MetaboNews

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In This Issue

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MetaboNews is a monthly newsletter published in a partnership between The Metabolomics Innovation Centre (TMIC) and Metabolomics Society.

Metabolomics Society News

Members Corner

Early-career Members Network (EMN)

Mark your calendars! The EMN will host its next webinar on November 26th 2020, at 1 pm UTC, and the committee is thrilled to have Dr. Fabien Jourdan, who will present "Network based solutions to improve metabolic profile interpretation". Please stay tuned for the registration details and future EMN webinars, and find past webinars on the Metabolomics Society website.

International Affiliates Corner

Metabolomics Association of North America (MANA)

Visit https://metabolomicsna.org

MANA 2020 was a great success! From exciting plenaries to Interactive Forums to poster sessions where presenters and viewers could directly talk and interact, there was lots of great knowledge shared and hopefully great connections made. We had over 400 attendees. We would also like to congratulate the winners of our awards:

2020 MANA Young Investigator Award

- Sophia Lunt

2020 Best Poster Awardees

- Casey Chamberlain
- Russell Fling
- Manuel Garcia-Jaramillo
- Kehau Hagiwara
- Clayton Kranawetter
- Ken Liu
- Felicity Nielson
- Hannah Parks
- Markace Rainey
- Shao Thing Teoh

2020 Lightning Talk Awardees

- Mark McCann
- Arpana Vaniya

We thank the organizers, Alla Karnovsky and Kathleen Stringer from the University of Michigan, for their tireless efforts that led to MANA 2020.

As announced in the closing ceremony, we are excited that the MANA 2021 meeting will be held October 17-19, 2021, in Columbus, OH, at The Ohio State University.

METABOLOMICS SOCIETY

METABOLOMICS SOCIETY
EARLY- CAREER MEMBERS NETWORK

The Metabolomics Society is an independent non-profit organisation dedicated to promoting the growth, use and understanding of metabolomics in the life sciences.

General Enquiries
info@metabolomicssociety.org
Membership Enquiries

Metabolomics Society News

More details will be posted in the next few months at the conference website: https://u.osu.edu/mana2021/

Also, we are also excited to announce that MANA's interest groups are seeking new members to help lead various initiatives across North America. Please visit https://metabolomicsna.org/index.php/resources/interest-groups to learn more about these interest groups and join!

Swiss Metabolomics Society (SMS)

Visit www.swiss-metabolomics.ch

The Swiss Metabolomics Society (SMS) is very happy to announce that the **Prof. Pablo Sinues** from the University of Basel, vice-president of the SMS, is the well-deserved recipient of the 2020 SGMS Award.

The Swiss Group for Mass Spectrometry (SGMS) award is awarded to a promising scientist working in Switzerland or a promising Swiss scientist working abroad, for outstanding independent research in the field of mass spectrometry. Prof Sinues was selected by an international award panel, with the following motivation: "Pablo has combined the expertise gained in his cross-disciplinary academic training in chemistry for his M.Sc. from the University of Murcia, Spain and Ghent University, Belgium, and his research on electrospray ionization mechanisms at the University Carlos III, Madrid, that was the subject of his Ph.D. thesis in mechanical engineering, with the experience he accumulated devising new methodologies for small metabolite analysis and applying these to clinical studies, work that led to his Habilitation in analytical chemistry, at the ETH."

Prof. Sinues made "key contributions to the analysis of exhaled breath by ambient mass spectrometry," during its former research projects and has continued to be innovative and productive since obtaining his position in Basel in 2017. Dr. Sinues has a strong publication record that spans a broad range from fundamentals in mass spectrometry ionization processes and hardware, to clinical applications of MS- based breath analysis for diseases such as COPD, pulmonary fibrosis, cardiovascular disorders, and breast cancer, to metabolism in plants.

Prof. Serge Rudaz, President of the Swiss Metabolomics Society

METABO INTERVIEW

Dr. Matej Orešic

Professor of Medical Sciences with Specialization in Systems Medicine
Örebro University, Sweden

Short Biography

Matej Orešic holds a PhD in Biophysics from Cornell University. He is Professor of Medical Sciences with Specialization in Systems Medicine at Örebro University (Sweden), Group Leader in Systems Medicine at Turku Bioscience Centre (Finland), and Guest Professor in Lipids and Nutrition at the Oil Crops Research Institute of the Chinese Academy of Agricultural Sciences in Wuhan. As of 2016, he was made a Lifetime Honorary Fellow of the Metabolomics Society. He is one of the founders of the Nordic Metabolomics Society and currently its Chair of the Board. Dr. Orešic currently also serves on the Board of Directors of the Metabolomics Society. In 2019, he co-chaired the 1st Gordon Research Conference on 'Metabolomics and Human Health'. Prof. Orešic's main research areas include metabolomics applications in biomedical research and systems medicine. He is particularly interested in the identification of disease processes associated with different metabolic phenotypes and the underlying mechanisms linking these processes with the development of specific disorders or their co-morbidities, with a central focus on both type 1 diabetes and non-alcoholic fatty liver disease. Prof. Orešic also initiated the popular MZmine open-source project, which led to the development and release of popular software for metabolomics data processing.

Interview Q&A

How has your work changed since 2013?

I have established new research team at Örebro University (Sweden) while also growing my team at University of Turku (Finland). I am currently dividing my time between the two sites. In the current times, such an arrangement presents a practical challenge, but on the other hand, we have been used to working and communicating via regular videoconferences between the two teams for years, preceding the current pandemic.

Overall, research has continued along the same lines, and with similar projects, as in 2013. We have over the past years advanced in the ways we analyze and model the data, and considerably expanded and improved our analytical platforms, which now also include platforms for comprehensive analysis of environmental chemicals.

What was the most unexpected success or outcome?

Perhaps the major finding was related to my research on early metabolic disturbances preceding the onset of islet autoimmunity and type 1 diabetes, which has been going on for nearly 15 years. I have previously identified specific metabolic disturbances, particularly decreased phospholipids, in children who later went on to progress to clinical type 1 diabetes (Oresic M *et al.* J Exp Med 2008 Dec 22;205(13):2975-84). These lipid disturbances can be observed even at birth (cord blood) (Oresic M *et al.* Diabetes 2013 Sep;62(9):3268-74 and La Torre D *et al.* Diabetes 2013 Nov;62(11):3951-6), and are primarily seen in those children who progress to the disease early in life (< 4 years of age).

For years, we did not understand what the causes of these lipid changes could be. Recently, when

studying the impact of prenatal exposure to per- and polyfluoroalkyl substances (PFAS) on postnatal lipid levels, together with Profs. Tuulia Hyötyläinen and Mikael Knip, we surprisingly found that prenatal exposure to PFAS decreased the same lipids in newborn babies as those previously found decreased in children who later progressed to type 1 diabetes. We then went on to focus our investigations of PFAS exposures on type 1 diabetes, including with exposure studies in experimental model of type 1 diabetes (NOD mouse) and verification in another prospective clinical cohort, and indeed found that prenatal exposure increases risk of islet autoimmunity and thus type 1 diabetes, while also causing the previously-observed lipid changes (McGlinchey A *et al.* Environ Int 2020 Jul 4;143:105935). Our findings are potentially also relevant for understanding incidence trends of type 1 diabetes in Finland and elsewhere. In Finland, where the incidence of type 1 diabetes is the highest in the world, the rising incidence has started to stabilize about 15 years ago. This time coincides with the tighter regulation of PFAS in Europe. Therefore, our findings may offer an explanation for this so-far unexplained phenomenon.

Clearly more work needs to be done on this topic, including large-scale studies of exposures to PFAS, and other environmental chemicals, on the incidence of type 1 diabetes and other autoimmune diseases, as well as on understanding the role that genetic risk of type 1 diabetes plays in mediating the impact of chemical exposures. Also, further mechanistic studies are needed to establish the link between the exposures, metabolic and immune disturbances, and the onset of clinical disease. This is on my current and future research agenda.

What key metabolomics initiatives are you currently pursuing at your research centre or institute?

In addition to type 1 diabetes, there are three main other projects I have been pursuing.

a. Identification of blood-based markers of traumatic brain injury (including concussions, i.e., mild TBI), for determining severity of injury as well as to predict patient outcomes, and potentially to offer new insights about the pathogenesis of TBI. I have teamed up with the large European cohort CENTER-TBI, where we have recently performed large-scale metabolomics/lipidomics study. TBI is one of the most challenging areas of clinical metabolomics, because due to the nature of the injury, metabolite data is heavily confounded.

b. Identification of biomarkers for different stages of non-alcoholic fatty liver disease (NAFLD). We are, e.g., part of the LITMUS consortium (IMI project by European Commission), which aims to develop, validate and qualify better biomarkers for testing NAFLD. In this project, I co-lead a task force to develop plasma lipid markers, which can be used in the clinic.

c. Studies of metabolic profiles associated with progression of psychotic disorders, with particular interest in the development of metabolic co-morbidities including obesity, NAFLD and type 2 diabetes. Our data suggest that the lipid signature of NAFLD may identify psychotic patients who are at highest risk of developing cardiometabolic complications. Based on data by us and others, we also believe that the endocannabinoid system may be the underlying link between the psychosis and the associated metabolic co-morbidities. Therefore, our current goal is to better understand the peripheral and central endocannabinoid systems in psychosis.

Unrelated to my own research, I have been also among the initiators of the Nordic Metabolomics Society, which was established in 2017, and where I currently serve as chair of the board. The society aims to promote metabolomics in the Nordic region, i.e., Denmark, Finland, Iceland, Norway and Sweden.

How has the metabolomics research landscape in your country changed over the last six years?

In the Nordic region, metabolomics has grown considerably over the past years, particularly in Denmark and Sweden. In several of the leading institutions, there are now multiple metabolomics groups active, covering different aspects of the field including technology and applications, including clinical. Several companies have emerged, some of them are already globally known, such as Nightingale in Finland (using blood-based NMR metabolomics as a key platform for personalized medicine). Having such a vibrant community was the primary reason why the Nordic Metabolomics Society was established. We first considered kicking off the Society at the 2011 Metabomeeting in Helsinki, but at the time there was not enough 'critical mass' to get the initiative started. On November 26-27 this year, the Society will be holding a networking meeting (http://www.nordicmetsoc.org/NMSnet2020_Virtual.html), which will highlight metabolomics research across the Nordic regions. All research teams in the region are invited to present themselves and their projects.

How do you see your work in metabolomics being applied today or in the future?

When it comes to applications of metabolomics, including in the clinic, research is being increasingly integrated with other areas, such as immunology, microbiology, and exposome research. Being an integral part of such systems biology (or systems medicine, in the clinical context) approaches, the way the metabolomics data are analyzed and interpreted also requires use of integrative methods that can contextualize the metabolism at different levels. As an example, genome-scale metabolic modeling is being increasingly used in metabolomics, because it can capture the cellular/tissue metabolism at the genome scale, while also enabling integration of gut microbiome (e.g., shotgun metagenomics sequencing) and metabolome data. As an emerging area that is still in its nascent stage, modeling of lipids is likely to play a key role in contextualizing lipidome data in relation to spatial and temporal complexity of lipid ensembles dynamics (e.g., in lipid bilayers, lipoprotein particles, exosomes) in biological systems. While we have done some early, and relatively simple, work on the topic of integrating lipidomics data and molecular dynamics simulations, computational lipidomics tools are now becoming available that, I expect, will transform the field of lipidomics and related metabolic research.

As you see it, what are metabolomics' greatest strengths?

While metabolomics research is increasingly being integrated with other related research areas, it is also increasingly recognized that metabolites play key roles in the regulation of the immune system, and in mediating the impact the gut microbiome and the exposome (particularly chemical exposome) have on host physiology. Thus, the metabolome can serve on a level where these different layers are integrated, making metabolomics a key platform for systems biology. While being an accurate readout of host physiology has always been a 'pitch' for metabolomics, evidence about the underlying mechanisms has grown considerably over the past years, and there is not a week without a new study reporting the roles of specific metabolites in the regulation of, e.g., immune system. Combining this with methodological improvements that enable reliable detection, identification and quantification of metabolites, as well as their study in dynamic (e.g., tracer studies) and spatial (e.g., imaging MS), one can foresee a bright future for the field.

What do you see as the greatest barriers for metabolomics?

As a scientific approach, I think the 'sky is the limit' for metabolomics. As a minor threat one could perhaps see that the need for increased integration may also lead to some silos within specific areas of metabolomics, to keep one's own subfields somehow distinct. However, analytical platforms are improving and may become less chemically selective in the future. Powerful informatics tools have been developed across all areas of metabolomics, addressing many common methodological challenges. Thus, both on the analytical and bioinformatics fronts, we are likely to see more integration within metabolomics and with other related areas, with perceived 'barriers' being only related to the specific scientific questions being asked.

When it comes to applications of metabolomics in the clinic, the key barrier is identification and development of clinically useful biomarkers. While there may be many studies reporting metabolic changes associated with specific indications, producing reproducible diagnostic tools is another matter. In addition to the obvious need for validation, accurate quantification of targeted metabolites would be essential, if one is to develop diagnostic signatures that are reproducible across different laboratories and could be considered for regulatory approvals. The area of lipidomics has been somewhat ahead of the curve here, since in lipidomics it has always been a common practice to use multiple internal standards to quantitate the lipids, and further progress is currently being made in the efforts for reliable identification and accurate quantification of lipids. The challenges are certainly bigger for the metabolome as a whole, due to chemical diversity, but lessons could already be learned from the studies of molecular lipids.

What improvements, technological or otherwise, have helped metabolomics grow over time?

While analytical technologies used to characterize the metabolome have fundamentally not changed over the past decades, we still rely mainly on MS and NMR, technologies in which considerable advances have been made. Better sensitivity, resolution, mass accuracy, speed of data acquisition, better separation (new chromatographic columns), emergence of ion mobility MS and MS imaging, ability to identify position of double bonds (e.g., in lipids, which is set to be applicable in lipidomics), have all advanced metabolomics by enabling more accurate detection (identification, quantification) of metabolites. My impression is that we still have not come to terms with all that the analytical advances over the past years have brought to us. We are likely to see more and more applications of metabolomics in the future by utilizing innovative approaches, even in clinical settings.

Additionally, on the bioinformatics side, emergence of molecular networking, availability of large-scale metabolite and spectral databases, and improvements of open source metabolomics data processing tools, have all enabled us to extract meaningful data from metabolomics studies and improved our ability to compare data across different studies, a persistent challenge common to most 'omics' fields.

How does the future look in terms of funding for metabolomics?

In Nordic countries and Europe in general, much of the funding for projects involving metabolomics is allocated for applied projects, focusing on specific questions, where metabolomics may or may not play a central role. While this is in line with a general trend of using more integrative approaches in the life and medical sciences, it does make it more challenging to acquire funding for much needed methodological advances in the field.

Recent Publications

Recently published papers in metabolomics

Workshop report: Toward the development of a human whole stool reference material for metabolomic and metagenomic gut microbiome measurements

Metabolomics Profiling of Critically Ill Coronavirus Disease 2019 Patients: Identification of Diagnostic and Prognostic Biomarkers

Gut Microenvironment and Bacterial Invasion in Paediatric Inflammatory Bowel Diseases

Personalization of Aspirin Therapy Ex Vivo in Patients with Atherosclerosis Using Light Transmission Aggregometry

Lyophilized fecal short-chain fatty acid and electrolyte determination by capillary electrophoresis with indirect UV detection for assessment of pediatric inflammatory bowel disease

Maternal Diet and the Serum Metabolome in Pregnancy: Robust Dietary Biomarkers Generalizable to a Multiethnic Birth Cohort

Chemically informed analyses of metabolomics mass spectrometry data with Qemistree

A novel metabolic function of Myc in regulation of fatty acid synthesis in prostate cancer

Deep phenotyping of myalgic encephalomyelitis/chronic fatigue syndrome in Japanese population

The maturity in fetal pigs using a multi-fluid metabolomic approach

Perspective: A potential role for NUS in metabolite-based in vitro diagnostics

Urinary metabolic signatures reflect cardiovascular risk in the young, middle-aged, and elderly populations

Metabolomics Events

14 Sep - 4 Dec 2020

Metabolomics: Understanding Metabolism in the 21st Century

Venue
Online

Overview
Metabolomics is an emerging field that aims to measure the complement of metabolites (the metabolome) in living organisms. The metabolome represents the downstream effect of an organism's genome and its interaction with the environment. Metabolomics has a wide application area across the medical and biological sciences. The course provides an introduction to metabolomics, describes the tools and techniques we use to study the metabolome and explains why we want to study it. By the end of the course you will understand how metabolomics can revolutionise our understanding of metabolism.

Course Link
https://www.birmingham.ac.uk/facilities/metabolomics-training-centre/courses/2020/metabolomics-mooc.aspx

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30 Nov - 18 Dec 2020

Quality Assurance and Quality Control in Metabolomics

Venue
Online, Birmingham Metabolomics Training Centre, University of Birmingham, United Kingdom

Overview
The application of quality assurance and quality control in the metabolomics field is vital to ensure the collection of high quality data. In this course you will explore the importance of quality assurance and quality control in both untargeted and targeted metabolomics studies. We will explain the difference between quality control and quality assurance and how to apply in your studies and laboratories. You will evaluate the types of quality control samples that can be applied in metabolomics, what is the most appropriate quality control sample to use in your research, and how to apply the data in your quality assurance procedure to produce robust and reproducible data.

Metabolomics Events

Topics Covered

- What are quality assurance and quality control and how do they differ
- What is the importance of quality assurance in metabolomics
- The types of quality assurance and quality control in untargeted and targeted metabolomics
- The importance of quality control samples
- The types of quality control samples applied in untargeted and targeted metabolomics
- Preparation of quality control samples in untargeted and targeted metabolomics
- Analytical studies including untargeted and targeted metabolomics
- Processing data in untargeted and targeted metabolomics
- Recommended quality assurance procedures in untargeted and targeted metabolomics
- Reporting quality assurance procedures in untargeted and targeted metabolomics

Course Link

https://www.birmingham.ac.uk/facilities/metabolomics-training-centre/courses/2020/Quality-Control-and-Quality-Assurance-in-Metabolomics.aspx

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15 & 17 Dec 2020

Biowaivers and Bioequivalence Studies

Venue

Webinar Training Session

Overview

The objective of this training is to familiarize R&D directors, responsible for galenic or clinical development, the people from regulatory affairs to the concepts of bioequivalence for a generic.

Webinar Link

http://metabolomicssociety.org/images/events/Flyer%202020-Biowaivers.pdf

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12 & 14 Jan 2021

Targeted Therapies and Companion Diagnostic Tests - From Development to "Market Access"

Venue

Webinar Training Session

Overview

- Understand the definitions and regulatory framework governing these products. Impact of new European DM regulations and DMDIV
- How to proceed with the analytical validation
- How to demonstrate clinical validity and prove clinical utility
- What development strategy to adopt

And much more.

Webinar Link

http://metabolomicssociety.org/images/events/Flyer%202021Test-Diagnostiques-Compagnons.pdf

Metabolomics Events

1-4 Feb 2021

5th HBP Student Conference on Interdisciplinary Brain Research

Venue
Virtual

Registration will open from September 2020 free of charge.

Call for Submissions
We invite original high-quality submissions describing innovative research in all disciplines addressed in the HBP. These contributions can emphasize theoretical or empirical works relating to a wide spectrum of fields including but not limited to: neuroscience, computer science, robotics, medicine, psychology, cognitive science or philosophy. We particularly encourage submissions with a potential to inspire collaboration in the research community by introducing new and relevant problems, concepts, and ideas, even if the work is at an early stage of development.

Registration deadline: 14 January 2021.
View announcement here.
Further information on abstract submission and the conference.
For any further questions, please contact education@humanbrainproject.eu.

Postponed Until 2021

The Third Annual Canadian Metabolomics Conference

Venue
Edmonton, Alberta, Canada

Overview
The Third Annual Canadian Metabolomics Conference has been postponed until 2021. The conference will highlight work by leading researchers, including new technologies and approaches for metabolomics research, and applications in various fields. The conference will feature networking opportunities and a poster session designed for trainees to present their work. Our goal is to highlight the exceptional metabolomics science that is being done in Canada and abroad, and foster Canada's leadership role in the global research community.

We look forward to seeing you in 2021!

Conference link
https://www.canmetcon.ca/

Metabolomics Events

6-7 April 2021

Targeting CNS Tumor Metabolism Symposium

Venue
NIH Campus, Bethesda, Maryland

Overview
This is the first conference that focuses on the tumor metabolism and it is expected to be a didactic and collegial learning environment. Metabolic investigations for these tumors have been conducted in isolation and the goal of this meeting is to bring together the clinicians with the experts in metabolism to increase the utilization of metabolic investigations in the clinical settings. This will, in turn, enhance partnerships and advance the treatment for patients.

In addition to oral and poster presentations selected from the submitted abstracts, the conference will feature invited lectures from an internationally recognized faculty, including keynote talks from Craig Thompson, MD (President and CEO of Memorial Sloan Kettering Cancer Center) and Paul Mischel, MD (Distinguished Professor, University of California San Diego).

Abstract submission deadline is Tuesday, December 1, 2020, 11:59pm CST.

Course link
https://www.soc-neuro-onc.org/SNO/2020METAB/Home.aspx

15-16 Apr 2021

Data Analysis for Metabolomics

Venue
Wageningen Campus, The Netherlands

Overview
Event postponed from June 4-5, 2020 to now April 15-16, 2021

Metabolomics experiments based on mass spectrometry (MS) or nuclear magnetic resonance (NMR) produce large and complex data sets. This course will introduce approaches to process and analyze data and design high-quality experiments. Through hands-on workshops and lectures highlighting the different concepts you will get a thorough basis for tackling the challenges in metabolomics data analysis.

Course link
https://www.wur.nl/en/Education-Programmes/Wageningen-Academy/Plant/Course-Data-analysis-for-Metabolomics.htm

Metabolomics Jobs

If you have a job you would like posted, please email Ian Forsythe (metabolomics.innovation@gmail.com).

Jobs Offered

Job Title	Employer	Location	Posted	Closes	Source
Various Positions			26-Oct-20		Metabolomics Association of North America Jobs
Postdoctoral Scholarship - Metabolomics in Diabetes Research	Lund University	Lund, Sweden	24-Nov-20	Until Filled	Lund University
FAPESP Postdoctoral Scholarship - Research on the Relationship between Postprandial Metabolism and Inflammation	The Food Research Center, University of São Paulo	São Paulo SP, Brazil	6-Nov-20	10-Dec-20	FAPESP
Post Doc Metabolomics - Advanced Mass Spectrometry Analysis and Data Evaluation	Boehringer Ingelheim Pharma GmbH & Co.	Biberach, Germany	4-Nov-20	Until Filled	Boehringer Ingelheim
Postdoctoral Fellow – Biosensors Device Development	University of Alberta	Edmonton, Canada	23-Oct-20	Until Filled	Wishart Research Group
Postdoctoral Position in Nuclear Magnetic Resonance (NMR) Spectroscopy	University of Alberta	Edmonton, Canada	23-Oct-20	Until Filled	Wishart Research Group
Laboratory Assistant/ Technician – Biosensors Device Development	University of Alberta	Edmonton, Canada	23-Oct-20	Until Filled	Wishart Research Group
Senior Bioinformatician/ Cheminformatician Position	University of Alberta	Edmonton, Canada	23-Oct-20	Until Filled	Wishart Research Group
Junior Scientist in Metabolomics	Fundación MEDINA	Granada, Spain	15-Jul-20	Until Filled	MEDINA
Postdoctoral scholar	University of California San Francisco (UCSF)	San Francisco, CA, USA	24-June-20	31-Dec-20 or Until Filled	Metabolomics Society Jobs
Postdoctoral Fellowship in MALDI Imaging Mass Spectrometry	U.S. Food and Drug Administration	Jefferson, AR, USA	6-May-20	Until Filled	Metabolomics Society Jobs
Postdoctoral Associate	Yale School of Public Health	New Haven, CT, USA	5-Feb-20	Until Filled	Metabolomics Society Jobs

Jobs Wanted

This section is intended for very highly qualified individuals (e.g., lab managers, professors, directors, executives with extensive experience) who are seeking employment in metabolomics.

We encourage these individuals to submit their position requests to Ian Forsythe (metabolomics.innovation@gmail.com). Upon review, a limited number of job submissions will be selected for publication in the Jobs Wanted section.

- Dr. Nara Consolo - Seeking a position involving the application of NMR-based metabolomics in animals/animal production; it could be a Researcher position or an Assistant Professorship