

YoungBMC Symposium 2026

Antwerp, Belgium

Monday, 21 September 2026

Dear participants,

Thank you very much for registering for the YoungBMC Symposium 2026. It's a pleasure to have you here. Events like these provide a fantastic opportunity to come together, share ideas, learn from one another, and foster connections.

Exchange. Learn. Explore.

Our Mission

YoungBMC fosters connections among early-career researchers passionate about metabolomics across Belgium, the Netherlands, and Luxembourg (Benelux).

Join. Connect.

Learn. Collaborate.

The goals of these events are to get to know each other in a low-key manner, learn from one another, expand your own network, explore new collaborations, and find your next research partners.

***Connecting the Next
Generation of Metabolomics
Researchers.***

Wish you a wonderful time!

The YoungBMC committee

Committee members



Kristian Serafimov

Brussels
BE



Wei Yang

Maastricht
NL



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Amsterdam
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Alejandro Mendoza Cantu

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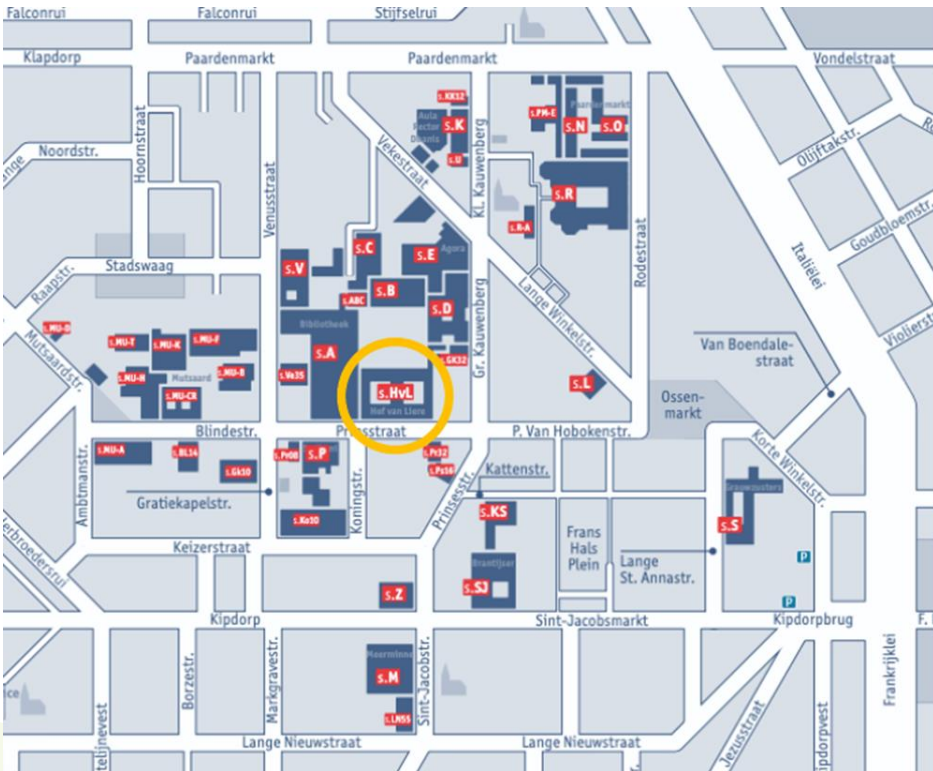


Janne Heirman

Antwerp
BE



Google Maps Hof van Liere



How to reach University of Antwerp?

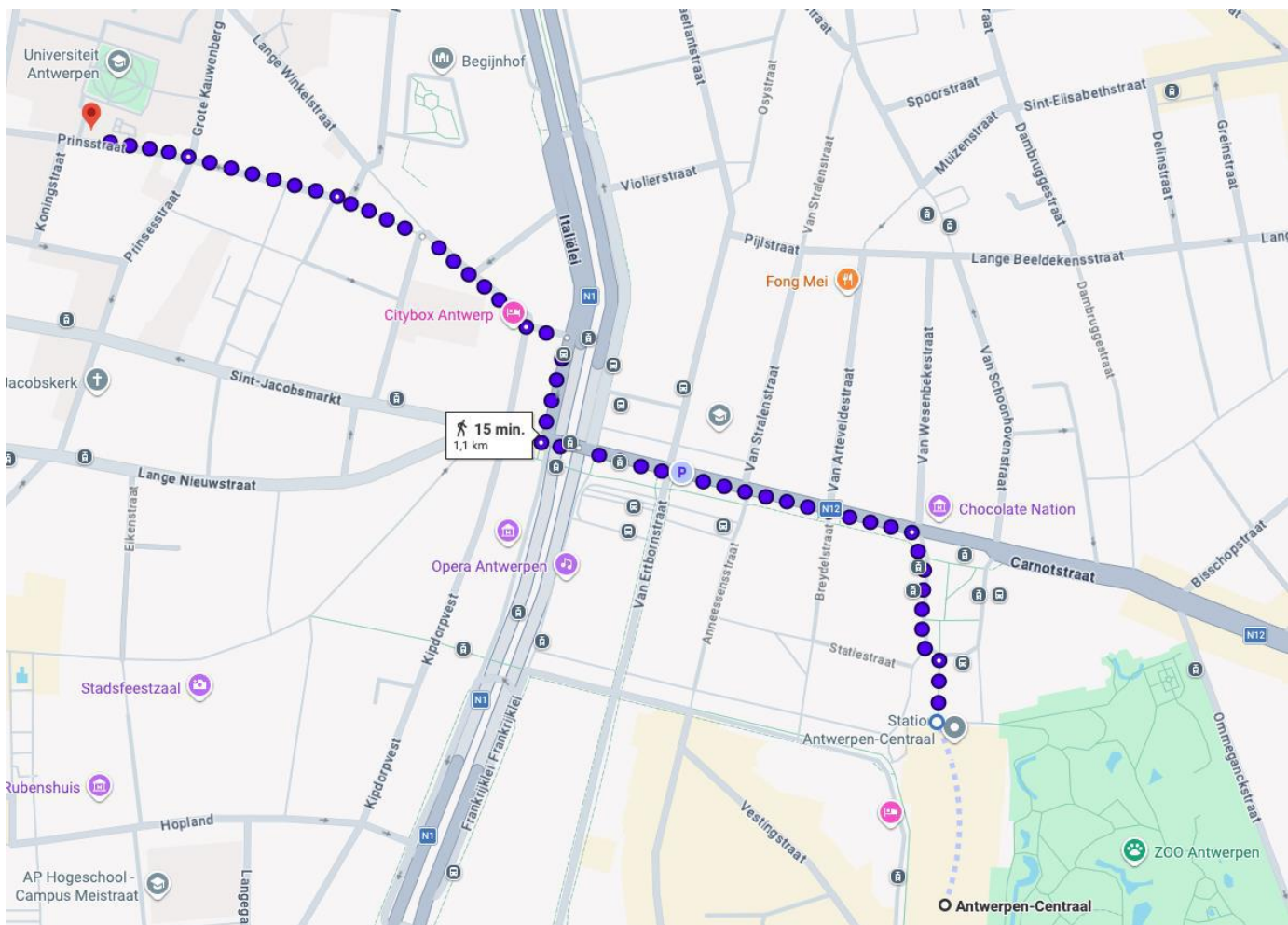
From Antwerpen-Centraal train station:

Walk 15 min

Bike 5 min

Tram 11 min: Take tram 11 for 2 stops, get off at **Antwerp St James** (**Antwerpen Sint-Jacob** in Dutch), then walk 4 min to the university

[Google Maps Hof van Liere](#)



Social event from 18:00

Location of the social event:

Spéciale Belge Taproom

Regine Beerplein 1

2018 Antwerpen, Belgium

[Google Maps Spéciale Belge Taproom](#)

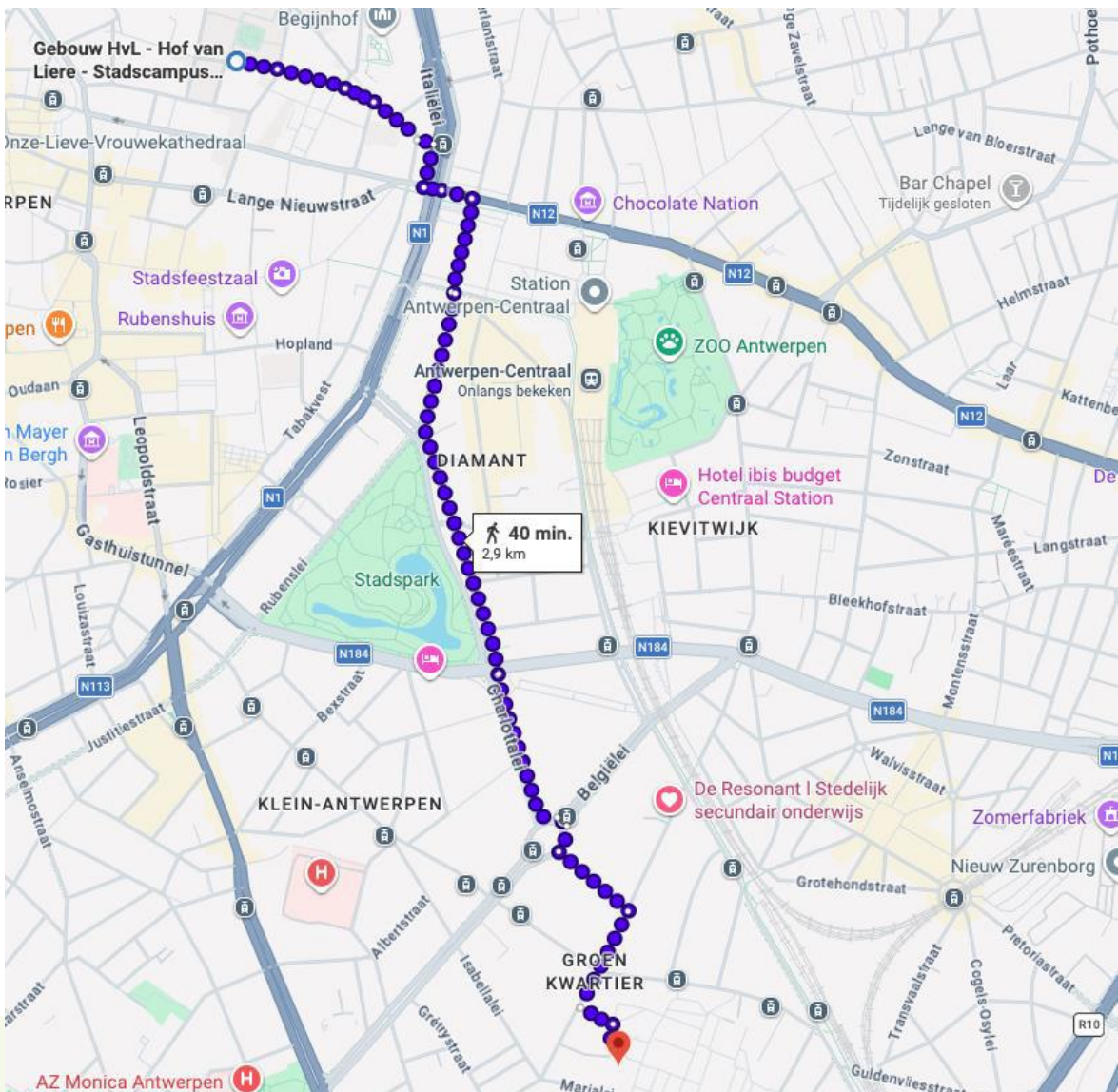
From symposium location:

Walk 40 min

Bike 11 min

Bus/Tram 26 min

Nearest train station: Antwerpen-Berchem



Getting around

Bike

- ❖ **Velo**
 - ❖ 300+ bike stations across the city
 - ❖ Day pass: €5
 - ❖ Week pass: €12
 - ❖ Buy a pass online or via the app
-
- ❖ **Donkey Republic**



Bus & Tram (De Lijn)

- ❖ €3 per ride
- ❖ Tap to pay when boarding or buy a ticket via the app before boarding



Program

Time	Presenter	Title of Presentation
9:30 - 10:00	All	Walk-in
10:00 - 10:10	YoungBMC committee	Welcome and Introduction
SESSION 1: Computational Metabolomics CHAIR: Wei Yang		
10:10 - 10:40	Keynote 1: Prof. Dr. Wout Bittremieux	Teaching AI to Understand Chemical Differences from Tandem Mass Spectra
10:40 - 11:00	Alejandro Mendoza Cantu	Fermentation-Induced Molecular Remodeling in South African Indigenous Tubers: Cassava and Cocoyam
11:00 - 11:15	Poster presenters	Poster pitches
11:15 - 11:35	All	Coffee break
SESSION 2: Cancer Metabolism & Therapeutics CHAIR: Victoria Pozo Garcia		
11:35 - 12:05	Keynote 2: Prof. Dr. Johannes Swinnen	Lipidomics as a Tool to Uncover Novel Therapeutic Vulnerabilities in Cancer
12:05 - 12:25	Layla Alnoumas	The Metabolic Response of Breast Cancer Cells to Capecitabine
12:25 - 12:40	Poster presenters	Poster pitches
12:40	All	Group photo
12:40 - 14:00	All	Lunch + poster session
SESSION 3: Metabolomics Across Biological Systems CHAIR: Yorrick Jaspers		
14:00 - 14:20	Michel Driessen	Hypoxia in T-Cell Immunity: A Barrier to Overcome or a Tool to Harness?
14:20 - 14:40	Maria Elisabetta Collaro	Microcystin-Specific Mass Spectrometry Query Language (MassQL) Queries Enable Comprehensive LC-HRMS/MS Screening of Known and New Variants
14:40 - 15:00	Markéta Macho	Towards Plant Pan-Metabolome; Metabolic Diversity of 3000 Plant Species
15:00 - 15:20	All	Coffee break
15:20 - 17:00	Alejandro Mendoza Cantu and Janne Heirman	Workshop (please bring your own laptop)
17:00 - 17:10	YoungBMC committee	Wrap-up
From 18:00	All	Evening event at Spéciale Belge Taproom

Keynote presentations: 25 min talk + 5 min (Q&A)

Oral presentations: 15 min talk + 5 min (Q&A)

Poster pitches: 3 min per poster pitch

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University of Antwerp

Abstracts Keynote presentations

Keynote 1

Teaching AI to Understand Chemical Differences from Tandem Mass Spectra

Prof. Dr. Wout Bittremieux

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Mass spectrometry-based metabolomics has transformed our ability to study the chemical complexity of biological systems, yet a fundamental challenge remains: the vast majority of tandem mass spectra cannot be confidently annotated. In this talk, I will present how bioinformatics and AI can move metabolomics beyond the limitations of traditional spectral libraries and enable large-scale, chemically informed discovery.

I will first introduce the nearest neighbor suspect spectral library, an open resource generated through repository-scale molecular networking of more than 500 million MS/MS spectra. By capturing relationships between known compounds and their structural analogs, this resource routinely doubles annotation rates across diverse applications, including human metabolomics, natural products, and environmental studies, revealing previously inaccessible regions of chemical space.

Next, I will present SIMBA, a transformer-based deep learning model that learns chemical relationships directly from MS/MS spectra. Rather than relying on simple spectral similarity scores, SIMBA learns complex fragmentation patterns associated with structural differences, enabling the discovery of molecular analogs that remain invisible to conventional approaches. Importantly, its predictions provide interpretable insights into how chemical modifications shape observed fragmentation patterns.

Finally, I will introduce Spectrawl, a deep learning approach that directly connects experimental MS/MS spectra to chemical structure databases. By shifting from searching existing spectral libraries to predicting and ranking candidate structures, this approach opens the door to discovering molecules that have never been measured before.

Together, these advances demonstrate a new paradigm for metabolomics: teaching AI not merely to recognize spectra, but to understand the chemical relationships encoded within them. By combining large-scale data resources with interpretable machine learning, we can transform unknown signals into actionable chemical knowledge and expand the frontiers of untargeted metabolomics.

Abstracts Keynote presentations

Keynote 2

Lipidomics as a Tool to Uncover Novel Therapeutic Vulnerabilities in Cancer

Prof. Dr. Johannes V. Swinnen

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Recent advances in lipidomics, encompassing bulk, spatial, single-cell, and stable isotope tracer approaches, have created unprecedented opportunities to investigate lipid metabolism in complex diseases. These complementary technologies enable not only the comprehensive characterization of lipid composition, but also the interrogation of metabolic fluxes and their spatial organization within heterogeneous tissues. As a result, lipidomics is increasingly emerging as a powerful platform for studying metabolic heterogeneity and plasticity in an integrated disease context.

In this lecture, we will discuss the capabilities and current challenges of these rapidly evolving technologies and highlight how their integration provides unique insights into disease biology. Using examples from cancer research, we will demonstrate how multimodal lipidomics approaches can uncover metabolic dependencies that remain inaccessible to conventional profiling strategies. By resolving the spatial and functional heterogeneity of lipid metabolism within tumors, these approaches reveal previously unrecognized therapeutic vulnerabilities and candidate drug targets, underscoring the growing potential of lipidomics to advance our understanding of cancer biology and inform precision oncology strategies.

Abstracts oral presentations

Fermentation-Induced Molecular Remodeling in South African Indigenous Tubers: Cassava and Cocoyam

Alejandro Mendoza Cantu¹, Motseoa Lephtsi², Yusuf Abass², Ndiko Ludidi³, Peter Bamidele⁴, Fidele Tugizimana², Julia M. Gauglitz¹, Wout Bittremieux¹

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Cassava and cocoyam are dietary staples across multiple countries in Africa, where natural fermentation has long been used to improve their safety, digestibility, and flavor. While previous studies have documented changes in proximate composition and microbial counts during fermentation, the molecular-level transformations remain understudied. Untargeted metabolomics offers a way to capture these changes, though annotation rates typically remain low when relying on standard spectral matching alone.

In this work, we applied a comprehensive computational metabolomics pipeline to characterize the molecular profiles of raw and fermented cassava and cocoyam. Samples were analyzed using LC-MS/MS, and features extracted using MZmine. We then employed SIRIUS with CSI:FingerID for in silico annotation, feature-based molecular networking through GNPS, metabolic pathway analysis using mummichog, and biotransformation prediction with BioTransformer. This pipeline generated 149 unique high-confidence structural identifications and 1,158 high-confidence class classifications out of 2,452 total features with MS/MS information.

Principal component analysis showed separation between control and fermented samples for both tubers, indicating that natural fermentation alters the chemical fingerprint of both substrates. However, the two tubers responded differently (log₂ fold change > 1, $p < 0.05$). In cassava, fermentation was depleting: 706 of 750 significant features were down-regulated. In cocoyam, the pattern was more balanced (329 up, 434 down), indicating increased metabolic complexity alongside degradation. Pathway enrichment also revealed distinct transformation routes; for example, chrysenes and benzoxazolones were enriched in cocoyam but absent in cassava ($p < 0.05$). Molecular networking further highlighted these differences, with spectrally related features clustering into matrix-specific families.

These results suggest that fermentation activates distinct microbial enzymatic pathways depending on the substrate, despite both being starchy tubers. This computational pipeline enabled a more interpretable picture of how fermentation reshapes their metabolic landscape.

Abstracts oral presentations

The Metabolic Response of Breast Cancer Cells to Capecitabine

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Background: Breast cancer comprises a heterogeneous group of biologically and molecularly diverse diseases that disproportionately affect women worldwide. An estimated 2 million new breast cancer cases are diagnosed globally each year, with more than half a million deaths reported worldwide, positioning breast cancer as a major global public health concern and underscoring the urgent need to develop more effective treatment strategies. Impaired DNA damage response and repair pathways are among the key hallmarks of breast cancer and contribute to genomic instability, tumour progression, and therapeutic resistance. To investigate the cellular consequences of disrupting DNA synthesis, our study employs an untargeted metabolomics approach to characterise the in vitro metabolic response of breast cancer cells to capecitabine. Capecitabine is an oral prodrug of 5-fluorouracil, which inhibits thymidylate synthase, impairing DNA synthesis and cell proliferation.

Methods: We exposed MCF-7, MDA-MB-231, BT-20, and BT-549 cells to incremental doses of capecitabine to measure cell line dependent sensitivity to these agents using MTS assay. Cells were then dosed at half maximal inhibitory concentration (IC₅₀) for a 4-day exposure time and analysed by an untargeted metabolomics using a Thermo Exploris 240 coupled to binary Vanquish Ultra High-Performance Liquid Chromatography system. Acquired mass spectral raw data was processed in Compound Discoverer 3.3 SP3 drawing a comparison between control and treated groups to visualize and interpret the clustering of metabolite features to observe global differences and identify significantly upregulated and downregulated metabolic features in each group. We then derived the pathway enrichment analysis of key metabolic changes occurring upon drug treatment using MetaboAnalyst 5.0.

Results: Our findings indicated a dose-dependent differential sensitivity in the studied breast cancer cell lines after exposure to capecitabine. We found overlapping metabolic features across all cell lines, including altered arginine, proline, alanine, beta-alanine, aspartate, and glutamate biosynthesis. While treatment with capecitabine affected vitamin B6 metabolism in BT-549 and MCF-7 cells, BT-20 showed changes specifically in phenylalanine, tyrosine, glyoxylate and dicarboxylate metabolism. Histidine metabolism was altered in both BT-20 and BT-549 cells, while lysine degradation and biosynthesis of cysteine and methionine were specific to MCF-7 cells. We also validated these findings by matching the detected features to our in-house metabolite database, enhancing the confidence level of detected compounds annotation.

Discussion and Conclusions: The observed amino acid perturbation seen in selected breast cancer cell lines upon treatment with capecitabine, suggests increased tumour amino acid utilisation to compensate for DNA synthesis blockade. Exposure to capecitabine also altered glucose metabolism of breast cancer cells, suggesting their reliance on aerobic glycolysis for energy production, known as the Warburg effect. Our global metabolomics profiling of various breast cancer cell lines corresponds to distinct metabolite that can be promising diagnostic biomarkers or therapeutic targets to be validated in future using targeted analytical approaches.

Abstracts oral presentations

Hypoxia in T-Cell Immunity: A Barrier to Overcome or a Tool to Harness?

Driessen M¹, Akoto JS¹, Zandhuis ND¹, Butt YA¹, van der Zwaan C^{2,3}, Hoogendijk AJ^{2,3}, Foskolou IP^{1,3}

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T cells expressing chimeric antigen receptors (CARs) have revolutionised immunotherapy. However, CAR-T cells are ineffective against solid tumours partly due to the immunosuppressive tumour microenvironment (TME). Infiltrating immune cells face many challenges within the TME, such as low availability of nutrients and oxygen. Although, hypoxia (low oxygen) in the TME is associated with T cell dysfunction, recent findings suggest that short hypoxic exposure can enhance T cell efficacy. In accordance with previous results, we find that short-term (24h) activation under 1% O₂ can shape T cell differentiation and function. To elucidate the mechanism behind these changes, we performed integrated multi-omics combining ATAC-seq, RNA-seq, proteomics, and metabolomics. We found that genes consistently altered across transcriptomic and proteomic datasets were associated with lipid, amino acid, and one-carbon metabolism, suggesting that metabolic adaptation might be responsible for the hypoxia-dependent enhanced T cell function. Functional validation of these metabolic pathways is underway to define their role in T cell efficacy and ongoing integration of metabolomic and chromatin accessibility data will further define the regulatory basis of this rewiring. Together, these findings identify metabolic rewiring as a powerful approach to enhance CAR-T efficacy in the immunosuppressive TME.

Abstracts oral presentations

Microcystin-Specific Mass Spectrometry Query Language (MassQL) Queries Enable Comprehensive LC-HRMS/MS Screening of Known and New Variants

M. E. Collaro¹, V. Miele¹, L. Tartaglione¹, S. Iliakopoulou^{2,3}, S.-K. Zervou², A.-I. Gialleli³, T. M. Triantis², A. Hiskia², J. Koreivienė⁴, J. Karosienė⁴, H. Mazur-Marzec⁵, R. Konkel⁵, T. Kaloudis^{2,3}

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Cyanobacteria produce a diverse array of potent toxins, among which microcystins are of primary global concern for water quality and public health. Rapid and accurate determination of these hepatotoxins in complex environmental and biological matrices is essential for hazard assessment and environmental monitoring. Liquid chromatography coupled with high-resolution mass spectrometry (LC-HRMS) is the method of choice for this purpose, with compound identification commonly relying on matching experimental LC-HRMS/MS spectra against reference spectral libraries. However, the remarkable structural diversity of microcystins, with more than 300 congeners described to date, together with the continuous discovery of new variants, limits the coverage of existing spectral libraries, often resulting in missed or uncertain annotations, underscoring the need for improved detection strategies.

To address this analytical gap, we developed a novel computational workflow for targeted screening of microcystin variants using Feature-Based Molecular Networking (FBMN) and microcystin-specific Mass Spectrometry Query Language (MassQL) queries implemented in the Global Natural Products Social Molecular Networking (GNPS2) platform. Microcystins were systematically classified into structurally related groups according to the identity and positional distribution of conserved amino acid residues within the cyclic peptide scaffold. Group-specific MS/MS fragmentation patterns were then used to design dedicated MassQL queries using a minimal set of highly informative diagnostic features, including characteristic fragment ions, immonium ions, and neutral losses, defined as required or excluded criteria.

The workflow was designed to maximize sensitivity while maintaining high specificity, thereby minimizing both false negatives and false positives. The resulting collection of microcystin-specific MassQL queries provides a robust, complementary, and transferable strategy for screening proprietary libraries and large public metabolomics repositories. By complementing conventional spectral library matching, this approach enables detection of both known microcystins and structurally related analogs that are absent from current reference libraries, offering a powerful tool for environmental monitoring, cyanotoxin research, and public health surveillance.

Abstracts oral presentations

Towards Plant Pan-Metabolome; Metabolic Diversity of 3000 Plant Species

Markéta Macho¹, Regina Wendenburg¹, Aleksandra Ivanova², Stefka Bogdanova², Mihail Angelov², Pietro M. Niccolini³, Riccardo Marconi⁴, Kateřina Krninská⁵, Helena Romero⁶, Ludvík Bortl⁷, Petr Hanzelka⁷, Klára Lorencová⁷, Romana Rybková⁷, Eva Smržová⁷, Eduardo de la Peña⁶, Tomáš Procházka⁸, Jana Navrátilová⁹, Lubomír Adamec⁹, Vlastimil Rybka⁸, Tsanko Gechev², Alisdair R. Fernie^{1,2}, Saleh Alseekh^{1,2*}

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Introduction

Plant secondary metabolites play key roles in development, defence, and environmental adaptation, contributing to extensive chemical diversity shaped by evolution, ecology, and genetic regulation. Despite over 300,000 plant metabolites reported so far and estimates of up to 15 million total, most plant species remain chemically uncharacterized, with research skewed toward medicinal, crop, and industrial plants. Expanding this knowledge is essential for discovering bioactive compounds, improving crop resilience, and broadening our understanding of the phytochemical landscape and the factors that influence it.

Approach

We established one of the most comprehensive plant metabolomics datasets to date, sampling nearly 3,000 species across 14 major embryophyte classes including mosses, ferns, conifers, monocots, and eudicots spanning 280 families and 85 orders. We collected primarily leaf tissue from international botanical gardens and research institutes, including rare, endemic, understudied, or traditionally used species. Untargeted UPLC-MS/MS profiling yielded over 6,000 MS/MS spectra, forming a rich resource for future comparative studies.

Outlook

This dataset enables large-scale investigations into the phylogenetic patterns of metabolite production, ecological drivers of chemical diversity, and the evolutionary origins of biosynthetic pathways. By covering underrepresented lineages, it supports mapping plant chemical diversity across the tree of life. Future analyses will link metabolite profiles to ecological and phylogenetic data, aiding discovery of novel compounds and informing conservation strategies for chemically unique species.

Abstracts poster presentations

Studying Non-Volatiles from Plant-Based Ingredients by LC-MS and NMR-Based Metabolomics

Mengqiu Zhang¹, Herwig Bachmann², Bas Teusink², Sofia Moco¹

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Plant-based proteins have been a key component in the development of sustainable and nutritious food alternatives. Besides their protein content, plant-based foods contain many non-volatile compounds that influence their flavour, function, and safety. Among the classes of described non-volatiles compounds, glycoalkaloids and saponins are associated to bitterness and may reduce the overall palatability of plant-based products.

A comprehensive metabolic map of all previously reported glycoalkaloids and saponins in soy, potato, oat, and faba bean was compiled. Both biosynthesis and degradation pathways based on current literature and databases were included, describing metabolites and (putative) enzymes. These metabolite lists will aid in metabolite identification in the analyses of non-volatile glycoalkaloids and saponins by liquid chromatography-mass spectrometry (LC-MS) and / or nuclear magnetic resonance-based metabolomics.

In addition to the chemical characterisation of glycoalkaloids and saponins in plant ingredients, we aim to monitor the non-volatile composition during fermentation by LC-MS / NMR metabolomics and potentially unravel novel degradation pathways.

We believe this approach will contribute towards better-tasting and safer plant-based food products through the targeted control of undesirable non-volatile compounds.

Abstracts poster presentations

The Brain Lipidome Reflects Treatment Efficacy in Metachromatic Leukodystrophy

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Introduction: Metachromatic leukodystrophy (MLD) is an inherited metabolic disorder caused by pathogenic variants in the gene encoding the lysosomal enzyme arylsulfatase A (ASA). ASA deficiency leads to sulfatide accumulation in myelin, resulting in demyelination and neurodegeneration in both the central and peripheral nervous systems. Identification of reliable biomarkers for MLD are essential for monitoring disease activity and evaluating therapy. As myelin consists of over 70% lipid, lipidomic analysis of brain tissue may provide mechanistic insights into disease pathology and facilitate the discovery of novel biomarkers.

Approach: Lipidomic analysis using UPLC-MS was applied to post-mortem frontal white matter samples from five MLD patients (two untreated, three treated with hematopoietic stem cell transplantation (HSCT)) and four young controls. Lipids were identified based on accurate mass and retention time, then semi-quantified using appropriate internal standards. Data were processed using an in-house R/MATLAB pipeline. Statistical differences between groups were assessed using Student's t-test or one-way ANOVA.

Results: Principal component analysis revealed clear separation between subgroups. Untreated MLD patients showed increased complex glycosphingolipids and sulfatides, and decreased ether lipids. In HSCT-treated patients, these alterations were partially reversed, with near normalisation in the neurologically stable patient.

Discussion: Brain lipidomics distinguished controls, untreated MLD, and HSCT-treated patients, showing that HSCT induces partial normalisation of disease associated lipid alterations. Importantly, these changes correlated with the clinical phenotype, indicating that the brain lipidome reflects treatment efficacy in MLD.

Abstracts poster presentations

Integrated Metabolomics Workflow Enables Systems-Level Insights into Early-Stage Metabolic Reprogramming during Potato Tuber Infections

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Introduction: Early-stage plant-pathogen interactions involve extensive metabolic perturbations that occur before visible symptom development. However, translating large-scale metabolomics datasets into biologically meaningful insights remains a major challenge. This study aimed to develop an integrated metabolomics workflow for systems-level investigation of the early and progressive stages of infection in potato tubers.

Approach: Untargeted metabolomics profiling was performed using complementary GC-MS and LC-MS platforms to capture diverse classes of primary and secondary metabolites associated with fungal and bacterial infections in potato tubers. Data preprocessing and feature extraction were conducted using XCMS and MS-DIAL, followed by statistical, pathway, and network-level analyses using MetaboAnalyst and integrative computational approaches.

Results: The integrated workflow enabled robust discrimination between asymptomatic and infected tuber states and improved the prioritization of metabolite features across analytical platforms. Early infection stages showed pronounced perturbations in central carbon metabolism, amino acid metabolism, and lipid-associated pathways, indicating coordinated metabolic reprogramming during disease establishment. Multi-platform integration further enhanced pathway-level biological interpretation and systems-level understanding of infection-associated metabolic responses.

Discussion: This study demonstrates the value of integrated metabolomics workflows for decoding complex plant-pathogen interactions and identifying biologically relevant metabolic signatures during asymptomatic disease stages. The proposed framework supports systems-level interpretation of large metabolomics datasets and contributes toward improved strategies for early disease detection in crop systems.

Abstracts poster presentations

Microbial Indoles Modulate Hepatic CYP2E1 Activity

Fanny Beekman¹, Fabrice Blankenzee¹, J. Chris Vos¹, Stefan J. Dekker¹, Jacqueline E. van Muijlwijk-Koezen¹ and Sofia Moco¹

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Cytochrome P450 2E1 (CYP2E1) is a member of the P450 superfamily responsible for the oxidation of a wide range of endogenous compounds and xenobiotics, such as arachidonic acid, ethanol and acetaminophen. CYP2E1 is also known to have a high electron uncoupling capacity, leading to the production of reactive oxygen species (ROS), and thereby contributing to oxidative stress and ultimately to liver disease progression. Therefore, modulation of CYP2E1 activity represents an interesting target for reducing oxidative damage. Gut microbiota-derived indoles are potential modulators through the gut–liver axis. Recent studies have shown that indoles, including indole-3-carboxylic acid (I-3CA), inhibit CYP2E1 activity and reduce formation of reactive metabolites such as N-acetyl-p-benzoquinone imine (NAPQI, a product of acetaminophen overdose). However, the inhibitory potential and mechanism of the different microbial indoles remain poorly understood.

In this study, recombinant human CYP2E1 was successfully expressed in *E. coli* and membrane fractions were isolated. Enzyme integrity was confirmed by carbon monoxide (CO) difference spectroscopy (highly specific for heme proteins), and catalytic activity was verified using 7-methoxy-4-(trifluoromethyl)coumarin (MFC) as a fluorescence probe substrate. Screening an array of microbial indole derivatives (skatole, indole, tryptamine, and the indole-3-acetic, -lactic, -aldehyde, -carboxylic, and -propionic acids) revealed concentration-dependent CYP2E1 inhibition and allowed for structure–activity relationships. Skatole, indole, and tryptamine were identified as the most potent inhibitors, with $IC_{50} < 20 \mu M$. The most potent inhibitors were further assessed in human liver microsomal incubations using LC–MS-based metabolite analysis. Time-dependent inhibition experiments showed limited additional loss of activity after preincubation, suggesting predominantly a reversible inhibition, rather than a mechanism-based inactivation.

Taken together, these findings identify microbial indole derivatives as potential CYP2E1 modulators and provide insight into how gut microbiota-derived metabolites may influence hepatic xenobiotic metabolism.

Abstracts poster presentations

Challenges in Tandem Mass Spectrometry-Based Resolution of Isotopomers of Glutamic Acid

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Stable isotope-resolved metabolomics (tracer metabolomics) enables detailed analysis of metabolic pathway activity by introducing labeled substrates (e.g., ¹³C, ¹⁵N) and tracking their incorporation into downstream metabolites via mass spectrometry. This reveals pathway connectivity and relative fluxes. Data are typically analyzed at multiple levels, including metabolite abundances, isotope incorporation, and isotopologue distributions. While these provide insights into pathway activity, isotopomer analysis, which captures the positional distribution of labels, offers higher specificity, as it more directly reflects the underlying metabolic routes.

Currently, isotopomer data are not extensively used due to the lack of technologies capable of accurately distinguishing them. The most straightforward tool for this purpose is NMR spectroscopy, but its use is limited to very abundant metabolites and requires large sample quantities. Another promising, yet not fully explored, technology for resolving isotopomers is tandem mass spectrometry (MS/MS).

Full tandem mass spectrometry-based isotopomer resolution requires a sufficient number of informative fragments, defined by the available parent–daughter transitions. In this work, glutamic acid was used as a model metabolite due to its central role in metabolism and its ability to ionize in both positive and negative modes. Different fragmentation strategies were applied to increase fragment coverage, but accurate isotopomer resolution remained tricky due to fragment ambiguity, peak picking limitations, and isotopic effects. To address these challenges, we developed in-house software that improves peak picking precision and enables more reliable isotopomer analysis, leading to better biological insights.

Abstracts poster presentations

Toward a Rule-Based Framework for De Novo Reconstruction of RiPPs from MS/MS Data

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Ribosomally synthesised and post-translationally modified peptides (RiPPs) are a rapidly expanding and structurally diverse class of natural products produced across all domains of life, exhibiting a wide range of bioactivities including antimicrobial, antiviral, cytotoxic, and signalling functions, which make them valuable across biomedical, ecological, and biotechnological contexts. However, *de novo* structural reconstruction of RiPPs from tandem mass spectrometry (MS/MS) data remains a significant bottleneck. Most existing tools are optimised for linear peptides, while the extensive chemical diversity introduced by post-translational modifications in RiPPs requires specialised analytical approaches.

This project aims to develop a rule-based computational framework for the *de novo* reconstruction of RiPP directly from MS/MS data. The system will aim to interpret characteristic fragmentation patterns and modification signatures through explicit rules. As an initial step, a curated dataset of RiPP MS/MS spectra and compound metadata is being compiled from public repositories. Preliminary analysis has identified key obstacles in RiPP bioinformatics, including inconsistent data formats across repositories, incomplete structural annotations, and limited availability of high-quality, experimentally verified spectra. These early findings will inform the design of a structured, interpretable rule set for fragmentation analysis, laying the groundwork for a *de novo* RiPP builder capable of generating candidate peptide structures from spectral data.