



# RECETOX Doctoral Conference 2024

For a healthy future

29. – 30.  
May



MUNI | RECETOX

# Planning

**Wednesday, May 29, 2024, RCX1**

9:30

Luděk Bláha – Welcome and introduction to PhD Conference

9:35 – 10:00

Barbara Kubíčková – Translating skills from my PhD studies to jobs in the non-academic sector

## SDE

10:00 – 12:30

State Doctoral Exams

- SDE01 ➤ **10:00 Gregor Petr** - Assessment of exposure to chemicals and their impact on human health
- SDE02 ➤ **10:30 Dvořák Tadeáš** - Urban Stress and Its Biomarkers: Investigating the Effects of Exposure to Built and Natural Environments
- SDE03 ➤ **11:00 Edebali Özge** - Characterising the link between indoor air, dust and textile contamination
- SDE04 ➤ **11:30 Seličová Hana** - Automated functional metabolomics and application to case-control disease studies
- SDE05 ➤ **12:00 Contini Thomas** - Deciphering the human prenatal chemical exposome using high-resolution mass spectrometry

12:45

Wrap-up & Voting // Announcement of the results

13:00

Pizza and Poster session – Category A

# Planning

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13:00 – 14:30	Category A (students in years of study 1-2)
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- P01 ➤ **Böhm Jan** - Multi-omic integration of four datasets: Insights into Barrett's esophagus and esophageal carcinoma
  
- P02 ➤ **Březina Adam** - Investigation of aromatic amines in municipal wastewaters using Stir Bar Sorptive Extraction with derivatization
  
- P03 ➤ **Capelli Diego** - Exploring Non-Canonical Amino Acid Integration in Fibroblast Growth Factors
  
- P04 ➤ **Pluskal Daniel** - IRrIS: The first BRET-based bioluminescent system engineered in nature's image
  
- P05 ➤ **Řehůrková Eliška** - Advancing Male Reproductive Toxicology with Innovative 3D hiPSCs-based Models of Testicular Steroidogenesis
  
- P06 ➤ **Skřídlová Soňa** - External Exposome Factors and Cancer Incidences
  
- P07 ➤ **Verma Naina** – Unraveling the conformational dynamics of staphylokinase
  
- P08 ➤ **Vykypělová Michaela** – Behind the BPA-free label

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15:00	Best Poster announcement (Category A)
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# Planning

**Thursday, May 30, 2024, RCX1**

9:30 - 9:35	Luděk Bláha – Welcome to 2nd day of PhD Conference
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## SDE

9:35 – 11:30	State Doctoral Exams
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- SDE6 ➤ **9:35 Kohout Pavel** - Generative Machine Learning in Protein Engineering
- SDE7 ➤ **10:00 Mičan Jan** - Molecular Modeling and Bioinformatics in the Study of Neurological Disorders
- SDE8 ➤ **10:30 Vašková Aneta** - Biochemical and structural studies of Apolipoprotein E in health and disease
- SDE9 ➤ **11:00 Mičůchová Natálie** - Microbiome and pharmacotherapy in patients with gastrointestinal disorders

11:45	Wrap-up & Voting // Announcement of the results
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12:00	Pizza and Poster session – Category B
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# Planning

## Poster Session

12:00 – 14:30

Category B (students in years of study 3-4)

- P09 ➤ **Divinová Renata** - Introducing MetaboPeak
- P10 ➤ **Haddadi Faraneh** - Capturing Protein Dynamics and Their Determinants Using Explainable Artificial Intelligence
- P11 ➤ **Holotová Simona** - Potential biomarkers of bone and adipose inter-tissue crosstalk in obese bariatric patients
- P12 ➤ **Horáčková Jana** - Shedding Light on the Secrets of Nanoluc its Mechanism and Allosteric Behaviour
- P13 ➤ **Kouba Petr** - Machine Learning for Dynamics-Aware Protein Sequence Design
- P14 ➤ **Strada Rebeca** - Investigating the Structure-Property Relationships of Croconaine Dyes
- P15 ➤ **Brenner Daniela** - Elucidation of the impact of Poly-and perfluorinated compounds (PFAS) on the liver metabolome and associated diseases using a 3D advanced in vitro model
- P16 ➤ **Hrežová Eliška** - Mediterranean diet score linked to cognitive functioning in women: evidence from the Czech Republic
- P17 ➤ **Jebli Akrem** - Automated sequential derivatization for GC-MS based metabolite profiling of human blood

# Planning

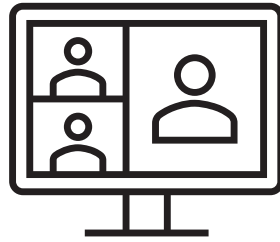
- P18 ➤ **Marcinekova Paula** - Association between building characteristics and plasticisers in indoor settled dusts
- P19 ➤ **Sapunova Daria** - Revealing bisphenol exposure in Czechia: disparities across decades and significant determinants
- P20 ➤ **Suchankova Lenka** - Multiannual characterization of PM1 aerosol optical properties and size distribution at the urban atmospheric site ATOLL in Lille
- P21 ➤ **Svobodova Petra** - Time trends of flame retardants additives in cars
- P22 ➤ **Čarnogurská (Hrivňáková) Martina** - One for all...? Morphology-resolved search for mutations in non-responders to anti-EGFR therapy in colorectal carcinoma
- P23 ➤ **Pivrcová Eliška** - Assessment of Viable Bacterial Communities in Fresh and Stored Human Milk
- P24 ➤ **Vyklická Kateřina** – Toxicological analysis in patients with inhalation injury during their hospitalization  
– ONLINE POSTER ONLY

15:00

Best Poster announcement (Category B)

**DAY 1**  
**29.05.2024**

# Day 1: Link for Participation Online



29.5.2024: [Připojit se ke schůzce hned](#)



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Poster Evaluation Link

- <https://forms.office.com/e/VAUrtMFK7p>

RECETOX PhD Conference:  
Day 1

Poster Evaluation Form

29th May 2024





# Invited speaker

Barbara Kubíčková



Technical Expert  
Global Science Delivery – Toxicology  
Syngenta UK, Jealott's Hill International Research Centre,  
Bracknell, Berkshire, United Kingdom



## Translating skills from my PhD studies to jobs in the non-academic sector

How do you know what you want to do after graduating (or not)? How do you navigate a job market and align your job search with your skills/expertise and interests? Is it possible or feasible to pursue multiple “targets”, like professional ambitions, international work experience, and family? What does it take? How Do you know if a workplace gives you the right environment to strive professionally and personally – ideally before starting the job?

### **Biography**

In 2017 I was awarded a Marie Skłodowska-Curie Fellowship in the “NaToxAq” Initial Training Network for my PhD studies at RECETOX, which I successfully concluded in 2022. My work investigating human health hazards associated with cyanobacterial blooms in surface waters, utilising *in vitro* test systems and exploring applicability towards human health risk assessment was honoured with the Rector’s Award for an outstanding Doctoral Thesis in 2023.

During my PhD studies, in 2020 I took the opportunity of a PostDoc position with the UK Health Security Agency (formerly Public Health England), working on the EU-funded project “GOLIATH”. I worked as the project manager for *in vitro* test method development, refinement, and (pre-)validation with relevance to the OECD Test Guidelines Programme, focusing on test methods on metabolic/ endocrine disruption. I then took an opportunity to work as a Technical Expert in Toxicology with Syngenta in 2023, working primarily as a toxicology study manager, overseeing data generation and delivery with Contract Research Organisations for Crop Protection Research projects. I am a Mental Health First Aider, a member of the British Toxicology Society’s “Network for Early Stage Toxicologists” subcommittee, have recently applied to become a European Registered Toxicologist, and have two children.

# Abstracts

SDE01

## Assessment of exposure to chemicals and their impact on human health

Gregor Petr



This thesis aims to explore novel approaches for assessing the impact of selected chemical exposure and other exposome factors on biomarkers of effect and potential health risks in the human population. These exposures were assessed by external approach (environmental concentrations) or internal approach (chemical concentrations in human matrices - blood, urine, saliva, etc.). Their impact was investigated at the individual level by biomarkers of effects (e.g., thyroid disruption, DNA-damages, or epigenetic markers in human blood: in the CELSPAC-YA, CELSPAC-SPECIMEn, CELSPAC-FIREexpo cohort studies) and at the population level (e.g., cardiovascular disease, asthma). Emphasis was placed on employing advanced statistical evaluation methods, utilizing R software and the latest R scripts for exposure to priority chemicals and their effect assessment.

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SDE02

## Urban Stress and Its Biomarkers: Investigating the Effects of Exposure to Built and Natural Environments

Dvořák Tadeáš



Urban living has been associated with adverse health effects and stress. It is paramount to understand what parameters stimulate urban stress. My PhD thesis aims to establish how exposure to urban environments and their attributes affects stress biomarkers. In a set of in situ and laboratory experiments, participants are exposed to built and natural environments with different underlying characteristics. The objectives are to i) quantify urban environments by their environmental, functional and social attributes; ii) measure exposure effects using physiological and neurobiological methods (e.g. HRV, EDA, EEG, fMRI); iii) apply statistical models to test the link between urban attributes and changes in stress biomarkers. By uncovering the underlying factors of urban stress, this research can contribute to healthier urban environments.

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SDE03

## Characterising the link between indoor air, dust and textile contamination

Edebalı Özge



Recognizing the role of textiles as inadvertent indoor passive samplers, we characterized the uptake of Aromatic Amines (AAs) from the gaseous phase of indoor air by cotton, wool, and polyester textiles under controlled conditions. AAs uptake to textiles was investigated using a series of chamber experiments to quantify textile-air partitioning. Textiles were uniformly spiked with a mix of AAs and placed in a glass chamber to equilibrate with the air inside. The chamber design allowed for the controlled extraction of a known volume of air by a vacuum pump. The analytes present in the air were sampled on a Tenax sorbent tube, and textile-air partitioning coefficient was calculated based on the concentrations in both textile and the air.

# Abstracts

SDE04

## Automated functional metabolomics and application to case-control disease studies

Seličová Hana



Short-chain fatty acids (SCFA) are vital products of gut microbiota fermentation tightly linked to human health. The correlation of SCFA disbalance with metabolic diseases underscores the need for a streamlined and cost-effective assay. Gas chromatography-mass spectrometry (GC-MS) offers high sensitivity but often requires chemical derivatization of analytes, prolonging analysis time. We present a rapid, automated, derivatization-free method for SCFA quantification and further volatile profiling. The method is approximately 20 minutes sample-to-sample long and aims to quantify 6 SCFA and 3 branched-chain fatty acids (BCFA). A cartesian autosampler and GC-Q-MS in full scan-SIM mode are utilized and enhance throughput and sensitivity. The developed automated method helps to reduce human-prone errors and enables easier multi-site replication with accessible instrumentation.

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SDE05

## Deciphering the human prenatal chemical exposome using high-resolution mass spectrometry

Contini Thomas



The placenta is a key regulator between maternal system and the fetus. Combining advantageous aspects, this is a relevant matrix to study prenatal chemical exposures. However, being relatively underexplored compared to other matrices (blood, urine), some questions remain to be answered before using the organ at cohort-scale.

This project implements a standardized methodology to apply non-targeted analyses, using HRMS to evaluate the intra- and inter-individual variability of the metabolome and the chemical exposome.

A collection of 25 placentas was made in France. Eighteen samples were taken from each placenta, at different distances and depth from the cord insertion site. Using LC and GC coupled to HRMS, we hope to provide relevant new insights regarding metabolome variability and placental chemical exposome.

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# Abstracts

P01

## Multi-omic integration of four datasets: Insights into Barrett's esophagus and esophageal carcinoma

Böhm Jan



**Objective:** Our study aimed to integrate and compare multiple omic datasets to identify differences between Barrett's Esophagus (BE) and Esophageal AdenoCarcinoma (EAC).

**Methods:** Data were processed using specific criteria for each omic type, including aggregation levels, normalization methods, and inclusion thresholds. We employed the DIABLO framework for the integration and analysis of these diverse datasets, focusing on the identification of discriminative features.

**Results:** In contrast to metatranscriptomic data, transcriptomic data demonstrated the highest discriminative power, effectively differentiating between paired BE/EAC pathological and adjacent esophageal tissues, as well as between diagnoses. Pathological samples displayed significant metagenomic variability (16S rRNA sequencing) compared to paired adjacent tissues.

P02

## Investigation of aromatic amines in municipal wastewaters using Stir Bar Sorptive Extraction with derivatization

Březina Adam



Aromatic amines (AAs) are significant environmental pollutants, suspected of being mutagenic, often entering water bodies through industrial discharge or municipal wastewater. Despite treatment efforts on wastewater treatment plants (WWTPs), AAs persist, posing risks to both the environment and human health. Objective of this is to develop method for monitoring aromatic amines in wastewater and sludge. This study introduces Stir Bar Sorptive Extraction (SBSE) pose an efficient method for monitoring AAs in wastewater and activated sludge. Different SBSE coatings are tested, along with various desorption methods, instrumental analyses, and two different derivatization approaches, using acetic anhydride and benzoyl chloride, to enhance extraction efficiency. This approach shows promise for analyzing and monitoring primary amines in wastewater and activated sludge from WWTPs.

# Abstracts

P03

## Exploring Non-Canonical Amino Acid Integration in Fibroblast Growth Factors

Capelli Diego



Fibroblast Growth Factors (FGFs) regulate numerous mechanisms within complex organisms, including cell proliferation, differentiation, and survival, sparking interest for applications like wound healing and cancer treatment. This PhD project aims to address the challenge of expanding the genetic code through the incorporation of non-canonical amino acids (ncAAs), enhancing stability and activity of FGFs. Two state-of-the-art methods will be employed: Selective Pressure Incorporation (SPI) and Stop Codon Suppression (SCS). Through SPI, we will globally replace natural amino acids with their non-canonical counterparts to evaluate the impact of ncAAs on FGFs. With SCS, we will use site-specific incorporation to introduce ncAA that will act as a handle for immobilisation or interaction with other biological entities.

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P04

## IRrIS: The first BRET-based bioluminescent system engineered in nature's image

Pluskal Daniel



The emission of visible light by living creatures is not only a fascinating phenomenon but also a valuable tool for biotechnology and biomedicine. This project focuses on studying molecular principles of bioluminescence and developing tuneable and autonomous light-emitting systems employing Renilla-type bioluminescence resonance energy transfer (BRET). This is enabled by our previous discoveries in marine bioluminescence, which this project aims to transfer into a useable technology, allowing not only ultrasensitive, noninvasive real-time bioimaging of biological processes and molecular events but also the treatment of cancer or other diseases through photodynamic therapy or the creation of independently bioluminescent organisms such as plants and trees. Such nature-inspired biosystems could ultimately help light up city streets and highways, reducing the need for electricity.

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P05

## Advancing Male Reproductive Toxicology with Innovative 3D hiPSCs-based Models of Testicular Steroidogenesis

Řehůřková Eliška



Rising concerns over male reproductive health have underscored the importance of understanding disruptions in the process of androgen production within Leydig cells, a phenomenon known as testicular steroidogenesis. Environmental pollutants and drugs are often responsible for such disruptions. However, current in vitro models used to study the effects of these substances lack human relevance. To address this gap, I have developed an innovative model that utilizes differentiated human induced pluripotent stem cells to create human Leydig-like cells. This approach allows us to investigate Leydig cell development during critical developmental windows in vitro and identify the effects of chemicals on this process. Additionally, the model is being adapted for three-dimensional conditions to better mimic the in vivo microenvironment.

# Abstracts

P06

## External Exposome Factors and Cancer Incidences

Skřídlová Soňa



This study explores the impact of external exposure factors on cancer in Czech communities. A novel approach is being incorporated to investigate the impact of chemical exposures on cancer incidences in the detailed spatial municipal resolution across the Czech Republic. By utilizing the comprehensive health outcome data from over 6,258 municipalities, collected over two decades, we meticulously explore the relationship between environmental factors and cancer occurrences. Special attention is given to developing a methodology ensuring estimations of radon indoor concentrations and their association with lung cancer outcomes. By employing advanced statistical tools (LME, GEE), latest EU ASR standards, and confounding factors this research aims to rigorously assess localized impacts such as targeted prevention. Further explorations will include the influence of additional environmental factors like drinking water quality and air quality.

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P07

## Unraveling the conformational dynamics of staphylokinase

Verma Naina



Seeking new thrombolytics, a small bacterial protein, Staphylokinase (SAK) is highly promising due to its high fibrin specificity and low cost. This research primarily focuses on the conformational dynamics of SAK with the main aim of understanding its in-solution behavior in apo and holo forms. Additionally, it aims to study the alterations in dynamics due to mutations that are designed through a rational protein engineering approach.

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P08

## Behind the BPA-free label

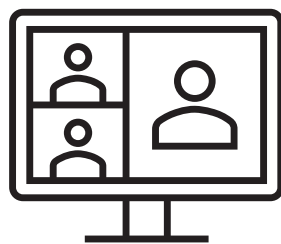
Vykypělová Michaela



Plastic additive bisphenol A (BPA) was proven to be an endocrine disruptor with estrogenic activity. Further, the tolerable daily intake was lowered 10 000x due to the impact of the immune system. The health concerns and following restrictions have led to the development of alternative chemicals (e.g. BPS), that also show similar endocrine disruption and other adverse health effects. For these alternatives, toxicity data are currently unavailable. We aim to investigate the long-term effect of BPA-alternatives on the immune system, particularly on the host gut microbiome-immunity axis. With zebrafish as a model, we will employ approaches that link the intestinal microbiome and markers of deregulated immunity in intestinal and blood tissue.

**DAY 2**  
**30.05.2024**

# Day 2: Link for Participation Online



30.5.2024: [Připojit se ke chůzce hned](#)

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Poster Evaluation Link

- <https://forms.office.com/e/WLeNVZAHDe>





# Abstracts

SDE6

## Generative Machine Learning in Protein Engineering

Kohout Pavel



Proteins are the fundamental building blocks of life and play vital roles in numerous biological processes with vast application potential in diverse fields, ranging from medicine to biotechnology. Nevertheless, utilizing the available extensive reservoir of protein data for successful protein design or unraveling the fundamental mechanisms that drive their evolution poses a daunting task. My current research focuses on the challenge of studying proteins using advanced machine-learning techniques. Namely, I employ state-of-the-art neural networks to construct interpretable low-dimensional representations to analyze various protein data modalities and explore the ways of incorporating structural properties encoded in these representations to design novel proteins that exhibit improved properties.

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SDE7

## Molecular Modeling and Bioinformatics in the Study of Neurological Disorders

Mičan Jan



We studied three neurological disorders that present a large medical burden on the aging population: stroke, Alzheimer's disease, and epilepsy. We designed stroke thrombolytics by mutagenesis of alteplase and staphylokinase by various structural bioinformatics methods. Mainly, we obtained their complexes with interacting proteins using protein-protein docking and molecular dynamics, and predicted the effect of mutations on their binding. For Alzheimer's disease, we describe current hypotheses and therapeutic strategies, as well as our computational modeling of amyloid beta 42 dynamics with a potential medicine using Markov state modeling by VAMPNets. For epilepsy, we describe the PredictNeuro web server for assessing mutation effects on epilepsy, precision-targeted therapy, and structural bioinformatics methods used in the server that we are developing.

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SDE8

## Biochemical and structural studies of Apolipoprotein E in health and disease

Vašková Aneta



This work summarizes research exploring the role of Apolipoprotein E in Alzheimer's disease and other neurodegenerative disorders, focusing on the distinct behaviours of its isoforms, particularly APOE4, and their implications in disease pathogenesis. Our study delves into APOE's involvement in lipid metabolism, its genetic variations, and its contributions to neurodegenerative processes such as protein aggregation, fragmentation, and DNA-binding ability. This research is conducted in collaboration with Biovendor, supporting the industry-academia PhD framework that combines practical industry experience with academic research. We also investigate therapeutic approaches to mitigate APOE4-related pathologies, aiming to develop targeted treatments based on genetic risk profiles. This comprehensive study enhances our understanding of APOE's role and advances potential personalized therapeutic interventions.

# Abstracts

SDE9

## Microbiome and pharmacotherapy in patients with gastrointestinal disorders

Mlčůchová Natálie



The role of microbiota is discussed as a crucial factor in the etiopathogenesis of several gastrointestinal disorders. In my dissertation project, I focus on microbiome, risk factors, or proton pump inhibitor treatment in patients with esophageal adenocarcinoma, pancreatic cancer, and colorectal carcinoma.

Objectives of this project are i) to analyse gastrointestinal microbiome by 16S rRNA sequencing in patients with gastroesophageal reflux disease and its complication, and also in patients with pancreatic cancer, and colorectal adenocarcinoma; ii) to identify bacterial biomarkers that could serve as a non-invasive diagnostic and predictive tool; iii) perform human genome analysis for a more comprehensive understanding of gastrointestinal cancers; and iv) to focus on metabolization of the most prescribed drugs for gastrointestinal disorders – proton pump inhibitors.

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# Abstracts

P9

## Introducing MetaboPeak

Divinová Renata



As global climate models forecast shifts in environmental conditions, understanding their impacts on forest ecosystems becomes imperative. Leveraging environmental metabolomics, this study employs LC-MS non-target analyses, exploratory statistics, and pathway analyses to unveil dynamic processes and stimuli. However, handling LC-MS data can be daunting. MetaboPeak, a new R package, addresses this challenge by automating processes, offering in-depth data insights, and facilitating file linking and data filtering. Designed to work with data from mass spectrometry software commonly used in metabolomics, MetaboPeak empowers even entry-level researchers to delve deeper into the intricacies of metabolomic data analysis, providing easy-to-follow insights and unlocking new possibilities for statistical analyses through preprocessing.

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P10

## Capturing Protein Dynamics and Their Determinants Using Explainable Artificial Intelligence

Haddadi Faraneh



Molecular dynamics is essential for unraveling the movements of biomolecules and their connection to biological mechanisms. Yet, traditional approaches to their analysis struggle with data complexity. Our project follows an alternative route and harnesses artificial neural networks and explainable artificial intelligence (XAI) to analyze two case studies: the dynamics of luciferases and interactions of Apolipoprotein E with a potential drug candidate. Our analysis revealed discrepancies between computational B-factors and residue relevancies in luciferases. We also identified regions of Apolipoprotein E critical for changes in its dynamical patterns due to the presence of the small molecule.

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P11

## Potential biomarkers of bone and adipose inter-tissue crosstalk in obese bariatric patients

Holotová Simona



Obesity's impact on bone health is complex, involving mechanical and biochemical factors influenced by various variables. We conducted a study on 32 severely obese patients who underwent bariatric surgery, analyzing serum and adipose tissue samples using advanced proteomics techniques and dual-energy X-ray absorptiometry (DXA). We found 41 serum proteins positively and 37 negatively correlated with bone mineral density (BMD). Comparing these proteins with those altered in adipose tissue, six were identified as potential mediators of adipose-bone communication: Adipsin and Alkaline Phosphatase - Tissue-Nonspecific Isozyme (AP-TNAP) showed positive correlations, while Tcadherin, MCAM, CD44 Antigen, and Integrin Alpha-2 (ITGA2) exhibited negative correlations with BMD.

# Abstracts

P12

## Shedding Light on the Secrets of NanoLuc its Mechanism and Allosteric Behaviour

Horáčková Jana



NanoLuc is a tiny but exceptionally bright bioluminescent enzyme designed in 2012 from a deep-sea shrimp luciferase. Despite its widespread use in biotechnology and biomedicine, the mechanism behind NanoLuc's light emission remained unclear, posing a barrier to advancing bioluminescent technologies. To study NanoLuc's catalysis, we combined laboratory and computational techniques, including crystallography, kinetic measurements, molecular docking, and molecular dynamics simulations with enhanced sampling. Our findings reveal that NanoLuc is monomeric in solution but is packed as a crystallographic homotetramer in some crystals. We identified two substrate binding sites: the catalytic site buried in NanoLuc's core and an allosteric site on the oligomerization interface. Finally, we enhanced the bioluminescent reaction in the active site by modifying the allosteric site.

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P13

## Machine Learning for Dynamics-Aware Protein Sequence Design

Kouba Petr



The problem of finding a protein sequence for a required protein backbone structure, also known as 'inverse folding', is of high importance for protein design and protein engineering. Recent methods tackled the core problem with success. However, the experimental validation of these methods brought a new question. Do the inverse folding models overoptimize for the recovery of the original structure at the cost of losing the protein's native flexibility? Apart from structure, dynamics is another important characteristic of a protein that should be accounted for - especially for enzymes as it allows them to perform or attend biochemical reactions. In this work, we try to address such need for dynamics-aware inverse folding.

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# Abstracts

P14

## Investigating the Structure-Property Relationships of Croconaine Dyes

Strada Rebecca



Croconaines are dyes structurally similar to cyanines, characterized by the presence of a five-membered central ring derivative of croconic acid. Croconaines are employed in several applications, including biomedicine. However, little is known about their steady-state and excited-states dynamics. We investigated the effects of functional groups on the dyes' photophysical properties using steady-state spectroscopy where, e.g. an increase of the fluorescence quantum yield was observed with increasing solvent viscosity. We investigated aggregation and acid-base equilibria in aqueous media. Finally, transient absorption spectroscopy and fluorescence upconversion (FLUPS) revealed details of their excited state behavior.

P15

## Elucidation of the impact of Poly-and perfluorinated compounds (PFAS) on the liver metabolome and associated diseases using a 3D advanced in vitro model

Brenner Daniela



Poly- and Perfluorinated compounds (PFAS) are persistent substances extensively employed in applications. Exposure to PFAS is associated with metabolic dysfunctions. This research aims to analyse the feasibility to investigate the impact of PFAS mixtures on the liver metabolome employing an advanced 3D-HepG2 in vitro model in long-term dynamic cultivation combined with  $^1\text{H}$  nuclear-magnetic-resonance spectroscopy (NMR). Matured liver spheroids were exposed for 7 days to a reconstituted real-life PFAS mixture. Post-exposure extraction of non-polar and polar metabolites, from both media and cells, was conducted using a multiple-solvent extraction method.  $^1\text{H}$  NMR measurements resulted in a metabolic fingerprint of 30-40 metabolites. Concluding, the used advanced in vitro model combined with NMR metabolomics enables the assessment of PFAS mixtures on the liver metabolome.

P16

## Mediterranean diet score linked to cognitive functioning in women: evidence from the Czech Republic

Hřežová Eliška



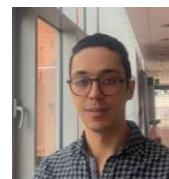
Evidence suggests that adherence to the Mediterranean diet (MED) may be beneficial in preventing cognitive decline. We aimed to explore this association in the Czech arm of Health Alcohol and Psychosocial factors in Eastern Europe study. MED score was calculated based on nine food groups from food frequency questionnaire. Cognitive function was assessed by four tests from which single z-scores were computed. The composite score of cognitive function was computed as the mean of z-scores. The cross-sectional associations between MED and composite score of cognitive function were analyzed using multivariate linear regression. Higher adherence to the MED was associated with better cognitive functioning in verbal memory and composite cognitive score in Czech females.

# Abstracts

P17

## Automated sequential derivatization for GC-MS based metabolite profiling of human blood

Jbebli Akrem



Sample preparation is a crucial step in the analysis of chemicals in biological fluids. However, it is time-consuming, limiting application to large-scale population studies. Reduced manual handling can also minimize bias and enhance method robustness. An automated sequential direct derivatization approach has been developed Utilizing a cartesian robotic autosampler. The developed method comprises 35 minutes derivatization, and evidence significantly increased sample throughput. The procedure has been applied to various human blood matrices (serum, plasma, dried blood spots of venous and capillary blood) followed by GC-[EI]-Orbitrap MS analysis with the use of cost-effective material for quality assurance and quality control (QA/QC). So far, the method enables reproducible measurement for ~80 confirmed analytes, with hundreds more putative features detected.

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P18

## Association between building characteristics and plasticisers in indoor settled dusts

Marcineková Paula



Phthalates, ubiquitous plastic additives, pose health risks, especially to children, who are exposed to dust particles via ingestion and inhalation. Though DEHP, DBP, DIBP, and BBP are restricted in many consumer products since July 2020, they are detected in household dusts in  $\mu\text{g/g}$ . We sampled dust from 120 Czech households with young children (< 5 y.) in summer 2022, analyzing 15 phthalates, 8 with 50% detection frequency. Phthalates primarily originate from vinyl flooring, PVC pipes, toys, packaging, cosmetics, and personal care products. We found that reconstruction, notably new flooring and carpeting, significantly influenced phthalate levels. Our study underscores the complexity of factors influencing indoor phthalate levels, emphasising the need for comprehensive understanding and management strategies.

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# Abstracts

P19

## Revealing bisphenol exposure in Czechia: disparities across decades and significant determinants

Sapunova Daria



Bisphenol A (BPA) and its substitutes, bisphenols S and F (BPS and BPF), are synthetic compounds commonly used in plastics and epoxy resins. Concerns arise from their endocrine-disrupting properties, given their widespread presence in consumer goods. Our study analyzed data from three Czech cohorts: CELSPAC (school children and young adults) and DEMOCOPHES (mothers with children). We attempted to estimate associations between the concentrations and questionnaire data that could reflect potential sources of exposure. Results show lower BPA levels but higher BPS and BPF levels in the CELSPAC 2019-2020 cohort compared to DEMOCOPHES 2011-2012. Cosmetics and beverages predicted BPS and BPF exposure in young adults and school children, with makeup cosmetics significantly contributing to BPS levels among Czech female young adults.

P20

## Multiannual characterization of PM1 aerosol optical properties and size distribution at the urban atmospheric site ATOLL in Lille

Suchánková Lenka



Atmospheric aerosols belong to short-lived climate forcers with high spatial and temporal variability. Although their radiative effects are greatest on regional scales, changes in aerosol emissions can induce long-term global climate effects. Thus, measuring aerosol properties is essential to better understand aerosol's impact on health and climate. Although several international projects and platforms have been monitoring aerosols worldwide (GAW, WMO, ACTRIS, EMEP, EUCAARI, etc.), only PM10/PM2.5 cutoff sizes have been used for measurements, and information about PM1 particles is missing. This study aims to present aerosol scattering, absorption properties and particle number size distribution in PM1 in 2018-2022 at the urban atmospheric site ATOLL in Lille, France.

P21

## Time trends of flame retardants additives in cars

Svobodová Petra



Vehicles, full of synthetic materials, which contain a complex mixture of additive chemicals. There is significant external impacts through variations in temperature and radiation that can influence the emission, degradation and fate of plastic additives.

We investigate the presence of brominated and organophosphate flame retardant (FR) additives in vehicles and evaluate the influence of vehicle age on the profile and levels of FRs detected. Vehicle dust was used as a surrogate matrix to indicate FR use in vehicle parts. Ten individual vehicles (1996-2021), two models of a Czech brand were tested.

We found that the levels of pentaBDE have decreased and there is no evident replacement of decaBDE. We assume the possible impact of recycling and degradation on substance levels.

# Abstracts

P22

## One for all...? Morphology-resolved search for mutations in non-responders to anti-EGFR therapy in colorectal carcinoma

Čarnogurská Martina

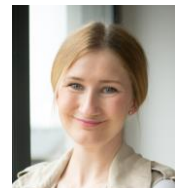


Colorectal cancer (CRC) is a significant global health concern, with limited therapeutic options for metastatic cases. This study delves into the genetic mutations present in primary tumors of 39 KRAS wild-type metastatic CRC patients undergoing anti-EGFR therapy. By employing deep next-generation sequencing of morphology-defined tumor regions and whole tumor samples, we analyzed 142 samples, revealing distinct mutational patterns between responders and non-responders, with the latter group exhibiting a higher mutational burden. Furthermore, BRAF mutations align with serrated and mucinous morphologies, while KRAS mutations (p.Lys147Glu and p.Ala146Thr, not clinically tested) are associated with mucinous and desmoplastic morphologies. Examination of genes linked to therapy response unveils substantial variability within tumors, underscoring the challenge of tumor heterogeneity in genetic profiling for treatment decisions.

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## Assessment of Viable Bacterial Communities in Fresh and Stored Human Milk

Pivrcová Eliška



This study investigated the viable bacterial communities in human milk and how different storage conditions affect them. The 16S rRNA metagenomic analysis of human milk samples from lactating mothers revealed that treating milk with propidium monoazide (PMA) resulted in fewer viable bacterial variants and diversity than untreated samples. While cold storage did not significantly change the overall bacterial diversity, it affected the viability and abundance of specific genera such as Streptococcus and Staphylococcus. Moreover, the presence of contaminants from pumping equipment and reagents underscored the need for standard collection and processing protocols. These findings highlight the importance of storage practices on the microbial composition of pumped human milk and its potential impact on infant health.

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## Toxicological analysis in patients with inhalation injury during their hospitalization

Vyklická Kateřina



Inhalation injury (INHI) may be caused by inhalation of hot stream and/or toxic compounds, such as polycyclic aromatic hydrocarbons (PAHs). In this prospective case series study, we aimed: i) to determine the PAHs in bronchoalveolar lavage (BAL) and hydroxy-PAHs (OH-PAHs) in urine, ii) to describe the dynamic changes of these toxic compounds throughout hospitalization in BAL and urine, and iii) to correlate these findings with clinical variables of the INHI patients. The highest levels of OH PAHs were found in the first day of the hospitalization, especially in patients with high-grade of INHI. In patients with INHI, the OH-PAHs in urine correlated with some of the clinical variables; thus, a determination of the OH-PAH sum in urine has a potential to serve as a prognostic marker in these patients.



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