

European RFMF Metabomeeting 2020

JANUARY 22 - 24, 2020

TOULOUSE, FRANCE

WITH THE PARTICIPATION OF EUROPEAN REGIONAL NETWORKS



ORAL AND POSTER ABSTRACTS



European RFMF Metabomeeting 2020

We are very pleased to welcome you to the 2020 European RFMF-Metabomeeting conference in Toulouse. This conference gathers together two metabolomics and fluxomics networks, the RFMF (French-speaking Metabolomics and Fluxomics Network) and the MPF (Metabolic Profiling Forum) with more than 10 years of existence. MPF and RFMF share the same objectives which are to catalyze metabolomics and fluxomics research, organize conferences and promote early career scientists. Both networks also put forward networking and social aspects as strong leverage to achieve cutting edge science. For all these reasons we decided to organize this joint event.

With the growing interest in metabolomics, several regional and national networks have been created across Europe (and affiliated islands) within the last years. That is the reason why we decided to also include them in the organization of this event. They were particularly instrumental in creating a high-level scientific program and providing travel grants (a staggering 21 travel grants!).

We expect this conference to demonstrate the recent breakthroughs in metabolomics and fluxomics in a wide range of application fields. We made the choice to keep the scope of the conference as broad as possible (in terms of techniques and applications) since we think that interactions between communities is key in creating new paradigms, collaborations and scientific hypothesis.

One of our aims in this conference is to promote early career scientist participation. That is the reason why we did our best to keep registration prices as low as possible. As mentioned, networks made a strong effort to offer travel grants. Early careers were also strongly involved in the scientific organization of the conference. In fact, an early career committee was set up, led by Alison Woodward, and selected the early career presentations that you will see during the conference. They also proposed and organized workshops and social events. Finally, they will co-chair sessions with the (less early career) scientists.

Good science is generally the outcome of hard work within a friendly and supportive environment. All organisers agreed on the fact that this friendly atmosphere is of utmost importance for the organization of the conference. That is the reason why we did our best to have exciting social and networking events before and during the conference. We also aim at following RFMF mantra of “Good food Good science” with a very local and original gala dinner.

Finally, we would like to acknowledge all the academic and industrial sponsors for supporting this event and previous ones. We also thank all the people involved in the scientific and practical organization of this conference. MetaboHub-Metatoul metabolomics and fluxomics facility contribution was outstanding and our warmest thoughts go to Justine Bertrand Michel and Floriant Bellvert for their hard work and unbreakable optimism.

We wish you a fruitful scientific, human and enjoyable conference!

Jules Griffin (MPF)
Fabien Jourdan (RFMF)



European RFMF Metabomeeting 2020

Tuesday January 21st 2020				
Workshop day				
University of Toulouse				
9:00 am - 12:00 pm	W1: Interactive tutorial - How to process LC-MS data with workflow4metabolomics.org			
12:00 pm - 1:00 pm	LUNCH BREAK - ON YOUR OWN			
Parallel Workshop A (room TBA)		Parallel Workshop B (room TBA)		
1:00 pm - 3:45 pm	W2: metaRbolomics hackathon plus	2:45 pm - 4:00 pm	W5: How to chair sessions	
4:00 pm - 6:00 pm	W4: Advanced approaches for the analysis of metabolomics data			
6:00 pm - 6:30 pm	BREAK			
6:30 pm - 8:00 pm	Social event : Toulouse walking tour			
8:30 pm - 10 pm	W6: Meet the editor			

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Wednesday 22nd 2020		
Auditorium Marthe Condat		
8:00 am - 9:00 am	Registration open	
9:00 am - 9:30 am	Opening Ceremony	
Methodological & Technological developments		
Chairs: Justine Leenders & Marta Cascante		
9:30 am - 10:15 am	Plenary 1: From analytical chemistry to clinical metabolomics: reflections on the experimental workflow using adrenal cancer and hypervitaminosis A case studies <i>Rick Dunn, UK</i>	
10:15 am - 10:35 am	O1: Compact NMR spectroscopy and advanced pulse sequences: the perfect match for the online and real-time monitoring of bioprocesses <i>Jonathan Farjon, France</i>	
10:35 am - 11:00 am	Coffee break	
Microbiology & Biotechnologies		
Chiars: Alison Woodward & Karl Burgess		
11:00 am - 11:20 am	O2: ScalaFlux: a scalable approach to quantify fluxes in metabolic subnetworks <i>Pierre Millard, France</i>	
11:20 am - 11:40 am	O3: Rational optimization of a novel synthetic pathway for methanol utilization in <i>E. coli</i> <i>Camille Peiro, France</i>	
11:40 am - 11:55 am	F1: Characterising the bidirectional biomolecular interactions between the intestinal microbiota and host drug metabolism <i>Marine Letertre, UK</i>	
	F2: Rapid kinetics of lipid second messengers controls secretion in <i>Toxoplasma</i> parasites <i>Nicholas Katris, France</i>	
	F3: Searching for differential metabolites between <i>Mycobacterium tuberculosis</i> and the MTBVAC vaccine using non-targeted approach metabolomics <i>Caridad Díaz Navarro, Spain</i>	
11:55 am - 12:10 pm	S1: Sciex : A New Tool in Metabolomics: SWATH® Acquisition Analysis for Global Profiling and Quantitation <i>Joerg Schlotterbec, Sciex</i>	
12:10 pm - 1:00 pm	Lunch & Posters	
1:00 pm - 1:45 pm	Lunch & Posters	Career information
1:50 pm - 2:20 pm	Lunch & Posters	S2: Bruker lunch seminar. TBA
Agriculture & Food		
Chairs: Loic Mervant & Steffen Neumann		
Chair:	Plenary 2: Physical inactivity and preservation of muscle mass: Lessons from hibernation <i>Etienne Lefai, France</i>	
3:15 pm - 3:35 pm	O4: Mass Spectrometry Imaging (MALDI-MSI) and LC-MS/MS reveal spatial distribution of metabolic responses to <i>Leptosphaeria maculans</i> infection in stems of <i>Brassica napus</i> <i>Anani Amegan Missinou, France</i>	
3:35 pm - 4:05 pm	Keynote 1: Insights from integration of metabolomics data in large-scale plant metabolic models <i>Zoran Nikoloski, Germany</i>	
4:05 pm - 4:20 pm	F4: Elicitor-specific reprogramming of potato's metabolome <i>Rafaela Martin, France</i>	
	F5: Biosource-guided network annotation and visualization for untargeted metabolomics <i>Santiago Codesido, Switzerland</i>	
	F6: Recommending substructures for unknown tandem mass spectra <i>Youzhong Liu, Belgium</i>	
4:20 pm - 5:00 pm	Coffee break	
Statistical & Computational developments		
Chairs: Sara Tortorella & Lorraine Brennan		
5:00 pm - 5:20 pm	O5: Mix it up! How to combine multiple LC-MS modes and design of experiments to understand multifactorial biological phenomena <i>Victor Gonzalez Ruiz, Switzerland</i>	
5:20 pm - 5:35 pm	EC1: ASICS: identification and quantification of metabolites in complex 1H NMR spectra <i>Gaëlle Lefort, France</i>	
5:35 pm - 5:55 pm	O6: Modelling intrahepatic metabolic rewiring during the onset of obesity using arterio-venous blood metabolomics profiles <i>Nathalie Poupin, France</i>	
5:55 pm - 6:10 pm	S3: Shimadzu . Profiling experiments with DIA on the Ultra-Fast Q-TOF LCMS-9030 <i>Thierry Legoupil</i>	
6:10 pm - 8:00 pm	Welcome drinks & Posters	

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Thursday 23rd 2020 <i>Auditorium Marthe Condat</i>	
Methodological & Technological developments Chairs: Jordi Capellades & Pietro Franceschi	
9:00 am - 9:45 am	Plenary 3: Spatial metabolomics in untargeted and quantitative studies <i>Ingela Lanekoff, Sweden</i>
9:45 am - 10:05 am	O7: Coupling metabolomic information coming from both LC-MS and Imaging-MS to characterize experimental induction of coral larvae metamorphosis <i>Alain Paris, France</i>
10:05 am - 10:25 am	O8: NMR metabolomics: a new tool in forensic sciences <i>Emanuela Locci, Italy</i>
10:25 am - 10:40 am	EC2: Machine learning-based classification to improve Gas Chromatography-Mass Spectrometry data processing <i>Yoann Gloaguen, Germany</i>
10:40 am - 11:05 am	Coffee break
Human health Chairs: Corentine Goossens & Matej Oresic	
11:05 am - 11:35 am	Keynote 2: Unveiling the metabolic phenotypes and vulnerabilities underlying metastasis and drug resistance <i>Marta Cascante, Spain</i>
11:35 am - 11:50 am	EC3: High throughput untargeted surface metabolite profiling of formalin-fixed paraffin embedded (FFPE) brain tumour tissue microarrays (TMA) using LESA-MS/MS and OrbiSIMS <i>Joris Meurs, UK</i>
11:50 am - 12:05 pm	EC4: Computational modeling of p53 metabolic functions <i>Carlo De Blasio, France</i>
12:05 pm - 12:20 pm	F7: Towards precision diagnostics: Untargeted metabolomics for the diagnosis of inborn errors of metabolism in individual patients <i>Kulkarni Purva, NL</i>
	F8: Metabolic maturation in the first two years of life in resource-constrained settings and its association with postnatal growth <i>Natasa Giallourou, UK</i>
	F9: Rapid LA-REIMS and comprehensive UHPLC-HRMS for metabolomics of biofluids in metabolic disorders <i>Lieven Van Meulebroek, Belgium</i>
12:20 pm - 1:30 pm	Lunch & Posters
1:30 pm - 2:00 pm	<div>Lunch & Posters</div> <div>S4: Thermo lunch seminar Escape the Identity Crisis with Intelligence Driven Mass Spectrometry <i>Amanda Souza, Marketing Manager, Life Sciences Mass Spectrometry & Anas Kamleh, Sales Support Expert - Thermo Fisher Scientific</i></div>
Environmental science & Plants Chairs: Sylvain Dechaumet & Anne-Emmanuelle Hay	
2:00 pm - 2:30 pm	Keynote 3: Environmental Cheminformatics: Case Study of Thirdhand Smoke in House Dust <i>Emma Schymanski, Luxembourg</i>
2:30 pm - 2:50 pm	O9: Relating metabolomics and yield in a network of experiments <i>Sylvain Prigent, France</i>
2:50 pm - 3:10 pm	O10: Understanding the regulation of proline content in source leaves of winter oilseed rape by using transcriptomic and 15N-isotope tracing approaches <i>Younes Dellero, France</i>
3:10 pm - 3:25 pm	S5, Waters: Multi-dimensional Metabolomics using Ion Mobility Workflows – Future Advances <i>Sarah Lennon, Waters</i>
3:25 pm - 4:00 pm	Coffee break
Methodological & Technological developments Chairs: Youzhong Liu & Patrick Giraudeau	
4:00 pm - 4:45 pm	Plenary 4: Micro-NMR for Metabolomic Observation of Microfluidic Culture Systems <i>Marcel Utz, UK</i>
4:45 pm - 5:05 pm	O11: Coupling UPLC-MS with Microdialysis for Metabotyping Burn Injury <i>Elizabeth Want, UK</i>
5:05 pm - 5:20 pm	EC5: Proton detected 31P NMR methods for metabolomics <i>Neil Cox, France</i>
5:20 pm - 5:40 pm	O12: The power of LC-MS based multiomics to explore human adipogenesis <i>Evelyn Rampler, Austria</i>
5:40 pm - 7:15 pm	Posters Session
8:00 pm - 12:00 am	Gala Dinner

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Friday 24th 2020	
Auditorium Marthe Condat	
Environmental science	
Chairs: Natasa Giallourou & Serge Rudaz	
9:00 am - 9:30 am	Keynote 4: Prenatal chemical exposure modulates neonatal serum phospholipids, increasing later risk of type 1 diabetes <i>Tuulia Hyötyläinen, Sweden</i>
9:30 am - 9:50 am	O13: TheWormJam 2019 vintage - New developments in the international research community for <i>C. elegans</i> systems biology and metabolic modelling <i>Horst Joachim Schirra, Australia</i>
9:50 am - 10:05 am	EC6: Child multi-omics signatures of the early life exposome <i>Léa Maitre, Spain</i>
10:05 am - 10:35 am	Coffee break
Human health	
Chairs: Kate Gallagher & Justine Bertrand Michel	
10:35 am - 11:20 am	Plenary 5: Lipidomics signatures of metabolic diseases <i>Maria Fedorova, Germany</i>
11:20 am - 11:40 am	O14: Optimisation of Biofluid and Tissue Metabolite and Lipid Extraction for Clinical Metabolic Phenotyping <i>Andrew Southam, UK</i>
11:40 am - 12:00 pm	O15: Integrated metabolomics and transcriptomics analysis of intra-tumour heterogeneity in paediatric brain tumours <i>Alison Woodward, UK</i>
12:00 pm - 12:20 pm	O16: Identifying novel activators of regulatory T-cell metabolism <i>Celia Berkers, The Netherlands</i>
12:20 pm - 12:35 pm	Closing Ceremony & Awards
O: Oral Presentation - EC: Early Career oral presentation - F: Flash presentation (180 seconds) - S: Sponsor presentation	

POSTER LIST

Poster 001: P001

Revealing age-related sex differences in human lipidome: Metabolic phenotyping of Lausanne population

Poster 002: P002

Untargeted metabolomic analysis for the discovery of treatment response biomarkers in breast cancer patients through Hotelling T2 multivariate profiling

Poster 003: P003

Metabolomic investigation of immune cell activation by Liquid Chromatography coupled with High Resolution Mass Spectrometry (LC-HRMS)

Poster 004: P004

GH-OMICS: applying metabolomics to the fight against hormonal doping

Poster 005: P005

NMR metabolomics for understanding the role of alkaline phosphatase in neurotransmission and inflammation processes

Poster 006: P006

A multiplatform approach: HPLC, GC and NMR for urinary metabolomic analysis of muscle-invasive bladder cancer

Poster 007: P007

NMR metabolic profiling can help discriminate between normal primary hepatocytes and diverging hepatic cancer cell lines

Poster 008: P008

Quantitative metabolomics analysis reveals altered lipid profile in women with endometriosis: a pilot case-control study

Poster 009: P009

Steroid profile in human seminal fluid: is it linked to sperm quality?

Poster 010: P010

Combination of two semi-targeted approaches to detect toxicological biomarkers as a tool to understand the relation between red meat consumption and colorectal cancer promotion

Poster 011: P011

Mre11 nuclease activity removes the replication blocking nucleoside analogue Gemcitabine from the nascent strand during DNA replication

Poster 012: P012

Metabolic characterization of *Leishmania mexicana*-infected macrophages

Poster 013: P013

A comprehensive analysis of metabolome and lipidome in different sleep deprivation models using a multiplatform technique of chromatography-mass spectrometry

Poster 014: P014

Study on Alterations of Metabolome by Blood Transfusion using LC-Q-TOF and GC-MS

Poster 015: P015

Dried Blood Spots for the Determination of Reduced to Oxidized Glutathione Status

Poster 016: P016

Preliminary investigations of alkaloid composition from *Thalictrum isopyroides* plant of Azerbaijan Flora

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Poster 017: P017

Serum targeted and untargeted metabolomics-based analyses in infants with Ureteropelvic Junction Obstruction

Poster 018: P018

Investigating urinary and faecal metabolic differences among native Africans, African Americans and Alaskans using mass spectrometry

Poster 019: P019

Alterations in plasmatic levels of metabolites involved in purine, urea cycle and tryptophan metabolic pathways during right ventricular remodeling in chronic thromboembolic pulmonary hypertension

Poster 020: P020

Molecular networking-based mass spectrometry to decipher tumor cells metabolism

Poster 021: P021

“-Omics- sciences and therapeutic”

Poster 022: P022

Metabolomic study of commercial mistletoe extracts used in alternative anticancer therapy

Poster 023: P023

Optimization of the untargeted metabolomics workflow for studying the impact of dysbiosis on the host

Poster 024: P024

Rapid extraction and High-Resolution Tandem Mass Spectrometry analysis of the acylCoA metabolome

Poster 025: P025

Serum metabolic profiling following traumatic brain injury in rats using ¹H Nuclear Magnetic Resonance spectroscopy

Poster 026: P026

Surface analysis of lipids in rat mesenteric fat tissue sections by MALDI-MS imaging to understand the impact of obesity

Poster 027: P027

Combined transcriptomics–metabolomics profiling of the heat shock response in the hyperthermophilic archaeon *Pyrococcus furiosus*

Poster 028: P028

Alternative carbon sources for the central metabolism of *Trypanosoma brucei* procyclic form

Poster 029: P029

Characterization of bioherbicidal compounds stemming from micro-algae diversity by differential metabolomic and spectral similarity network assisted dereplication (ALL DREAM)

Poster 030: P030

Threonine metabolism in *Leishmania*

Poster 031: P031

Fluorinating Putida: Annotating Novel and Undesired Metabolites

Poster 032: P032

Analysis of metabolome time-variations of an endophytic fungal strain of *Botryosphaeria mamane* through untargeted LC-MS profiling

Poster 033: P033

Study of the production of (phyto)hormones by mycorrhizal fungi

Poster 034: P034

Metabolites characterization of nine cyanobacteria isolated from thermal mud.

Poster 035: P035

Metabolomics in plant-microbe interactions: “MetaboHUB-MetaToul-plant metabolites” platform facilities

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Investigating the effects of future climate scenarios in soft fruit: application of HPLC-PDA-MS metabolite profiling in blackcurrant cultivated under increased temperature and altered light regimes

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The role of food polyphenols in energy metabolism

Poster 038: P038

Study of dietary polyphenols metabolites by a top-down metabolomics approach

Poster 039: P039

NSP19 an original eco-extract from *Dioscorea villosa* with neuroprotective effects in in vitro Alzheimer's disease models

Poster 040: P040

Digging out the terroir influence on bioactive polyphenols from grape stems: A correlation_network_ driven approach to spatialize metabolomics data.

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Development of a UHPLC-MS/MS targeted method in various matrices for the quantification of toxicologically relevant aldehydes produced from lipid peroxidation

Poster 042: P042

LC-MS based untargeted metabolite profiling of wholegrain spelt (*Triticum spelta*) cultivated in Switzerland

Poster 043: P043

Isotope Labelling and Molecular Networking to Identify New Fungal Secondary Metabolites

Poster 044: P044

Specific derivatization with isotopic labeling introduction and mass spectrometry to monitor lipid peroxidation carbonyl compounds in the intestinal lumen by both targeted and non-targeted approaches.

Poster 045: P045

Characterization of *A. thaliana* responses to plant defence elicitors using untargeted metabolomics

Poster 046: P046

Metabolomics implemented to the Equine Biologic Passport (EBP) for doping control.

Poster 047: P047

Unravelling the impact of the antidepressant venlafaxine on the metabolome of meagre fish

Poster 048: P048 Comparison of effects produced by the exposure of bisphenol A and estradiol in zebrafish embryos (*Danio rerio*) using an untargeted metabolomics approach

Poster 049: P049

Let's talk about POEMS !! Photosynthetic Organisms from Atmospheric Ecosystem in a Multiscale Study

Poster 050: P050

Developing a multi-omics approach for chemical grouping

Poster 051: P051

Microbiome and metabolome analyses of the medaka fish gut during a chronic exposure to toxic cyanobacterial blooms

Poster 052: P052

High-Throughput Targeted Lipidomics Analysis of Dihydroceramide Desaturase-1 (DES1) Knockout Mice

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In Vivo Microdialysis of Endogenous and ¹³C-labeled TCA Metabolites in Rat Brain: Reversible and Persistent Effects of Mitochondrial Inhibition and Transient Cerebral Ischemia

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Ion source optimization in liquid chromatography time-of-flight mass spectrometry for metabolomics studies using the design of experiments

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A novel multi-targeted quantitative approach for nutrimetabolomics research

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FOBI: An ontology to represent food intake data and associate it with metabolomic data

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Comparison of different methods for lipidic extraction

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Development of an untargeted metabolomics workflow for investigating drug-induced cardiotoxicity using cardiac microtissues.

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A metabolomics-like approach for chemical forensic: preliminary study and perspectives

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Simultaneous measurement of absolute metabolite concentration and isotope incorporation by mass spectrometry

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Evaluation of pure shift NMR method in metabolomics

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A high throughput fluxomic workflow for exploration of metabolic phenotypes

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Metabolomic fingerprint of aging on red blood cells

Poster 064: P064

Intelligent Acquisition for Comprehensive Metabolome Coverage in Plants, Mammals, and Bacteria

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Novel MALDI imaging solution empowered by a dual-source Q-TOF and a dedicated bioinformatics pipeline for identification of peaks from tissue

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Establishing a Spectral Library and Accurate Mass Retention Time (AMRT) Database for Pediatric Metabolomics Analysis

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Investigation of mevalonate pathway by quantitative metabolomics and isotopologue profiling

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High-throughput metabolite profiling of cell media for improved antibody production utilizing a dual separation/mass spectrometry system

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The development of selective sorbent for isolation of catecholamines and their metabolites from biological fluids

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Data processing workflow to study the exposome by suspect screening

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Development of an untargeted approach based on isotope profiling of metabolic networks by high resolution mass spectrometry

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Improving lipid annotation coverage using intelligent precursor selection software on an Orbitrap-based mass spectrometer

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Comparison of normalization techniques for untargeted metabolomics of urine samples.

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Comparison of two sampling and extraction protocols to perform metabolomic studies on human adherent cells

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Development of a System Suitability QC Sample for Nano-Electrospray Direct Infusion Mass Spectrometry Metabolomics

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Evaluation of U-13C *Spirulina* (*Arthrospira platensis*) for stable isotope assisted untargeted metabolomics and liquid chromatography-isotope dilution mass spectrometry (LC-IDMS)

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Increased throughput and coverage for the annotation of Saponins using a structurebased MSn approach on a Tribrid Orbitrap mass spectrometer

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Application of 13C flux analysis in diagnosis of metabolic disorders

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Study on Intracellular Tracking of 13C isotope - labeled Volatile Cancer Markers

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Metabolomics profiling urine by Benchtop NMR

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Multi-platform and multi-matrix analytical development

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A comparison between a targeted and an untargeted approach in the frame of a pilot biomonitoring study

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AlpsNMR: an R package for fully untargeted NMR-based metabolomics workflow

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Costs and benefits of switching from vendor-based to open source pipelines for untargeted LC-MS metabolomics

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Volatile Biomarker discovery in flatus by GC-MS and GC-IMS to diagnose digestive disorders and diseases.

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MetExplore: Omics data analysis in the context of metabolic networks

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BARSA: Bidimensional nmR Spectra Annotation

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Uniting metabolomics data processing and highly confident annotation across six MS instrumental set ups: MetaboScape 5.0

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Integrated workflow with quality control for large cohort and clinical metabolomics research using robust hardware and signal correction

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Automatic annotation in untargeted metabolomics: a proof of concept protocol based on recurrent experiments

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Metabolomics results interpretation using recommender system embedded in metabolic network visualization

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Technological developments and opportunities with Workflow4Metabolomics

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Taxonomically informed metabolite annotation enhances confidence in specialized metabolomes annotation

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Improving prediction of essential genes using context-specific metabolic network ensembles

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Showcasing Longitudinal Metabolomic Datasets: Accessible, Fast and Simple

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Developing methods for targeted metabolomics by LC-MS

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The SMRT dataset for machine learning-based metabolite retention time prediction.

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LC-MS/MS data analysis with xcms

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FoodomicsGR National research infrastructure for the comprehensive characterisation of Foods

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SWATH® Acquisition Allows a Deeper Level of Comprehensive Metabolite Quantitation

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Using metabolomics to investigate the role of the gut microbiota in mediating the effects of diet on appetite in humans

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