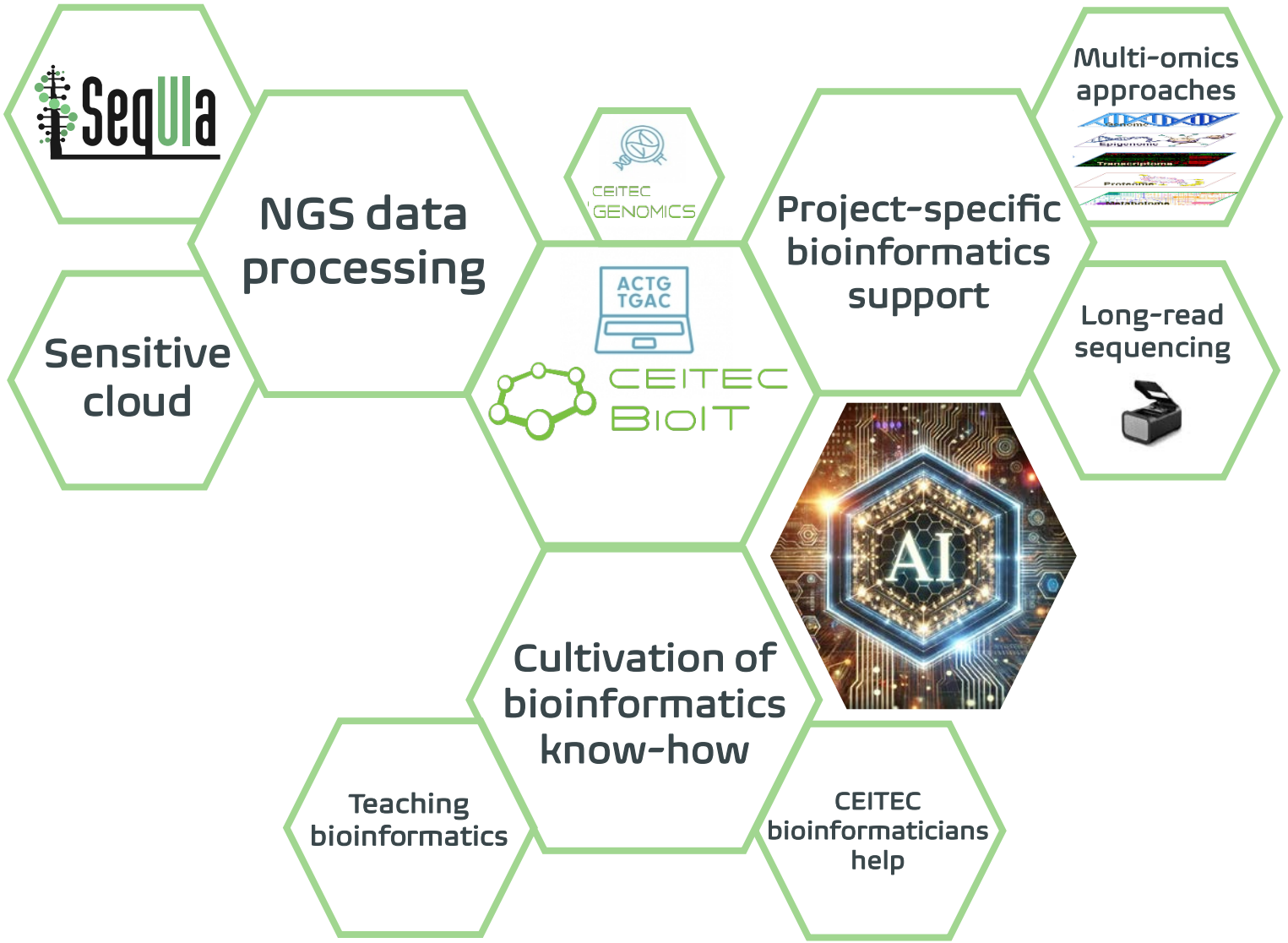

SeqUla
NGS data processing
Sensitive cloud
CEITEC GENOMICS
ACTG TGAC
CEITEC BioIT
Project-specific bioinformatics support
Multi-omics approaches
Long-read sequencing
Cultivation of bioinformatics know-how
Teaching bioinformatics
CEITEC bioinformaticians help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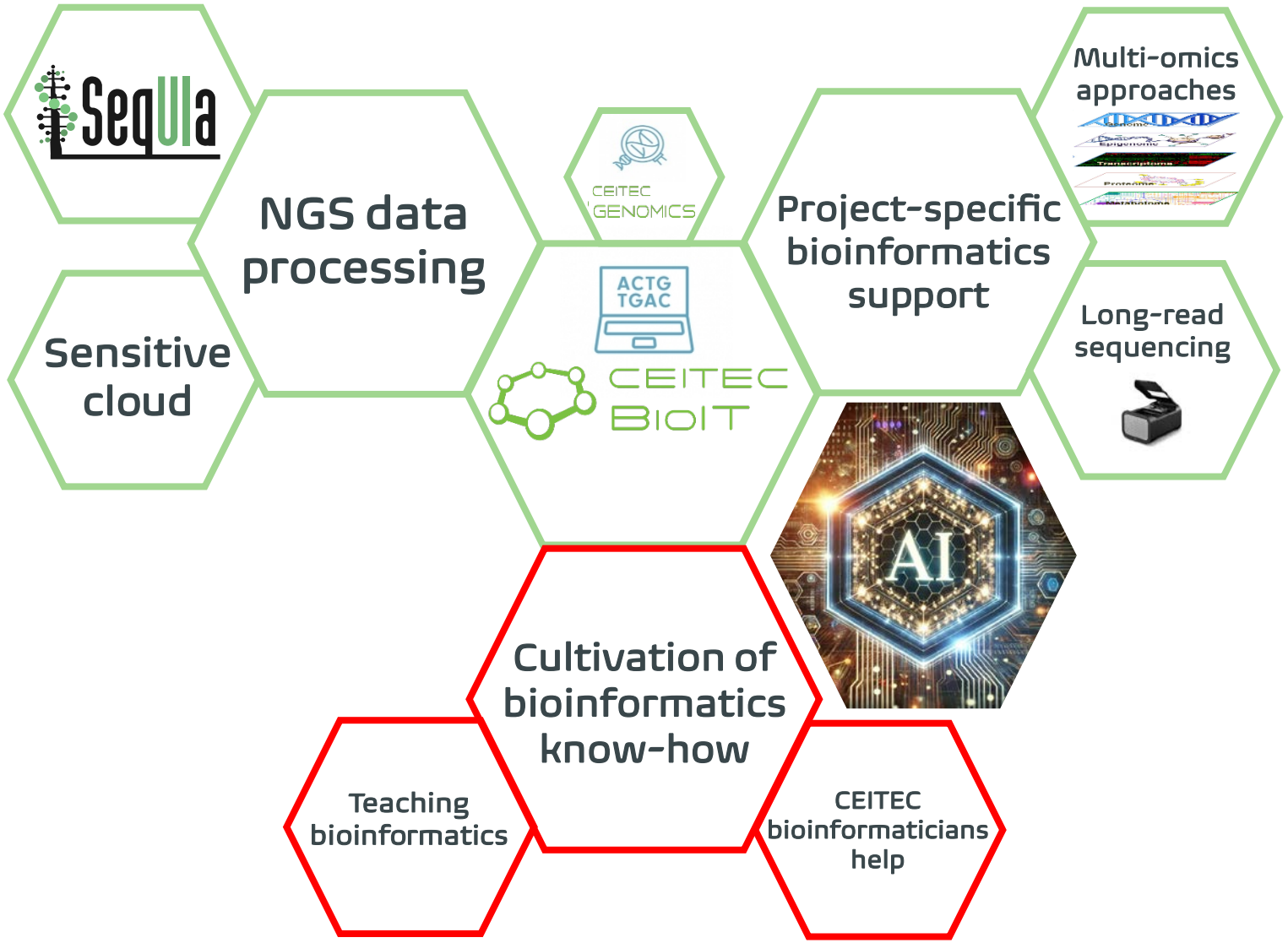
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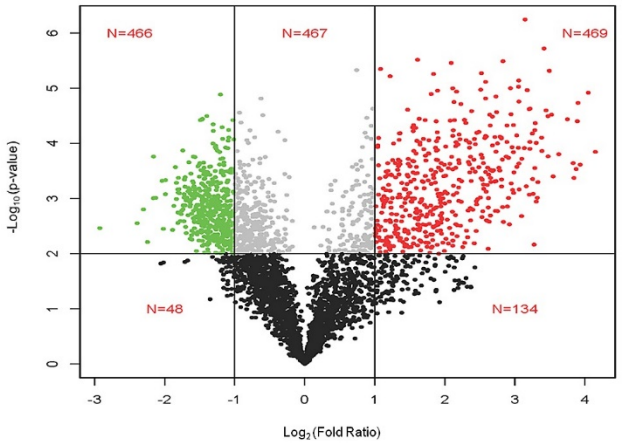
Teaching bioinformatics
CEITEC bioinformaticians help

Genes	LogFC	FDR	Genes	LogFC	FDR
RNASE2	−4.2668	1.25E-24	LMO2	−2.02467	1.26E-04
CLC	−4.94929	1.05E-13	CD24	−2.24512	1.65E-04
PRG3	−3.90837	2.93E-12	MRC1	−2.06384	2.36E-04
RNASE3	−4.31871	5.08E-12	CRISP3	−2.73151	2.55E-04
PRG2	−5.93443	1.01E-09	MS4A3	−2.17214	2.61E-04
MPO	−2.52454	8.15E-09	ZNF358	2.042213	2.66E-04
DEFA4	−2.22389	1.70E-08	MS4A6A	−2.21587	3.54E-04
ELANE	−4.39842	1.94E-08	IL4R	−2.1392	3.74E-04
EPX	−3.18113	9.02E-08	PXDC1	−2.08509	4.67E-04
ARMC7	2.314169	2.21E-07	CD320	2.241042	4.83E-04
CAMP	−3.0549	9.82E-07	CD163	−2.52643	5.17E-04
IGHG1	−3.7307	2.23E-06	LUM	−3.58203	5.20E-04
CTSH	−2.87845	3.55E-06	CXCL8	−2.40243	5.26E-04
AIF1	−2.16656	4.43E-06	NOD2	−2.95453	5.26E-04
LST1	−2.19262	8.38E-06	S100A8	−2.70373	5.61E-04
IGLJ3	−4.49176	1.13E-05	CXCL2	−2.71229	5.61E-04
CLPP	2.32109	1.65E-05	IGHD	−4.07084	5.84E-04
LTF	−3.89554	1.65E-05	HMOX1	−2.36868	5.99E-04
FABP4	−2.79511	3.18E-05	MS4A4A	−3.38126	6.11E-04
LYVE1	−2.9819	3.18E-05	HIF1A	−2.13129	6.18E-04
NRP1	−2.08155	3.34E-05	VNN2	−2.4071	6.18E-04
S100A12	−2.16333	3.34E-05	MAFB	−3.4547	6.41E-04
CEACAM8	−3.52708	4.20E-05	ALDH1A3	−2.01185	6.80E-04
IGLV1-44	−4.8402	6.64E-05	LHFP	−2.18934	6.98E-04
KCTD12	−2.56891	6.99E-05	S100A9	−2.3273	8.20E-04
CD14	−3.15551	7.82E-05	MNDA	−3.14832	9.14E-04
RPS11	2.079562	8.44E-05	HLA-DPA1	−2.64283	9.63E-04
IGK	−3.99784	9.70E-05	TGFBI	−2.93660	9.89E-04
P2RY13	−2.46684	1.05E-04	MAGEA4	2.361871	9.92E-04
DTX2	2.071491	1.05E-04	MROH7	−2.03615	9.95E-04

FC, fold change; FDR, false discovery rate.



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GitHub Copilot

https://github.com/education

Join GitHub Education >

Genes	LogFC	FDR	Genes	LogFC	FDR
RNASE2	−4.2668	1.25E-24	LMO2	−2.02467	1.26E-04
CLC	−4.94929	1.05E-13	CD24	−2.24512	1.65E-04
PRG3	−3.90837	2.93E-12	MRC1	−2.06384	2.36E-04
RNASE3	−4.31871	5.08E-12	CRISP3	−2.73151	2.55E-04
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DEFA4	−2.22389	1.70E-08	MS4A6A	−2.21587	3.54E-04
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ARMC7	2.314169	2.21E-07	CD320	2.241042	4.83E-04
CAMP	−3.0549	9.82E-07	CD163	−2.52643	5.17E-04
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CTSH	−2.87845	3.55E-06	CXCL8	−2.40243	5.26E-04
AIF1	−2.16656	4.43E-06	NOD2	−2.95453	5.26E-04
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CLPP	2.32109	1.65E-05	IGHD	−4.07084	5.84E-04
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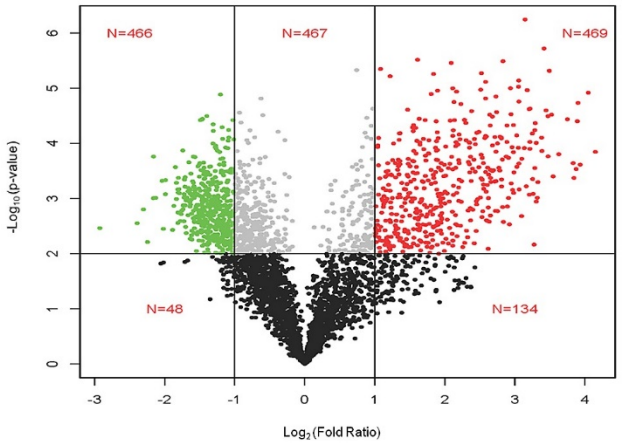
FABP4	−2.79511	3.18E-05	MS4A4A	−3.38126	6.11E-04
LYVE1	−2.9819	3.18E-05	HIF1A	−2.13129	6.18E-04
NRP1	−2.08155	3.34E-05	VNN2	−2.4071	6.18E-04
S100A12	−2.16333	3.34E-05	MAFB	−3.4547	6.41E-04
CEACAM8	−3.52708	4.20E-05	ALDH1A3	−2.01185	6.80E-04
IGLV1-44	−4.8402	6.64E-05	LHFP	−2.18934	6.98E-04
KCTD12	−2.56891	6.99E-05	S100A9	−2.3273	8.20E-04
CD14	−3.15551	7.82E-05	MNDA	−3.14832	9.14E-04
RPS11	2.079562	8.44E-05	HLA-DPA1	−2.64283	9.63E-04
IGK	−3.99784	9.70E-05	TGFBI	−2.93660	9.89E-04
P2RY13	−2.46684	1.05E-04	MAGEA4	2.361871	9.92E-04
DTX2	2.071491	1.05E-04	MROH7	−2.03615	9.95E-04

FC, fold change; FDR, false discovery rate.



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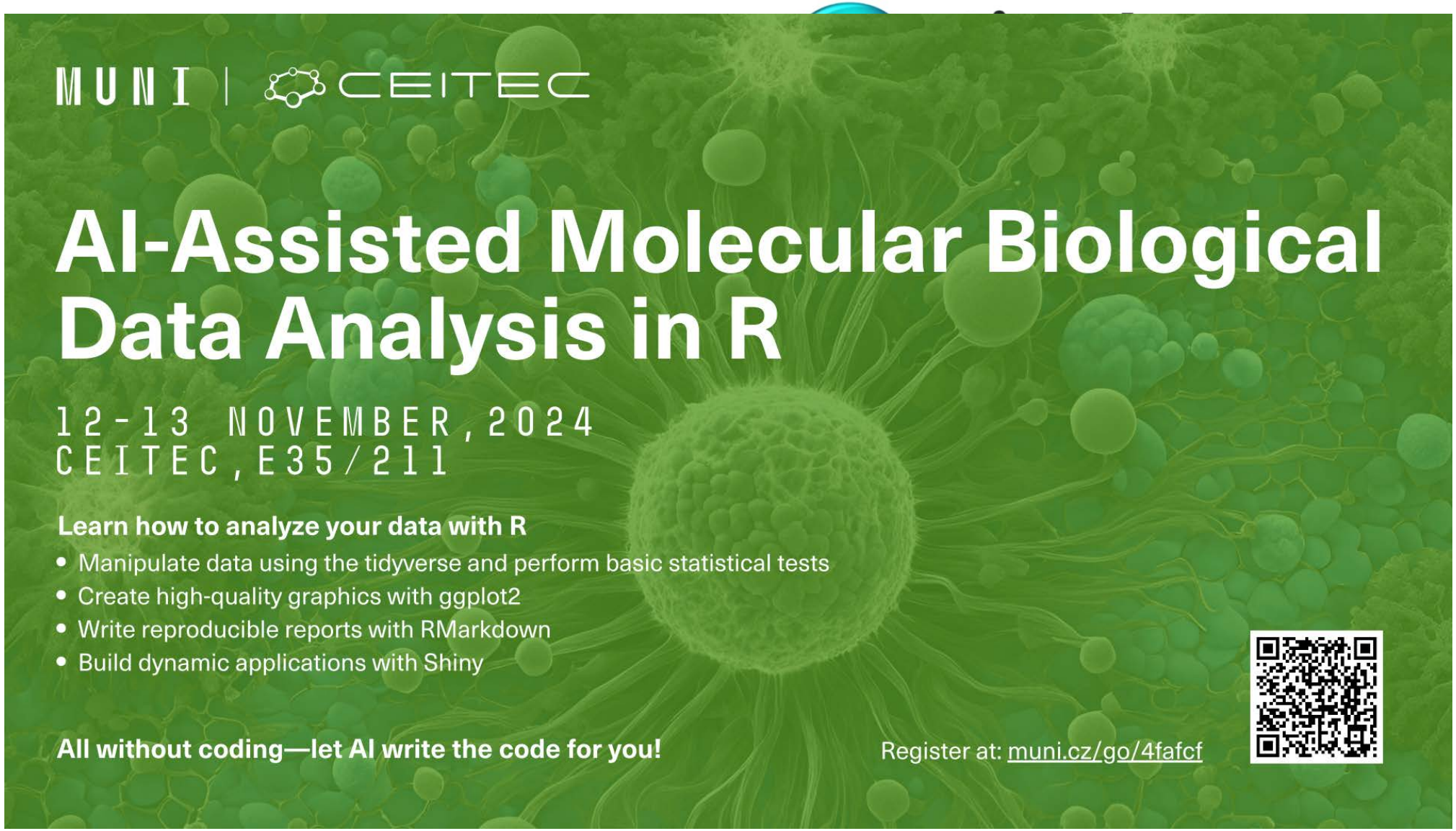

FC, fold change; FDR, false discovery rate.

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All without coding—let AI write the code for you!

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FC, fold change; FDR, false discovery rate.

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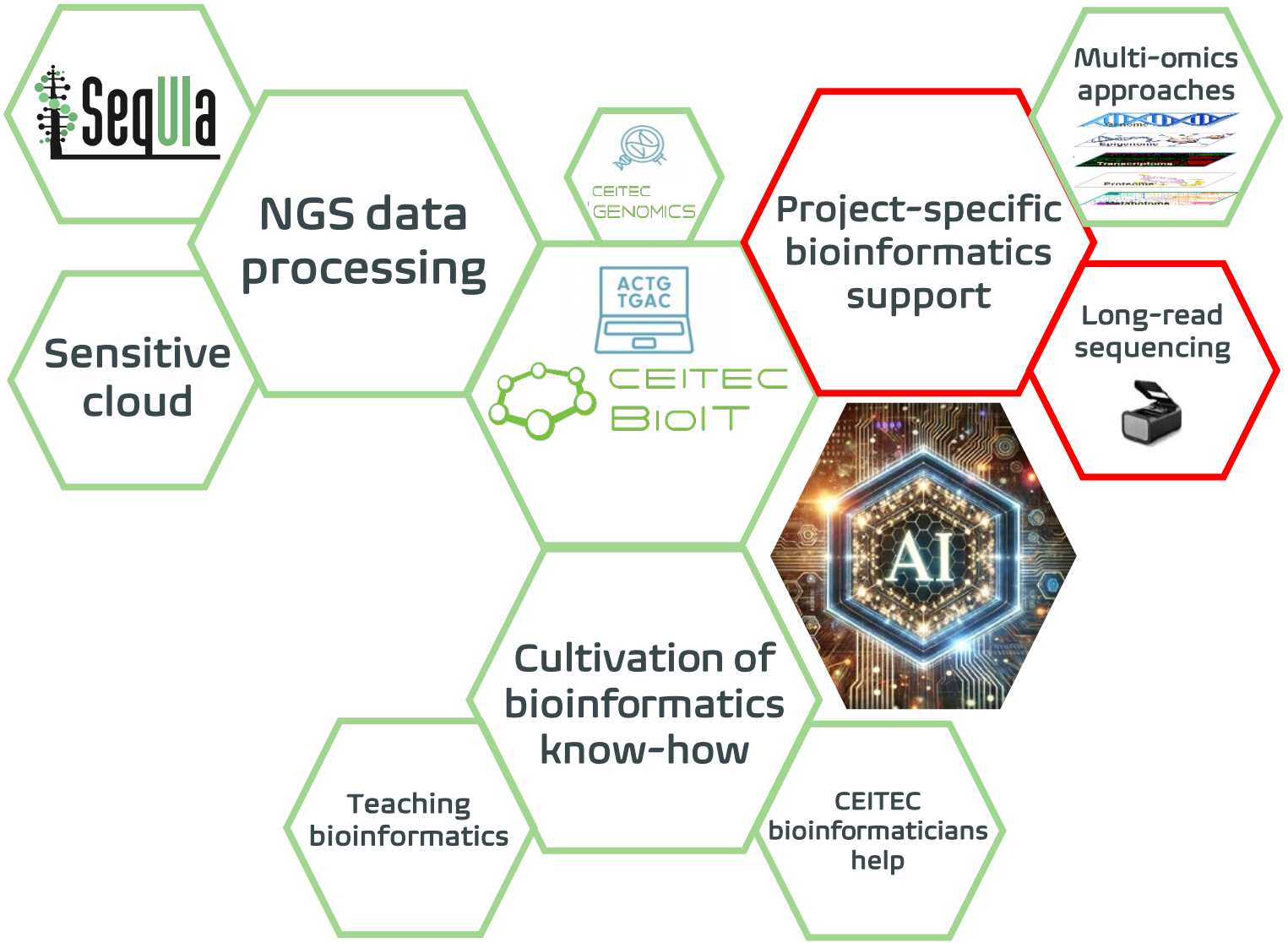
SeqUla
NGS data processing
Sensitive cloud
CEITEC GENOMICS
ACTG TGAC
CEITEC BioIT
Project-specific bioinformatics support
Multi-omics approaches
Long-read sequencing
AI
Cultivation of bioinformatics know-how
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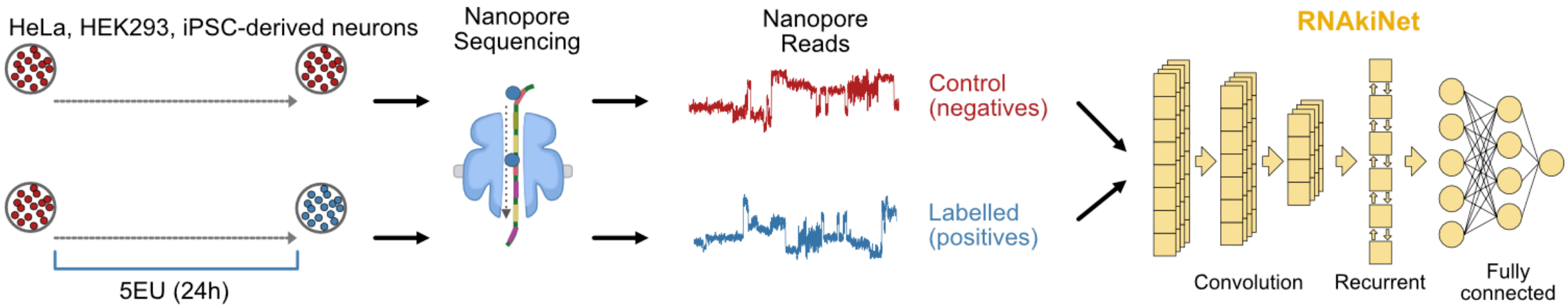

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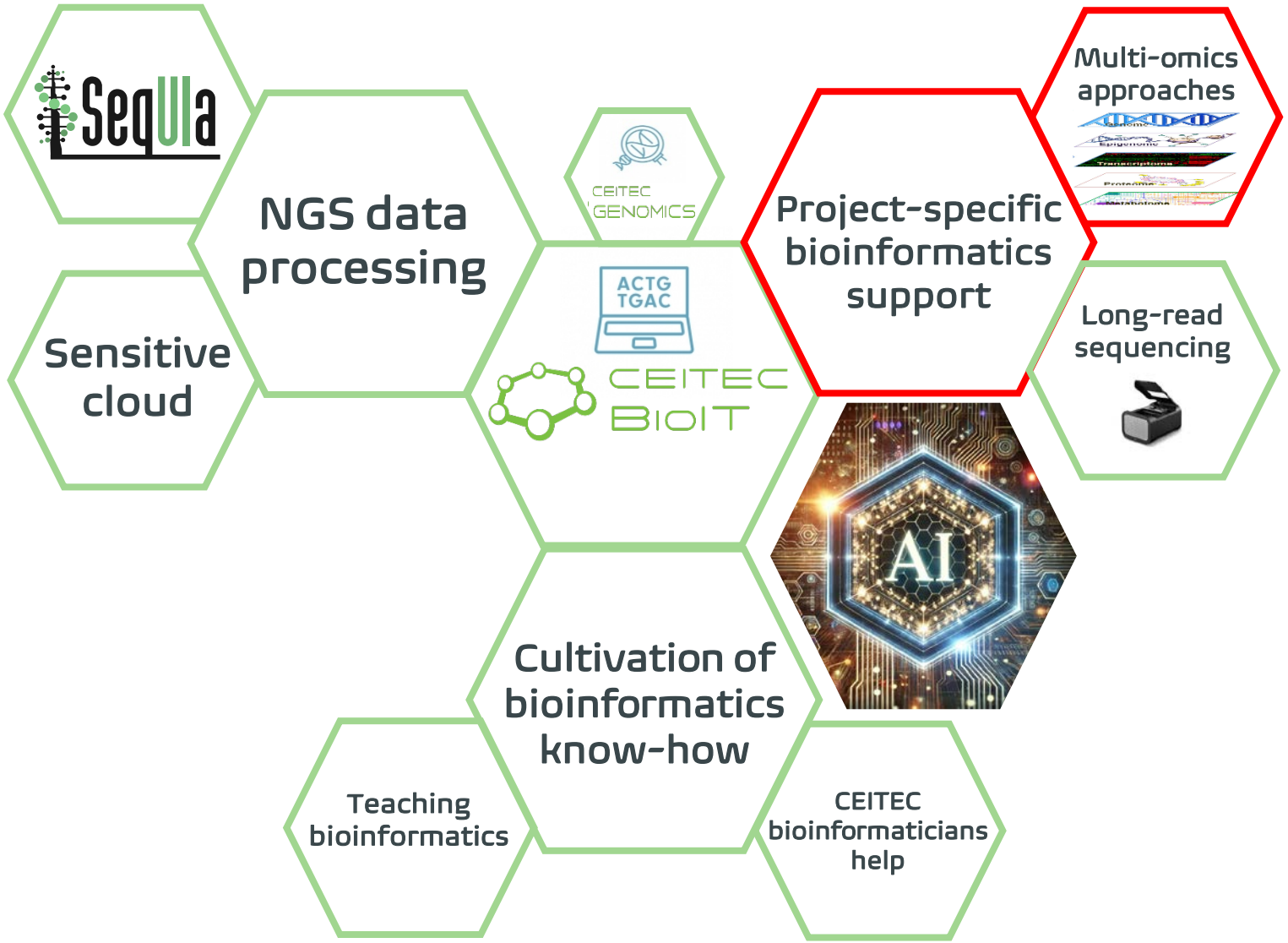
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Protein sequence
Arg
Arg
Gly
Met
Ile
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Gln
Arg
Arg
Gly
Arg

AlphaFold

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Protein sequence
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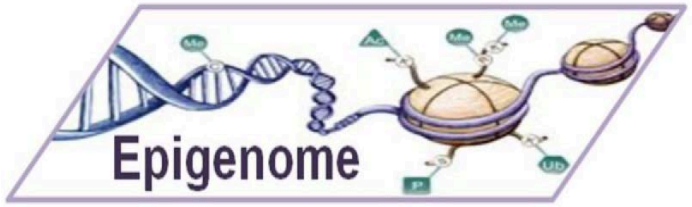
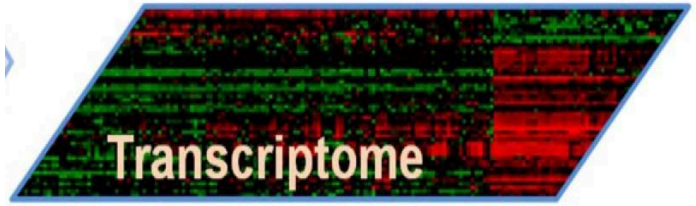
Gln
Arg
Arg
Gly
Arg

AlphaFold

Genome


Epigenome


Transcriptome

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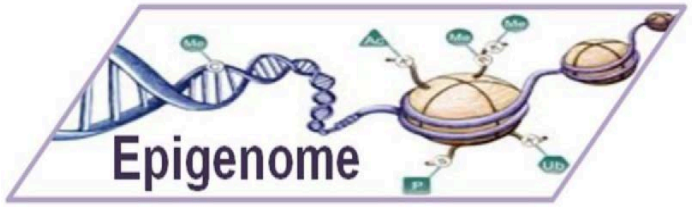
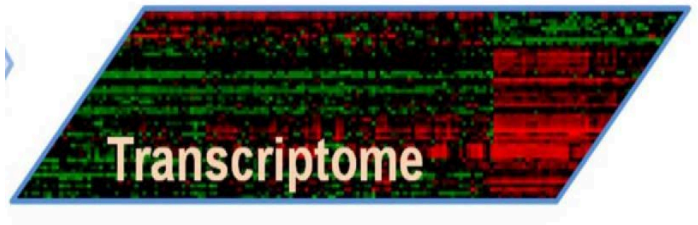
DNABERT_2

[ICLR 2024] DNABERT-2: Efficient Foundation Model and Benchmark for Multi-Species Genome



EpiGePT: a Pretrained Transformer model for epigenomics

Zijing Gao,[1,#] Qiao Liu,[2,#*] Wanwen Zeng,[2] Rui Jiang,[1,*] and Wing Hung Wong[2,3,*]



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Article | Published: 06 June 2024

Large-scale foundation model on single-cell transcriptomics

Minsheng Hao, Jing Gong, Xin Zeng, Chiming Liu, Yucheng Guo, Xingyi Cheng, Taifeng Ma, Xuegong Zhang & Le Song

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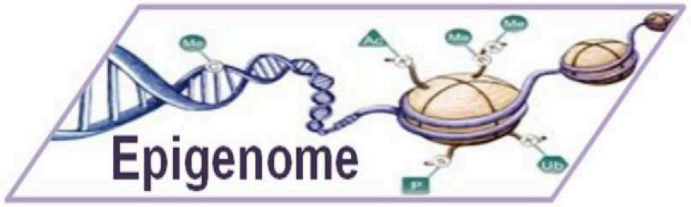

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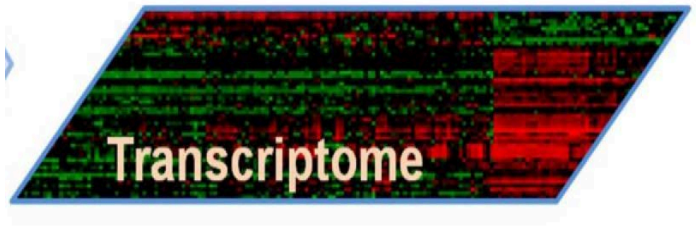

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Differential Expression

Differential
Expression

Differential
Expression

Differential
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Expression

SeqUla

NGS data processing

Sensitive cloud

CEITEC GENOMICS

ACTG TGAC

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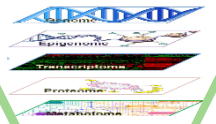

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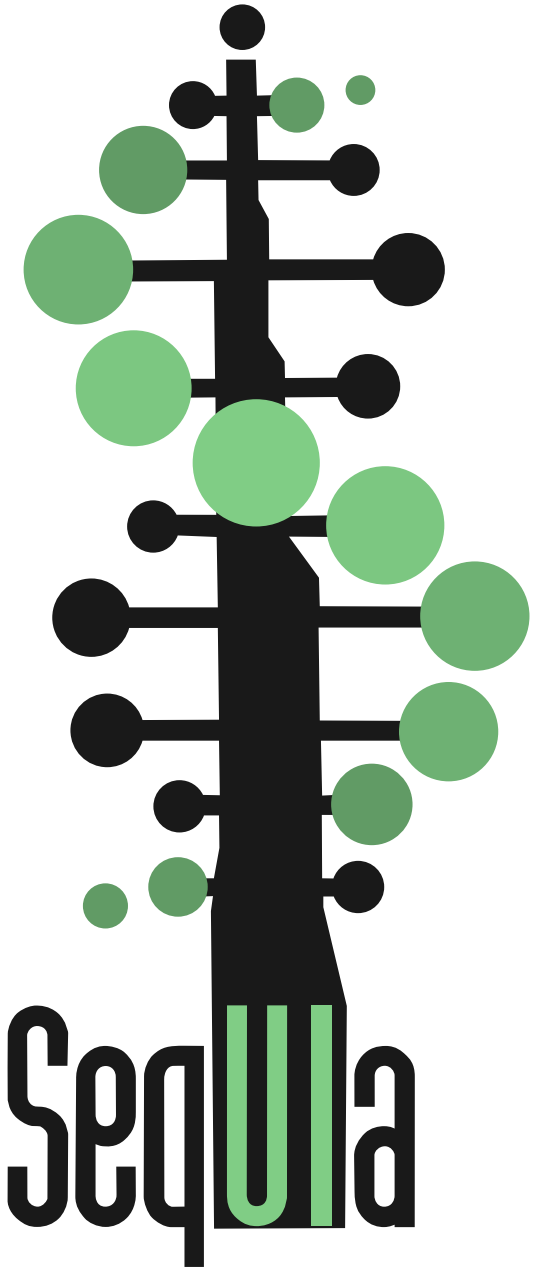

SeqUla Sequencing kits Index kits Samples Libraries Runs Projects Patients | Analysis Tasks Users Groups Sequencers Workflows Help Logout *Bystrý Vojtěch*

Runs | Add run | Download runs outputs | Run outputs

Runs

Run name	Libraries	Last edit	Paired output - name	Paired output - flowcell	Status	Action
NS_200_20241011	Dvorak_qSeq Analysis processing; BRONCO110_NovaSeq Analysis processing; ALL8-WES-ZV-NovaSeq_P2 Analysis processing; ALL1-WES-ZV-copied Analysis success; ALL8-WES-ZV-NovaSeq_P1 Analysis processing; ALL8-WES-ZV-NovaSeq_P3 Analysis processing; digiMLPA_ALL20_ZV Analysis processing; TP53_20240823-copied Analysis processing; Zita_miRNA_Nextflex_v4_NEW_INTERVALS Analysis success; Brazdil_FCD_sRS07_NovaSeq Analysis error; 11102024_Flurothyl_shivani_spike_additional Analysis success; GBOseq_opt_11_10 Analysis success; Fabian_10x-copied Analysis success	2024-10-15	ALL_WES_ZV_241011	HWHYHDSX7	Analysis error	
CMBG_MGI_300_20241018	Next_tM_NHA Run assigned; Next_tN_NHA Run assigned; Next_tO Run assigned; Next_tP Run assigned	2024-10-15	*--- click to pair ---*		Libraries assigned	
CMBG_MGI_300_20241011	Next_tK Analysis success; Next_tL Analysis success; A153 Analysis success; AMP111 Analysis success; Navrk95 Analysis success	2024-10-13	CMBG_MGI_30020241011	F350038847	Analysis success	
BabyFox_003	BabyFox_003 Run data paired	2024-10-10	BabyFox_003	HKCLMDRX5	Data paired	
BabyFox_002	BabyFox_002 Run data paired	2024-10-09	BabyFox_002	HKFJYDRX5	Data paired	
	Navrk93 Analysis success					

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SeqUlla

new sequencers data processing

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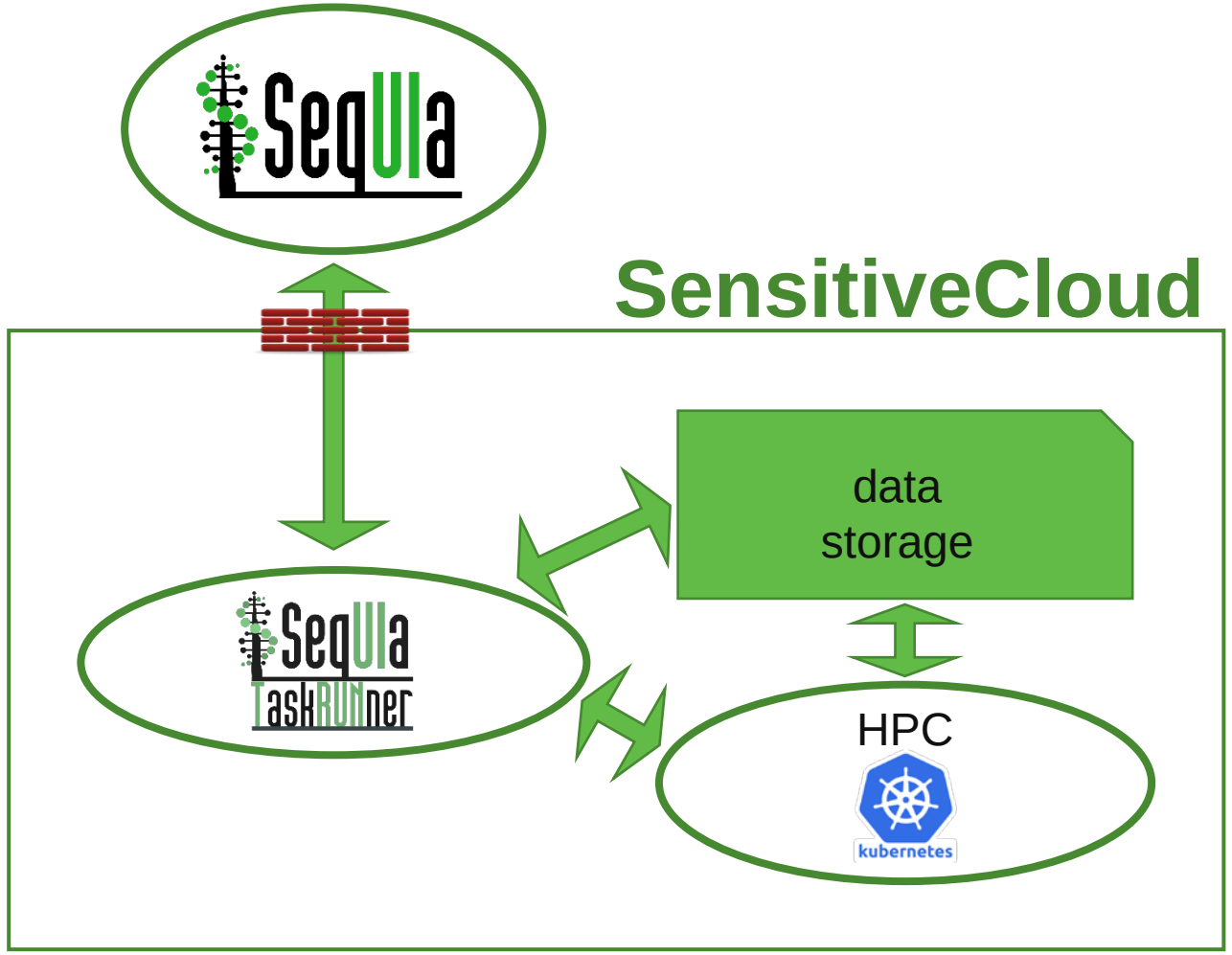
SeqUla



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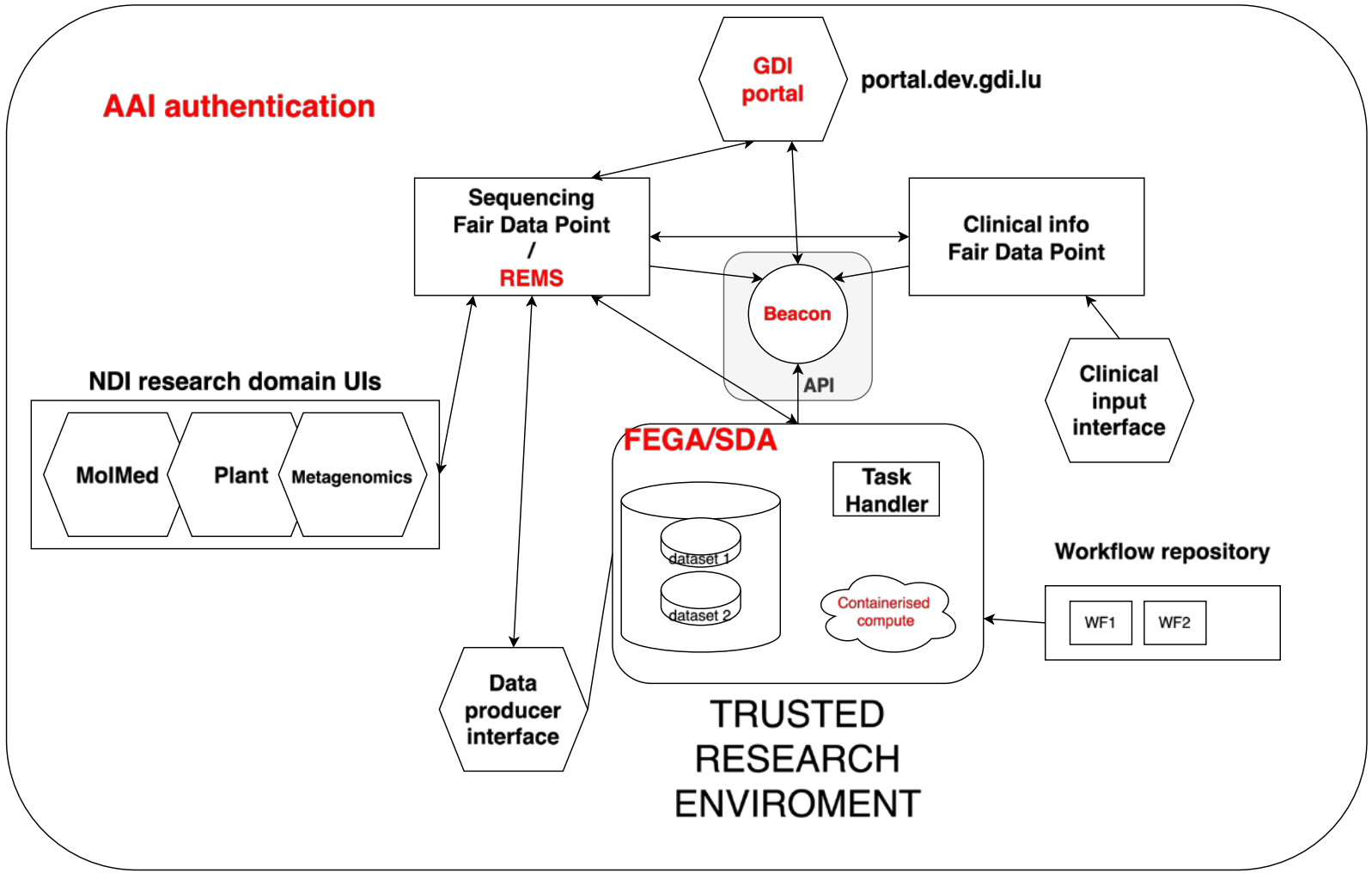

EUROPEAN OPEN SCIENCE CLOUD

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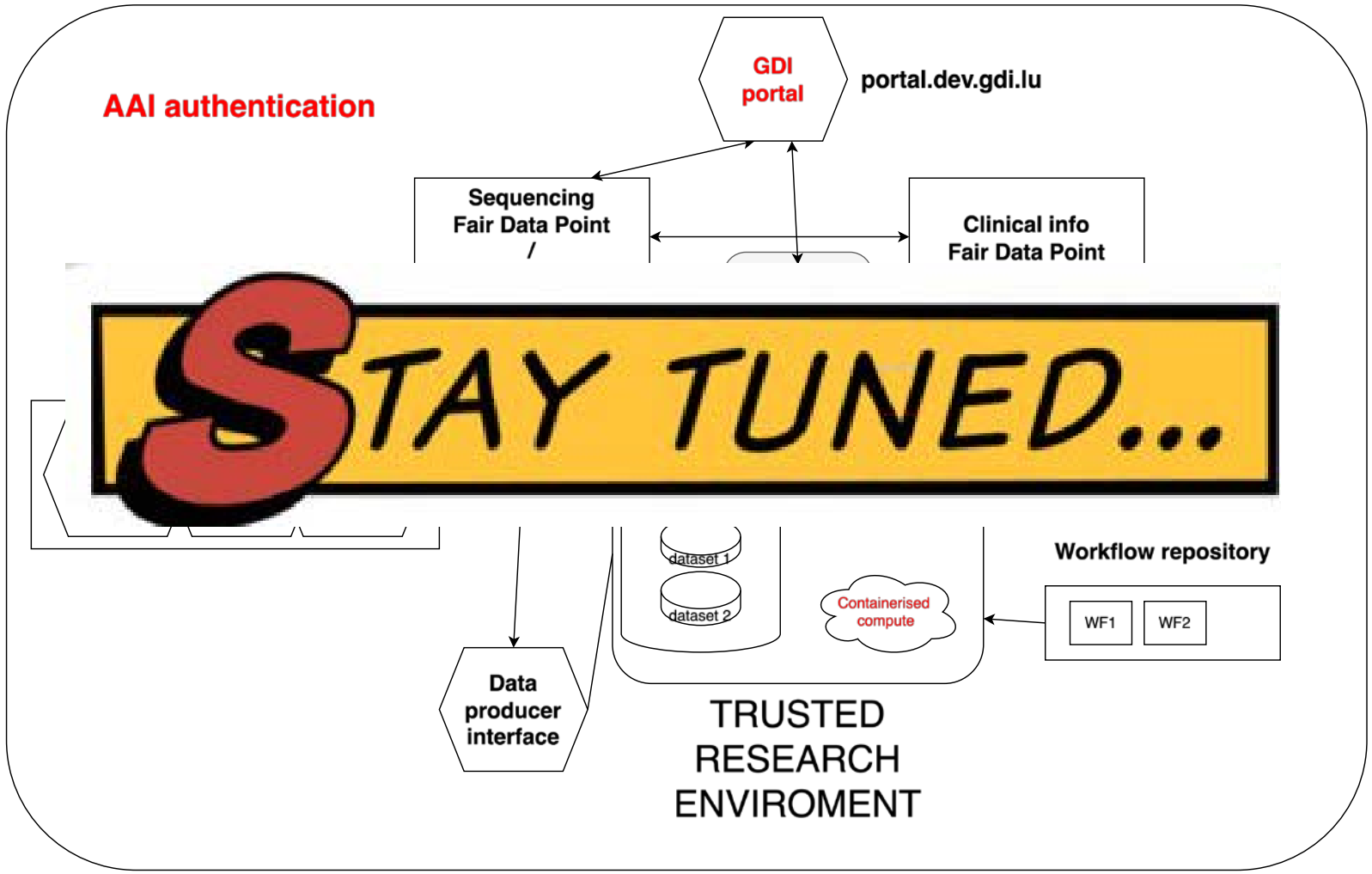

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NCMG

Acknowledgement text – NCMG

- *„We acknowledge the CF Bioinformatics supported by the NCMG research infrastructure (LM2023067 funded by MEYS CR) for their support with the bioinformatics analysis of scientific data presented in this paper.“*

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Core Facility Day 2024
Life Sciences

16 OCTOBER, 2024
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SensitiveCloud as an Environment within e-INFRA CZ

CEITEC Core Facility Day Life Sciences 2024
2024-10-16

Michal Růžička <ruzicka@ics.muni.cz>, Petr Holub <hopet@ics.muni.cz> et al.
Prepared in cooperation with the EOSC CZ Secretariat

Co-funded by the European Union

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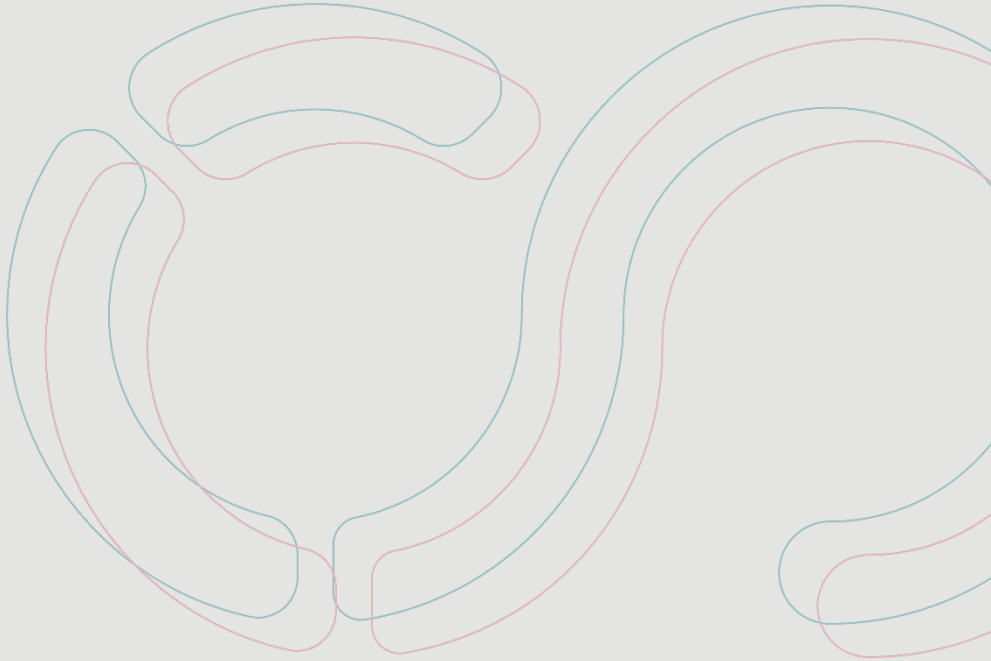
SensitiveCloud

Infrastructure for Sensitive Data within e-INFRA CZ



Motivation

- Security is an increasingly emphasized area.
  - Users are gradually placing more and more emphasis on the security of their data.
  - Various parts of the university (Med, CEITEC, RECETOX, CERIT-SC, ...) work with medical and other sensitive data.
- Two “hot topics” in data management and processing.
  - Open and FAIR data – The principles of Open and FAIR data (Findable, Accessible, Interoperable, Reusable, ...) are needed as the simple availability of data does not guarantee its usability.
  - Sensitive Data – Primarily in Health and Life Science, which creates a clear demand for processing sensitive data.
- A strategic goal of CERIT-SC / e-INFRA CZ – Supporting life-science and high-value users.

Our Team

- Selected specialists from CERIT-SC team.
  - Technical implementation (storage and computation software and hardware, data networks, datacenters personnel, …).
  - Compliance, risk management, ...
  - Service design.
  - Legal consultation.
  - Security research (forensic readiness).

Environment Design and UX

- Higher security == worse UX.
- Higher security == requirement for higher service maturity (ITIL, ISO, ...).
- Environment design based on:
  - “General security best-practice”.
  - User interviews and testing.
- Developed semi-formal framework:
  - On-boarding process for users: first contact, interview(s), contract signing, access and training, deployment.
  - Description of the environment.
  - User rights and responsibilities.
  - Contract template.
  - General conditions of use of the service.

Implementation

- Two components:
  - SensitiveCloud Compute (including GPUs).
  - SensitiveCloud Storage.
- SensitiveCloud Compute is provided as a PaaS built on Kubernetes with Rancher:
  - The user only manages the application, not the entire VM.
  - Ideal SaaS – R-Studio, Jupyter Notebook, ...
- SensitiveCloud Storage.
  - Integration within computing via NFS-CSI.
- Separate network, WireGuard VPN access, Perun AAI with multi-factor, iron behind the lock with camera surveillance, ...

General Security Best Practice

- Rational search for possible vulnerabilities, attacks and countermeasures.
  - From formal risk analysis to wise men over coffee meetings...
- ISO 27k:
  - Not a prerequisite, not a sufficient condition.
  - By itself, addressing process maturity and higher security de facto is a by-product.
  - SensitiveCloud certified in summer 2023.
- BUT:
  - The correct solution implicitly must necessarily be ISO 27k compliant.
- Forensic readiness.
  - The security methods research applied to SensitiveCloud infrastructure.

Continuous Process

- ISO 27k is about continuous planning, monitoring and improvements.
- In the process of applying for projects planning to use SensitiveCloud.
  - Possible extension of hardware resources.
  - Possible new integrations with infrastructures.
  - Possible new use-cases.
- Continuous improvements of processes, technical security measures, onboarding process, and SensitiveCloud public presentation, ...
- Thinking of SensitiveCloud 2.0, 3.0, …
  - Full virtual machines, virtual desktops in the secure environment.
  - Dedicated Kubernetes/OpenStack platform deployed on-demand.

SensitiveCloud Infrastructure

- SensitiveCloud up and running.
  - ISO 27k certified.
  - Onboarding process, processes, technical measures, service agreement template, …
- Continuous process of improvements.
  - Projects in progress, FEGA.
  - Thinking of SensitiveCloud 2.0, 3.0, …

1.

We find out whether SensitiveCloud fulfils your requirements.

2.

We explore all the specifics of your use case and, if necessary, make appropriate changes.

3.

We sign an agreement confirming our duties and expectations.

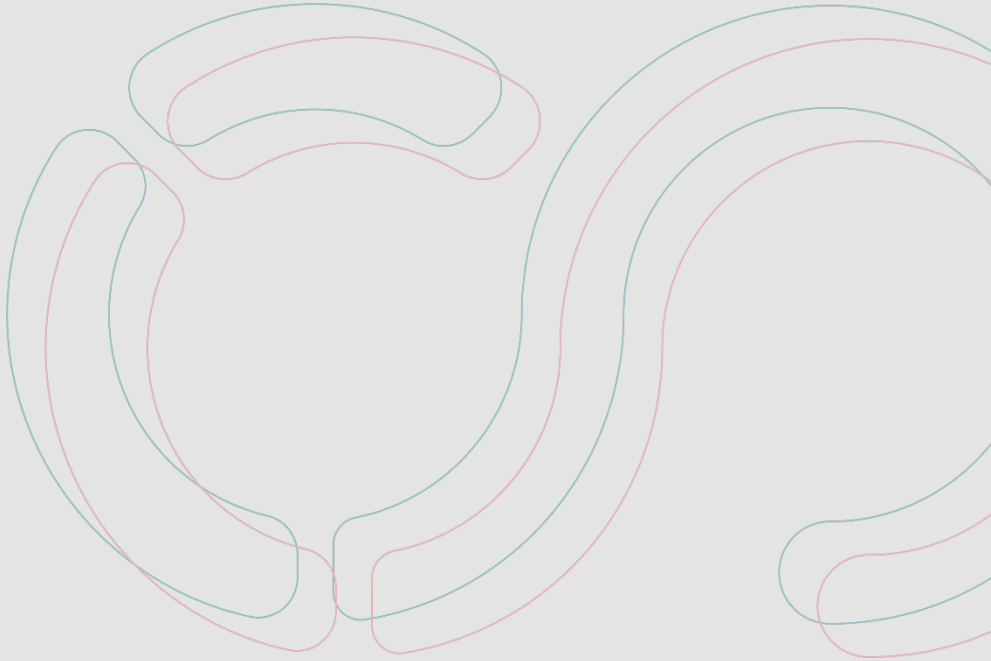
4.

We train you to harness the most of the environment.

5.

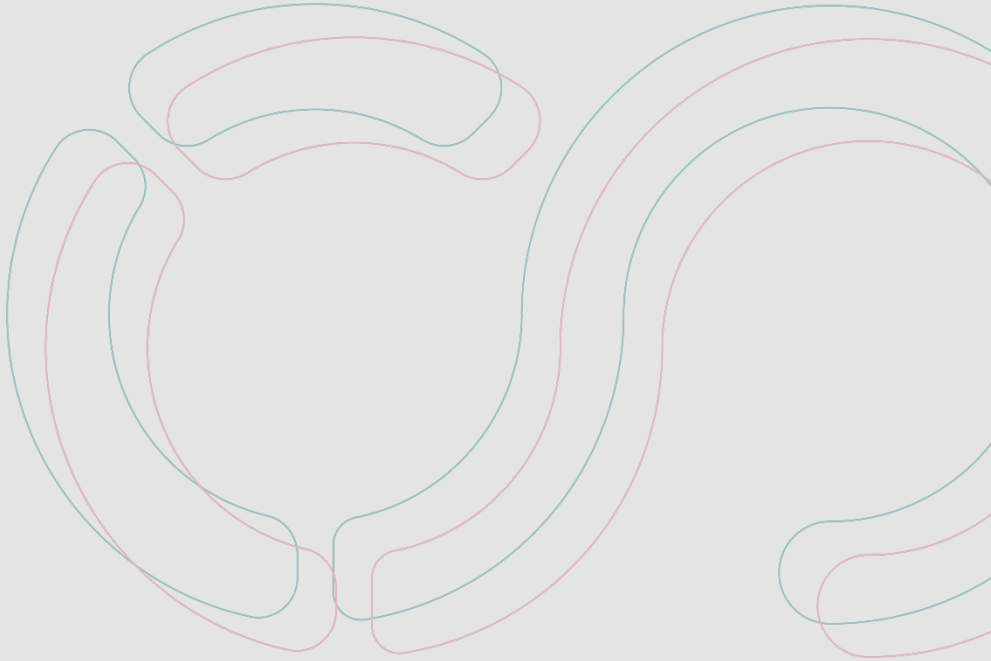
You work on your research, and we continuously monitor your needs and satisfaction.

https://www.cerit-sc.cz/infrastructure-services/sensitivecloud



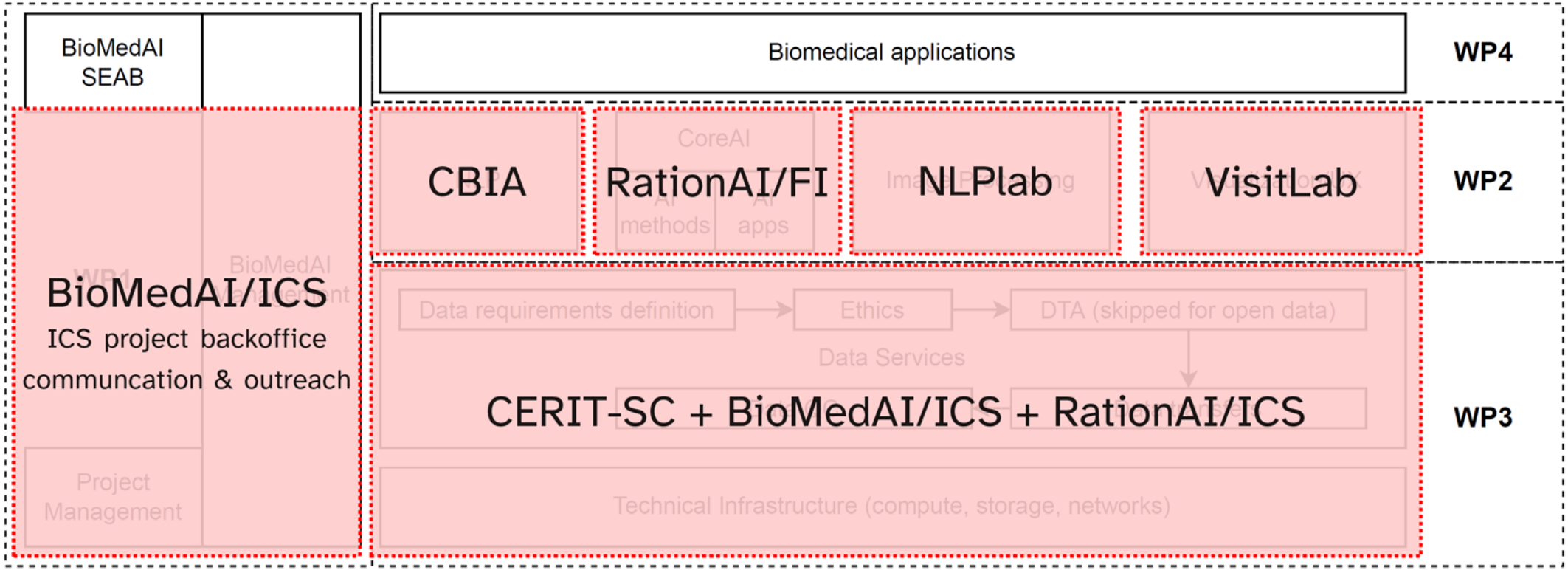
RationAI

SensitiveCloud Use-Case



RationAI Use of SensitiveCloud

- RationAI: Research group at FI/ICS MUNI.
  - Main focus: Rational application of AI in biomedical domain – primarily those with clinical impact.
- BioMedAI Center: Infrastructure, data, and research groups (MU, MMCI, FN Brno, BBMRI.cz, …).



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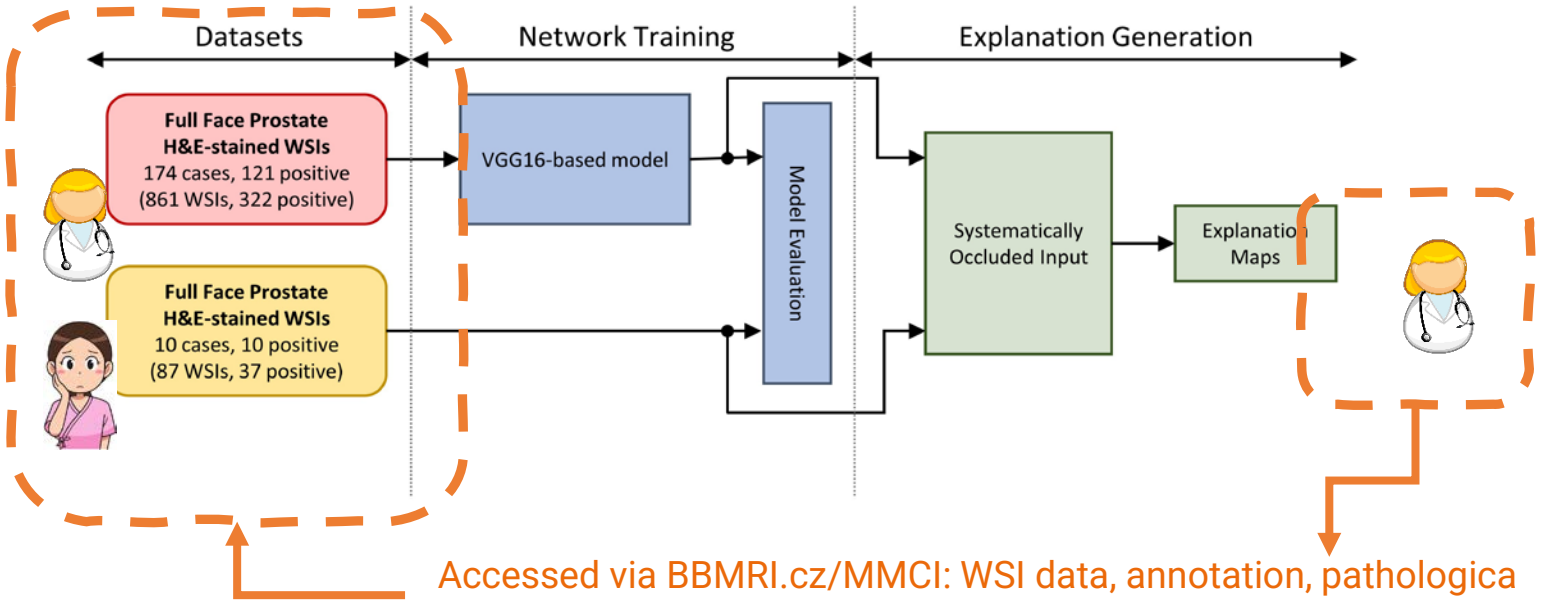
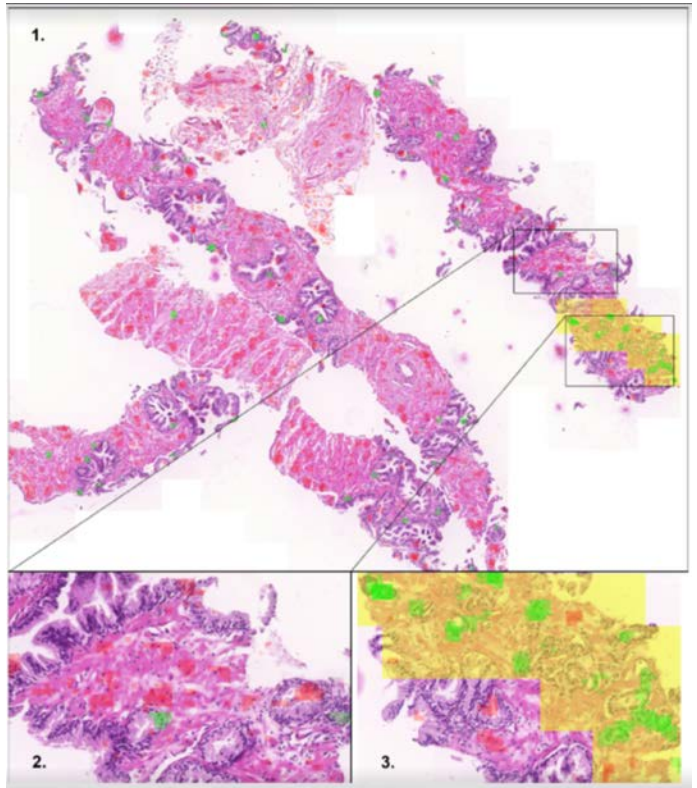
RationAI Use of SensitiveCloud: Selected Results

- Prostate cancer diagnosis support using explainable AI.
  - Developed using supervised training of AI models with robust application of explainability.
  - Internal clinical validation and use at MMCI.





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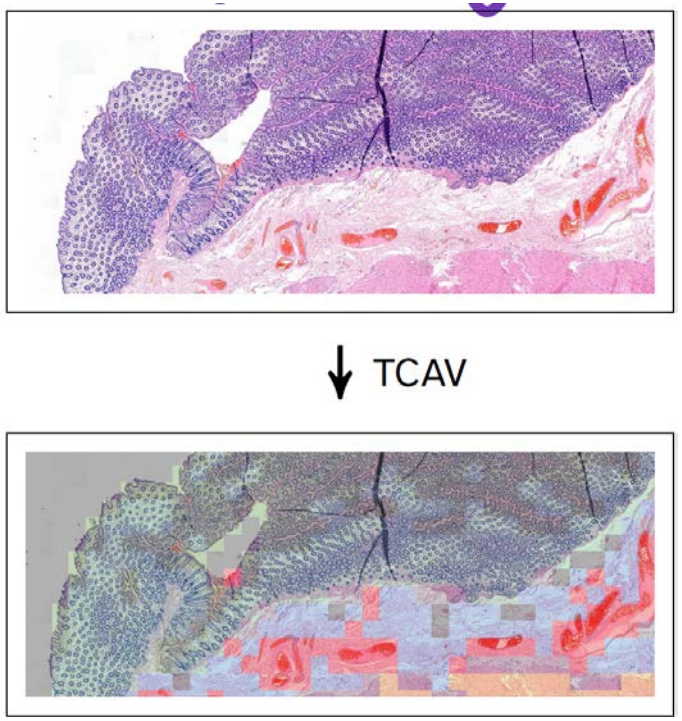
RationAI Use of SensitiveCloud: Selected Results

- Ki67 model trained entirely on real-world clinical data without any additional manual annotations.
- Model for deduplication and cleanup of National.
- Oncology Register in collaboration with UZIS.
- Extracting “knowledge” from existing models.
  E.g., Testing with Concept Activation Vectors (TCAV).
- Explainable models for blood glucosis level predictions – collaboration with 1st Faculty of Medicine, Charles University.



RationAI Contributing to the Infrastructure

- Reusable Mlflow-based pipeline system for development of AI models in SensitiveCloud.
  - RatioPath – training and inference pipelines for digital pathology and management of experiments.
  - RatioViz – visualization system for digital pathology, including WSIs, annotation, results and exploration of AI models.
  - RatioCast – training, inference and visualization system for time series data.
- Methods for sharing digital pathology data as anonymous data published in Nature Comms.
- QC algorithms for working with digital pathology data.
- Provenance information infrastructure for documenting history of data and AI models.

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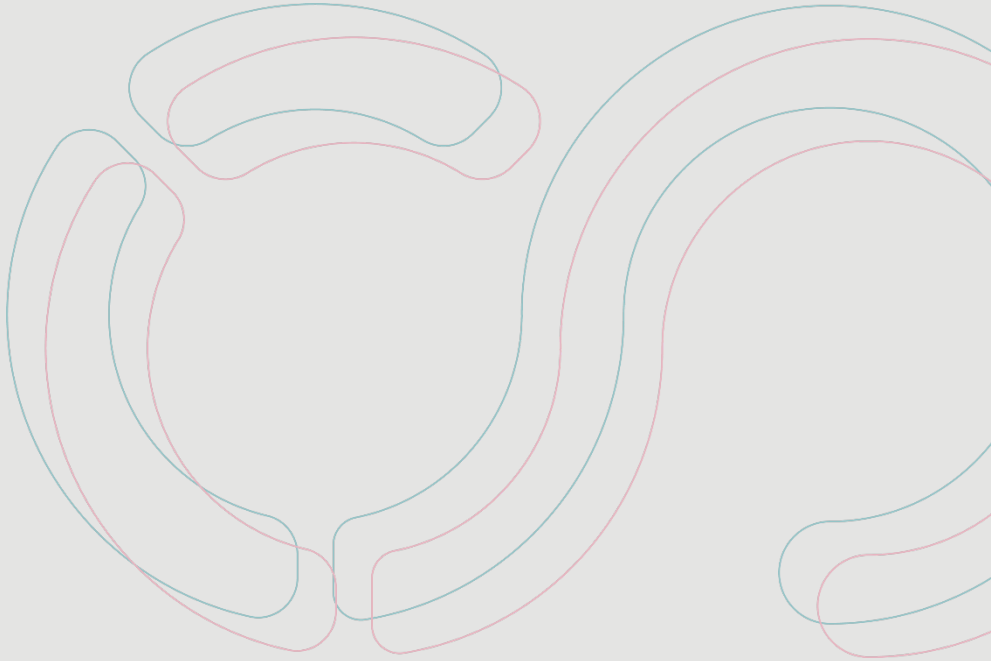
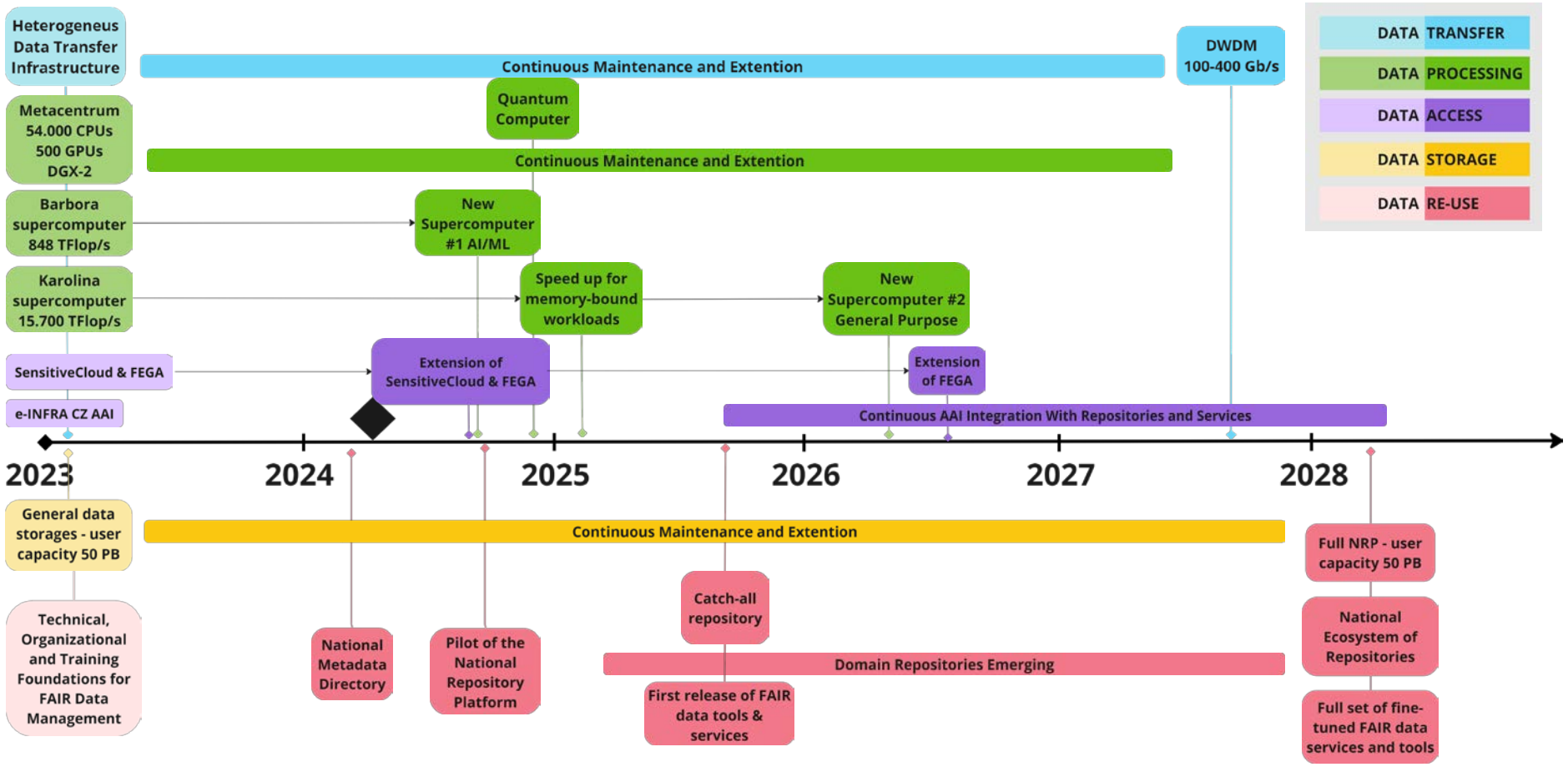
EOSC Implementation in the Czech Republic



EOSC Services in Wider Context



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From Storage to Repositories

26 November 2024
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Registration for on-line stream still open!

https://www.eosc.cz/

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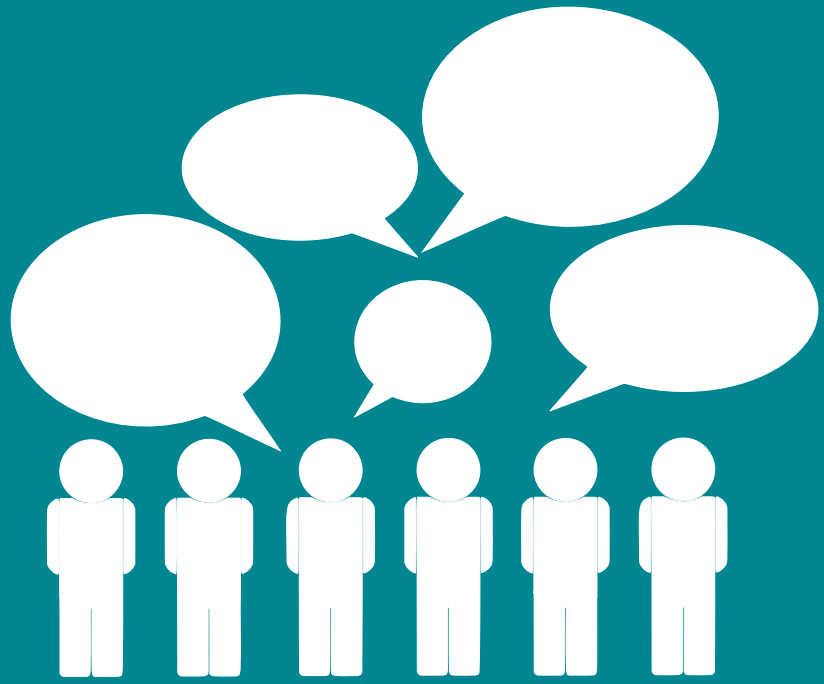

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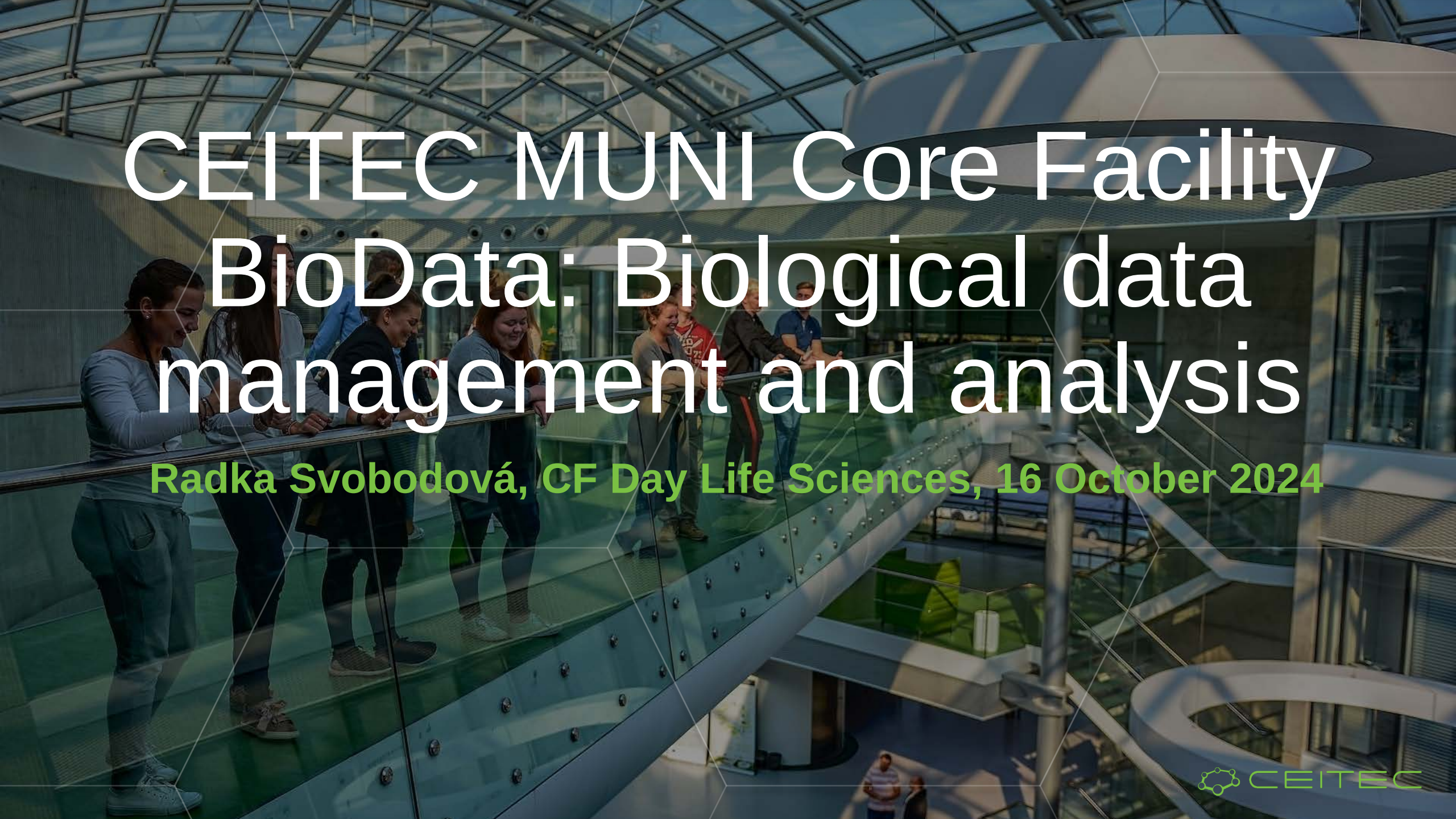


CEITEC MUNI Core Facility BioData: Biological data management and analysis

Radka Svobodová, CF Day Life Sciences, 16 October 2024

CEITEC

BioData overview

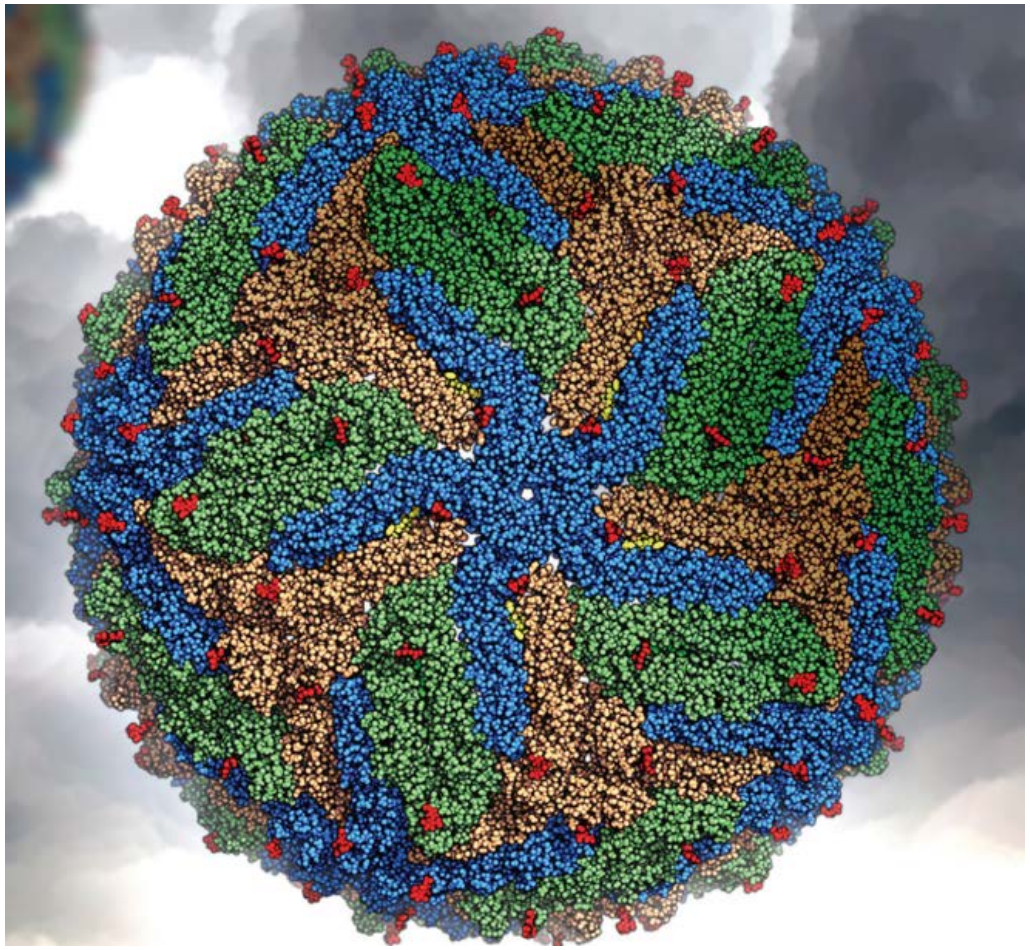
Why data management?

Biological data are:

- Interesting
- Expensive
- Larger and larger
- We have them more and more…

The data deserve to be:

- **F**indable
- **A**ccessible
- **I**nteroperable
- **R**eusable



About BioData CF

- **Mission:** Analysis and management of biological data

- **Expertise:**
  - Computer science
  - Data management
  - Structural bioinformatics

- **Members of ELIXIR and EOSC research infrastructures**

BioData services

Data

Data management

- Data repositories
- Access to ICT data resources
- Booking support
- **EOSC networking**

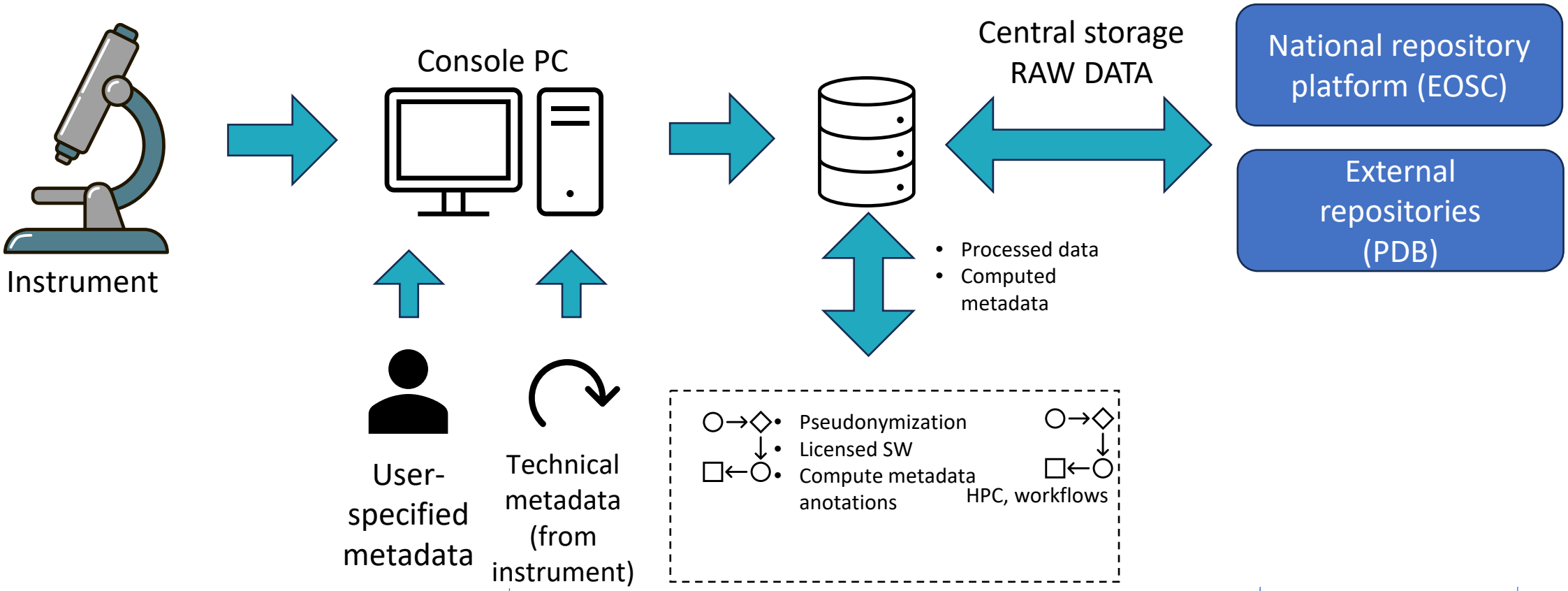
Bio

Structural bioinformatics

- Analyses of protein structures
- Validation and deposition
- AlphaFoldology
- Tools and databases
- **ELIXIR networking**

Our Data services + examples

Data: Data repositories



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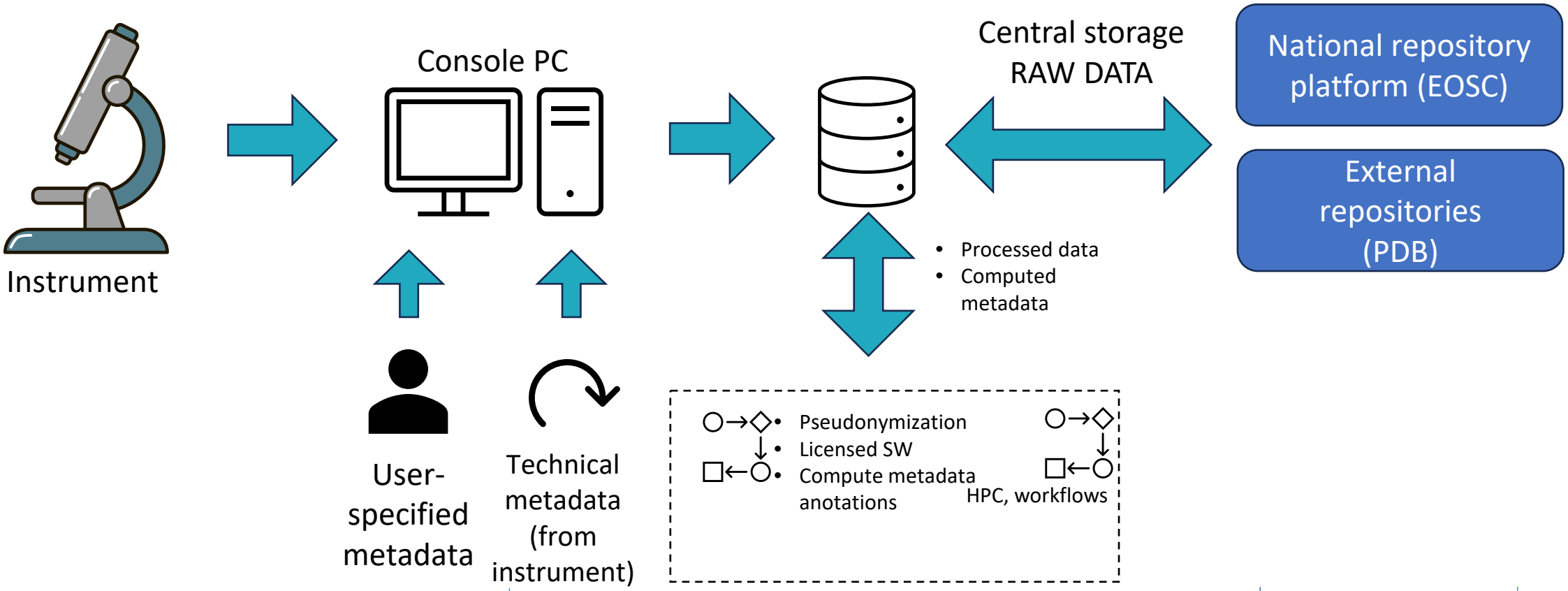
Data: Data repositories



Laboratory notebooks

DAREG

Data management systems

ONEDATA

Onedata4Sci

Central repositories

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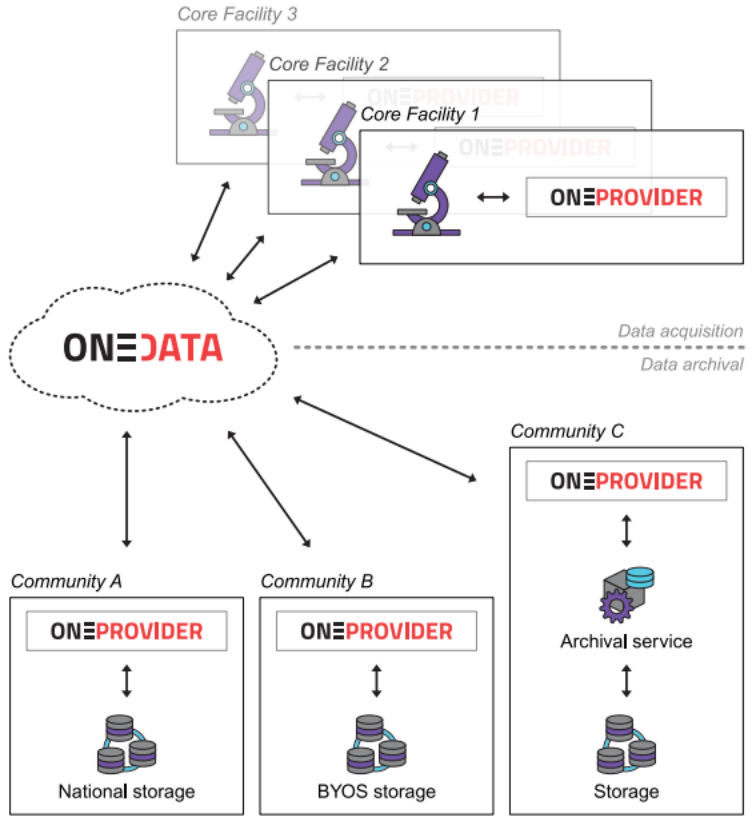
Data: Data repositories – our tools

Onedata4Sci: Life science data management solution based on Onedata

Svoboda T., Raček T., Handl J., Sabo J., Rošinec A., Opioła L., Jesionek W., Ešner M., Nováček J., Pernisová M., Valasevich N. M., Křenek A., Svobodová R.: *Onedata4Sci: Life science data management solution based on Onedata*,

https://doi.org/10.48550/arXiv.2311.16712



DAREG: Dataset Registry

A web portal that allows users to manage their datasets, stored using Onedata, and enrich them with metadata.
https://dareg.biodata.ceitec.cz/

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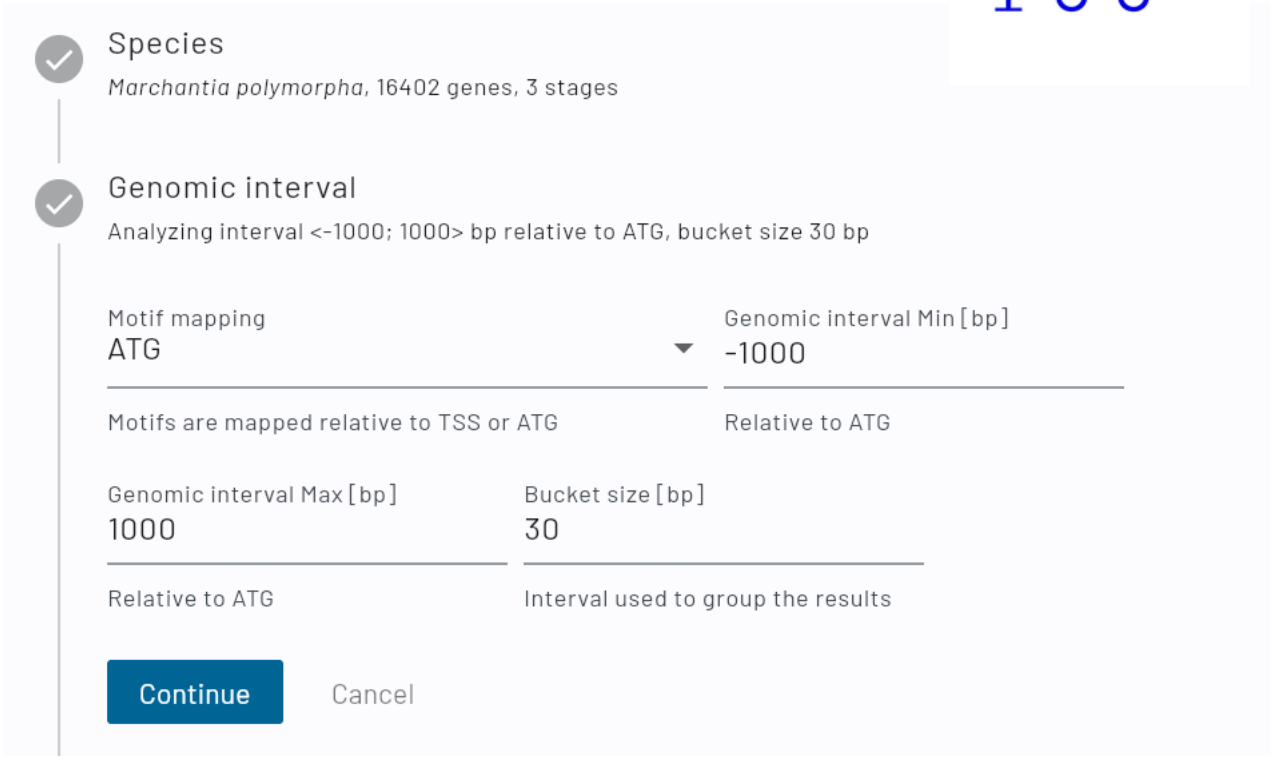
Data: Data repositories – examples

- RG of prof. Rektor
- CF Plant sciences
- CF Cellular imaging
- CF Multimodal and Functional Imaging (MAFIL DB)
- CF Biomolecular Interactions and Crystallization

Data: Access to IT resources of MU

- Web servers
- Virtual machines
- Compute
- Storage



Data: Access to IT resources of MU

- **Web servers**
- **Virtual machines**
- Compute
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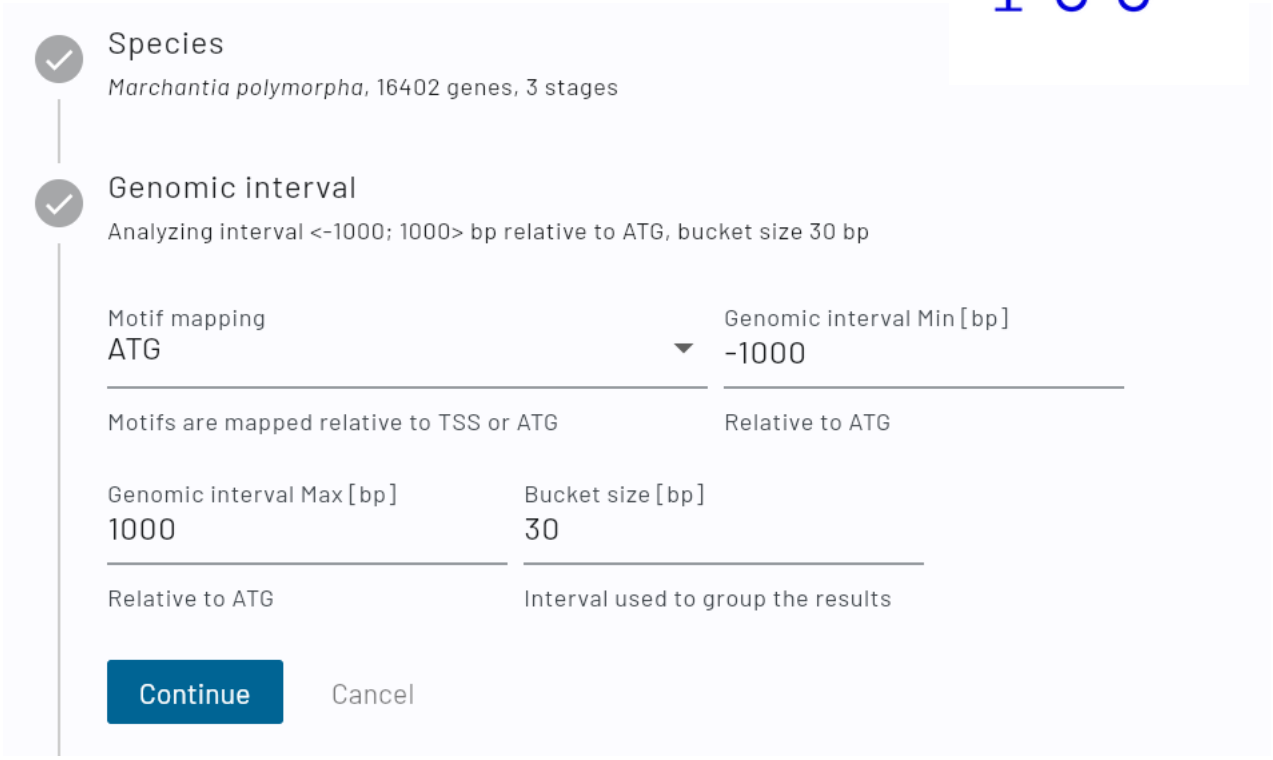
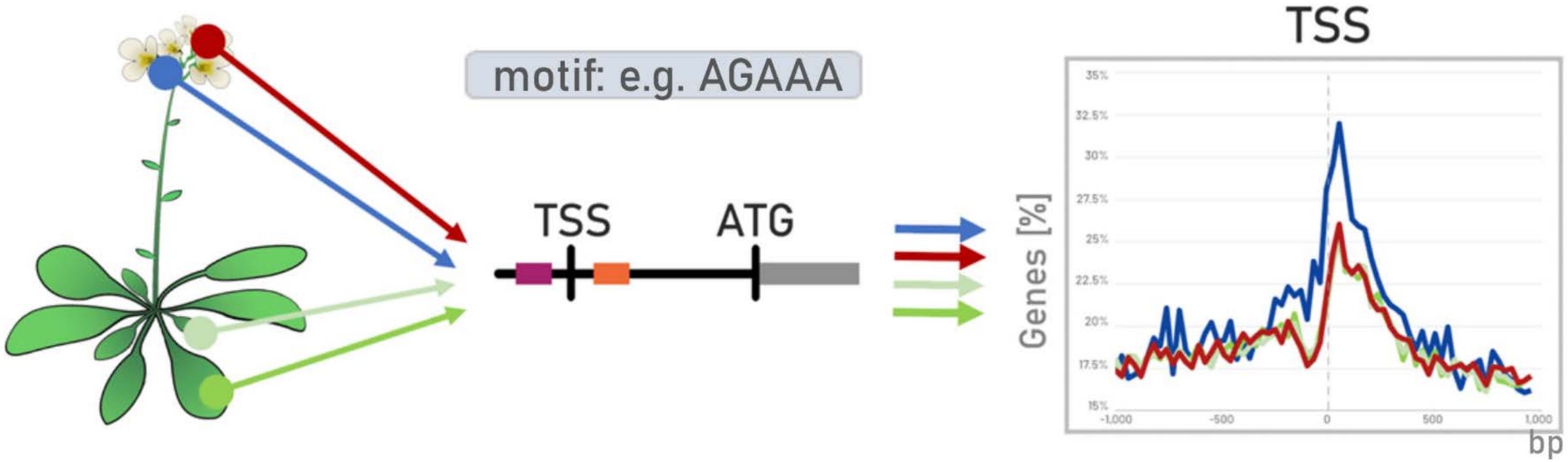


Data: Access to IT resources of MU – examples
GOLEM

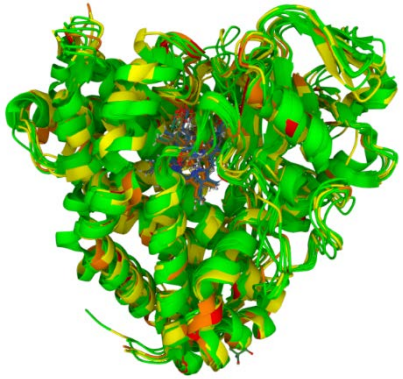


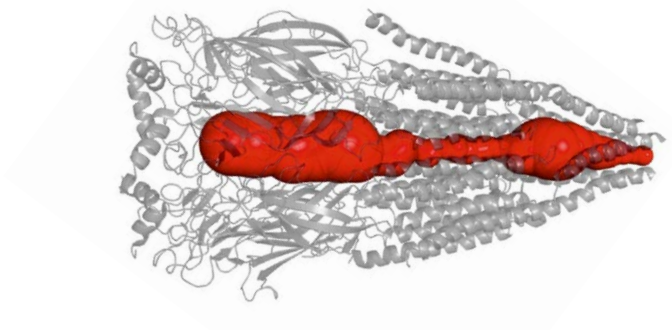
Nevosád L., Klodová B., Honys D., Svobodová R., Raček T., **Procházková Schrumpfová P.**: *A tool for visualizing the distribution of Gene regulatOry eLEMents within the plant promoters with a focus on male gametophyte*, in review (The Plant Journal)

Our Bio services + examples

Bio: Structural bioinformatics support

- Analyses of protein structures
- Validation and deposition
- AlphaFoldology
- Structural bioinformatics training

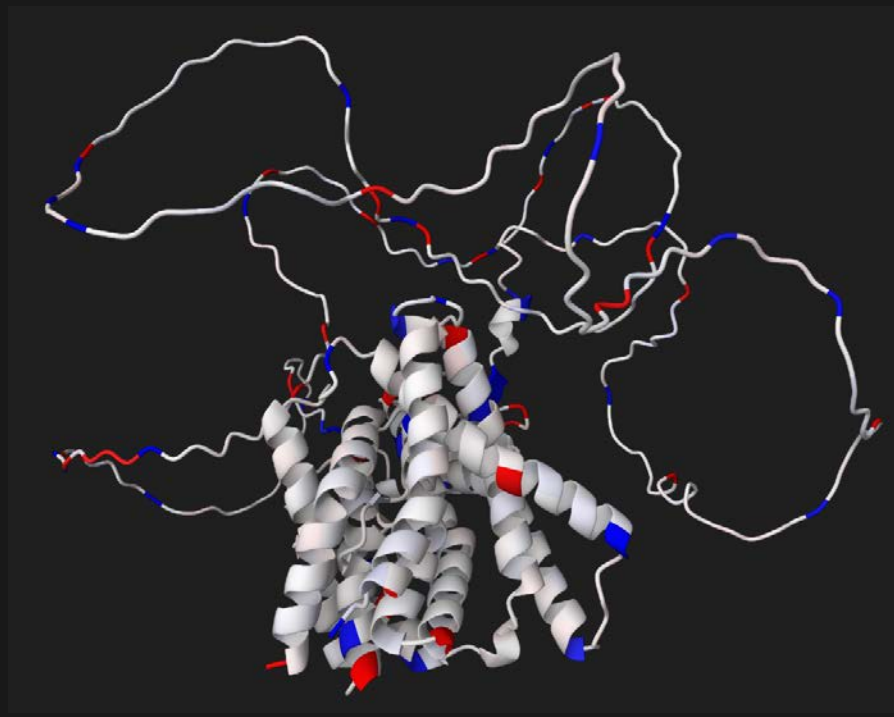




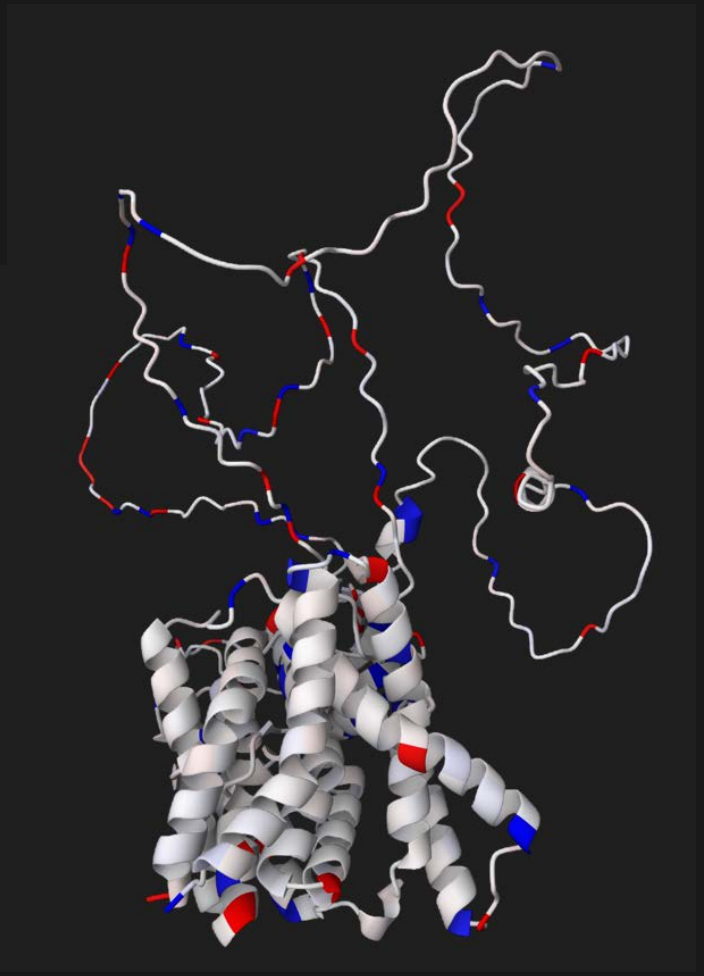
PDBe
Protein Data Bank in Europe

EMBL-EBI

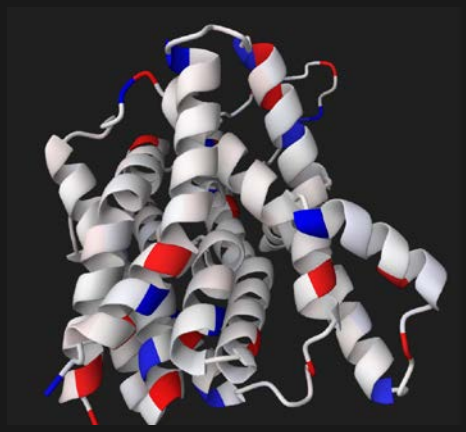
Bio: Structural bioinformatics support - example
PIN anatomy



PIN3

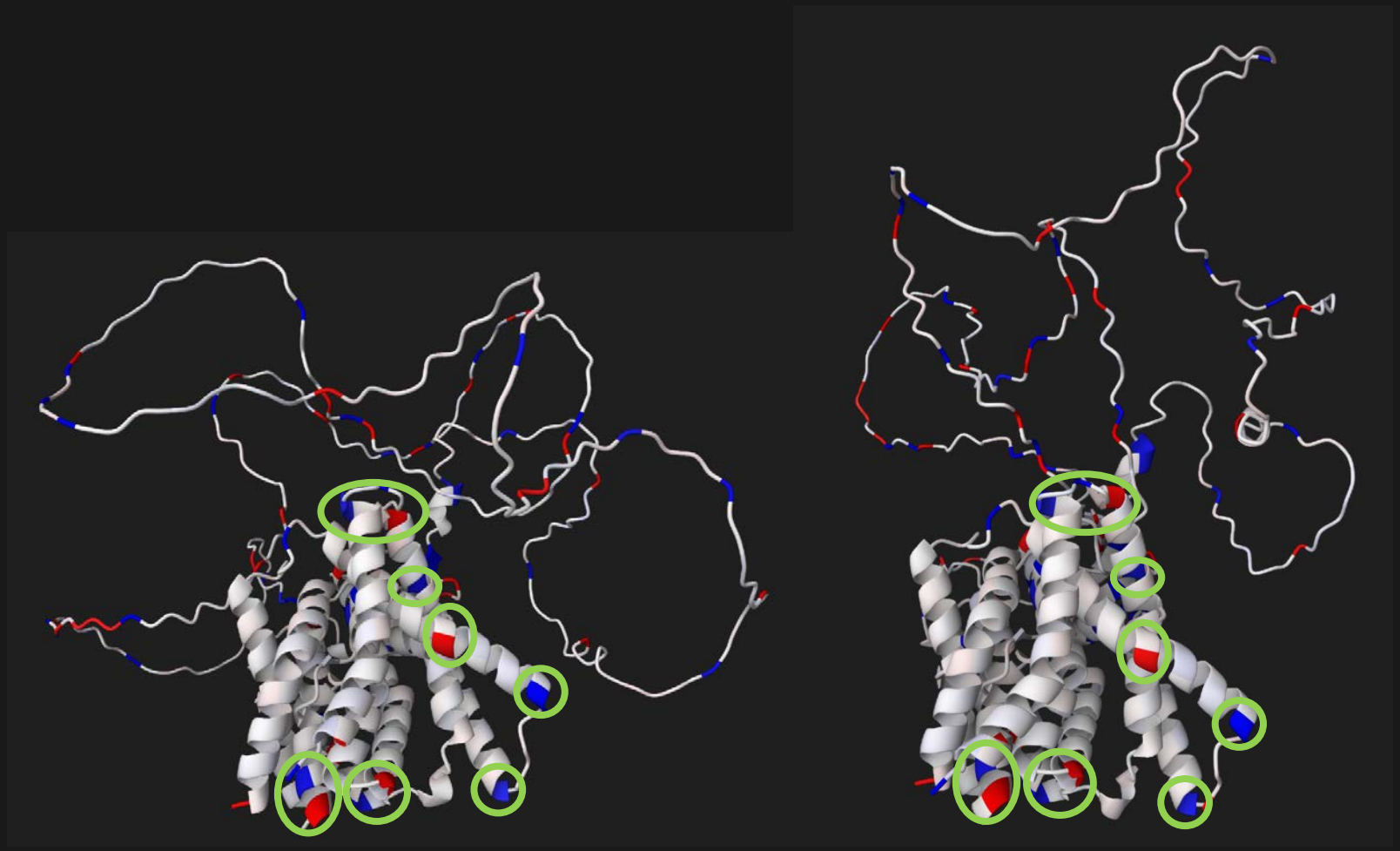


PIN7



PIN5

Bio: Structural bioinformatics support - example
PIN anatomy



Legend:
Similar charges
Different charges

PIN3

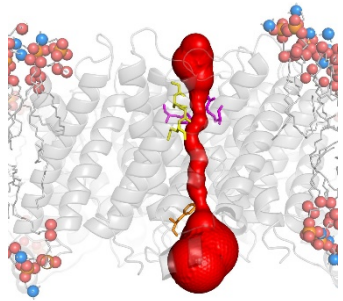
PIN7

PIN5

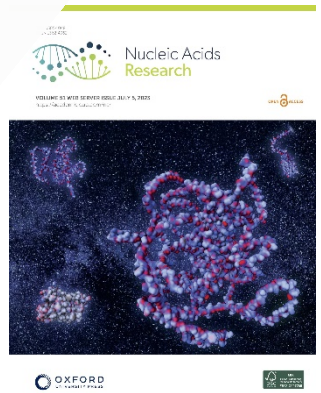
Bio: Structural bioinformatics tools – new

AlphaFind (https://alphafind.fi.muni.cz):
Searching of similar proteins in AlphaFold DB

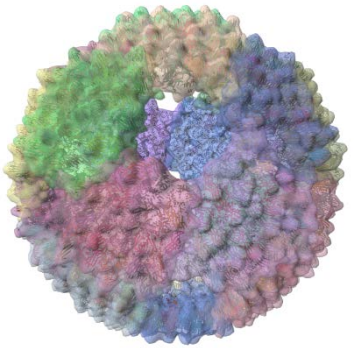
aCharges (https://alphacharges.ncbr.muni.cz)
Web application for calculation of partial atomic charges on AlphaFold2 structures



ChannelsDB (https://channelsdb.biodata.ceitec.cz)
Database of channels and pores in proteins



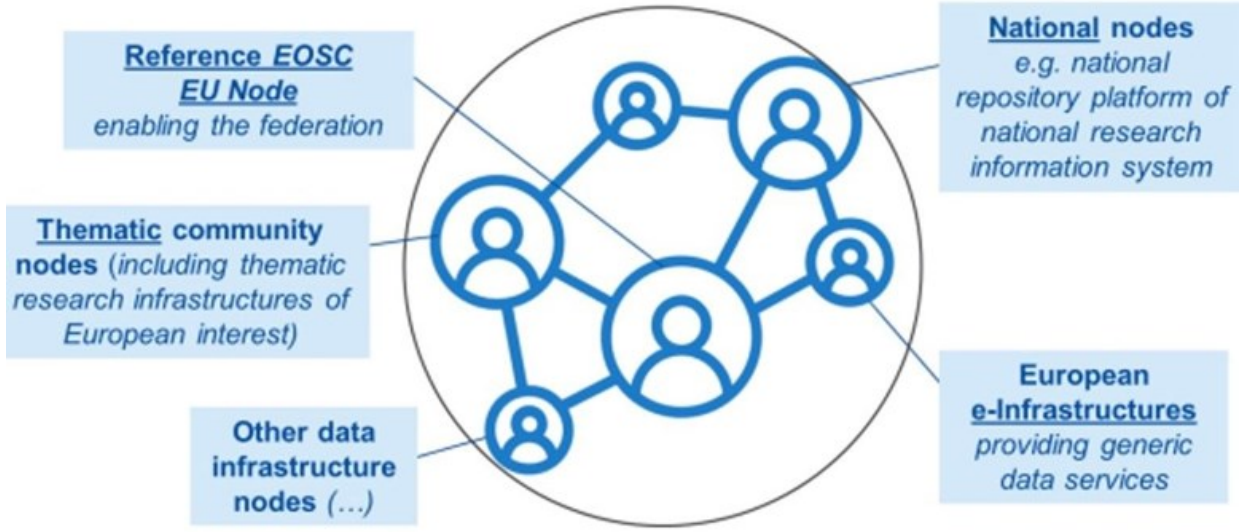
Mol *VS (https://molstarvolseg.ncbr.muni.cz)
Web application for visualization and interpretation of cell imaging data



All published in **Nucleic Acids Research 2023-2024**

Bio: ELIXIR networking

Data: EOSC networking



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Other information

Cooperation & Funding

- **ELIXIR & ELIXIR CZ**
  - Node at Masaryk university
  - funding 2023 - 2026
- **EOSC**
  - National repository platform (KA5)
  - Bio/Health/Food cluster
  - funding from 03/2024
- **EMBL-EBI**
  - Cooperation with Protein Data Bank, CATH, etc.

People

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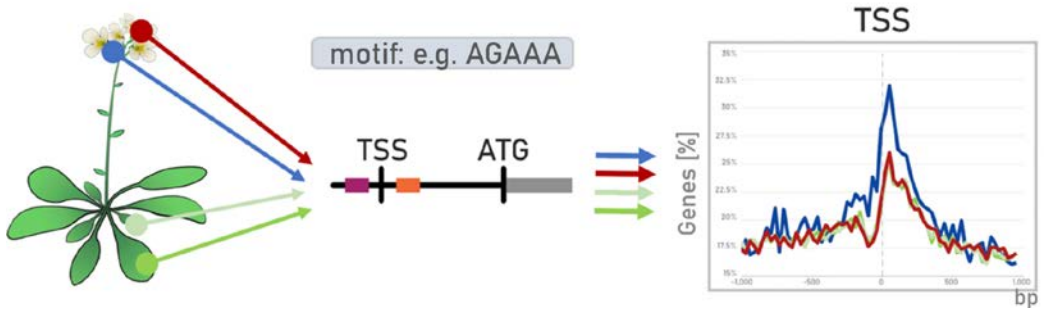
Acknowledgement text

- *„Biological Data Management and Analysis Core Facility of CEITEC Masaryk University, funded by ELIXIR CZ research infrastructure (MEYS Grant No: LM2023055), is gratefully acknowledged for supporting the research presented in this paper.“*

Summary

- **For researchers:**
  - We can help you to **store / make accessible / publish** your data



- **For students:**
  - Join us and **do research / build infrastructure** with us

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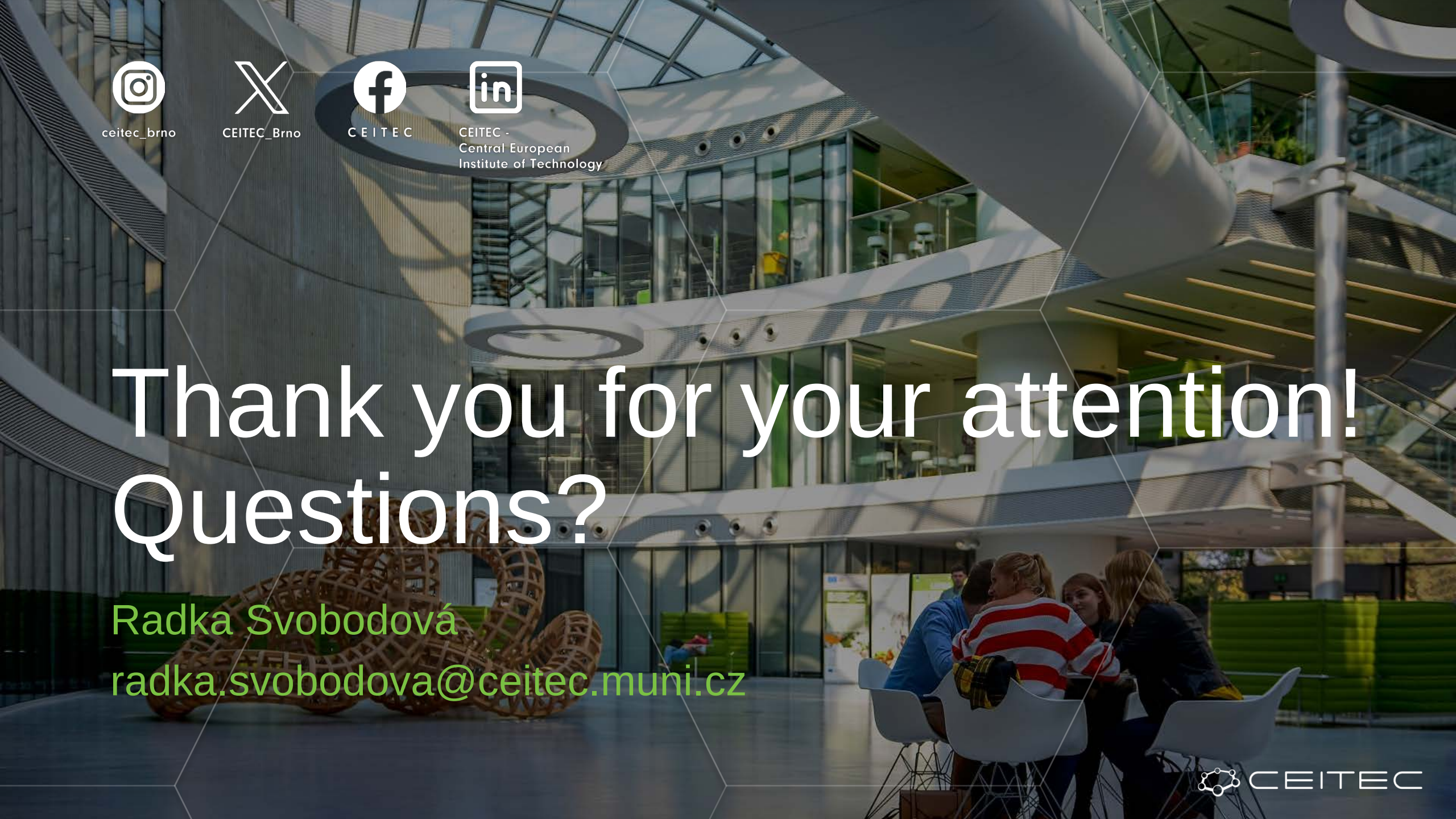

Thank you for your attention!
Questions?

Radka Svobodová
radka.svobodova@ceitec.muni.cz

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Core Facility Day 2024
Life Sciences

16 OCTOBER, 2024
CEITEC, E35/211+ATRIUM

Curious about what expert services are available to researchers on campus? What instruments can you use in shared mode and under what conditions? Do you want to see everything for yourself?

Register at: muni.cz/go/fba265

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CERIT-SC (part of e-INFRA CZ)

Luděk Matyska
CERIT-SC director
Institute of Computer Science MU

Who we are? A little bit of history

- Till 2019, CERIT-SC has been a separate Large Research Infrastructure, together with CESNET and IT4Innovations
- Since 2020, these three LRIs created an e-INFRA CZ consortium and work together as a complex (and unique) large national research e-infrastructure
- CERIT-SC is also founding member of ELIXIR CZ, Czech node of ELIXIR
- Collaboration with other LRIs

So, who we are? e-Infrastructure!

- Part of the MetaCentrum
- Resources
  - Compute capacity
  - Including GPUs
  - Storage capacity
- Service and tools layer
  - Batch processing (more at other parts of e-INFRA CZ)
  - OpenStack Cloud
  - Containers and Cubernetes
  - Jupyter notebooks
  - AAI

So, who we are? e-Infrastructure with expertise

- Efficient use of the resources and tools
  - Lukáš Hejtmánek, Viktoria Spišaková, Radek Polášek and the whole cloud team
- Optimization of algorithms and analyses
  - Aleš Křenek group
- GPU acceleration and
  - Jiří Filipovič research group
- General data analytics
  - Tomáš Rebok research group

What we have?

- 9000 CPUs
  - 3500 within Kubernetes environment
- 80 GPUs
  - 39 within Kubernetes environment
- Almost 15 PB storage capacity
  - 2,6 PB within the Kubernetes environment
  - Additional 4 PB on the way
  - Not repository features (e.g. guaranteed data retention)

Cloud, Containers, Kubernetes

- OpenStack cloud environment
  - Whole virtual machines/clusters
- Kubernetes and Containers support
  - Containers support reproducibility of computations/analyses
  - Kubernetes the management environment for containers
  - Very flexible environment (see next slide)
  - Extensible application catalogue

    Rancher applications: Ansys, Matlab, Rstudio, VMD, UI for LLM, …

Containers and Kubernetes applications

- Static always running applications, e.g. webs and portals
- HPC workflows (batch processing), including long-term running applications
- Interactive workloads
  - Jupyter Hubs, virtual desktops, GUIs, …
- But also semi-interactive HPC workflows (e.g. CryoEM sw)
- Bursty workloads

- Ability to restart applications, increased reliability of the environment

JupyterHub

- https://hub.cloud.e-infra.cz
- Integrated with e-INFRA CZ storage
  - Integration with Onedata datasets in progress
- No explicit runtime limit
- Set of prepared applications already available
- Allows to spawn additional jobs from the notebook (cascading)
- Notebook environment for advanced users
  - https://binderhub.cloud.e-infra.cz
  - Build notebook image from source
  - Possible to request special resources (RAM, CPU, GPU, …)

Aplhafold

- Web UI for Apphafold tools
- Supports several different tools
  - Alphafold, Colabfold, Omegafold, Emsfold
- Colabfold
  - Running our mmseqs server (no rate limits)
  - Added possibility to limit number of models
- Integrated Mol* viewer and e-INFRA CZ storage

- Also collaboration on the development and support for AlphaFind

Aleš Křenek group

- Building application specific computational environments for scientific data processing, analysis, and interaction with data repositories
  - CryoEM, MD, protein similarities
- Joint development of advanced computational techniques in scientific data processing using ML and quantum computing
  - Mass spectroscopy, MD
- Operation and development of Galaxy service, generic environment for FAIR data processing
  - https://usegalaxy.cz

Jiří Filipovič Group

- Methods for Automatic Code Optimization
  - OpenCL and CUDA Autotuning with kernel Tuning Toolkit
  - Optimization of Computation Kernels Granularity
- Application in Computation Chemistry and Biology
  - Caverdock 2.0
  - Optimization and acceleration of EM software (Xmipp sw package)
- Related areas of research interest
  - Runtime systems
  - Performance Engineering
  - Performance Prediction Methods
  - Real-time simulations

Tomáš Rebok Group

- Data analytics environment for heterogeneous and multisource unstructured data
  - Central processing, personal datasets and „assistents“, …
- Originally developed for Police
  - Need of high privacy, personal data processing
  - Highly unstructured data combined with structured ones
- Work with Institute for Global Change (CzechGlobe)
- Currently offered as the Core Data Center facility and services for the eLTER-ERIC under preparation

CERIT-SC interaction with EOSC

- Coordinating the EOSC-CZ project
  - Partners are CESNET and VSB-TUO (IT4Innovations)
  - The strategic project of OP JAK
  - To oversee, monitor and support the EOSC implementation in CR
  - Hosting EOSC CZ secretariat
- Collaborating with CARDS project (NTK)
  - Mirek Bartošek one of the major architects for PNG
- Member of NRP for research data project
  - Coordinated by CESNET
  - CERIT-SC leading service oriented workpackages there

CERIT-SC interaction with EOSC

- Collaborating with UK on preparation of the Open Science II project
  - Helping to coordinate MU involvement

- Providing also wider Open Science support at MU
  - MU Open Science strategy
  - Support for Open Access
  - Coordinating the OpenAccess/Open Science managers at MU
  - Cultivating support and environment for the Data Curators

Summary for CERIT-SC

- CERIT-SC provides resources together with the advanced expertise for their use
  - From batch processing to highly interactive tasks
  - Indirect support for AI (LLM) processing on GPUs
- Part of large research infrastructures
  - Formally e-INFRA CZ and ELIXIR CZ
  - eLTER(-ERIC) in progress
- Collaboration with other LRIs
  - BBMRI CZ, RECETOX, CzeCOS, …
-

Thank you for your attention

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