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CEISAM
Chimie et Interdisciplinarité Synthèse, Analyse, Modélisation

NMR metabolomics symposium

June 16 – 18, 2025

Nantes Université - UFR Sciences et Techniques, building n°2, Amphi Pasteur

SUMMIT

Nantes Université

Welcome word

Dear colleagues,

We are delighted to welcome you to this 3-day symposium on NMR based metabolomics in Nantes, France.

This unprecedented 3-day event is dedicated to the development and application of NMR methods for metabolomics, at the interface between NMR methodology (including high-field and compact NMR, MRI and hyperpolarization), analytical chemistry and applications in various fields. NMR metabolomics has recently undergone major research breakthroughs from all over the world, and we believe that it is timely to provide a forum to exchange on the most recent advances in the field.

We are glad and honored that 12 international leading specialists have accepted our invitation to give a lecture. Oral communications have been selected from submitted abstracts and a large part of the symposium will be dedicated to formal and informal discussions.

The event takes place on 16-18 June 2025 in the vibrant city of Nantes, close to the beautiful Atlantic coast of South Brittany. The symposium takes place on the Nantes Université campus located 15 min from the town center by public transportation.

We sincerely hope that you will enjoy this exciting event!

The organizing committee:

Jean-Nicolas Dumez, Jonathan Farjon, Karine Gautier, Patrick Giraudeau, Marine Letertre.

Thanks

The symposium is funded by the ERC SUMMIT research program which focuses on hyperpolarized and 2D NMR methodological developments for metabolomics.

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We are grateful to the CEISAM research institute and to our host institutions, Nantes Université and CNRS for supporting this event.

NMR metabolomics symposium - June 16-18, 2025

Program

	Monday 16		Tuesday 17		Wednesday 18
	8.30 registration				
Chair: M. Letertre	9.00 Opening (P. Giraudeau)	Chair: P. Giraudeau	9.00 David Wishart	Chair: M. Letertre	9.00 Rafael Bruschweiler
	9.20 Elaine Holmes		9.40 Sahithya Phani Babu Vemulapalli		9.40 Silke Heinzmann
	10.00 Styliani Chasapi		10.00 Sakshi Kamboj		10.00 Jan Sykora
	10.20 Joao Duarte		10.20 Pilar Alonso Moreno		10.20 Antoine Bruguière
	10.40 Coffee break		10.40 Coffee break		10.40 Coffee break
	11.20 Morgan Hayward		11.20 Ilona Dudka		11.20 Claire Cannet
	11.40 Daniel Raftery		11.40 Marco Tessari		11.40 Edern Cahoreau
	12.00 Jose-Luis Izquierdo-Garcia		12.00 Peter Vermathen		12.00 Tone Bathen
	12.40 - 14.00 Lunch break		12.40 - 14.00 Lunch break		Group photo Lunch break
Chair: J. Farjon	14.00 Pascal de Tullio	Chair: J.-N. Dumez	14.00 Paola Turano	Chair: J.-N. Dumez	14.00 Irene Marco-Rius
	14.40 Jérémy Marchand		14.40 Ricardo Conde		14.40 Indrek Reile
	15.00 Stéphane Beaudercq		15.00 David Castejon		15.00 Manon Campas
	15.20 Han Wang		15.20 Sofia Moco		15.20 Sofia Mariasina
	15.40 Coffee break		15.40 Coffee break		15.40 Coffee break
	16.20 Fabien Torralba		16.20 Joris Mandral		16.20 Florence Fauvelle
	16.40 Luciano Liao Morais		16.40 Plamen Chorbadzhiev		16.40 Christopher Wall
	17.00 Mathilde Lerche		17.00 Elizabeth O'Day		17.00 Oscar Millet
					17.40 Closing remarks
	Free evening		**Free evening**		**Gala dinner (19h45 - 23h) (upon registration only)**

Invited lectures: 30’ + 10’ Q&A

Oral communications: 15’ + 5’ Q&A

Gala dinner – practical informations

The gala dinner will be held on **June 18th**.

The address for the gala dinner is Quai de la Motte Rouge, place Waldeck Rousseau, Nantes – the closest tram station on line 2 is Motte-Rouge, then cross the river.

The **boarding time is 19h45**, with a departure at 20h30 and back to Nantes at 23h. **Please be on time, the boat will not wait!**

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The Role of NMR in Molecular Phenomics and Precision Medicine

Elaine Holmes * [1]

[1] Murdoch University, Western Australia Imperial College London

Metabolic profiling of biofluids such as urine, plasma or fecal water in combination with multivariate statistical modeling tools, can provide a window for investigating the impact of disease on human health and can be used to define metabolic phenotypes associated with a wide range of physiological and pathological conditions. The growing demand for sensitive, high quality disease diagnostics has facilitated the development of new technological and statistical methods for extracting biomarkers from spectral data. Analytical pipelines for monitoring metabolic events, utilising a combination of spectroscopic methods focusing on specific molecular properties, are required to enable the assembly of panels of biomarkers that are associated with human clinical conditions e.g. inflammation, cardiovascular disease risk or gut microbial functionality. Tailored approaches to spectral acquisition can be combined with statistical methods for processing and modeling the spectral data with a view to achieving downstream diagnostic assays that are clinically translational. This lecture will explore analytical pipelines for augmenting current medical diagnostic and discovery methods.

*Speaker

Urine Metabolomics for Early-Stage Diagnosis and Etiological Differentiation of Chronic Kidney Disease

Styliani Chasapi * [1]

[1] Department of Pharmacy, University of Patras, GR-26504, Patras Greece – Greece

Chronic kidney disease (CKD) is a significant public health concern, as its progression can lead to end-stage kidney failure requiring replacement therapy. Early and accurate diagnosis, along with appropriate treatment, can significantly delay CKD progression. This study investigates whether CKD etiology can be reflected in urine metabolomics during its early stages.
Metabolomics, particularly nuclear magnetic resonance (NMR)-based urine metabolome profiling, provides a promising approach to uncover the biochemical landscape of CKD. Our aim was to characterize the urinary metabolic profile of CKD patients and assess whether disease etiology can be distinguished through metabolomic analysis during early-stage progression.

Urine samples were collected from 108 CKD patients diagnosed with the three most common etiologies: chronic glomerulonephritis (IgA and membranous nephropathy), diabetic nephropathy (DN), and hypertensive nephrosclerosis (HN). Patients were further stratified into five groups based on CKD stage. Untargeted NMR spectroscopy was employed to analyze urinary metabolic fingerprints and explore metabolic fluctuations across CKD subtypes and disease progression.

Preliminary results revealed a moderate clustering of glomerulonephritis subtypes, characterized by distinct metabolic profiles that reflect differences in etiology. Specifically, the urine metabolome of IgA nephropathy patients exhibited a unique metabolic signature, highlighting its distinct pathophysiology. Conversely, DN and HN patients did not exhibit specific metabolic patterns, consistent with their overlapping clinical presentations.
These findings underscore the potential of urine metabolomics in improving the understanding of CKD pathophysiology and providing insights for more precise diagnostic and prognostic approaches.

*Speaker

Evidence-based denoising optimization for accurate brain GABA estimation by ^{13}C NMR spectroscopy in vivo at 14.1T

Kelley M. Swanberg [1,2], Iben Lundgaard [1,2], Joao M.N. Duarte * [1,2]

[1] Department of Experimental Medical Science, Faculty of Medicine, Lund University – Sweden
[2] Wallenberg Centre for Molecular Medicine, Lund University – Sweden

GABA turnover estimation is key for understanding regulation of this inhibitory neurotransmitter. GABA signals in brain ^{13}C NMR spectra are generally 4-fold smaller than glutamate, and methods to improve GABA quantification are warranted. Spectral denoising techniques potentially, but do not necessarily, improve the reliability of metabolite concentration estimates by NMR spectroscopy when spectral signal-to-noise ratio (SNR) is limited. Using synthetic data enabling accuracy calculations and *in vivo* spectra, we quantified the effects of three denoising methods on GABA concentration estimates derived from rat brain ^{13}C spectra. Localized ^{13}C spectra from the rat brain (400 μL) were acquired using a localized DEPT sequence at 14.1 T with a linearly polarized ^{13}C coil and quadrature surface ^{1}H coil. A noiseless *in-vivo*-like spectrum was generated via realistic amplitude scaling and 0.03 ppm Lorentzian line-broadening, and 500 uncorrelated complex noise patterns were added in time domain. Linear combination modeling was conducted in LCModel for ^{13}C fitting. Apodization (AD) denoising was controlled by LCModel parameter NUNFIL. Singular value decomposition (SVD) and wavelet transform (WT) denoising were conducted in Python using 1D Spectrum Denoiser and DESPERATE, respectively. Denoising methods yielding the 97th percentile of mean spectral SNR and magnitude accuracy on GABA C2, C3 and C4 on a single sample were applied to the full N=500 synthesized spectra. The highest-SNR, highest-accuracy, and highest-precision techniques thereof were then applied to spectral *in vivo* data. This approach is expected to improve accuracy in the estimation of GABA neurotransmitter synthesis rates using compartmentalized modeling of brain energy metabolism.

*Speaker

CcpNmr AnalysisMetabolomics: A versatile graphical tool for reference-based profiling of 1D^{1}H NMR-based Metabolomics data

Morgan Hayward * [1], Marie Phelan [2], Edward Brooksbank [1], Geerten W. Vuister [1], Luca Mureddu [1], Victoria Higman [1], Gary Thompson [2]

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[2] Biochemistry, Cell and Systems Biology [University of Liverpool] – United Kingdom
[3] Department of Biological Sciences [Kent] – United Kingdom

The AnalysisMetabolomics program is a recent development of the CcpNmr Analysis Version 3 package: a freely-available software suite for biomolecular NMR for visualisation and interpretation of NMR data, written in the Python programming language. AnalysisMetabolomics contains tools for interactive graphical identification and quantification of metabolites, aka profiling, of 1D^{1}H NMR spectra via reference to accurate simulated metabolite standards.
Metabolite profiling in AnalysisMetabolomics is flexible and fully interactive and can be performed manually and semi-automatically. It is supported by the Ccpn Analysis Simulated Metabolomics DataBase (CASMDB), a remediated collection of simulated 1D^{1}H metabolite standards data for 1938 distinct metabolites, gathered from three publicly available repositories: the HMDB, BMRB and GISSMO libraries. AnalysisMetabolomics also provides tools for users to quickly build their own simulated references for custom libraries to support profiling, in addition to the references provided in the CASMDB.
Furthermore, AnalysisMetabolomics is also backed up with extensive user support through the CCPN user forum, clear graphical tutorials and YouTube Video tutorials.

*Speaker

Modeling Blood Metabolite Homeostasis Reduces Unexplained Variance and Reveals Basal Metabolism Levels and Network Relationships

Daniel Raftery * [1]

[1] University of Washington – United States

Blood metabolite levels are affected by numerous factors, including demographic, clinical, genetic, as well as pre-analytical factors such as collection methods and geographical sites. This variance has caused deleterious consequences for many metabolomics studies, including the discovery and validation of potential metabolite biomarkers for various diseases, and thus represents a major challenge in metabolomics. It is important to understand the factors that cause the unwanted variance and develop methods and models that can reduce it. However, to date, the lack of suitable mathematical models for blood metabolite levels under homeostasis has hindered progress. We describe the development of quantitative models of blood metabolite levels in healthy adults based on multisite sample cohorts that reflect the current challenge. Four cohorts of samples obtained across three geographically distinct sites were investigated, focusing on approximately 50 metabolites that were quantified using ^{1}H NMR spectroscopy. A dramatic reduction in the site-to-site and sample to sample variation of metabolite levels was achieved based on modeling each metabolite using demographic and clinical factors and especially other metabolites. From PCA, the predicted variation of 303 test samples across all 4 sites based on a model built using 101 samples from only two sites was reduced by 96% (PC1), 94% (PC2) and 70% (PC3). Several metabolites that contributed disproportionately to such variation were associated with biosynthesis and degradation. The study demonstrates an intriguing, cross-pathway network effect of metabolites that can be utilized to better define basal homeostatic metabolite levels, which may have implications for improved health monitoring.

*Speaker

From HR-NMR to benchtop NMR-based metabolomics: Bridging the gap to clinical translation

Jose Izquierdo García * [1,2], Jesús Ruiz-Cabello [3,2], José Ángel A. Lorente [4,2], Pilar Alonso Moreno [1], Patricia Comella [5], Germán Peces-Barba [6,2]

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[2] Centro de Investigación Biomédica en Red Enfermedades Respiratorias – Spain
[3] Centro de Investigación Cooperativa en Biomateriales – Spain
[4] Getafe University Hospital = Hospital Universitario de Getafe – Spain
[5] Vall d'Hebron Research Institute – Spain
[6] Instituto de Investigación Sanitaria Fundación Jiménez Diaz [Madrid] – Spain

Nuclear Magnetic Resonance (NMR)-based metabolomics offers a powerful, non-invasive approach to disease diagnosis by capturing specific metabolic fingerprints in biofluids. Although high-resolution (HR) NMR spectroscopy has demonstrated effectiveness in identifying and monitoring pathologies, its high cost, large footprint, and demanding maintenance requirements constrain widespread clinical adoption. Benchtop NMR spectrometers represent a promising alternative, as they provide sufficient sensitivity and resolution at a fraction of the cost, enabling near-patient testing even in resource-limited settings.

This presentation explores the clinical translation of benchtop NMR-based metabolomics across various applications, including TB diagnosis, pediatric TB, and COVID-19 patient stratification in Intensive Care Units (ICUs). Comparative analyses with HR-NMR data reveal that benchtop instruments can achieve robust performance in differentiating diseased from healthy states, facilitating rapid and accurate detection of key biomarkers. Furthermore, we demonstrate the potential of benchtop NMR to support personalized medicine, such as predicting treatment outcomes or identifying metabolic signatures that correlate with severity.

By validating these methods in multi-site, large-scale studies, we show that benchtop NMR-based metabolomics can be easily integrated into existing clinical workflows without prohibitive costs or infrastructure requirements. This technology thereby enhances the feasibility of implementing omics-driven diagnostics in diverse healthcare environments, ultimately improving patient care and outcomes. Our findings underscore benchtop NMR as a critical stepping stone in bridging the gap between research-grade metabolomics and practical, cost-effective clinical tools.

*Speaker

NMR as a Key Enabler of Metabolomics Integration into Clinical Chemistry

Pascal de Tullio * [1]

[1] Liège University – Belgium

Medical practice is undergoing a paradigm shift toward more personalized, precise, and patient-centered approaches. In this evolving landscape, clinical metabolomics emerges as a highly promising tool. Positioned at the intersection of genetics, environment, physiology, and pathology, metabo-lomics offers a unique window into the patient's phenotype and thus represents a powerful interface for personalized care.
Despite its potential, significant challenges must be addressed before metabolomics can fully transition from research settings to routine clinical use. Among these, the selection of the most adapted biofluids, the development of robust analytical and data management methodologies, the standardization of pre-analytical processes, the establishment of Biological Variation (BV) and Least Significant Change (LSC) for metabolites and the deeper understanding of the metabolome, including its physiological and pathological variabilities and functionalities, are key hurdles to overcome.
In this context, analytical platforms play a central role. Nuclear Magnetic Resonance (NMR) spectroscopy, due to its inherent strengths, particularly its robustness and quantification capabilities, stands out as a powerful tool in overcoming these obstacles. NMR's suitability for reproducible and high-throughput metabolic profiling positions it as a critical technology in the clinical translation of metabolomics.
This presentation will explore the major steps and challenges on the path to clinical implementation of metabolomics, with a particular focus on the contributions of NMR technology to the development of reliable protocols, sample analysis, and biological interpretation. Special attention will be given to matrix selection, pre-analytical standardization, and the characterization of temporal dynamics of the human metabolome.

*Speaker

Practical applications of NMR method for better resolved and more sensitive metabolomics

Jérémy Marchand * [1], Estelle Martineau [1], Virginie Silvestre [1], Benoît Charrier [1], Jonathan Farjon [1], Jean-Nicolas Dumez [1], Marine P.M. Letertre [1], Patrick Giraudeau [1]

[1] Nantes Université – CNRS,Chimie Et Interdisciplinarité: Analyse, Synthèse et Modélisation (CEISAM), UMR 6230 – France

NMR is a technique of choice for metabolomics, thanks to its very high reproducibility, the simplicity of sample preparation and its ability to provide both quantitative and structural information. However multiple characteristics associated with this technique can be challenging for the analysis of complex metabolomic samples, such as its low sensitivity compared to MS or a high degree of signal overlap from the widely-applied 1D ^{1}H NMR experiments.
Over the years, various developments have been initiated at CEISAM in order to overcome these limitations by developing better resolved and more sensitive data acquisition methods.
In order to improve signal dispersion, we have developed targeted and untargeted metabolomics workflows based on fast 2D methods such as ultrafast spectroscopy and non-uniform sampling. In parallel, methodological development for dissolution DNP resulted in a dramatic increase in sensitivity, allowing metabolomics studies at natural ^{13}C abundance. In this presentation, these works will be illustrated through concrete example of metabolomics studies that have benefited from these progresses. These include 2D metabolomics or lipidomics studies on complex biological extracts, as well as hyperpolarized metabolomics of biofluids, with particular focus on quantitative analysis. In addition, the multiple efforts that have been made to bring these innovative approaches to the metabolomics community will be discussed, such as the organization of the first quantitative interlaboratory ring-test based on fast 2D NMR through the national metabolomics and fluxomics infrastructure MetaboHUB

*Speaker

Metabolomic insights into the impact of shipping noise on blue mussels using ^{1}H-NMR and mass spectrometry

Stéphane Beauclercq * [1], Delphine Veillard [2], Nathan Ghafari [1], Dror E. Warschawski [3], Lekha Sleno [1], Réjean Tremblay [2], Isabelle Marcotte [1]

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[3] Chimie Physique et Chimie du Vivant, CPCV, CNRS UMR 8228, Sorbonne Université, École normale supérieure, PSL University – Chimie Physique et Chimie du Vivant, CPCV, CNRS UMR 8228, Sorbonne Université, École normale supérieure, PSL University – France

Underwater noise pollution from maritime traffic has been doubling every 11.5 years, posing a growing threat to marine organisms. Among them, blue mussels (*Mytilus edulis*) - key species in coastal ecosystems and aquaculture in North America - are particularly vulnerable since adult individuals are sessile and cannot escape noisy environments. While noise serves as a cue for the settlement of mussel larvae, it also notably delays metamorphosis and increases metabolic costs. However, its impact on adult mussels remains understudied.
To address this gap, we investigated the effect of maritime noise on the metabolism of adult *M. edulis*. Mussels were exposed for 15 days to varying ship noise intensities recorded in the Gulf of St. Lawrence. The metabolomes of the digestive gland, gills, and muscle were analysed by ^{1}H-NMR, complemented by mass spectrometry (MS), with multiblock modelling enhancing metabolic pathway interpretation.

^{1}H-NMR screening revealed strong metabolic disruptions in the digestive gland and gills, with lower impacts in the muscle. Both low and high noise exposure induced osmotic and oxidative stresses, along with alterations in energy metabolism, particularly affecting betaine, β-alanine, methionine, and nucleotide metabolism. Additionally, glycine and serine pathways, critical for biosynthesis and antioxidative capacity, were impacted in gills. Combining NMR with MS significantly improved the discriminant and predictive power of the models, demonstrating their complementarity in metabolomics.

Altogether, this study shows that maritime noise induces substantial metabolic shifts in adult mussels, potentially compromising their physiological resilience. These findings underscore the importance of regulating shipping noise in coastal environments.

*Speaker

^{1}H NMR Pure Shift Metabolomic Analysis of Black Tea

Han Wang * [1], Laura Castañar [2], Ralph Adams [1], Stephen Fowler [1], Gareth Morris [1], Mathias Nilsson [1]

[1] University of Manchester – United Kingdom
[2] Complutense University of Madrid – Spain

Pure shift NMR provides a significant improvement in resolution, by suppressing homonuclear scalar couplings, but at the cost of sensitivity. This work compares the untargeted metabolomic analysis results obtained using different pure shift methods (PSYCHE, TSE-PSYCHE, and 2DJ-PSYCHE) with those from conventional 1D ^{1}H and 2D J-resolved experiments. The comparison was made on a selected set of black teas from four regions and of two cultivars. The efficiency of these spectra for tea classification and metabolite identification was evaluated with chemometric methods including principal component analysis (PCA), fold change (FC) analysis, and *t*-test in order to find potential biomarkers for sample classification. PCA suggests that despite the lower sensitivity, the enhanced resolution of PSYCHE gave similar classification power of the different varieties of black tea to standard 1D ^{1}H NMR. PSYCHE also makes relative quantification possible even in the most crowded region of the conventional ^{1}H NMR spectrum. The feasibility of using 1D projections of 2DJ-PSYCHE spectra for an NMR metabolomics study was evaluated for the first time. A pure shift 1D ^{1}H NMR spectrum and a phase-sensitive 2D J-spectrum can be obtained in a single experiment using the 2DJ-PSYCHE method; this approach is particularly attractive for NMR metabolomic studies.

*Speaker

On the classification of ^{1}H NMR plants spectra (at an industrial scale) with a combined machine learning and metabolomic approach

Fabien Torralba * [1,2], Guillaume Hoffmann [2], Asma Bourafai Aziez [2], Christophe Morell [1]

[1] Evear Extraction – Université Lyon 1 – France
[2] Université Claude Bernard Lyon 1 – Université de Lyon – France

This presentation will include the results obtained during an ongoing research project of my PhD thesis (in partnership with University of Lyon, France and an industrial partner, EVEAR extraction), on the modeling and intelligent classification of NMR spectroscopic data, using NMR spectra and AI models trained on 4 Nvidia L4 GPUs. The main goal is to develop a classification of plants extract from their NMR spectra database (4000 spectra), aiming to specifically identify the plants studied among a defined set.This methodology relies on detecting the unique characteristics present in each spectrum, allowing for accurate recognition of the molecules comprising the sample. First a similarity study I presented, from this, early results on a machine learning workflow based on a random forest (RF) algorithm have been obtained. On a side note, a comparison with several other machine learning models will be presented, mainly Support Vector Machines (SVM) and Decision Tree, where some algorithms enhance the results and provide further good predictions. This project promises to significantly improve the speed and accuracy of chemical compound identification on key industrial steps, offering potential applications in various scientific and industrial fields. It represents a notable advancement in the use of NMR spectroscopy, opening new perspectives for the exploration of spectroscopic data in research and beyond.

*Speaker

NMR and chemometrics for studying the aging process of cachaças stored in barrels made from native Brazilian woods

Luciano Morais Lião * [1], Karla C.r.c. Morais [1], Kariny P. Silva [1], Gerlon A.r. Oliveira [2], Eduardo S.p. Nascimento [3], Vinícius S. Pinto [1]

[1] Federal University of Goiás – Brazil
[2] Universidade de Brasilia = University of Brasilia [Brasília] – Brazil
[3] Bruker BioSpin MRI GmbH [Ettlingen, Germany] – Germany

The aging process in the Brazilian beverage industry predominantly relies on imported oak barrels, leading to increased final product costs. Therefore, identifying alternative native Brazilian woods suitable for cachaça aging is highly relevant. This study investigates the chemical profile of cachaças aged in casks made from white Sucupira (*Pterodon emarginatus*), black Sucupira (*Bowdichia virgilioides Kunth*), and black Angico (*Anadenanthera peregrina*) using ^{1}H Nuclear Magnetic Resonance (^{1}H NMR) spectroscopy. The metabolic chemical profiles of the cachaças were monitored using ^{1}H NMR at 3, 6, and 12-month intervals and compared with non-aged samples. Although cachaça exhibits a complex spectral profile, with signals spanning nearly the entire spectrum, 38 compounds were identified and classified into alcohols, esters, organic acids, aldehydes, amino acids, and carbohydrates. Principal Component Analysis (PCA) revealed a clear distinction between aged and non-aged samples, mainly due to the increasing concentration of phenolic compounds during aging. A hierarchical cluster analysis (HCA) indicated similarities between the samples aged in black Angico and black Sucupira. Forming maturation-related compounds further supports the feasibility of using these woods as viable alternatives to imported casks. These findings highlight the untapped technological potential of Brazilian native woods, particularly for applications in the beverage industry. Acknowledgments: The authors are grateful to CAPES and FAPEG for financial support.

*Speaker

Bridging Cellular Pathways and In Vivo Metabolism with Quantitative dDNP-NMR

Mathilde Lerche * [1]

[1] Technical Universiy of Denmark – Denmark

NMR spectroscopy plays a pivotal role in metabolomics, yet its sensitivity constraints often limit its reach across biological scales. In this presentation, I will introduce a quantitative dissolution dynamic nuclear polarization (dDNP) workflow that enables high-sensitivity, isotope-resolved NMR of complex metabolite mixtures from cellular extracts to in vivo translation.
Our approach combines stable isotope labeling, extraction-based sample preparation, and hyperpolarized ^{13}C NMR to deliver reproducible and quantitative data on central metabolic pathways.
Crucially, the insights gained in vitro can inform, and ultimately be validated by, non-invasive hyperpolarized MRSI studies in animal models, forming a translational bridge from mechanistic understanding to metabolic imaging. This continuum, from cells and tissue to pathways and on to whole organisms, positions dDNP-enhanced NMR as a versatile tool for metabolomics across biological complexity.

*Speaker

Automating and Accelerating NMR Metabolomics

David S. Wishart * [1]

[1] Depts. of Biological Sciences and Computing Science University of Alberta, Edmonton, AB, Canada T6G 2E9 –Canada

For nearly two decades my lab has been developing tools, kits and software to support quantitative metabolomics. In this presentation I will describe our efforts in both automating and accelerating NMR-based quantitative metabolomics via 1D NMR spectroscopy. In particular, I will highlight some of the early efforts we undertook (Chenomx, Bayesil) and then focus on our most recent efforts with MagMet. I will describe how MagMet works, how it has been applied and its current capabilities for analyzing biofluids (serum, plasma, CSF, stool samples, milk) and beverages (beer, wine and juice). MagMet is particularly unique because of its support for full automation (phasing, baseline correction, water removal, chemical shift referencing, linewidth adjustment, peak picking, spectral deconvolution, quantification). MagMet is currently capable of automatically identifying and quantifying >80 metabolites in as little as 3 minutes. It is now being adapted to work at multiple field strengths (400-800 MHz). We are also developing low-cost robotic systems (built out of 3D printers) to automate sample preparation and when coupled with automatic sample changers and MagMet, the entire NMR process is not only faster but is nearly hands free. Our other efforts aimed at accelerating NMR metabolomics are based on using machine learning to enhance the signal-to-noise of 1D NMR spectra. This work potentially shortens spectral collection times by a factor of 2 or more. Overall, we believe these efforts to automate and accelerate NMR-based metabolomics will make it much more accessible to a far wider number of NMR labs.

*Speaker

Advancing Marine Dissolved Organic Matter Characterization: Unveiling Molecular Diversity Through NMR Spectroscopy

Sahithya Phani Babu Vemulapalli * [1], Christian Griesinger [2], Thorsten Dittmar [1]

[1] Marine Geochemistry, ICBM, Carl von Ossietzky University of Oldenburg – Germany
[2] NMR-Based Structural Biology, Max Planck Institute for Multidisciplinary Sciences – Germany

Marine dissolved organic matter (DOM), accounting for approximately 660 Pg C, represents the largest carbon reservoir on the Earth's surface, comparable in size to atmospheric CO. Even minor changes in the composition and dynamics of marine DOM can significantly impact marine biogeochemical cycles. Therefore, unraveling its molecular composition across diverse aquatic environments is crucial for understanding its role in global carbon cycles, particularly in a warming climate. Marine DOM is an intricate mixture of hundreds of thousands of individual molecules, present at extremely low concentrations, as identified by Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS). However, mass spectrometry fails to distinguish between numerous isomeric structures corresponding to a single molecular formula, making DOM from different locations appear similar on the molecular formula level. In this regard, nuclear magnetic resonance (NMR) spectroscopy is a powerful tool for the structural characterization of complex mixtures and is well established across various scientific fields. However, it remains underutilized in DOM research. In this study, we employ advanced NMR techniques to structurally characterize marine DOM from both surface and deep ocean waters. Our findings reveal that the molecular composition of marine DOM is far more diverse than previously estimated using ultrahigh-resolution mass spectrometry. This study underscores the importance of technological and methodological advancements in DOM characterization, providing deeper insights into its molecular composition and dynamics.

*Speaker

Tracing gut microbial tryptophan metabolism by ^{19}F NMR

Sakshi Kamboj * [1], Oona Rössler [2], Bohdan Holoborodko [3], Till Strowig [2], Jonathan Jantsch [4], Katja Dettmer [1], Peter J. Oefner [1], Wolfram Gronwald [1]

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[4] Institute for Medical Microbiology, Immunology, and Hygiene, and Center for Molecular Medicine Cologne (CMMC), University Hospital Cologne and Faculty of Medicine, University of Cologne, Cologne, Germany – Germany

The immune homeostasis of the host is largely influenced by gut microbiota, with many effects mediated by the binding of metabolites to the ligand activated aryl-hydrocarbon receptor (AhR). Planar aromatic compounds such as tryptophan and derived metabolites may act as a ligand for the AhR. Therefore, profiling of these metabolites can provide a better understanding of AhR function and related disease mechanisms. Even though ^{1}H NMR has been extensively used in medical research for metabolic profiling, it has its limitations in the presence of high background and narrow chemical shift range, which hampers metabolite identification and quantification. This limitation may be overcome by labelling tryptophan with a stable NMR isotope such as ^{19}F that shows high sensitivity and large chemical shift range, thereby eliminating unrelated signals and facilitating identication and quantification. Here, we used 5-fluoro-L-tryptophan for studying the metabolism of tryptophan by different human gut microbial species in a time dependent and quantitative manner. Also, cecum content of both germ-free and specific pathogen-free (SPF) mice fed with ^{19}F-labeled tryptophan was analyzed. Furthermore, *Salmonella enterica* was used as an exemplary system as it could be cultivated on minimal medium. One major challenge was the assignment of resulting NMR signals to specific metabolites. To this end, we combined one- and two-dimensional NMR data, information from high-resolution mass spectrometry with measurements of standards and chemical shift predictions to derive a catalogue of tryptophan metabolites with their corresponding ^{19}F spectral positions. Finally, we investigated the effect of the ^{19}F label on enzymatic rates.

*Speaker

Benchtop nuclear magnetic resonance-based metabolomics for rapid caprine tuberculosis diagnosis

Pilar Alonso Moreno * [1,2], Paula Ortiz [1], Javier Ortega [3,4], Carlos Velasco [3], Alba López [1], Javier Bezos [3,4], Jose L. Izquierdo-García [1,2,5]

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[3] VISAVET Health Surveillance Centre, Complutense University of Madrid, Madrid, Spain. – Spain
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[5] CIBER de Enfermedades Respiratorias (CIBERES), Instituto de Salud Carlos III, Madrid, Spain. – Spain

Goats represent an important source of tuberculosis (TB) in animals. The *ante-mortem* diagnosis is challenging due to the limited sensitivity of existing diagnostic methods and the potential for false-positive results associated with other mycobacterial infections. NMR-based metabolomic provides a unique metabolic fingerprinting of the disease's status, making it a promising diagnostic tool. However, conventional NMR spectrometers have several limitations in veterinary practice, including high costs and large size. Benchtop NMR (bNMR) spectrometer is proposed as a compact, cost-effective alternative for use in livestock farms.
The study aims to evaluate NMR-metabolomics as a diagnostic tool and transfer this technology for use with a bNMR spectrometer in animal settings.

Serum samples were collected from TB-infected (n=26), paratuberculosis-infected (PTB, n=16) and healthy control (n=25) goats. PTB is a non-tuberculous mycobacterial disease that produces similar clinical signs and diagnostic interferences. Samples were analyzed using NMR spectroscopy (700 MHz Bruker AVIII and 80 MHz Magritek NMR spectrometers), and the data underwent multivariate statistical analysis.
Principal Component Analyses (PCA) indicated significant metabolic differences among the groups, identifying 12 metabolites that differed significantly between groups in both HR-NMR and bNMR spectra. Partial Least Squares Discriminant Analysis (PLS-DA) achieved perfect separation between groups for both datasets, demonstrating 100% accuracy and robust cross-validation metrics. These findings confirm the diagnostic potential of the identified metabolomic biomarkers and demonstrate that bNMR spectroscopy can offer performance comparable to high-field instruments. Consequently, this approach could substantially enhance livestock health management by providing a reliable, cost-effective diagnostic method for tuberculosis and other mycobacterial infections.

*Speaker

Metabolomic profiling of prostate cancer tissues for improved risk stratification and personalized treatment

Ilona Dudka * [1], Kristina Lundquist [1], João Figueira [1], Verena Van Loon [1], Pernilla Wikström [2], Anders Bergh [2], Gerhard Gröbner [1]

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Prostate cancer is a multifocal and heterogeneous disease, making accurate diagnosis and risk stratification challenging. Current diagnostic methods rely on histopathology, which is limited by sampling constraints. Metabolomic profiling offers a promising approach with high diagnostic value for molecular level tumor characterization and to monitor tumor-instructed normal tissue responses, potentially enhancing diagnostic accuracy and treatment decisions.

Here, high-resolution magic angle spinning nuclear magnetic resonance (HR MAS NMR) was applied to intact biopsy samples from prostatectomy-treated patients (1,2). Distinct metabolic patterns were found between tumor subtypes based on Ki67 proliferation index and PSA expression. Seven key metabolites - choline, phosphocholine/glycerophosphocholine, glycine, creatine, glutamate/glutamine (Glx), taurine, and lactate - were significantly altered between these tumor subtypes. Additionally, benign tissues near high-grade tumors exhibited distinct metabolic alterations compared to those near low-grade tumors. Notably, myo-inositol, lysine, serine, and lysine/leucine/ arginine were elevated, while ethanolamine and lactate were decreased in benign tissues near high-grade tumors. Furthermore, metabolic differences in benign tissues varied with their proximity to the nearest tumor, with eight metabolites - including glutathione, glutamate, Glx, glycerol, inosine, ethanolamine, serine, and arginine - differentiating tissues close to versus far from the tumor.

This dual-study approach highlights the power of HR MAS NMR-based metabolomics in identifying cancer-specific metabolic profiles and uncovering tumor-induced metabolic adaptations in benign tissues. These findings support the potential of metabolomic biomarkers for improved PC diagnosis, risk stratification, and personalized treatment strategies.

1. Dudka et al. *J Transl Med; 21*, 2023
2. Dudka et al. *Front Mol Biosci;12, 2025*

*Speaker

Semi-targeted NMR metabolomics via Parahydrogen Induced Hyperpolarization

Marco Tessari * [1], Thom Posthumus [1], Ruud Aspers , Floris Rutjes [1]

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Non-hydrogenative Parahydrogen Induced Hyperpolarization (nhPHIP) has proven a powerful tool for the enhanced detection of several classes of metabolites in complex mixtures. Particularly, compounds carrying a alfa-amino acid motif have been previously detected and quantified in biological samples and natural extracts at sub-micromolar concentrations using 2D nhPHIP NMR spectroscopy. This technique is here applied to a semi-targeted metabolomics NMR study on urine from patients suffering from Pyridoxine-Dependent Epilepsy (PDE). A statistical model able to discriminate PDE patients from a control group was obtained via multivariate analysis of nhPHIP data.The signal enhancement, combined with the resolving power of 2D nhPHIP, result in a superior sensitivity to metabolic composition compared to conventional ^{1}H NMR, demonstrating the potential of this hyperpolarization technique in NMR-based metabolomics.

*Speaker

NMR Techniques applied in the clinical environment: Investigations on cellular dynamics, heart transplant quality and more

Peter Vermathen * [1]

[1] University of Bern – switzerland

NMR studies performed in the clinical environment will be presented. The main part of the talk will focus on investigations of cell cultures in an NMR Bioreactor. This includes cell immobilization techniques and Bioreactor setup. Techniques developed to separate intra- and extracellular metabolite contributions in fibroblasts, methods to determine oxygen concentrations and consumption rates which are essential for the interpretation of metabolic changes, cell viability measurements, and studies on fibroblasts with mitochondrial defects will be presented.
In addition, a brief overview will be provided of other NMR studies performed in the clinical environment in Bern, primarily studies assessing the quality of heart transplants from perfused hearts in Donation After Cardiac Death (DCD), as well as NMR studies investigating physical properties besides the metabolome.

*Speaker

Metabolomics meets bioinorganic chemistry

Paola Turano * [1]

[1] Università degli Studi di Firenze – Italy

Here, we describe the use of NMR-based metabolomics to evaluate the changes induced by metal-based compounds in ovarian cancer cell lines. The clinically established platinum(II) agents cisplatin, carboplatin and oxaliplatin show very similar effects when administered under the same toxicity conditions (1). In contrast, gold(I) and gold(III) compounds represent a structurally diverse class of cytotoxic metallodrugs that typically exhibit DNA-independent mechanisms of action, while interacting preferentially with intracellular protein targets (2). Post-treatment NMR profiling allowed the clustering of the members of this small library as a function of key target pathways and the establishment of correlations between cellular effects and the chemical nature of the gold complex.2 NMR was also used to establish the invariance in the mechanism of action of these drugs when conjugated to protein nanocarriers for targeted delivery (3,4).

1. Ghini V, Magherini F, Massai L, Messori L, Turano P. Dalton Trans. 2022; 51:12512.
2. Ghini V, Tristán AI, Di Paco G, Massai L, Mannelli M, Gamberi T, Fernández I, Rosato A, Turano P, Messori L. J Proteome Res. 2025; 24:813.
3. Cosottini L, Massai L, Ghini V, Zineddu S, Geri A, Mannelli M, Ciambellotti S, Severi M, Gamberi T, Messori L, Turano P. J. Drug Deliv. Technol. 2023; 87:104822
4. Cosottini L, Geri A, Ghini V, Mannelli M, Zineddu S, Di Paco G, Giachetti A, Massai L, Severi M, Gamberi T, Rosato A, Turano P, Messori L. Angew Chem Int Ed Engl. 2024; 63:e202410791.

*Speaker

Metabolomic Insights into Cardiometabolic Health: Bridging the Gap Between Metabolic Dysfunction and Cardiovascular Disease risk

Ricardo Conde * [1], Rubén Gil-Redondo [1], Maider Bizkarguenaga [1], Angela De Diego [1], Beatriz González-Valle [1], Tammo Diercks [1], Alain Ibañez De Opakua [1], Daniel Jardon [1], Chiara Bruzzone [1], Ignacio Verde [2], Amaia Zabala-Letona [3,4,5], Miguel Unda-Urzaiz [3,4,6], Claire Cannet [7], Hartmut Schäfer [7], Arkaitz Carracedo [3,4,5,8,9], Tobias Madl [10,11], Luca Valenti [12,13], Julien Wist [14,15], Jeremy Nicholson [14,16,17], Shelly C. Lu [18], Nieves Embade [1], José M. Mato [1,19], Oscar Millet [1,19]

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[16] Medical School, Faculty of Health and Medical Sciences, University of Western Australia, Department of Endocrinology and Diabetes, Fiona Stanley Hospital, Perth, WA 6150, Australia – Australia
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Cardiovascular disease (CVD) remains the leading cause of global mortality, underscoring the urgent need for enhanced risk assessment strategies. Cardiometabolic health profiling has emerged as a promising tool for early intervention and prevention, offering insights into the intricate relationship between metabolic dysregulation, inflammation, and disease risk. This

*Speaker

study leverages advanced metabolomic profiling to explore age- and sex-dependent metabolic patterns and their association with cardiometabolic health and inflammation. Using a large cohort of serum samples (n > 30,000), participants were stratified into metabolically healthy and unhealthy profiles, revealing distinct metabolic signatures across the lifespan. Key findings highlight the interplay between metabolic dysregulation, inflammation, and cardiometabolic risk, with specific metabolic pathways reflecting insulin resistance, energy metabolism imbalances, and oxidative stress. The study identifies metabolic markers associated with both detrimental and protective effects on cardiometabolic health, emphasizing the role of inflammation as a critical mediator in the progression of metabolic syndrome and CVD. Furthermore, the integration of metabolomic data with traditional CVD risk factors enhances risk stratification, supporting the development of personalized, metabolism-driven interventions. These findings underscore the clinical relevance of metabolic profiling in refining CVD risk assessment and highlight the importance of sex-specific and metabolism-targeted strategies to mitigate cardiometabolic risk across the lifespan. By elucidating the complex interplay between metabolic health, inflammation, and disease, this study provides a foundation for innovative approaches to reduce the global burden of CVD and metabolic syndrome.

Metabolomic Profiling of Tenebrio molitor Frass: A ^{1}H-NMR HRMAS Study

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[2] ICTS Complutense Bioimaging. Complutense University of Madrid – Spain

In the framework of circular economy strategies and the valorization of agrifood by-products, *Tenebrio molitor* larvae play a key role in biotransforming organic residues into valuable biomaterials, including frass, a promising organic fertilizer. However, its chemical composition is strongly influenced by the insect's diet, affecting its agronomic properties. To the best of our knowledge, this is the first study employing high-resolution magic angle spinning nuclear magnetic resonance (^{1}H-NMR HRMAS) spectroscopy to directly analyze frass composition without prior extraction. *T. molitor* larvae were reared for 60 days on five different diets: pure oat (M1), 66% oat and 33% polystyrene (M2), 66% polystyrene and 33% oat (M3), pure polystyrene (M4), and pure orange peel (M5). Multivariate data analysis was performed to classify the NMR data and identify distinct metabolic profiles associated with each diet. Pattern recognition analysis of the ^{1}H-NMR spectra successfully discriminated the five groups, separating M4 and M5 from the oat-containing samples, while further differentiating M1, M2, and M3 based on their oat content. Additionally, loadings plots identified key spectral regions (buckets) responsible for this classification, which were associated with specific metabolites. This study highlights the potential of HRMAS-NMR as a powerful tool for the direct metabolomic profiling of *T. molitor* frass, providing valuable insights into its compositional variability and reinforcing its role in sustainable agronomic applications.

*Speaker

Studying dynamics of cellular metabolism by real-time NMR metabolomics

Valentina Ferro , Mengqiu Zhang , Brian Van Der Kieft , Victoria Pozo Garcia , Sofia Moco * [1]

[1] Vrije Universiteit Amsterdam [Amsterdam] – Netherlands

Cellular metabolism is dynamic and time dependent. Bioactive compounds, such as pharmaceutical drugs, induce cellular metabolic changes. These metabolic alterations inform about the drug's mechanism-of-action or their metabolic fate. The dynamics of metabolite concentrations are then a proxy of their metabolism. NMR gathers several advantages in studying cellular metabolism: it allows screening many cellular metabolites in parallel, in a quantitative fashion, and it even allows to detect kinetic changes over time.
In our lab, we use a combination of NMR metabolomics approaches (1D, 2D) to study both metabolic fate of drugs (their xenobiotic metabolism), as well as the impact of drugs on cellular energy (their central carbon metabolism). Real-time NMR can effectively monitor metabolic shifts, offering a deeper understanding of drug metabolism, including the identification of metabolic intermediates or products.
Gathering biochemical information of drugs and their metabolism is essential for their development in drug discovery programs.

*Speaker

Pure shift NMR methods for the analysis of complex biological mixtures with a benchtop NMR spectrometer

Joris Mandral * [1], Jérémy Marchand [1], Marine P.M. Letertre [1], Jean-Nicolas Dumez [1], Patrick Giraudeau [1], Jonathan Farjon [1]

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The analysis of complex mixtures is challenging as they contain a wide variety of molecules of different nature, size and concentration. Nuclear magnetic resonance (NMR) spectroscopy is a powerful analytical tool capable of providing a wealth of information on these complex mixtures. Over the last decade, benchtop NMR spectrometers have become increasingly attractive for this purpose, due to their growing performance and capabilities, and the prospects of new applications have prompted the development of NMR methods on compact systems. Indeed, benchtop NMR spectra of complex mixtures are hampered by ubiquitous peak overlap, which calls for the implementation of methods capable of better separating analyte signals at the data acquisition stage. We have implemented solvent-suppressed pure shift (PS) NMR strategies on an 80 MHz benchtop NMR spectrometer. PS NMR consists in eliminating the signal multiplicity induced by homonuclear J-couplings observed in 1D ^{1}H NMR, thus simplifying the spectral information. These strategies were evaluated with similar acquisition parameters on a model mixture in pure water, to compare their performance with respect to important analytical criteria: sensitivity, resolution, spectral purity and repeatability. Our most performant PS strategy provided the highest sensitivity (27% of solvent-suppressed 1D ^{1}H sensitivity), repeatability (CV = 4%) and spectral purity (no baseline distortions and limited strong coupling artefacts). Then, as a proof of concept for fraud detection, we evaluated this PS NMR strategy on bergamot essential oils (BEO) adulterated with cheaper orange essential oils (which is common in the industry), using a metabolomic workflow approach.

*Speaker

Unraveling the Wild: NMR and LC-MS Metabolomic and HetCA-Guided Exploration of Wild Ales

Plamen Chorbadzhiev * [1,2], Plamena Staleva [1], Zhanina Petkova [1], Konstantina Priboyska [1], Ralitsa Chimishirova [1], Dessislava Gerginova [1], Svetlana Simova [1]

[1] Institute of Organic Chemistry with Centre of Phytochemistry - IOCCP (Sofia, Bulgaria) – Bulgaria
[2] University of Chemical Technology and Metallurgy – Bulgaria

Wild ales are a unique class of spontaneously fermented beers, considered the closest modern equivalent to the beers originally brewed thousands of years ago. Unlike conventional beers, which rely on controlled yeast strains, wild ales ferment naturally with indigenous yeasts and bacteria, leading to complex sensory and bioactive profiles. Extended aging further enhances their distinct composition, shaped by microbial metabolism and environmental factors. This study employs an integrated analytical approach combining ^{1}H NMR and LC-MS metabolomics with antioxidant and phenolic content assays, supported by chemometric analysis and statistical spectroscopy (STOCSY, HetCA and SHY). ^{1}H NMR provides structural and quantitative insights into alcohols, sugars, organic acids, amino acids, and nucleosides, while LC-MS enhances the detection of phenolic compounds and additional amino acids, offering a broader metabolic perspective. Antioxidant activity is assessed through DPPH and FRAP assays, while total phenolic content (TPC) is measured to evaluate polyphenolic contributions. Chemometric tools are used to distinguish the samples, based on their geographical origin.
By integrating these techniques, we achieve a comprehensive metabolic perspective of wild ales, providing valuable insights into their chemical diversity, bioactivity, and the influence of spontaneous fermentation on their metabolite composition. This study highlights the potential of advanced metabolomics and chemometrics in characterizing complex fermented beverages, contributing to a deeper understanding of wild ale production and quality.

*Speaker

Leveraging Metabolomics and Machine Learning to Launch NMR-Based Clinical Diagnostics

Elizabeth O'Day * [1]

[1] Olaris, Inc – United States

There is an unmet clinical need to develop better monitoring tools for kidney transplant recipients. The current blood-based rule out assays have limited utility and there is a need for rule-in assays that allow for early detection and course correction before irreversible damage is done to the graft. Here we will describe the biomarker discovery engine, myOLARIS-Toolbox, which was used to elucidate a urine-based metabolomic signature to detect graft injury. The platform leverages the use of Navigators or molecules that monitor sample quality and software that combines statistics, ML/AI and linking back to biology. Finally, we will discuss the analytical validation approach required to launch the assay as a laboratory developed test (LDT). To the best of our knowledge this is not only the world's first rule-in assay for transplant injury, but the first NUS HSQC-based clinical diagnostic.

*Speaker

Seamless Integration of 1D and 2D NMR for the Automated Analysis and Quantification of Complex Metabolomics Samples

Rafael Brüschweiler * [1]

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In addition to strong peak overlaps, a major challenge in 1D ^{1}H NMR-based metabolomics studies is the occurrence of (even slight) shifts of the resonances of mixture compounds compared to the reference spectra in the metabolomics spectral databases due to variations in buffer conditions, temperature, and matrix effects. This can considerably hamper both the automated spectral deconvolution and metabolite quantification of crowded regions in 1D ^{1}H NMR spectra of complex mixtures whose analysis is particularly susceptible to such effects. 2D NMR-based metabolomics, on the other hand, is substantially more robust but much more demanding in terms of NMR spectrometer time.

A new web-server based platform will be introduced, termed COLMAR1d2d, which uses selected 2D ^{1}H–^{13}C HSQC and ^{1}H–^{1}H TOCSY NMR spectra of a subset of samples along with standard 1D ^{1}H NMR spectra collected for all samples to overcome this bottleneck. It relies on the extension of our 2D NMR-based platform COLMARm using 2D ^{1}H–^{13}C HSQC and 2D ^{1}H–^{1}H TOCSY spectra as input measured for a representative subset of samples to unambiguously and comprehensively determine the metabolite composition and the exact peak positions of the identified compounds under the sample conditions present. This information is then used to “correct” the chemical shifts of affected metabolites in the GISSMO NMR database allowing the reliable, automated analysis of a potentially large cohort of 1D ^{1}H NMR spectra using the COLMAR1d platform. It is demonstrated how this synergistic combination of 1D with selected 2D NMR spectra allows the analysis of a significantly larger number of metabolites than would be possible with 1D NMR alone. Moreover, COLMAR1d2d also improves quantitation, as is demonstrated for mouse urine and Pseudomonas aeruginosa biofilm. The COLMAR1d2d approach is particularly powerful for large-scale high-throughput metabolomics studies aiming at maximal metabolite coverage.

*Speaker

An improved NMR metabolomics workflow for quantification and metabolite assignment in longitudinal human urine metabolomics studies

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Metabolomics studies provide valuable insights into metabolic alterations and biomarker discovery, yet challenges remain in accurate quantification and metabolite identification. This work presents an improved NMR workflow that integrates a peak quantification method with metabolite assignment approach utilizing the CLASSY algorithm, facilitating higher confidence in both metabolite identification and quantification accuracy. Additionally, we introduce a framework for determining the biological origin of metabolites, enabling interpretable results in the context of metabolic changes. To support the analysis of longitudinal datasets, we provide a suite of statistical tools that allow for rigorous assessment of time-dependent variations, enhancing our ability to monitor dynamic shifts in the metabolome.
We applied our workflow to urine samples of the MARS500 study, a long-duration confinement experiment mimicking space exploration. By collecting daily 24-hr urine samples from a homogenous group of 6 males over 250 days, we mitigate interindividual variation, unveiling true metabolic uniqueness. We gradually refine our NMR-based metabolome dataset using unsupervised techniques to selection of relevant and well characterized metabolites for in-depth individual and time-resolved analysis. We define a personal phenotype in the absence of individual dietary and lifestyle choices based on few particular metabolites out of the whole metabolome. Going on, we characterize the nature of time-resolved factors that stem from the given dietary regime and individual adaptation to the confinement.
Our analysis holds the promise of advancing our understanding of the multifaceted interplay between genetics, lifestyle, and metabolism, providing critical insights to serve as a solid starting point in personalized healthcare.

*Speaker

An association of pancreatic cancer to diabetes mellitus and attempts to differentiate its stages

Jan Sykora * [1], Lenka Michalkova [1], Stepan Hornik [1], Bohus Bunganic [2]

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[2] Military University Hospital Prague – Czech Republic

Diabetes mellitus type 2 is, by some physicians, considered as a very first manifestation of pancreatic cancer as approximately 80% of PC patients are simultaneously diagnosed with DM or impaired glucose tolerance. This so-called pancreatogenic diabetes appears prior to pancreatic cancer within a period of three years and is accompanied by characteristic features such as absence of obesity or frequent infections. In our recent study, we applied ^{1}H NMR metabolomics to plasma samples of patients with pancreatic cancer, individuals with long term diabetes mellitus type 2 (lasting more than 5 years) and subjects of the risk group - patients with recently diagnosed diabetes mellitus (less than 3 years after diagnosis of DM). First two groups of patients served to establish a predictive model to classify the patients of the risk group to either of the previous groups. The health condition of identified at-risk individuals was then re-examined providing a valuable feedback on predictive power of the proposed model. Subsequently, we attempted to differentiate the individual PC stages. Unfortunately, the performance values were found rather low, only 71.5% accuracy was reached for discrimination of early and metastatic stage of PC. On the other hand, a classification of found at-risk individuals into this discriminant analysis provided some clue to distinguish individuals at high and moderate risk of PC development.

*Speaker

Dereplication strategy by ^{13}C-NMR using the MixONat software

Antoine Bruguière * [1], Séverine Derbré [1], Jules Leguy [2], Valentine Rahier [2], Frédéric Saubion [2], Pascal Richomme [1]

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MixONat is a free software that allows the dereplication of mixtures (mainly of natural products) by using ^{13}C-NMR (1,2). By comparing signals given by the sample with those contained in a database, MixONat can rapidly give the user an idea of the molecules that are inside the sample. In order to improve the quality of the propositions, DEPT 135 and DEPT 90 data can also be added to MixONat, allowing it to only keep results with appropriate carbon type (CH_3, CH_2, CH, C). It is also possible to add MS information to further filter the results by molecular weight.
The software has already been successfully used in several dereplication strategies (3,4,5). This presentation will explain how you can use it for your own applications through some examples of published work.

(1) Bruguière *et al.* Anal. Chem. 2020
(2) Bruguière *et al.* Planta Med. 2021
(3) Leong *et al.* Bioorg. Chem. 2023
(4) Meunier *et al.* Talanta 2023
(5) Herbert *et al.* Nat. Prod. Res. 2024

*Speaker

Lipoproteins and small molecules quantification using benchtop NMR Spectroscopy

Cannet Claire * [1]

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NMR Spectroscopy is well established for human metabolomics profiling, especially for lipoproteins and metabolites in plasma. High field NMR spectroscopy can give reliable quantitative and reproducible results with simple and low preparation cost per sample for its biomarkers panel and can be transfer to benchtop NMR Spectroscopy which opens new opportunities in precision medicine.

*Speaker

Microbiota - Host interactions during juvenile growth: exploration of interconnected metabolic networks

Edern Cahoreau * [1,2], Pavel Melentev [3], Hanna Kulyk [1,2], Lindsay Peyriga [1,2], Justine Bertrand-Michel [1,4], Pauline Le-Faouder [1,4], Cyrielle Clement [1,4], Ludovic Cottret [1,5], Rabemanantsoa Koloina [1,5], François Leulier [3,6], Floriant Bellvert [1,2]

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[4] Institut des Maladies Métaboliques et Casdiovasculaires – Université Toulouse III - Paul Sabatier, Institut National de la Santé et de la Recherche Médicale – France
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The gut microbiota influences animal growth in various nutritional environments. Despite recent progress, the molecular mechanisms behind this mutualism remain poorly understood. This is partly due to the complexity of the gut microbiota, mainly composed of bacteria, which form intricate nutritional and metabolic networks among themselves and with the host. Given this complexity, no study has yet determined to what extent and how the microbiota's metabolic activities contribute to the host's juvenile growth. The aim of MicroMetabo project, is to identify metabolic networks of the gut microbiota and determine how it influences the availability and allocation of the host's metabolic resources during juvenile growth, taking *Drosophila melanogaster* larva as host model. To do this, we are using a simple gnotobiotic model that allows full control over the diet, the host, and the members of its microbiota, and combine large-scale metabolomics, precise metabolite tracking, and genetic and biochemical approaches. Nuclear Magnetic resonance analyses were applied in combination with Mass spectrometry analyses to explore metabolic behavior of two model bacteria: *Acetobacter pomorum* and *Lactoplantibacillus plantarum*, naturally found in fly and larval gut. To explore metabolic interactions between the different actors, bacteria were cultivated alone and in co-cultivation, then in presence of the drosophila larvae. Exo and endo metabolome was explored and quantified by combination of NMR and MS for metabolic profiling and ^{13}C isotopic profiling.

*Speaker

Metabolic portraits of breast cancer

Tone F. Bathen * [1]

[1] Norwegian University of Science and Technology – Norway

Despite progress in early detection and therapeutic strategies, breast cancer remains a leading cause of cancer-related death among women globally. Due to the heterogeneity and complex tumor biology, breast cancer patients with similar diagnoses might have different prognoses and responses to treatment. Metabolomics is the branch of “omics” technologies that involves high-throughput identification and quantification of small-molecule metabolites in the metabolome. Cancer cells must be able to convert nutrients to biomass while maintaining energy production, which requires reprogramming of central metabolic processes. This phenomenon is increasingly recognized as a potential target for treatment, but also as a source for biomarkers that can be used for prognosis, risk stratification, and therapy monitoring. This talk will focus on NMR-based metabolo-mics research in breast cancer, covering aspects from risk assessment to cancer characterization, treatment monitoring and outcome predictions.

*Speaker

Hyperpolarization-enhanced NMR and MRI methods for tissue engineering applications

Irene Marco-Rius * [1]

[1] Institute for Bioengeneering of Catalonia – Spain

There is a need for non-invasive and reliable methods to diagnose, stage, and monitor treatment response in diseases like cancer and non-alcoholic fatty liver disease. Magnetic resonance (MR) techniques offer a way to identify metabolic biomarkers in real time. By combining carbon-13 spectroscopy to detect and quantify metabolites with imaging (MRI), MR enables simultaneous probing of spatial (biodistribution) and temporal (kinetics) aspects of metabolism in vivo.

This is made possible by hyperpolarized (HP) MR methods, such as Dynamic Nuclear Polarization (DNP), which transiently enhance carbon-13 MR signals by several orders of magnitude compared to traditional methods. DNP enables real-time measurement of enzymatic reactions in cell suspensions, tissue samples, and in vivo models. Multiple HP ^{13}C-labeled substrates have been successfully used to investigate key metabolic pathways, including glycolysis, the pentose-phosphate pathway, and cellular redox states.

In this presentation, I will demonstrate the potential of HP MR to study metabolism in various systems, from cell suspensions to animal models. I will also share recent progress at IBEC, including efforts to use HP MR to monitor metabolic processes in organ-on-chip platforms. These advances highlight how HP MR can provide transformative insights into disease mechanisms and therapeutic responses, paving the way for innovative approaches in precision medicine.

*Speaker

nh-PHIP hyperpolarization assisted analysis of dilute biomolecule mixtures on affordable spectrometers

Mateusz Urbańczyk [1], Kärolin Kork [2], Kerti Ausmees [2], Tomasz Ratajczyk [1], Indrek Reile * [2]

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NMR metabolomics is one of the best ways to study the complex network of biochemical processes that define living organisms. However, the most informative metabolomics studies have been conducted on complex high-end spectrometers. The cost of such instruments is often high enough to exclude adopting NMR in application fields that would otherwise benefit from the robustness and the easy to interpret NMR data - for instance point-of-care medical tests or horti- and agricultural analysis. The obvious solution would be to conduct NMR metabolomics on more affordable mid- and lower field (< 400 MHz) or even benchtop spectrometers. While the number of such studies is quickly increasing, they are held back by the sensitivity and resolution offered by affordable instrumentation. Herein, we demonstrate the pathway to overcome such limitations by **adopting parahydrogen based nh-PHIP hyperpolarization**, which has been previously used at 500 MHz and 800 MHz, **on 300 MHz and 80 MHz spectrometers**. We demonstrate the necessary method development and considerations when porting nh-PHIP to lower fields. At 300 MHz, we utilize hyperpolarization to resolve a spectrally congested biological mixture in an order of magnitude shorter analysis time, compared to regular NMR methods. At 80 MHz, we demonstrate analysis of a mixture of eight 100-200 micromolar concentration biomolecules - which proved to be unfeasible on a benchtop instrument without nh-PHIP. Therefore, we argue that nh-PHIP hyperpolarization can be used to expand the application scope of affordable NMR instrumentation in metabolite analysis and metabolomics.

*Speaker

The Metafollow project : A one-year longitudinal follow-up to assess intra-individual metabolites variations in healthy subjects

Manon Campas * [1], Cirillo Arianna [1], Matthieu Schoumacher [1,2], Pierre-Yves Sacré [3], Olivier Bruyère [4,5], Etienne Cavalier [1,2], Pascal De Tullio [1]

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In healthcare, most metabolomics' studies focus on pathologies by studying inter-individual and/or inter-group variations of metabolites concentrations. However, patients care paradigm is currently changing towards a more personalized approach. Thus, to integrate metabolomics into personalized medicine, understanding normal intra-individual metabolite variations is crucial to identify deviations that may indicate early pathological changes. Currently, our knowledge of these "normal" variations remains limited. To bridge this gap, it's essential to first study the metabolome of healthy individuals over a defined period.
For this purpose, we conducted a one-year longitudinal study involving 30 healthy volunteers. Blood, urine, and saliva samples were collected weekly for the first ten weeks, followed by monthly collections for ten months, according to the recommendations of the EuBIVAS (EFLM Working Group on Biological Variation). The analysis was first focused on blood samples and as metabolites quantification is absolutely required here, NMR appeared to be the most useful analytical tool. Over the ten-week period, metabolites were classified based on their variability, ranging from the least to the most fluctuating. A similar classification pattern emerged from the monthly samples, confirming the consistency of metabolite variability over time. Additionally, we applied an innovative approach, Metabolomic Informative Content (MIC), to stratify individuals based on the variation in their metabolome.
Our preliminary results enable the stratification of blood metabolites according to their short- and long-term variability. Ongoing urine and saliva analyses will further refine our understanding of normal metabolome variations, providing a more comprehensive foundation for the future application of metabolomics in personalized medicine.

*Speaker

Unraveling the Organismal Impact of Gene Inactivation Through NMR Metabolomics

Sofia Mariasina * [1], Olga Averina [1], Anastasia Bolikhova [1], Maria Khokhlova [1], Peter Sergiev [1], Vladimir Polshakov [1]

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Understanding the physiological roles of genes at the organismal level is a central goal of functional genomics. In this study, we applied NMR-based metabolomics to genetically modified mouse models to elucidate the systemic functions of several genes, including methyltransferases Thumpd2 and Mettl4, as well as small regulatory peptide Mitoregulin (Mtln). While our previous work demonstrated their roles in cellular processes, including RNA modification and mitochondrial regulation, their contributions to whole-organism metabolism remained unexplored.

We generated mouse models with targeted disruptions in Thumpd2, Mettl4, or Mtln genes and performed comprehensive NMR metabolomic profiling of serum and urine. Our findings revealed distinct metabolic perturbations associated with gene inactivation. Disruption of Thumpd2 led to alterations in kidney function, accumulation of uremic toxins, and symptoms associated with metabolic disorders, such as impaired glucose homeostasis and fatty degeneration of organs. Mettl4 deficiency resulted in abnormalities in energy metabolism. In *Mtln* knockout mice, we observed obesity, elevated serum triglycerides, and impaired mitochondrial substrate oxidation, accompanied by depletion of TCA cycle intermediates.

These findings bridge the gap between the cellular and organismal roles of Thumpd2, Mettl4, and Mtln, highlighting their importance in maintaining metabolic homeostasis. By integrating NMR metabolomics with functional genomics, we provide new insights into their systemic functions and their potential implications in metabolic diseases and mitochondrial dysfunction. This study underscores the power of metabolomics in advancing our understanding of gene function at the organismal level.

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*Speaker

An improved and earlier diagnosis of Parkinson's disease with a blood test?

Florence Fauvelle * [1], Vanille Millasseau , David Mallet , Sabrina Boulet [1]

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Parkinson's disease (PD) is an incurable neurodegenerative disorder that progresses silently over decades. By the time it becomes visible, through the well-known movement disorders, the brain damage is already irreversible, with around 70% of dopaminergic neurons having died, so it's too late to apply a curative therapy. Moreover, post-mortem studies show that current diagnostic tools are unreliable at the onset of these disorders. Diagnostic confirmation of the disease takes several years, from an average of 5 years onwards. Patients therefore experience diagnostic "wandering" during these years, with, what's more, a lack of diagnostic specificity compared with other, closely related Parkinsonian syndromes.

At the Grenoble Institute of Neuroscience, by combining the study of three complementary animal models of PD and two cohorts of newly diagnosed (*de novo*) Parkinson's patients, we have recently patented a 6 metabolites-blood biomarker (Patent BNT2304^{19}FR00; Mallet et al. JCI, 2022).

We are now working on two different axes:

- Firstly, to assess its performance in terms of specificity compared with other parkinsonian syndromes, and evaluate its predictability for PD before the irreversible brain damages,

- Secondly, to translate the biomarker to clinics using a Bruker 600 MHz IVDr system at Grenoble Hospital, dedicated to highthroughput metabolomics (all previous developments have been made at 950 MHz).
Early results show that our biomarker is not a global biomarker of neurodegenerative disease (e.g. compared to Alzheimer disease), but is specific of PD compared to Progressive Supranuclear Palsy and Multiple System Atrophy, two confounding parkinsonian syndromes, even at 600 MHz.

*Speaker

Applied Saliva NMR Metabolomics for Metabolic Profiling

Christopher Wall * [1]

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Saliva-based metabolomics offers a noninvasive approach to metabolic health assessment, yet its relationship with established cardiovascular risk factors and subjective wellbeing remains underexplored. Here, we employed Nuclear Magnetic Resonance (NMR) metabolomics to profile saliva samples from 121 individuals, quantifying 47 distinct metabolites. Concurrently, participants underwent comprehensive evaluation using gold standard Framingham cardiovascular risk markers including glucose, HbA1c, triglycerides, blood pressure, cholesterol, LDL, HDL, weight, height, and BMI. Self-reported quality of life was assessed using the RAND-SF36 questionnaire. Analysis revealed both anticipated and novel correlations between specific salivary metabolites and established blood-based biomarkers, underscoring the biological relevance of saliva in systemic metabolic assessments. Moreover, intriguing associations emerged between distinct metabolic profiles and self-reported wellbeing scores, suggesting a biochemical underpinning for subjective health perceptions. Our findings demonstrate the utility of saliva NMR metabolomics as a practical, informative tool for noninvasively characterizing individual metabolic status and wellness. This approach has potential applications in preventative medicine, personalized health interventions, and the routine monitoring of metabolic health.

*Speaker

Age and Gender Specific Lipoprotein Characterization for Improved Cardiovascular Risk Stratification

Oscar Millet * [1]

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Cardiovascular disease (CVD) remains the leading cause of mortality worldwide. Atherosclerosis, driven by dyslipidemia, plays a central role in CVD pathogenesis. While conventional lipid measurements such as LDL-C and HDL-C are widely used for risk assessment, they fail to capture the full complexity of lipoprotein metabolism. NMR spectroscopy enables the characterization of lipoprotein subparticles, providing a more detailed lipid profile with potential clinical relevance. This study analyzed a large dataset of more than 25.000 serum samples from healthy individuals using the B.I.LISA™ NMR-based platform, quantifying 112 lipoprotein parameters, including subclass size and concentration. A second cohort of 12.000 individuals with metabolic risk factors was used to identify lipoprotein parameters that differentiate CVD risk in an age- and sex-dependent manner. Lipoprotein parameters exhibit distinct sex- and age-dependent trajectories, with inflection points observed at 44 and 60 years in women and around 60 years in men, aligning with known aging acceleration models. Many NMR-derived parameters effectively distinguish between healthy and unhealthy metabolic profiles, with VLDL-associated parameters demonstrating the highest predictive value across a broad age range. Our findings highlight the added value of NMR-derived lipoprotein parameters in refining CVD risk assessment, emphasizing the importance of sex- and lipoprotein-specific therapeutic strategies. The study underscores the need for reference values tailored to age and sex, supporting the clinical integration of advanced lipoprotein profiling.

*Speaker

NMR metabolomics symposium - June 16-18, 2025

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BAY NORD Anders - University of Gothenburg - Sweden

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BERMON Muriel - CEISAM - France

BERTRAND Marylène - Centre de Biophysique Moléculaire - France

BIZKARGUENAGA Maider - CIC bioGUNE - Spain

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BRICENO Daniela - La Trobe University - Australia

BRUGUIÈRE Antoine - SONAS - France

BRUSCHWEILER Rafael - The Ohio State University - USA

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CASSANI Julia - Universidad Autonoma Metropolitana - Mexico

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THANK YOU ALL FOR

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