

#	Poster Title	Presenter First Name	Last Name	Organization	Theme
10	Use of untargeted LC-MS metabolome to discriminate Italian mono-varietal red Origin Wines: Polyphenols and N-containing metabolites were the main biomarkers	Panagiotis	Arapitsas	Fondazione Edmund Mach	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
13	Metabolomics Analysis Reveals a Time-Response Mechanism Underlying the Liver Toxicity in Mice	Chunzhen	Shi	Beijing Technology And Business University	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
17	Assessment of the Phenolic Compounds of Pearl and Finger Millets Obtained from South Africa and Zimbabwe	Zahra	Hassan	University Of South Africa	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
25	A high-resolution mass spectrometry platform revealed oxidized lipid modification in barley roots as an adaptation mechanism to salinity stress	Thusitha	Rupasinghe	SCIEX	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
31	Metabolomics reveals new biomarkers for processed meat intake	Roland	Wedekind	International Agency For Research On Cancer	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
41	Variations in the leaf metabolites profile between hydroponic and field grown <i>M. oleifera</i> genotypes	Lavhelesani Rodney	Managa	University Of Pretoria	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
43	Volatiles and cuticular compounds as a mean to combat the lesser mealworm pest, <i>Alphitobius diaperinus</i> (Coleoptera: Tenebrionidae)	Erika	Calla Quispe	PUCP	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
49	Non-target screening workflow of plant metabolomes to reveal changes caused by antiepileptic drug incubation	Rofida	Wahman	TUM	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
60	Discovery of serum and urine biomarkers of legumes by untargeted LC-MS metabolomics through nutrikinetic analysis and evaluation of their suitability in 24-h urine collections	Mar	Garcia-Aloy	Fondazione Edmund Mach	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
75	Metabolomics characterization and microbial diversity along the Rimac River, the highly polluted water source of Peru's Capital	Hammerly Jonathan	Lino Fuentes Rivera	Pontifical Catholic University Of Peru	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
77	Natural deep eutectic characteristics of honey improve the bioactivity of natural products	Shasha	Kong	Institute Of Chinese Materia Medica, China Academy Of Chinese Medical Sciences	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
83	Urine 1H-NMR-based metabolomics reveals in vivo effect of <i>Psidium friedrichsthalianum</i> fruit juice administration in oxidative metabolism in rats.	Alexander	Montoya-Arroyo	Institute of Nutritional Sciences, Department of Food Biofunctionality. University of Hohenheim	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
84	FOBI: an ontology to represent food intake data and associate it with metabolomic data	Pol	Castellano-Escuder	University Of Barcelona	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
86	Metabolomics profile of <i>Elaeis guineensis</i> and correlation with neuroprotective activity in <i>Caenorhabditis elegans</i>	Taiwo	Elufioye	University Of Ibadan	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
91	Exploring metabolism and biochemical profile in response to combined heat and drought stress in <i>Pinus pinaster</i>	Cristina	López-Hidalgo	University of Oviedo	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
96	Metabolomics meets white biotechnology: interdisciplinary approaches to resolve suboptimal biosurfactant production	Sven	Dierickx	Ghent university	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
107	Side-stream products of malting are a rich and neglected source of phytochemicals	Ville	Koistinen	University of Eastern Finland	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
108	Saffron formulations for clinical intervention studies: analytical pitfalls and critical considerations	Stella	Ordoudi	Aristotle University Of Thessaloniki	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
112	LC-MS/MS-based free amino acid determination in three honeybee products	Agnieszka	Klupczynska	Poznan University of Medical Sciences	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
113	Metabolite profiling of <i>Pinus pinaster</i> infected with <i>Bursaphelenchus xylophilus</i>	Ana Margarida	Rodrigues	ITQB NOVA	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms

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123	The Art of Storytelling in Metabolomics: Investigating ruminal metabolic changes of grazing heifers treated with 3-nitrooxypropanol (3-NOP)	Emily	Daubney	UQ	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
130	The metabotyping of an East African cassava diversity panel: a core collection for developing biotic stress tolerance in cassava	Laura	Perez Fons	Royal Holloway University of London	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
139	The metabolic response to infection with Wolbachia pipientes implicates the insulin/insulin-like-growth factor and hypoxia signalling pathways in Drosophila melanogaster.	Denni	Currin-Ross	The University of Queensland	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
140	The nutritional potential of the Australian Green Plum (Buchanania obovata)	Selina	Fyfe	The University Of Queensland	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
141	Characterisation of acute heat stress in Bos taurus with NMR-based metabolomics	Alexandra	Gloria	Centre for Advanced Imaging	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
148	Metabolite profiling of fermented cacao beans from different origins of Indonesia	Abu	Hanifah	Osaka University	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
149	GC-MS based metabolomics approach to evaluate shelf life-related metabolites in pineapple (Ananas comosus) ripening process	Muhammad Maulana Malikul	Ikram	Osaka University	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
150	Investigating the effect of sonication, temperature and prolonged fermentation to amino acid content in tempe via Response Surface Methodology	Hadi Akbar	Dahlan	Department of Biotechnology, Graduate School of Engineering, Osaka University	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
154	Non-targeted exploration of metabolic processes and xenobiotic metabolism in plants exposed to micropollutants using mass spectrometry imaging	Aiko	Barsch	Bruker Daltonics, Bremen	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
159	Optimization of intracellular metabolites extraction of the bacterium Brucella abortus for metabolomics studies	Joane	Mariela Miari Corrêa	UFMG	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
160	Validating biomarkers of dairy food intake in a free-living observational cohort	Katherine	Li	Wageningen University & Research	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
162	LC-MS-based metabolomics discriminates Varietal from Premium Chilean Cabernet Sauvignon wines	Vania	Sáez	Fondazione Edmund Mach	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
163	LC-MS Based Assays for the Absolute Quantification of Primary and Secondary Metabolites in Pine/Spruce Needles	Sudarshana Reddy	Bhumireddy	The University Of Alberta	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
164	Integration of the Microbial Natural Product Atlas in Mass Spectrometry-Based de novo Discovery and Screening Applications	Giorgis	Isaac	Waters Corporation	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
165	Exposure to 4-(Methylnitrosamino)-1-(3-pyridyl)-1-butanone during early development reveals metabolic and phenotypic alterations in zebrafish embryos	Carla	Merino Ruiz	MIL@B - CIBERDEM - URV	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
167	Comparative & Complementary Metabolite Annotation Strategies for Unknown Metabolite Identification on HR LC-MS/MS based Metabolomics Data	Biswapriya	Misra	Enveda Therapeutics India	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
168	Does water limitation or grafting affect the metabolite profiles of roots of Vitis genotypes?	Annick	Moing	INRAE	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
169	Metabolic changes in murine hair follicles treated with Procyanidine-B2 rich nutraceuticals studied by Magnetic Resonance Mass Spectrometry (MRMS)	Heino	Heyman	Bruker	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
173	A GC-MS Based Assay for the Identification and Quantification of Terpenes in Cannabis sativa L.	Yilin	Wang	University of Alberta	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
184	A GC-MS based metabolites profiling and sensory profiling of tempe from different legumes	Della	Rahmawati	Osaka University	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
186	Development of an innovative metabolomics approach combining NMR and LC-MS: application to the identification of Sharka disease biomarkers	Cedric	Bertrand	Université De Perpignan	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms

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192	Untargeted metabolomics study of phloem and xylem of aspen grown under different nitrogen fertilization	Magdalene	Reinkensmeier	Bruker Daltonik GmbH	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
193	FoodomicsGR National Research Infrastructure For The Comprehensive Characterisation Of Foods	Georgios	Theodoridis	Aristotle University Thessaloniki	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
198	Untargeted UPLC-ESI-QTOF/MS metabolomic determination of anti-inflammatory compounds of <i>Ocotea</i> sp. (Lauraceae)	Albert	Katchborian Neto	UNIFAL	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
199	Study of the system <i>Thaumastocoris peregrinus</i> – <i>Eucalyptus</i> : A metabolomic approach	Guillermo	Bragunde	Universidad De La República	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
201	Impact of cluster thinning on aromatic amino acid metabolites profile for Ribolla Gialla monovarietal sparkling wine production from different vineyard sites	Domen	Škrab	Fondazione Edmund Mach	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
202	The impact of soluble gas stabilization during packaging on cooked chicken breast: a metabolomics investigation	Oscar Daniel	Rangel-Huerta	Norwegian Veterinary Institute	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
204	UHPLC-DAD-(ESI)-HRMS and NMR-based metabolomics approach to access the seasonality of <i>Terminalia catappa</i> L. from Brazilian biodiversity	Ana Caroline	Zanatta	University Of Strathclyde	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
206	Untargeted metabolomic to explore changes in the microbial metabolome after in vitro incubation with Monacolin K $\beta$ -hydroxy acid	Rocío	Garcia Villalba	CEBAS-CSIC	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
219	Volatile biomarkers for insect-infested brown rice: GC-MS search and real-time MS verification	Fukuyo	Tanaka	Central Region Agricultural Research Center, National Agriculture And Food Research Organization (NARO)	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
220	GC/MS-based metabolomics approach and Quantitative Descriptive Analysis (QDA) exert the importance of size in white leg shrimp ( <i>Litopenaeus vannamei</i> )	Safira	Putri	Osaka University	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
221	Effects of ergotamine on the central nervous system using untargeted metabolomics analysis in a mouse model	Priyanka	Reddy	Agriculture Victoria Research	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
227	The Metabolomic Story of a Marine Microbial Love – Deciphering Microbial Chemical Mediation in a Marine Environment	Samuel	Bertrand	Université De Nantes	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
229	Mass Spectrometry-based Untargeted Metabolomics Approach for Differentiation of Beef of Different Geographic Origins	Ka-yi	Man	The Hong Kong Polytechnic University	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
232	Non-target ROIMCR LC-MS study of the disruptive effects over time of TBT on the lipidomics of <i>Daphnia Magna</i>	Jamile	Mohammad Jafari	Institute for Advanced Studies in Basic Sciences (IASBS)	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
235	Root endophytic fungus <i>Piriformospora indica</i> induces heavy metal and salt stress tolerance to <i>Stevia rebaudiana</i> Bertoni plants by metabolic reprogramming.	Nazima	Nasrullah	Jamia Hamdard	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
244	Development and validation of a simple UPLC-MS/MS method for the quantitative determination of ppGpp in enriched activated sludge microbial communities	Nay Min Min Thaw	Saw	Singapore Center For Environmental Life Science Engineering	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
245	Bilinear and Trilinear ROIMCR analysis of LC-MS untargeted metabolomic datasets obtained using an experimental design approach	Roma	Tauler	IDAEA-CSIC	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
256	Analysis of two-dimensional NMR spectra for identification of conjugated $\alpha$ -linolenic acid isomers in pot marigold seed oil	Natalia	Tyszkiewicz	Politechnika Wroclawska	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
258	Mass spectrometry based untargeted metabolomics enables the discovery of new advanced glycation end products after feeding rats with heat-treated skimmed milk powder	Xiaomin	Zhou	University Of Copenhagen	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
260	Metabolomics reveals the complexity of chemical-based interactions between <i>Daphne gnidium</i> and <i>Aegilops geniculata</i>	Monica	Scognamiglio	University Of Campania "Luigi Vanvitelli", DiSTABiF	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
261	<sup>1</sup> H NMR Metabolic Profiling of Wild Ruminant Bighorn Sheep to Inform Wildlife Conservation Efforts	Galen	O'Shea-Stone	Montana State University	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms

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264	Fluoroacetate Toxicity and Metabolism in an Adult Zebrafish Model	Casey	Chamberlain	Washington University in St. Louis	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
270	Metabolomic characterization of different honey designations by ultra-fast gas chromatography coupled with electronic nose	Juan Miguel	Torres Chávez	UASLP	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
274	WormJam and Drosophila Pate - lessons from metabolomics and genome-scale modelling of model organisms.	Horst Joachim	Schirra	The University Of Queensland	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
275	Use of multivariable data analysis in unravelling the metabolic differences between two varieties of Chamomile ( <i>Matricaria chamomilla</i> ).	DANA	Atoum	University Of Strathclyde	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
276	Toxicogenomic signatures suggest differential sensitivity of double-crested cormorants and Japanese quail following early-life stage exposure to chlorpyrifos	Elena	Legrand	McGill University	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
279	<sup>1</sup> H-NMR and LC-MS based metabolomics profile of wild and cultivated <i>Amaranthus</i> spp.	Nolitha	Nkobole	University of South Africa	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
280	Metabolic Profiling Provides Unique Insights to Accumulation and Biosynthesis of Key Secondary Metabolites in Annual Pasture Legumes of Mediterranean Origin	Sajid	Latif	Charles Strut University	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
286	<sup>1</sup> H-NMR-based metabolomics to investigate the effects of Phoenix dactylifera seed extracts in LPS-IFN- $\gamma$ -induced RAW 264.7 cells	Faridah	Abas	UPM	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
289	Systemic accumulation of secondary defense metabolites in pepper leaves in response to soil application of kale leaves	Jorge	Poveda	Csic	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
292	Metabolomics: PFAS Toxicology Endpoints	Georgia	Sinclair	Rmit University	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
293	Detection of Pork and Chicken Adulteration Using a Spectroscopy-based Sensor	George - John	Nychas	Agricultural University Of Athens	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
294	Identification of Lipid Species in the allergic cell model by UPLC-Q-Exactive	ZhiQiang	Yang	JiMei University	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
296	Lipidome Disturbances in Preadipocyte Differentiation Associated with Bisphenol A and Replacement Bisphenol S Exposure	Jun	Zeng	Jimei University	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
297	Effects of bisphenol A and replacement bisphenol S on differentiation of 3T3-L1 preadipocytes detected by UPLC-Q-Exactive	JunLi	Li	Jimei University	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
298	Screening and de-replication of fungal extracts using metabolomic tools	Gabriela	Cabrera	Universidad de Buenos Aires	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
299	Large-scaled Lipidome Profiling of <i>Epinephelus coioides</i> Spleens	Yue	Zhong	Jimei University	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
300	Symbiotic relationship between Micro algae & PGPB Bacteria and co product application	Haixin	Peng	Auburn University	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
313	METABOLIC IMPACT OF DIET INDUCED OBESITY IN DIFFERENT TISSUES IN MICE: A COMPARTMENTOMICS STUDY	Francisco J.	Rupérez	Universidad San Pablo - CEU	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
316	Quality control in the elaboration of chocolate, from the cocoa bean to the final product, using DART-MS	Stephanie	Michel	PUCP	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
319	Untargeted metabolite profiling-based identification of PAF-antagonistic neolignans from different plant-derived, unfractionated extracts.	Ericsson	Coy-Barrera	Universidad Militar Nueva Granada	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
322	Hepatic lipid signatures in little brown bats ( <i>Myotis lucifugus</i> ) and big brown bats ( <i>Eptesicus fuscus</i> ) with white nose syndrome	Evan	Pannkuk	Georgetown University	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms
328	HormonomicsDB: A new tool for analysis of plant growth regulators	Ryland	Giebelhaus	The University of British Columbia	Environmental, Plant, Animal, Agriculture, Food, and Model Organisms

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12	Discovery of an anti-obesogenic agent from the microbiome of a genetically modified mouse and other important genome to metabolic phenotype correlations	Jeremy	Everett	University Of Greenwich	Metabolomics in Health and Medicine
14	Identification of profiles of volatile organic compounds in exhaled breath by means of an electronic nose as a proposal for a screening method for breast cancer: a case-control study	Lorena	Díaz de León	Coordinación para la Innovación y Aplicación de la Ciencia y la Tecnología	Metabolomics in Health and Medicine
15	Time-Dependent Changes in Urinary Metabolome Before and After Intensive Phase Tuberculosis Therapy: A Pharmacometabolomics Study	Monique	Combrink	North West University	Metabolomics in Health and Medicine
28	AT Lipidomics Atlas – analytical strategies to generated reference tissue lipidome	Maria	Fedorova	Leipzig University	Metabolomics in Health and Medicine
30	Optimized isolation of human milk exosomes for lipidomic analysis	Victoria	Ramos-Garcia	Health Research Institute La Fe	Metabolomics in Health and Medicine
32	Associations of the serum metabolite profile with a healthy Nordic diet and risk of coronary artery disease	Stefania	Noerman	University Of Eastern Finland	Metabolomics in Health and Medicine
40	Linking the metabolic microenvironment of the human oocyte and early embryo to pregnancy potential	Arieh	Moussaieff	HUJI	Metabolomics in Health and Medicine
44	Antibiotic-induced changes in microbiome-related metabolites and bile acids in rat plasma	Philipp	Ternes	BASF Metabolome Solutions	Metabolomics in Health and Medicine
46	Application of in vivo metabolomics to evaluate the early pathways of toxicity triggered by human-relevant doses of 3,4-methylenedioxypropylvalerone in mice	Ana Margarida	Araújo	UCIBIO/requimte	Metabolomics in Health and Medicine
52	Data-dependent normalization strategies for untargeted metabolomics—a case study	Paula	Cuevas-delgado	Cambio - San Pablo Ceu University	Metabolomics in Health and Medicine
53	Multi-omics investigation of $\beta$ -adrenergic regulation on macrophage metabolism	Amanda	Peterson	Monash Institute Of Pharmaceutical Sciences	Metabolomics in Health and Medicine
54	Comparative metabolomics revealed key pathways associated with the synergistic killing of bacteriophage-polymyxin combination against multidrug-resistant <i>Klebsiella pneumoniae</i>	Meiling	Han	Monash University	Metabolomics in Health and Medicine
55	Characterization of mouse metabolic alterations following the selective inhibition of gut microbial $\beta$ -glucuronidases.	Marine	Letertre	Corsaire	Metabolomics in Health and Medicine
56	Relationships between metabolite and drug uptake and excretion by mammalian cell lines and their transporter expression profiles.	Marina	Wright Muelas	University Of Liverpool	Metabolomics in Health and Medicine
58	Connecting the DOTS: A two-dimensional view of pulmonary TB	Ilse	Du Preez	North-west University	Metabolomics in Health and Medicine
59	Pharmacometabolomic approach in gynaecological cancer patients using high-resolution mass spectrometry	Ye-Ji	Kang	Kyungpook National University College Of Pharmacy	Metabolomics in Health and Medicine
61	Towards a mid-infrared spectroscopy screening of liver grafts at the operating room	Guillermo	Quintas	Leitat	Metabolomics in Health and Medicine
62	Does the international classification of diseases relate with metabolic biomarkers?	Kalle	Kilk	University Of Tartu	Metabolomics in Health and Medicine
63	Shedding light on the effect of pasteurization on the lipid and metabolite composition of human milk	Isabel	Ten-Doménech	Health Research Institute La Fe	Metabolomics in Health and Medicine
71	UNDERSTANDING AYAHUASCA EFFECTS IN MAJOR DEPRESSIVE DISORDER TREATMENT THROUGH IN VITRO STUDIES AND MULTI-OMICS DATA INTEGRATION	Flávia	Zandonadi	Chemistry Institute-unicamp	Metabolomics in Health and Medicine
72	A Volatile 10-Biomarker Panel in Urine for an Improved Prostate Cancer Diagnosis	Ana Rita	Lima	REQUIMTE PT505722232	Metabolomics in Health and Medicine
78	Histone acetyltransferases as direct regulators of metabolic reprogramming	Evelina	Charidemou	University Of Cyprus	Metabolomics in Health and Medicine
79	Exploration of LC-MS approaches for DNA adductome mapping and modelling	Lieselot	Hemeryck	Ghent University	Metabolomics in Health and Medicine
81	Association of Insulin Resistance-Related Lipidomic Signature with Rapid Renal Function Decline in Individuals with Young-onset Type 2 Diabetes	Jiexun	Wang	Khoo Teck Puat Hospital	Metabolomics in Health and Medicine

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89	An open label, single dose, randomised, three-way cross over, oral administration of Andrographis paniculata 1000mg, 2000mg capsule and Metformin 1000mg tablet pharmacometabolomics study in 18 healthy volunteers under fasting condition. A preliminary results and challenges.	Khim Boon	Tee	Universiti Malaya	Metabolomics in Health and Medicine
93	Metabolic phenotyping for exploring metabolic phenotypes related to patient outcomes in sepsis	Humma	Hussain	Imperial College London	Metabolomics in Health and Medicine
94	Characterising the serum metabolic profile of HIV/TB co-infection in cohorts treated and untreated for HIV	Chandré	Liebenberg	North-West University	Metabolomics in Health and Medicine
95	A comprehensive study of metabolic changes in brain slices lifespan through a multiplatform metabolomics approach	Carolina	Gonzalez-Riano	University San Pablo CEU	Metabolomics in Health and Medicine
101	Postprandial serum bile acids are associated with plasma glucose in health but not type 2 diabetes	Chang	Chen	Chongqing Medical University	Metabolomics in Health and Medicine
103	Identification of breath-prints for the COPD detection associated with smoking and household air pollution exposure by electronic nose.	Maribel	Rodríguez Aguilar	Universidad Autonoma de San Luis Potosí	Metabolomics in Health and Medicine
104	Investigation of Diet-induced Metabolic Alterations in Mouse Plasma	Ioanna	Ntai	Thermo Fisher Scientific	Metabolomics in Health and Medicine
106	Proton NMR metabolic profiling of exhaled breath condensates and serum to understand the pathogenesis of hypersensitivity pneumonitis	Sanjukta	Dasgupta	IIT Kharagpur	Metabolomics in Health and Medicine
109	Dynamics of bile acid metabolism and impact of gut microbiome in progression to islet autoimmunity and type 1 diabetes	Santosh	Lamichhane	University Of Turku	Metabolomics in Health and Medicine
110	Identifying the metabolomic signature of a psychiatric disease: The right tool for the job	Lauren	Chaby	Cohen Veterans Bioscience	Metabolomics in Health and Medicine
111	Correlating differential endogenous metabolite profiles with the pharmacokinetics of Gefitinib and its associated drug metabolites using an ion mobility based approach	Lee	Gethings	Waters Corp	Metabolomics in Health and Medicine
114	Reprogramming of glutamine metabolism via glutamine synthetase silencing induces cisplatin resistance in ovarian cancer	Jing	Guo	Keio University	Metabolomics in Health and Medicine
115	- Identification of proton NMR metabolomic fingerprints in uterine fluid of women associated with idiopathic recurrent spontaneous miscarriage	Da Doma	Sherpa	Indian Institute Of Technology	Metabolomics in Health and Medicine
116	The MSTARs concept: Multimodal clinical mass Spectrometry to TArget treatment ReSistance	Álvaro	Fernández-ochoa	Max Delbrück Center For Molecular Medicine	Metabolomics in Health and Medicine
117	Variation in serum metabolome explain prothrombotic changes associated with combined oral contraceptive use	Albe	Swanepoel	North-west University AND University of Pretoria	Metabolomics in Health and Medicine
118	New Insights Into Acoustically-mediated Blood-Brain Barrier Disruption: A Metabolomics Investigation	Antoine	Presset	UMR 1253, Ibrain, Université De Tours, Inserm, Tours, France	Metabolomics in Health and Medicine
120	Chemoselective Probes with a Unique Bioorthogonal Cleavage Site for Improved Metabolomic Analysis	Weifeng	Lin	Uppsala University	Metabolomics in Health and Medicine
125	Metabolic Profiling of Human Plasma and Urine, Targeting Tryptophan, Tyrosine and Branched Chain Amino Acid Pathways	Andrea	Anesi	Fondazione E. Mach	Metabolomics in Health and Medicine
126	Serum metabolite profile is altered years prior to diagnosis of alcohol-related diseases	Olli	Kärkkäinen	University Of Eastern Finland	Metabolomics in Health and Medicine
128	Investigation of crosslinks between DJ-1 (Park7) mutation and murine faeces and serum metabolomics studied by 1.7 mm microprobe 1H-NMR spectroscopy	Laimdota	Zizmare	Eberhard Karls University of Tuebingen	Metabolomics in Health and Medicine
132	Effects of aspirin on rectal mucosal protein and metabolite profiles in a randomized, placebo-controlled, crossover trial in healthy humans	Sandi	Navarro	Fred Hutchinson Cancer Research Center	Metabolomics in Health and Medicine

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143	Characterization of the human exposome by a comprehensive and quantitative large scale multi-analyte metabolomics platform	Raul	Gonzalez Dominguez	Universidad De Barcelona	Metabolomics in Health and Medicine
144	SHR/NCrl rats as a model of ADHD can be discriminated from controls based on their brain, blood or urine metabolomes	Camille	Dupuy	Inserm U1253	Metabolomics in Health and Medicine
145	Two apples a day modulate human: microbiome co metabolic processing of polyphenols, tyrosine and tryptophan	Marynka	Ulaszewska	San Raffaele Scientific Institute, Center For Omics Sciences	Metabolomics in Health and Medicine
147	Metabolomic studies of Pseudomonas aeruginosa - 1H NMR analysis	Karolina	Mielko	Wroclaw University Of Science And Technology	Metabolomics in Health and Medicine
156	Exploring Gut Microbiota Metabolism – New Chemical Biology Tools for Metabolomics Analysis	Daniel	Globisch	Uppsala University	Metabolomics in Health and Medicine
158	Impaired beta-oxidation and increased vulnerability to Influenza A infection in a diabetic mouse model.	Sebastiaan	Van Liempd	CIC bioGUNE-BRTA	Metabolomics in Health and Medicine
170	The Maternal Serum Metabolome by Multisegment Injection-Capillary Electrophoresis-Mass Spectrometry: A High Throughput Platform and Standardized Data Workflow for Large-scale Epidemiological Studies	Meera	Shanmuganathan	Mcmaster University	Metabolomics in Health and Medicine
174	Establishment and characterization of cellular models to modulate breast cancer-associated macrophages	Ana Sofia	Dias	University Of Aveiro	Metabolomics in Health and Medicine
175	Identification of novel diagnostic biomarkers for classical homocystinuria through untargeted metabolomics/next generation metabolic screening.	Karlien	Coene	Radboudumc Nijmegen	Metabolomics in Health and Medicine
182	Measurement of neutrophils metabolism using 13C-metabolic flux analysis	Takeo	Taniguchi	Osaka university	Metabolomics in Health and Medicine
183	A recall-by-genotype study on the metabolomic signatures of body mass index	Si	Fang	University of Bristol	Metabolomics in Health and Medicine
185	Development of a Targeted Metabolomic LC-MRM/MS Method on Allergic Inflammation	David	Obeso Montero	San Pablo Ceu University	Metabolomics in Health and Medicine
187	The 1H NMR studies for rare changes in metabolic adaptations depend on the availability of oxygen and time for the fibrosarcoma cell line	Badr	Qasem	Wroclaw University of Science and Technology	Metabolomics in Health and Medicine
190	Implementing metabolomic tools to optimise the production of anti-biofilm metabolites of endophytic Hypoxylon rubiginosum isolated from Scottish marine Fucus vesiculosus	Saif Aldeen	Jaber	Strathclyde University	Metabolomics in Health and Medicine
191	Normalizing Untargeted Periconceptional Urinary Metabolomics Data	Ana	Rosen Vollmar	Yale University School Of Public Health	Metabolomics in Health and Medicine
194	Immunometabolic dysregulations in human macrophages exposed to pro-atherogenic compound 7-ketocholesterol	Luís	Mendes	University Of Aveiro	Metabolomics in Health and Medicine
195	A sound microbiota in a sound body through apolipoprotein A-I and HDL: from mouse models to humans - The OCTOPUS Consortium	Mariel	Garcia	MDC Berlin	Metabolomics in Health and Medicine
196	Polly-PeakML: A novel machine learning algorithm for metabolomics analysis	Richa	Mudgal	Elucidata	Metabolomics in Health and Medicine
197	Challenges and opportunities of metabolic analysis of urine and plasma samples from COVID-19 patients	Ulrike	Bruening	Max-delbrück Center Für Molekulare Medizin (mdc)	Metabolomics in Health and Medicine
205	Insight into first-trimester metabolic changes associated with Gestational Diabetes Mellitus development	Danuta	Dudzik	Center for Metabolomics and Bioanalysis (CEMBIO), Faculty of Pharmacy, San Pablo CEU University, Madrid, Spain	Metabolomics in Health and Medicine
209	Correlation of clinical types of Coronary Artery Disease with patients' metabolic profile - The CorLipid study	Olga	Deda	School of Medicine, Aristotle University Of Thessaloniki	Metabolomics in Health and Medicine

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213	COnsortium for METabolomics Studies (COMETS): Infrastructure for the Conduct of Large-Scale Metabolomics Studies	Steven	Moore	National Cancer Institute	Metabolomics in Health and Medicine
215	Suitability of Dust and Domestic Sludge Standard Reference Materials (SRMs) for Metabolomics Studies	Kehau	Hagiwara	National Institute Of Standards And Technology	Metabolomics in Health and Medicine
216	Metabolomic Analyses of Asthma Phenotypes across Multiple Cohorts	Kevin	Mendez	Harvard Medical School	Metabolomics in Health and Medicine
217	Monitoring the inflammatory profile of acute burn wound healing in adults: Implications for improved burn wound management	Monique	Ryan	Murdoch University	Metabolomics in Health and Medicine
223	On the gut microbial origin of human metabolites – Curation of data supporting evidence in the Exposome-Explorer database	Augustin	Scalbert	International Agency For Research On Cancer	Metabolomics in Health and Medicine
224	Identification of biomarkers for patient stratification in HDM-allergic asthma	Alma	Villaseñor	San Pablo Ceu University	Metabolomics in Health and Medicine
225	Inability to repair damaged forms of NAD(P)H leads to a mitochondrial impairment	Adhish	Walvekar	University Of Luxembourg	Metabolomics in Health and Medicine
226	Metabolomics: a novel approach in the study of cow's milk allergy	Tomás Clive	Barker Tejeda	Cembio, Universidad Ceu San Pablo	Metabolomics in Health and Medicine
228	Towards precision diagnostics: Untargeted metabolomics for the diagnosis of inborn errors of metabolism in individual patients	Purva	Kulkarni	Radboud University Medical Center	Metabolomics in Health and Medicine
233	Genetic ablation of lysoplasmalogenase (TMEM86B) modulates endogenous plasmalogens and is a potential therapy for non-alcoholic fatty liver disease	Sudip	Paul	Baker Heart and Diabetes Institute	Metabolomics in Health and Medicine
236	Baseline metabolic profiles of rheumatoid arthritis achieving sustained drug-free remission after initiating treat-to-target tocilizumab, methotrexate or the combination: insights from systems biology	Wei	Yang	Leiden University	Metabolomics in Health and Medicine
238	Pathway-based integration of multi-omics data reveals lipidomics alterations in mouse models of Alzheimer's Disease	Monica	Emili Garcia-segura	Imperial College London	Metabolomics in Health and Medicine
240	Impact of combined cytotoxic drug doxorubicin and metabolic agent on cancer cell fitness	Iman Wassime	Achkar	Weill Cornell Medical College in Qatar	Metabolomics in Health and Medicine
247	Changes in the lipidome in type 1 diabetes following low carbohydrate diet: a randomized crossover trial	Naba	Al-sari	Steno Diabetes Center Copenhagen	Metabolomics in Health and Medicine
249	Metabolic alternations in IgE-mediated allergic enteritis	Elisa	Zubeldia-Varela	San Pablo Ceu University	Metabolomics in Health and Medicine
251	Monitoring of the metabolome changes of cancer cells cultured with limited oxygen access. 1H NMR - based metabolomics studies.	Piotr	Mlynarz	Wroclaw University Of Science And Technology	Metabolomics in Health and Medicine
253	Metabolomic signatures of tumour tissue and plasma of colorectal cancer patients with different response to radiotherapy	Anna	Wojakowska	Institute of Bioorganic Chemistry Polish Academy of Sciences	Metabolomics in Health and Medicine
254	Metabolic switch of infants with congenital heart defect undergoing atrial septostomy	José David	Piñeiro-ramos	Neonatal Research Unit, Health Research Institute Hospital La Fe	Metabolomics in Health and Medicine
262	Inter-laboratory reproducibility of a targeted lipidomics platform for the analysis of human serum and plasma	Nyasha	Munjoma	Waters Corp	Metabolomics in Health and Medicine
263	Does the patient understand the importance of adherence to therapeutic recommendations?	Joanna	Dawidowska	Medical University of Gdańsk	Metabolomics in Health and Medicine
269	Metabolic Profiling of Urinary Sulfate Metabolites	Christopher	Fitzgerald	Australian National University	Metabolomics in Health and Medicine
277	Metabolomics Signatures Among Mothers with a Congenital Heart Defect-Affected Pregnancy	Ping-ching	Hsu	University Of Arkansas For Medical Sciences	Metabolomics in Health and Medicine
278	Multi-omics profiling of NGLY1 deficiency patients and cellular models to characterize molecular phenotypes	Songjie	Chen	Stanford University	Metabolomics in Health and Medicine
281	Prospective Metabolomic Biomarkers of Equine Osteoarthritis	Emily	Clarke	University Of Liverpool	Metabolomics in Health and Medicine
282	Gender and microbiota shape metabolism and epigenetic marks in the host	Joan	Miro-Blanch	Rovira I Virgili University	Metabolomics in Health and Medicine
283	1H NMR lipidomic analysis of synovial fluid in equine osteochondrosis	Eleanor	Rowland	University Of Liverpool	Metabolomics in Health and Medicine



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284	Profiling the Differentiating Myeloid Lineage in MDS with Low and High Bone Marrow Blast Counts	Theodora	Katsila	National Hellenic Research Foundation	Metabolomics in Health and Medicine
287	Investigation of metabolic responses in MCF-7 after treatment with 4-hydroxytamoxifen using time-series metabolomics	Kazuki	Nishimoto	Osaka University	Metabolomics in Health and Medicine
302	Lipid metabolism in early psychotic disorders	Alex	Dickens	University Of Turku	Metabolomics in Health and Medicine
305	The effect of JAK inhibition on the metabolome of neutrophils from patients with Rheumatoid Arthritis	Michele	Fresneda Alarcon	University Of Liverpool	Metabolomics in Health and Medicine
306	Investigating neurodegenerative diseases with the metabolomics approach	Federica	Murgia	University Of Cagliari	Metabolomics in Health and Medicine
310	A validation study in the Cork SCOPE birth cohort of a five-lipid biomarker panel predictive of preterm birth	Kirsten	Dowling	Infant Research Centre, University College Cork	Metabolomics in Health and Medicine
311	Lipidomics and redox lipidomics indicate early stage alcohol-induced liver damage	Wanying	Tan	Yale School Of Public Health	Metabolomics in Health and Medicine
312	Metabolomic profiling and gut microbiome analysis to investigate the role of aldehyde dehydrogenase 1B1 in subacute alcohol metabolism	Georgia	Charkoftaki	Yale School Of Public Health	Metabolomics in Health and Medicine
314	Metabolic Signatures of T cell Functional Suppression by Glioblastoma	Max	Colonna	University Of Georgia	Metabolomics in Health and Medicine
315	GC-MS metabolomic analysis for elucidating gastrointestinal stromal tumour resistance to imatinib treatment	Szymon	Macioszek	Medical University Of Gdansk	Metabolomics in Health and Medicine
317	A Comprehensive Analysis of the Metabolic Dysfunction and Gut Microbiome Dysbiosis in Familial Dysautonomia: Implications of Systemic Metabolic Deficits on the Gut-Brain Axis.	Stephanann	Costello	Montana State University	Metabolomics in Health and Medicine
320	Untargeted metabolomic approach in Cri-du-Chat Syndrome	Nilson	Assuncao	Unifesp	Metabolomics in Health and Medicine
321	A Metabolomic Approach to Non-Alcoholic Fatty Liver Disease (NAFLD): from Networks to Biomarkers	Aidan	Mcglinchey	Örebro University	Metabolomics in Health and Medicine
326	Salivary oxidized phosphatidylcholines increased in OSA patients negatively correlates with the surface tension of saliva	Jiyoung	Kim	Seoul National University	Metabolomics in Health and Medicine
327	Longitudinal monitoring of urinary metabolic patterns of infants with Hypoxic-Ischemic Encephalopathy	Julia	Kuligowski	Health Research Institute La Fe	Metabolomics in Health and Medicine
2	Symbolic Aggregate Approximation Improves Gap Filling in High-Resolution Mass Spectrometry Data Processing	Tobias	Schulze	Helmholtz Centre For Environmental Research	Technology, Systems Biology & Advancing the Field
3	SmartPeak automates targeted and quantitative metabolomics data processing	Douglas	McCloskey	Technical University of Denmark	Technology, Systems Biology & Advancing the Field
4	Towards accurate annotation of adducts and fragments from LC-HRMS metabolomics data	Wenyun	Lu	Princeton University	Technology, Systems Biology & Advancing the Field
5	An end-to-end open-source LC-MS/MS data analysis pipeline for metabolomics	Nouf	Alourfi	University Of Bristol	Technology, Systems Biology & Advancing the Field
7	A scalable and flexible infrastructure for mass spectrometry data in R	Johannes	Rainer	Eurac Research	Technology, Systems Biology & Advancing the Field
9	Development of A Combined Strategy for Accurate Lipid Structural Identification and Quantification in Ion-Mobility Mass Spectrometry based Untargeted Lipidomics	Xi	Chen	Chinese Academy of Sciences	Technology, Systems Biology & Advancing the Field
11	Spec2Vec: Improved mass spectral similarity scoring through learning of structural relationships	Justin JJ	van der Hoof	Wageningen University	Technology, Systems Biology & Advancing the Field
18	MetaboKit: a comprehensive data extraction tool for untargeted metabolomics	Pradeep	Narayanaswamy	Sciex	Technology, Systems Biology & Advancing the Field
22	Identification & Distribution of bile acids, sterols and carnitines by LC-MS in humans, mice and pigs - A Qualitative Analysis	Ambrin Farizah	Babu	University Of Eastern Finland	Technology, Systems Biology & Advancing the Field

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23	On sample preparation methods for fermented beverage VOCs profiling by GCxGC-TOFMS	Penghan	Zhang	Edmund Mach Foundation	Technology, Systems Biology & Advancing the Field
26	<sup>13</sup> C metabolic flux analysis revealed metabolic alterations induced by three-dimensional culture in human cancer cell line	Shingo	Noguchi	Daiichi Sankyo Co., Ltd.	Technology, Systems Biology & Advancing the Field
27	Evaluating the accuracy of automated metabolomic feature annotation	Matthew	Keller	University Of Tennessee, Knoxville	Technology, Systems Biology & Advancing the Field
29	LipidLynxX: data transfer hub linking experimental lipidomics with data integration solutions	Zhixu	Ni	Leipzig University	Technology, Systems Biology & Advancing the Field
33	Retention time variability and adduct formation in large scale HILIC-based untargeted metabolomics data set	Vinicius	Veri Hernandes	Eurac Research	Technology, Systems Biology & Advancing the Field
34	Differential Profiles of Gut Microbiota and Metabolites Associated with Host Shift of <i>Plutella xylostella</i>	Feiying	Yang	Fujian Agriculture And Forestry University	Technology, Systems Biology & Advancing the Field
36	Increasing reliability in non-targeted data pre-processing	Yasin	El Abiead	University Of Vienna	Technology, Systems Biology & Advancing the Field
37	The Virtual Metabolic Human Database and COBRA Toolbox for enabling personalised metabolic modelling of human-microbiome interactions and digital health applications.	Cyrille	Thinnes	National University Of Ireland Galway	Technology, Systems Biology & Advancing the Field
38	Untargeted Stable-Isotope Probing of Gut Microbiome Metabolome Using <sup>13</sup> C-Labeled Dietary Fibers	Pan	Deng	University of Kentucky	Technology, Systems Biology & Advancing the Field
39	Benchmarking non-targeted metabolomics using yeast derived libraries	Evelyn	Rampl	University Of Vienna	Technology, Systems Biology & Advancing the Field
42	ContInGEMC: A collaborative pipeline for open-source community-based curation of metabolic networks	Jake	Hattwell	University Of Queensland	Technology, Systems Biology & Advancing the Field
45	Salivary Metabolomics: A validated UHPLC-HRMS and rapid LA-REIMS method.	Kathleen	Wijnant	Ghent University	Technology, Systems Biology & Advancing the Field
47	Total Metabolome Extraction Method For GC-MS Metabolomics Analysis	Joy	Mongwe	North-west University	Technology, Systems Biology & Advancing the Field
48	Ranking metabolite sets by their activity levels	Joe	Wandy	Glasgow Polyomics, University of Glasgow	Technology, Systems Biology & Advancing the Field
57	Hyperparameter optimization of metabolomics datasets and the impact thereof on supervised modeling outcomes	Marilyn	De Graeve	Ghent University	Technology, Systems Biology & Advancing the Field
64	Critical assessment of chromatographic metadata in publicly available metabolomics data	Eva-Maria	Harrieder	Helmholtz Zentrum Neuherberg	Technology, Systems Biology & Advancing the Field
65	FlyMet: An online metabolomics atlas and resource for <i>Drosophila</i> tissues.	Karen	McLuskey	University of Glasgow, UK	Technology, Systems Biology & Advancing the Field
67	The nPYc-Toolbox, a Python module for the pre-processing, quality-control and analysis of metabolic profiling datasets	Caroline	Sands	Imperial College London	Technology, Systems Biology & Advancing the Field
69	Deep metabolome annotation of in vivo <sup>13</sup> C-labeled mouse urine	Annelaure	Damont	CEA	Technology, Systems Biology & Advancing the Field
70	A Framework for the Rapid Development of New Data-Dependent Acquisition Strategies	Vinny	Davies	University Of Glasgow	Technology, Systems Biology & Advancing the Field
74	A Comprehensive Workflow for Routine, Automated, Metabolite + Lipid Analysis of Mammalian Cells	Genevieve	Van de Bittner	Agilent	Technology, Systems Biology & Advancing the Field

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80	HILIC meets MS imaging: CCS values obtained by chromatographic separation coupled to trapped ion mobility-MS for unequivocal assignment of phospholipids in MALDI-MS imaging	Patrick Olaf	Helmer	Institute of Inorganic and Analytical Chemistry, University of Münster	Technology, Systems Biology & Advancing the Field
92	Multi-matrix optimization and validation of LA-REIMS for rapid metabolic fingerprinting of biofluids: evolving towards clinical point-of-care applicability	Vera	Plekhova	Ghent University	Technology, Systems Biology & Advancing the Field
97	High Speed untargeted 4D-Lipidomics LC-MS/MS workflows with Parallel Accumulation Serial Fragmentation (PASEF)	Nikolas	Kessler	Bruker	Technology, Systems Biology & Advancing the Field
98	Highly reproducible 4D-Metabolomics using PASEF on a timsTOF Pro	Lucy	Woods	Bruker	Technology, Systems Biology & Advancing the Field
99	SwissLipids, a knowledge resource to link lipids with biology	Lucila	Aimo	Swiss Institute of Bioinformatics	Technology, Systems Biology & Advancing the Field
102	mfapy: A Python toolbox for isotope-based metabolic flux analysis using mass spectrometry	Fumio	Matsuda	Osaka University	Technology, Systems Biology & Advancing the Field
105	A Comprehensive Targeted Metabolomic Assay for Urine Analysis	Jiamin	Zheng	University Of Alberta	Technology, Systems Biology & Advancing the Field
124	Characterising Time-Dependent Metabolite Behaviour in a Pooled Cross-Sectional Context	Luke	Husdell	Centre For Advanced Imaging UQ	Technology, Systems Biology & Advancing the Field
129	Optimization of sample preparation for metabolomics card construction using combined NMR and LC-HRMS	Cecile	Martias	Inserm	Technology, Systems Biology & Advancing the Field
134	Enhancing the chromatographic separation of polar metabolites using new generation HILIC columns	Katyeny Manuela	Da Silva	University of Antwerp	Technology, Systems Biology & Advancing the Field
136	The Chemical Composition of Cannabis	Mickel	Hiebert	University of Alberta	Technology, Systems Biology & Advancing the Field
137	Profiling the Lipidome: Quantitate up to 2000 Lipid Molecular Species in a Single Injection	Mackenzie	Pearson	Sciex	Technology, Systems Biology & Advancing the Field
142	Automatic and joint metabolite identification and quantification of a set of 1H NMR spectra	Gaëlle	Lefort	INRAE	Technology, Systems Biology & Advancing the Field
151	Integrating 4D peak picking of LC-TIMS-MS/MS data into GNPS feature based molecular networking for metabolomics and lipidomics analysis.	Florian	Zubeil	Bruker Daltonik Gmbh	Technology, Systems Biology & Advancing the Field
153	Integrated analysis of lipidomics and proteomics data reveals biomolecular processes associated with bladder cancer	Nobal	Dhruw	Elucidata Data Consulting Pvt. Ltd.	Technology, Systems Biology & Advancing the Field
155	Bi-modal variational autoencoder for mass spectra and chemical structures	Svetlana	Kutuzova	Technical University Of Denmark	Technology, Systems Biology & Advancing the Field
157	Expansion of MetaboQuan-R / LipidQuan-R: A Single High-Throughput UPLC-MS/MS Platform for Targeted Metabolomic, Lipidomic and Proteomic Studies (Targeted Multi-OMICS)	Billy	Molloy	Waters	Technology, Systems Biology & Advancing the Field
161	An in-silico comparison of DDA and DIA acquisition strategies for metabolomics	Simon	Rogers	University Of Glasgow	Technology, Systems Biology & Advancing the Field
166	Maternal rat metabolomics: placenta and amniotic fluid metabolic profiling workflows	Alexandra	Bourdin-Pintueles	Inserm U1253	Technology, Systems Biology & Advancing the Field
171	Supervised Topic Modeling for MS2 Metabolite Structural Characterization	Gabriel	Reder	Stanford University Bioengineering Department	Technology, Systems Biology & Advancing the Field
176	TidyMS: a Python library for preprocessing LC-MS data in untargeted metabolomics workflows	Gabriel	Riquelme	CIBION-CONICET	Technology, Systems Biology & Advancing the Field

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177	A Comprehensive Targeted Metabolomic Assay for Uremic Toxin Quantification	Lun	Zhang	University of Alberta	Technology, Systems Biology & Advancing the Field
179	Automated metabolomic profiling of 1D 1H NMR spectra with MagMet	Manoj	Rout	TMIC, University Of Alberta	Technology, Systems Biology & Advancing the Field
180	Pathway Size Matters: The Influence of Pathway Granularity on Metabolomics Enrichment Analysis	Peter	Karp	SRI International	Technology, Systems Biology & Advancing the Field
181	One integrated solution for advancing LC-PASEF based pharma, metabolomics, non-target screening and exposome research	Xuejun	Peng	Bruker	Technology, Systems Biology & Advancing the Field
188	Metabolite Profiling by Automated Methoximation and Silylation	Hans-Joachim	Huebschmann	CTC Analytics AG	Technology, Systems Biology & Advancing the Field
200	peakPantheR, an R package for large-scale targeted annotation and integration of metabolic features in LC-MS profiling datasets	Gonçalo	Correia	Imperial College London	Technology, Systems Biology & Advancing the Field
203	Spectra consolidation of high resolution tandem mass spectrometry data in LC-MS based non-targeted metabolomics and lipidomics	Liesa	Salzer	Helmholtz Zentrum Muenchen	Technology, Systems Biology & Advancing the Field
207	Ovarian Cancer Metabolomics: Targeted Microchip Capillary Electrophoresis-Mass Spectrometry to Track Disease Progression.	Samyukta	Sah	Georgia Tech	Technology, Systems Biology & Advancing the Field
210	Accurate MS/MS Spectral Prediction with CFM-ID 4.0	Fei	Wang	University Of Alberta	Technology, Systems Biology & Advancing the Field
214	CyProduct: Significantly Improved In Silico Cytochrome P450 Metabolism Prediction	Siyang	Tian	University Of Alberta	Technology, Systems Biology & Advancing the Field
230	Fecal sample preparation for untargeted and targeted metabolomics and a reproducibility study in the targeted platform	Andressa	de Zawadzki	Steno Diabetes Center Copenhagen Klinisk Forskning / Clinical Research	Technology, Systems Biology & Advancing the Field
234	The development of high-resolution optical infrared photothermal spectroscopy for measuring the metabolic activity of bacteria at the single cell level.	Roy	Goodacre	University Of Liverpool	Technology, Systems Biology & Advancing the Field
237	Development of a Metabolomics System Suitability Sample for MS-based Metabolomics	Tracey	Schock	NIST	Technology, Systems Biology & Advancing the Field
239	A QC procedure for untargeted LC-MS metabolomics for large-scale epidemiological studies	Pekka	Keski-Rahkonen	International Agency for Research On Cancer	Technology, Systems Biology & Advancing the Field
242	Development of a data processing platform for isotope tracer experiments in Garuda	Nobuyuki	Okahashi	Osaka University	Technology, Systems Biology & Advancing the Field
243	Metabolic profiles of whole, parotid and submandibular/sublingual saliva	Alberto	Spisni	University of Parma	Technology, Systems Biology & Advancing the Field
250	Improving interpretation of lipidomic and metabolomic data through comprehensive functional annotation and network approaches	Andrew	Patt	National Center For Advancing Translational Sciences/The Ohio State University	Technology, Systems Biology & Advancing the Field
252	Revealing Lipid Structure Insights with the Information-Dependent Electron Impact Excitation of Ions from Organics (EIEIO) Fragmentation	Eva	Duchoslav	Sciex	Technology, Systems Biology & Advancing the Field
255	MetaboAtlas21: A comprehensive atlas of the mouse metabolome in response to the metabolic challenge	Tomas	Cajka	Institute of Physiology of the Czech Academy of Sciences	Technology, Systems Biology & Advancing the Field
257	1H NMR metabolomics and full-length RNA seq reveal the effect of acylated and nonacylated anthocyanin extracts on hepatic metabolome and transcriptome in Zucker diabetic fatty rats	Kang	Chen	University Of Turku	Technology, Systems Biology & Advancing the Field
259	DoE approach in sample preparation procedure optimization for modified nucleosides and deoxynucleosides targeted metabolomics analysis	Małgorzata	Artymowicz	Medical University of Gdańsk	Technology, Systems Biology & Advancing the Field

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265	CCSP 2.0: An Open Source Jupyter Tool for the Prediction of Ion Mobility Collisional Cross Sections in Metabolomics	Markace	Rainey	Georgia Institute of Technology	Technology, Systems Biology & Advancing the Field
266	A Multimodal Analysis in Cancer: Revealing metabolic heterogeneity using DESI-MS imaging with Laser-microdissection coupled transcriptome approach	Emine	Kazanc	IMPERIAL COLLEGE OF LONDON	Technology, Systems Biology & Advancing the Field
267	WiNN: Batch and Drift Correction Method by White Noise Normalization for Metabolomic Studies that does not Rely on Quality Control Samples	Olga	Demler	Division Of Preventive Medicine, Brigham And Women's Hospital	Technology, Systems Biology & Advancing the Field
268	Is High-Resolution Fourier Transform Ion Cyclotron Resonance Mass Spectrometry Needed to Improve Metabolite Annotation?	Danning	Huang	Georgia Institute Of Technology	Technology, Systems Biology & Advancing the Field
271	Feature Selection Strategies for Unknown Metabolite Identification by In Silico NMR and Ion Mobility Collision Cross Section Prediction	Carter	Asef	Georgia Institute Of Technology	Technology, Systems Biology & Advancing the Field
272	Robust metabolomics workflows using a modified benchtop Orbitrap Mass Spectrometer	Mark	Schroeder	Thermo Fisher Scientific	Technology, Systems Biology & Advancing the Field
273	Five Easy Metrics of Data Quality for LC-MS Based Global Metabolomics	Daniel	Raftery	University Of Washington	Technology, Systems Biology & Advancing the Field
285	Mass spectrometry signal quantification using supervised deep learning	Ali	Rahnavard	George Washington University	Technology, Systems Biology & Advancing the Field
290	Quantification of Polar Metabolites in Urine using an Automated Parallel Derivatization Strategy and LC-SWATH-MS	G	Boehm	CTC Analytics	Technology, Systems Biology & Advancing the Field
291	EPA and DHA lipid mediators formation is enhanced by the use of acellular fish skin grafts during burn wound healing	Aristotelis	Kotronoulas	University of Iceland	Technology, Systems Biology & Advancing the Field
301	LC-MS/MS data processing and Molecular Networking with Workflow4Metabolomics	Yann	Guitton	Umr1329 - Laberca	Technology, Systems Biology & Advancing the Field
304	Tools for Analysis of MEtabolomic NMR: tameNMR	Marie	Phelan	University Of Liverpool	Technology, Systems Biology & Advancing the Field
308	Automated high-throughput evaluation of LC-HRMS data of in-vitro incubation experiments for improving the screening annotation level of pesticide metabolites in human biomonitoring	Carolin	Huber	Helmholtz Centre For Environmental Research - UFZ	Technology, Systems Biology & Advancing the Field
309	Applications of Machine learning (ML) Algorithms for Biomarker Identification and Patient Stratification: A Systematic Review of Mass Spectrometry Studies	Daragh	O'Boyle	University College Cork	Technology, Systems Biology & Advancing the Field