

Open Science Week

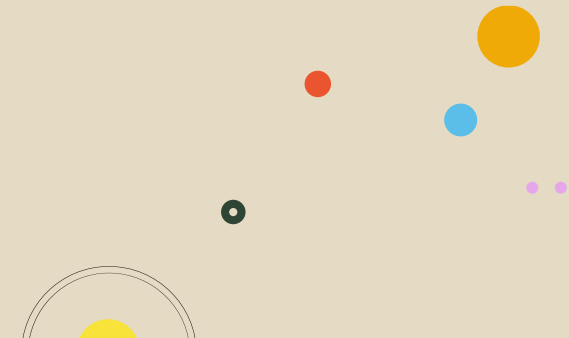
16.–20. 10. 2023



# Multiomická studie

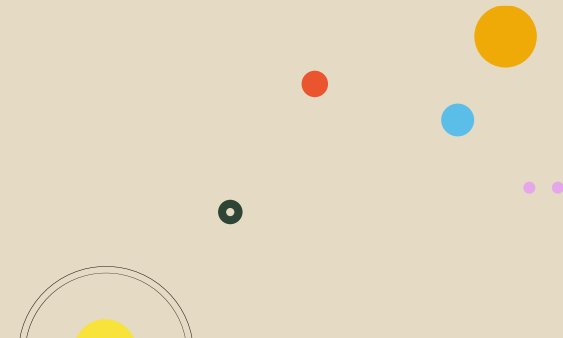
Jarmila Stanková, Ústav molekulární a translační medicíny, LF UPOL

International  
Open Access Week



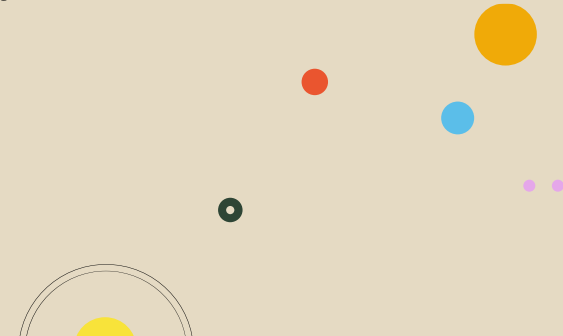
# Eatris+ projekt – Multiomická studie

- EATRIS (European Advanced Translational Research Infrastructure in Medicine)
- Projekt podpořený v rámci programu H2020
- 20 partnerů
- 2020 – 2023
- Efektivní rozvoj personalizované medicíny

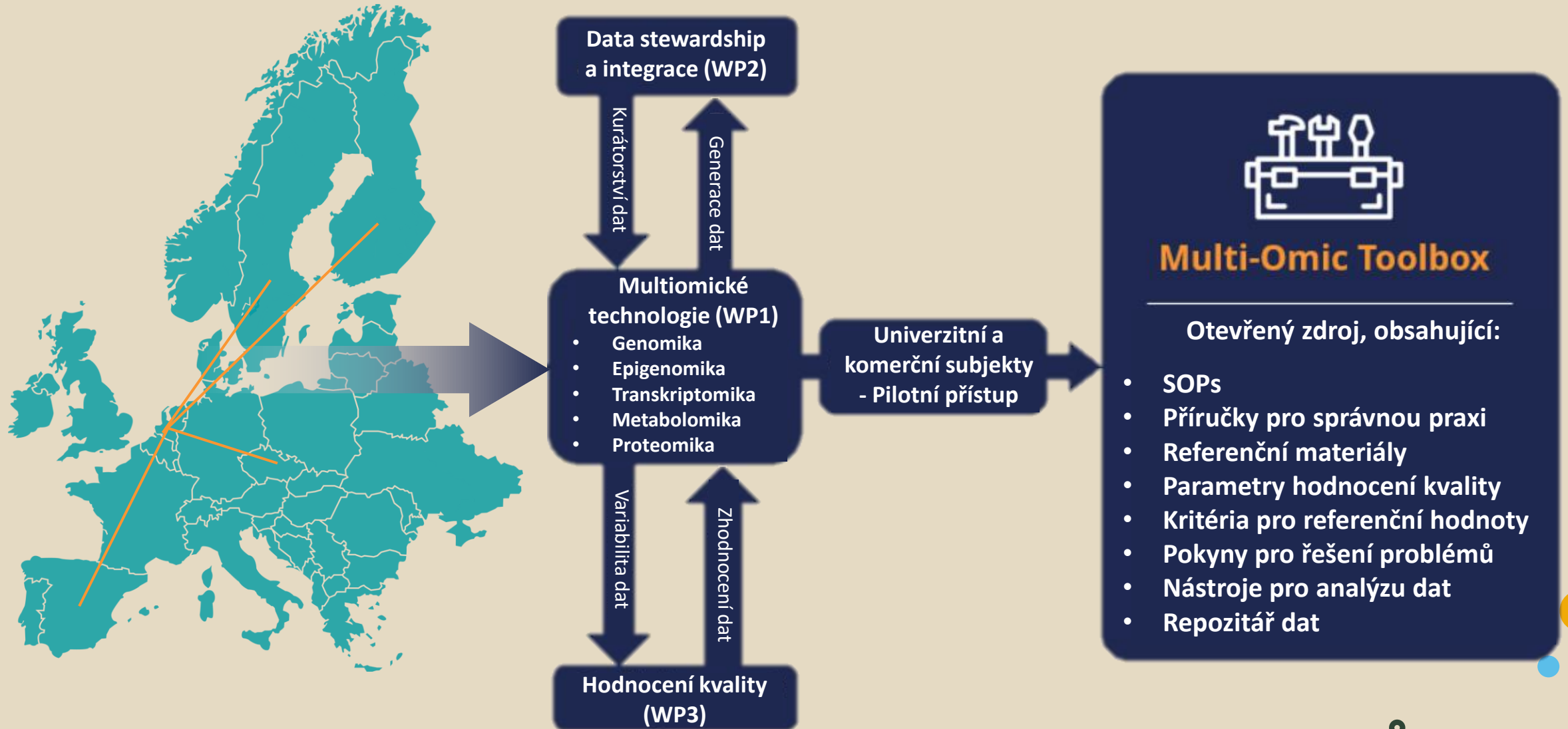


# Eatris+ projekt – Multiomická studie

- Základní myšlenky:
  - Vytvoření mostu mezi poznatky vědců a potřebami kliniků
  - Vytvoření multiomických přístupů a překonání systémových překážek ovlivňujících obor biomarkerů:
    - Nízká úroveň technologické a analytické harmonizace
    - Špatná správa dat a dodržování zásad FAIR (naležitelná, dostupná, interoperabilní a opětovně využitelná)
    - Nepochopení vztahu mezi genomovými biomarkery a downstream molekulárními markery
    - Nedostatek spolehlivých kontrolních referenčních hodnot pro tyto biomarkery u zdravé populace
    - Špatné pochopení klinických potřeb, které má za následek omezené klinické přijetí

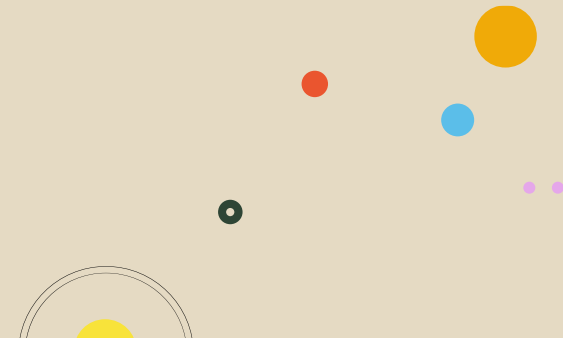


# Multiomický toolbox



# Multiomická studie - Proteomika

- Vypracování standardních operačních protokolů
- Mezilaboratorní a vnitro-laboratorní hodnocení kvality
- Zpracování a analýza vzorků pomocí proteomiky, definice kvalitativních kritérií pro datové výstupy
- FAIRifikace dat české kohorty a analytického procesu
- Návrh pracovního postupu pro společnou analýzu multi-omics dat



# SOPs

- Batch organization

The batch is started with SST Test (5 injections of BSA Standard), samples are released for analysis based on the results of SST. The plasma samples (5 samples in duplicate, 10 injections) and 1 BSA Standard are running repeatedly until 46 plasma samples is measured. The batch is ended with SST Test (3 injections of BSA Standard). In total 108 injections is acquired and then regular maintaining needs to be done.

- LC settings

- Flow rate 300 nl/min
- Temperature 35 °C
- Loading - Loading Buffer over the 5 minutes, flow 6 µl/min
- Injection - 10 µl of sample (1 µg of peptides, 100 fmol PROCAL peptides)
- Gradient - 0 min (98% A/ 2% B), 5 min (98% A/ 2% B), 65 min (65% A/ 35% B), 73 min (10% A/ 90% B), 95 min (98% A/ 2% B) - total time 95 minutes.

- MS settings

- Ionization - NSI type
- Acquisition - positive mode
- MS1 - Orbitrap at resolution 120 000, scan range 400-1500, injection time 50 ms
- Dynamic exclusion - after 1 times for 60 sec
- Data dependent type of acquisition, with cycle time 2 sec
- Fragmentation type - HCD (NCE 32)
- MS/MS detector - Orbitrap at resolution 15 000, injection time 22 ms

All detailed parameters of liquid chromatography and mass spectrometry settings are described below.

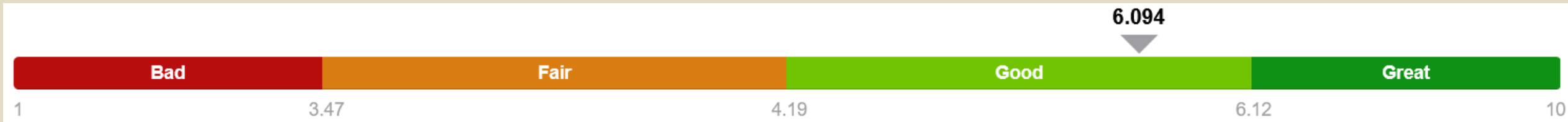
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Thermo Scientific SII for Xcalibur Method

---- Overview ----

# Mezi-laboratorní hodnocení kvality

- chinese-quartet.org - Quality Control and Data Integration of Multi-omics Profiling
- Zheng, Y., Liu, Y., Yang, J. *et al.* Multi-omics data integration using ratio-based quantitative profiling with Quartet reference materials. *Nat Biotechnol* (2023)

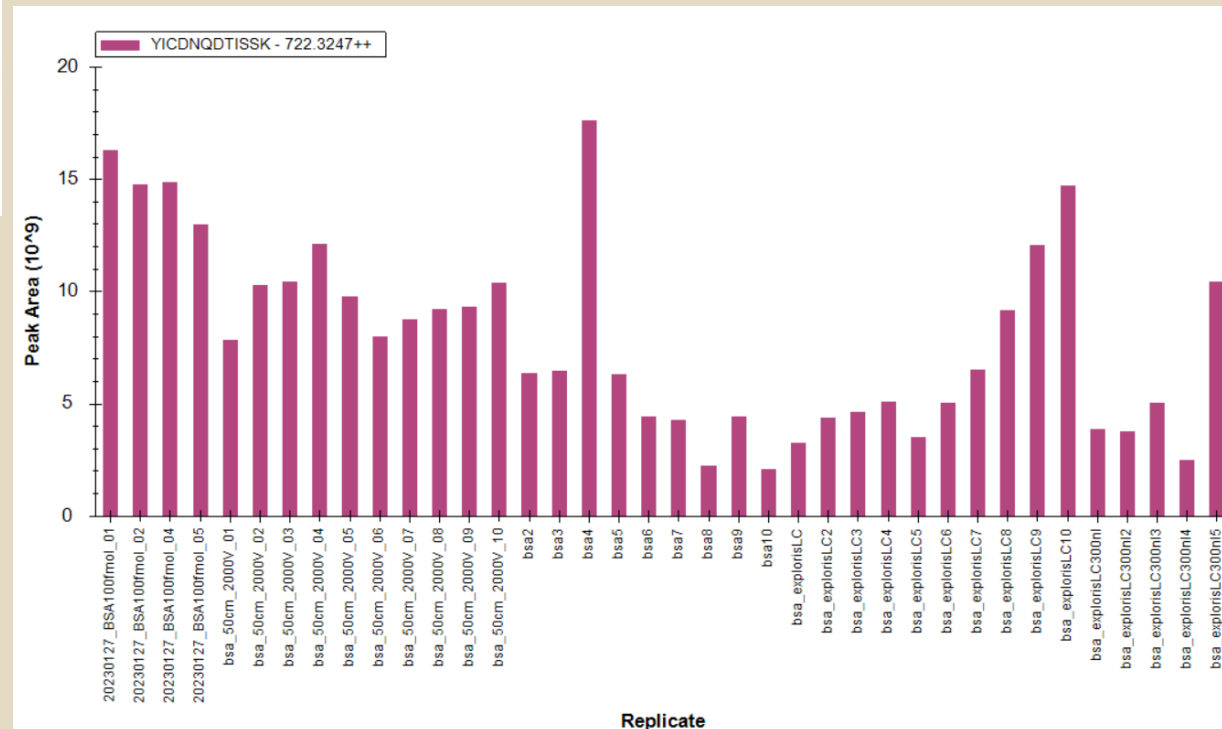


Quality Metrics	Value	Historical Value	Rank	Performance
Number of features	3708.000	4533.938 ± 838.623	28/33	Bad
Missing percentage (%)	6.877	24.382 ± 9.879	5/33	Great
Absolute Correlation	0.943	0.92 ± 0.033	8/33	Good
Coefficient of variation (CV, %)	1.206	22.52 ± 8.324	1/33	Great
Signal-to-Noise Ratio (SNR)	5.376	15.766 ± 8.094	28/33	Bad
Relative Correlation with Reference Datasets (RC)	nan	0.897 ± 0.082	nan	nan
Total Score	6.094	4.919 ± 2.185	9/33	Good

- NIST - National Institute of Standards and Technology (USA)

# Vnitro-laboratorní hodnocení kvality

- Pravidelné měření standardů (komerčních nebo vytvořených)
- Pravidelné vyhodnocení standardů
- SST test
- Pravidelná údržba přístrojů







Welcome to Ontobee!

Ontobee: A [link](#) dynamically [dere](#) Se

Newly processed Raw data in the List of reanalyzed 2546 2547 2549

ReanalysisInfo.txt

OLS / PRID

PI Ke

Short description - Processing was - Search with Se - PSM, Peptide a - Quantification S - Normalization

Proteomics\_readme.txt

Data

http://pu

Algorithm: MDS Hash: C194E8 Path: EatriPlus

MDEcheckum.txt

(59:50)

for ies.

Log in

sample properties

data file properties

study variables

source name	characteristics[organism]	characteristics[disease]	characteristics[phenotype]	...	assay name	comment[fraction identifier]	comment[label]	comment[data file]	factor value[phenotype]
sample 1	homo sapiens	gastric carcinoma	control		Run 1	1	label free	fileRAW_Control_F1.raw	control
sample 2	homo sapiens	gastric carcinoma	primary tumor		Run 2	1	label free	fileRAW_Tumor_F1.raw	primary tumor
....									

EatrisPlus\_Reanalysis\_normalizationandimputation\_proteins.txt

Confidence(Seq)

EatrisPlus\_Reanalysis\_normalizationandimputation\_peptides.txt

12

[BCO](#)

Biological Collections Ontology

L



Safe home for your scientific data.

Register

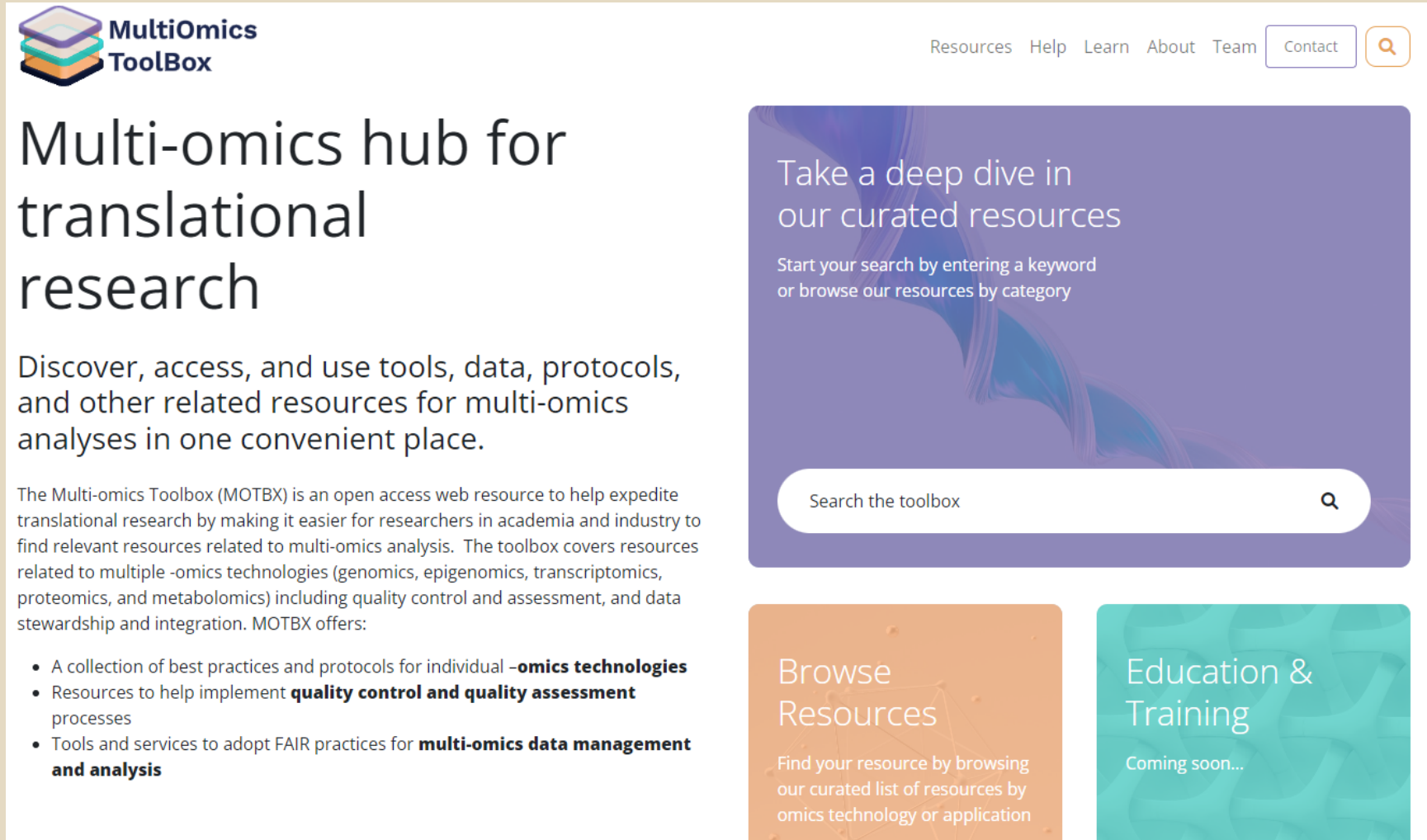
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# Multiomics toolbox

- <https://motbx.eatris.eu/>



The screenshot shows the homepage of the MultiOmics ToolBox. At the top left is the logo, which consists of three stacked squares in purple, teal, and orange, followed by the text "MultiOmics ToolBox". To the right of the logo is a navigation menu with links for "Resources", "Help", "Learn", "About", "Team", and "Contact", along with a search icon. The main heading reads "Multi-omics hub for translational research". Below this is a sub-heading: "Discover, access, and use tools, data, protocols, and other related resources for multi-omics analyses in one convenient place." A paragraph follows, describing the toolbox as an open access web resource to expedite translational research. Below the paragraph is a bulleted list of three key offerings. The right side of the page features a large purple banner with the text "Take a deep dive in our curated resources" and a search bar. Below the banner are two colored boxes: an orange one for "Browse Resources" and a teal one for "Education & Training".

**MultiOmics ToolBox**

Resources Help Learn About Team Contact 

## Multi-omics hub for translational research


Discover, access, and use tools, data, protocols, and other related resources for multi-omics analyses in one convenient place.

The Multi-omics Toolbox (MOTBX) is an open access web resource to help expedite translational research by making it easier for researchers in academia and industry to find relevant resources related to multi-omics analysis. The toolbox covers resources related to multiple -omics technologies (genomics, epigenomics, transcriptomics, proteomics, and metabolomics) including quality control and assessment, and data stewardship and integration. MOTBX offers:

- A collection of best practices and protocols for individual **-omics technologies**
- Resources to help implement **quality control and quality assessment** processes
- Tools and services to adopt FAIR practices for **multi-omics data management and analysis**

Take a deep dive in our curated resources

Start your search by entering a keyword or browse our resources by category

Search the toolbox 



**Browse Resources**

Find your resource by browsing our curated list of resources by omics technology or application

**Education & Training**

Coming soon...

- <https://motbx.eatris.eu/resource-category/proteomics/>

 Resources Help Learn About Team Contact 

# Proteomics

Includes a collection of guidelines, reference materials, sample processing workflows, data processing tools and material for technical and quality checks regarding proteomics data.

## Guidelines and best practices

Quality control in mass spectrometry-based proteomics

## Categories

Scroll for more filter options

Internal Quality Control

Missing something? Contribute to the Multi-omics Toolbox!

[Submit a resource](#)

Plasma sample preparation for HR-MS analysis

Protocol for processing plasma samples appropriately for High-Resolution Mass Spectrometry (HR-MS) proteomic analysis.

Tagged in: [EATRIS-Plus project](#) [sample preparation](#) [proteomics](#) [protocol](#)

[View this resource](#)

[Report broken link](#)

Raw data search in proteomics

HR-MS proteomic analysis with Thermo Orbitrap Fusion instrument setup

Guidelines and best practices

Raw data processing

Protocols

Technical and quality checks

Reference material

Samples processing

Tool

Metabolomics

Omics data management and analysis

Tags

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Děkuji za pozornost!

[jarmila.stankova@upol.cz](mailto:jarmila.stankova@upol.cz)

International  
Open Access Week

