



Scottish Metabolomics Network Newsletter

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Twitter updates: [#ScotMetNet](https://twitter.com/ScotMetNet)

Upcoming Events

This year's Scottish Metabolomics Network Symposium 2022 will take place on Thurs 3rd – Fri 4th November 2022. **Location:** P&J Live Aberdeen: <https://www.pandjlive.com/>

The Rattray Lab and the Strathclyde Centre for Molecular Bioscience (SCMB)



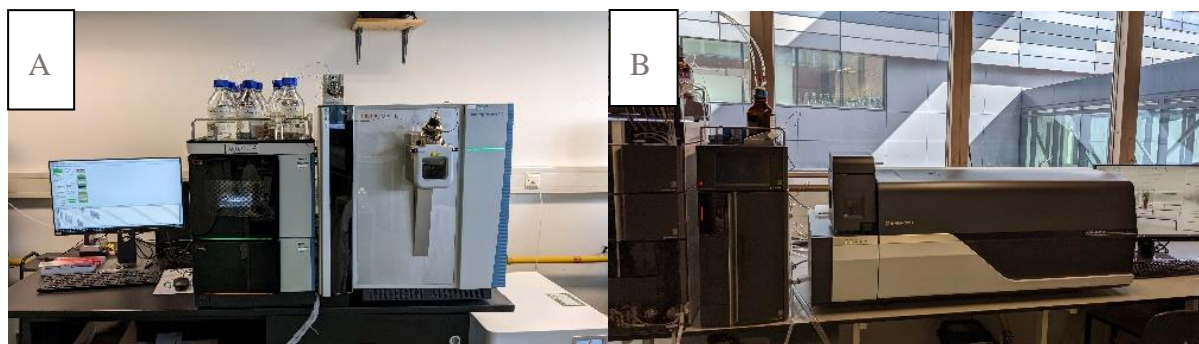
Strathclyde Centre for
**Molecular
Bioscience**

The Strathclyde Institute of Pharmacy and Biomedical Sciences (SIPBS) has always had a strong contribution to metabolomics research, with Dave Watson making a huge impact in the way high-resolution MS and HILIC-based chromatography have been used by the community. With Dave retiring, the Rattray group has looked to continue the way mass spectrometry instrument and separation technologies are implemented within metabolomics research. Working alongside colleagues within SIPBS and the Pure and Applied Chemistry department, we have formed a new collaborative and multi-disciplinary research centre that spans research groups across the Faculties of Science and Engineering – the Strathclyde Centre for Molecular Bioscience (SCMB). The centre's underlying ethos is to enhance our understanding of the molecular mechanisms of human disease to facilitate the development of new treatments in human healthcare, and metabolomics technologies sit as a core capability. A recent investment of £1.5M has seen us purchase a range of mass spectrometry instrumentation that will allow us

the centre to act as a point of convergence for a huge range of biomolecular analyses – with metabolites being a primary focus.

Installed in summer 2021, the main untargeted metabolomics instrument is a Thermo Exploris 240 set up with pos/neg switching C₁₈ and HILIC methodologies alongside the AquireX functionality (the system being akin to a next-generation Q-Exactive). It benefits from automatic exclusion list generation that allows deep-scanning identification of QC samples. The system also has an internal in-house library of over 600 metabolites embedded into each analysis as an inclusion list. Supporting this system, the centre also benefits from Shimadzu 8060-NX and 8050 instruments used for targeted LC-MS work with a focus on primary metabolism and toxicology workflows – with a Shimadzu G-CMS TQ-8050 being installed in July 2022. These instruments are also run alongside one of Dave’s old Exactive systems that still have life in the sogevac-pump yet!

The SCMB is supported by three full-time technical leads constantly developing new and bespoke methodologies that help accommodate the most diverse chemical needs. We are open to collaboration and fee-for-service analyses. Feel free to email any enquires to scmb@strath.ac.uk or check our website www.scmb.strath.ac.uk



A| The SCMB’s new Thermo Exploris 240 with Vanquish LC System that the SCMB uses for untargeted metabolomics alongside shotgun proteomics. B| A new Shimadzu 8060-NX with Nexeria LC-30 System that the SCMB uses for targeted metabolomics and toxicology assay design.

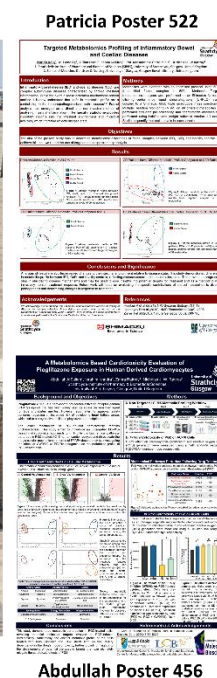
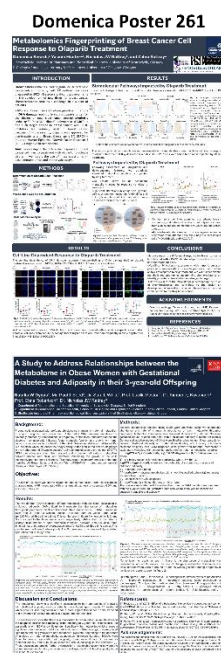
The Metabolomics Society Conference 2022



In July, the Metabolomics society 2022 meeting took place in Valencia Spain. Several groups from within the network were in attendance including representatives from the Burgess group (University of Edinburgh) and the Rattray group (University of Strathclyde), as well as Will (JHI). Standout presentations included the plenary lectures of Prof. Ron Heeren (Maastricht University, NL) on the advancements of MS imaging at greater speeds and resolutions than could be imagined five years earlier, and of Prof. Asaph Aharoni (Weizmann Institute, IL) on

the development of MS/MS and MSⁿ libraries for over 10,000 plant and microbial secondary metabolites, as well as MS imaging approaches in plant physiological studies.

Four PhD students from the Rattray group attended the Metabolomics Society Annual conference in Valencia. Domenica presented work on metabolomics used to understand metabolic rewiring in breast cancer upon drug treatment. Abdullah's poster described a metabolomics approach used to investigate off-target effects in pioglitazone treatment. Tricia's poster focused on developing new methodologies to analyse biological samples from Crohn's and colitis patients. Natalia presented work that described the implementation of general additive models in pediatric research. PI Nik gave a talk on the issues of translating biological models of the ageing metabolome into clinically relevant biomarkers.



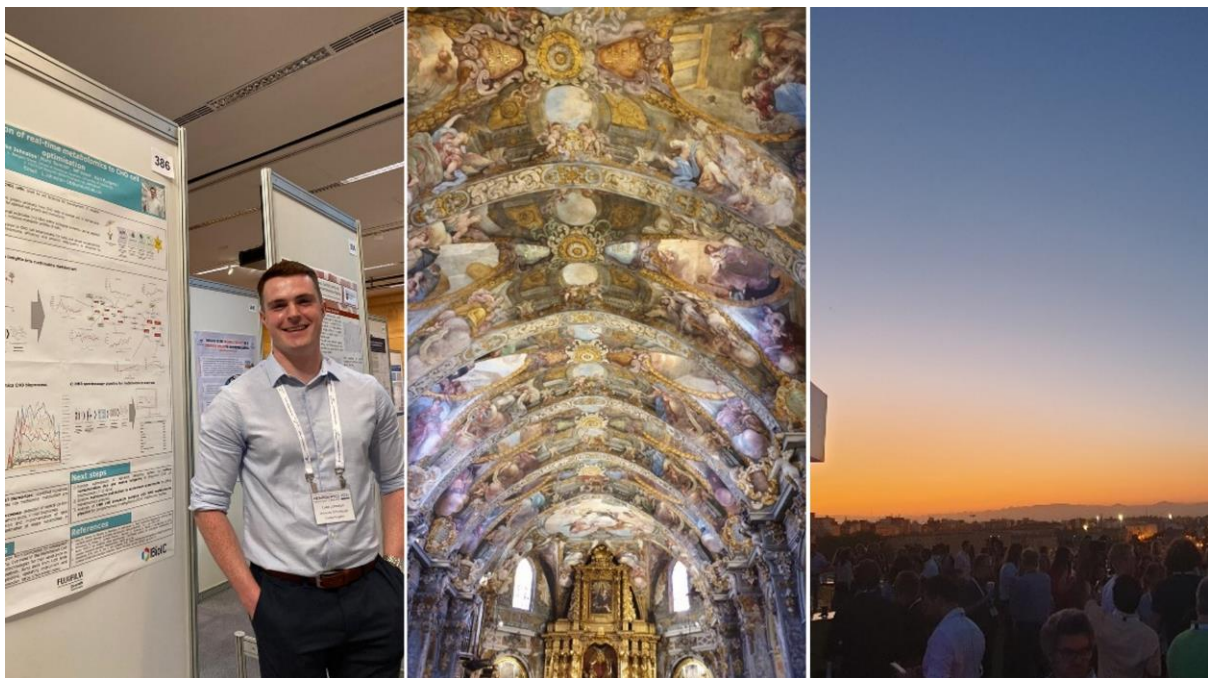
Picture from METSOC 2022 Valencia, Spain. Left to right; Domenica Berardi (3rd Year PhD student), Natalia Dygas (3rd Year PhD student), Patricia Kelly (1st Year PhD student), Abdullah Al Sultan (2nd Year PhD student)

Karl and Luke Johnston from the University of Edinburgh also attended, with Karl presenting on Mass Difference Networks at a workshop titled 'Hitchhikers' Guide to Networks in Metabolomics' which focused upon graphical and network interpretation of large metabolomics datasets. Luke presented a poster on his work applying real-time metabolomics bioprocess monitoring and untargeted, rapid ion mobility mass spectrometry to drive improved monoclonal antibody yield in Chinese hamster ovary cell bioprocesses.



Karl at the Metabolic Networking workshop. Many thanks to Elva-Maria Novoa del Toro for the photo and fantastic organisation of the workshop itself.

Karl was also excited to attend the Metabolomics Quality Assurance and Quality Control Consortium (MQACC) dinner, which was a great opportunity to meet the team (many of whom had previously just been voices over Zoom!) and discuss best practises for untargeted metabolomics.



Luke presenting his poster at the conference (left). The beautiful view inside Iglesia de San Nicolás de Bari y San Pedro Mártir de València, Valencia's very own "Sistine Chapel" (middle). Sunset over the conference dinner, hosted at Veles e Vents, Valencia (right).



Will from The James Hutton Institute presented his work upon nitrogen supplementation in oat grains which illustrated that whilst higher levels of nitrogen enhance yields, protein and beta-glucans, it negatively impacts the avenanthramides and a number of health beneficial secondary metabolites.

Will also attended the international affiliates meeting where he discussed the current activities of the SMN and how these activities can be linked with the wider networks, especially in the areas of training links and laboratory visits to representatives within the European affiliates such as the FRMF (France), NMC (Netherlands), SSMET (Spain), SMS (Switzerland), and others.

Will enjoying some downtime with Prof's Young Choi (Leiden University, middle) and Serge Rudaz (Geneva University and chair of the Swiss Metabolomics Society, left), as well as post conference relaxation in the shade of the botanic gardens of Valencia University.

The Nutrition Group, from the Institute of Aquaculture, University of Stirling

In June, the Nutrition group from the Institute of Aquaculture, University of Stirling, attended the International Symposium on Fish Nutrition and Feeding in Sorrento, Italy. Several group members gave both poster and oral presentations, with the role of lipids a key theme within the group's work.

A key development was the use of lipidomics to study the parity of oils derived from GM sources, with a poster illustrating whether isomeric alterations exist within the fish fed these novel diets and whether any lipid-wide alterations were detected within different fish tissues. This may potentially lead to alterations in inflammation, owing to the roles of lipids as inflammatory mediators. This forms a core part of both Dr Richard Broughton and Dr Monica Betancor's work within the fish nutrition field. The work was picked up by International Aquafeed magazine and will be published later this year, with a paper to follow shortly.



Picture from the International Symposium on Fish Nutrition and Feeding 2022 in Sorrento, Italy. Left to right; Stuart McMillan, Monica Betancor, Karla Fernandez Quiroz, Daniel Gonzalez Silvera.

The TALENT Commission Parliamentary Reception

Natalie Homer (Mass Spectrometry Core, University of Edinburgh) attended the TALENT Commission Parliamentary Reception. Natalie said, “On the evening of 24th May 2022, I was lucky enough to be invited to the TALENT Commission Parliamentary Reception hosted by the Research England-funded TALENT programme at the House of Lords. The TALENT Commission is the outcome of 20 months of in-depth research, stakeholder engagement and evidence gathering within the sector on technical skills, roles and careers. The Commission has generated new strategic insights into the UK’s technical community in higher education and research and sets out a vision for the future of the UK's technical talent. It makes 16 overarching recommendations to guide the delivery of this vision and a series of targeted recommendations for specific stakeholder groups, including employers, government policymakers, funders and professional bodies.

I was pleased to be able to represent the University of Edinburgh both as a core facility manager and as the Chair of the University of Edinburgh Technician Steering Committee and also to have a chance to talk to colleagues across the country. With the 16 recommendations, I am hopeful that the TALENT Commission report will make a real difference to technicians and those choosing a technical career.”



Cassandra Hodgkinson, University of Manchester (left) and Natalie Homer, University of Edinburgh (right) at the Cholmondeley Terrace of the Houses of Parliament. .

Clinical Trials Laboratory Services (CTLS) Online Congress - contribution of SMN members



Core
TECHNOLOGIES FOR
LIFE
SCIENCES

Core Technologies for Life Sciences ([CTLS](#)) is a European networking non-profit association that brings scientists together, technical and administrative staff working across the world in core facilities, research infrastructures and other shared resource laboratories. For the CTLS online congress from 13th-15th September 2021, Natalie

Homer (University of Edinburgh) co-chaired a session with Gabriel Martins. The session focussed on “*Methodological and technological development in core facilities*”, and in it, Phil Whitfield gave a presentation entitled “*Opportunities and Challenges in a Metabolomics and Lipidomics Facility*” where Phil gave a great run-down of the convergent approach to lipidomic analysis. Later in the week, Tessa Moses (from Edinomics, University of Edinburgh) and Natalie held a community workshop titled ‘The Importance of scientific

publications from core facilities’, which 23 people attended and where we conducted a poll and discussion-based workshop to highlight resources, guidelines and initiatives to recognise core facility contribution in publications. We would like to reach other audiences and have plans to build upon what we learnt from the workshop.



Congratulations!

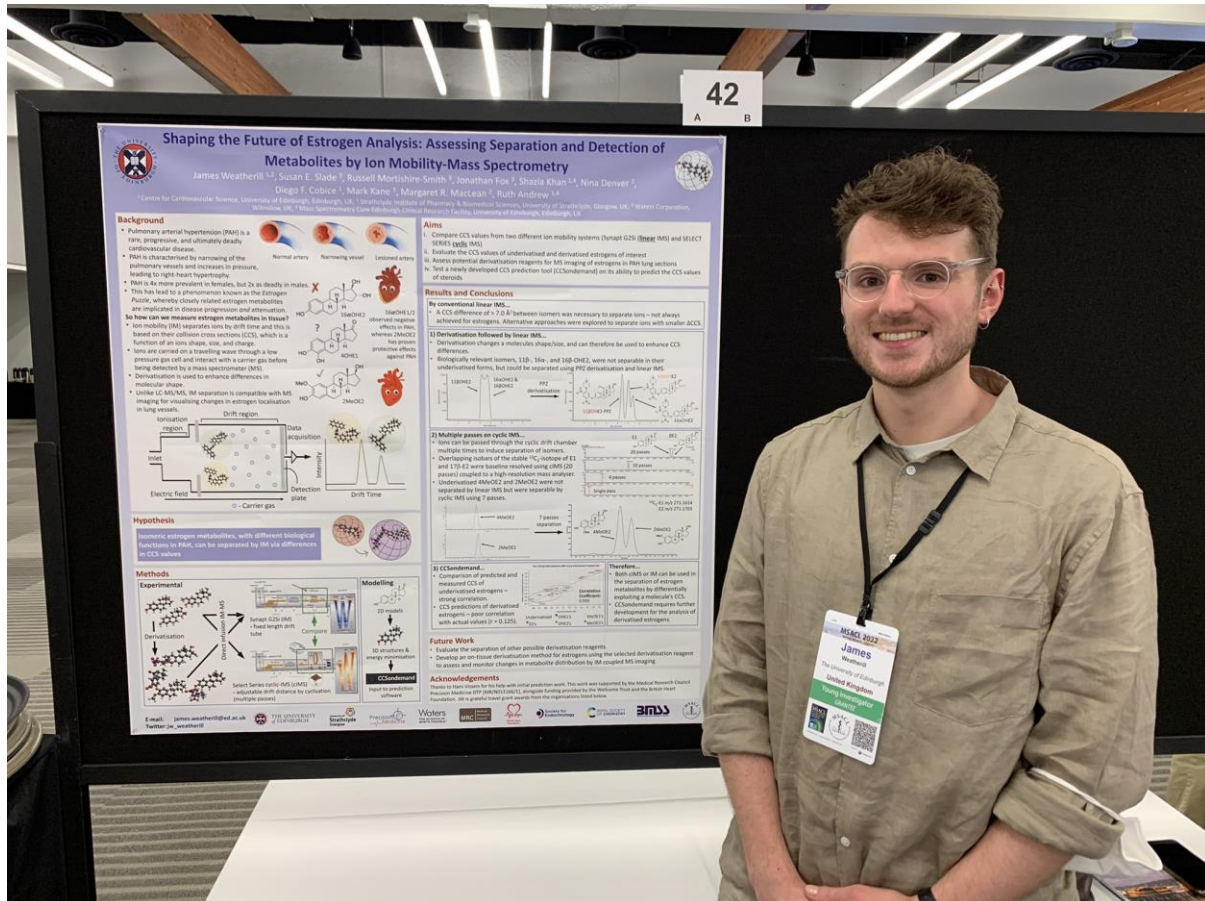
Congratulations to **James Weatherill** (University of Edinburgh), who won runner-up in the poster prize competition at the Mass Spectrometry & Advances in the Clinical Lab (MSACL) conference in Monterey, California, held on April 5th – 8th, 2022 - his first international face-to-face meeting! James's poster title was '*Shaping the Future of Estrogen Analysis: Assessing Separation and Detection of Metabolites by Ion Mobility-Mass Spectrometry*', and the authors included;

James Weatherill, Susan E. Slade, Russell Mortishire-Smith, Jonathan Fox, Shazia Khan, Nina Denver, Diego F. Cobice, Mark Kane, Margaret R. MacLean, Ruth Andrew.

The research was done in collaboration with Strathclyde University and Waters Corporation.

James said, “The MSACL conference 2022 was the first international conference that I have had the opportunity to attend during the course of my PhD. Set in the picturesque backdrop of Monterey, California; the conference had a packed, week-long programme full of interesting workshops, panel discussions, poster presentations, and plenary sessions, covering topics from

the development and applications of novel MS technologies in understanding the underlying mechanism of disease to how we can implement MS into clinical diagnosis. The conference organisers champion early-career development, so I was given the opportunity to co-chair the MS imaging session. Alongside this, I presented a poster on my work comparing ion mobility-MS approaches for the analysis of small molecules, for which I won second place in the poster competition! Having the chance to discuss (in-person) my research with such a diverse group of scientists and clinicians was an overwhelmingly positive experience.”



James Weatherill, at the MSACL conference 2022

Funding Success!

BBSRC BARIToNE - Barley Industrial Training Network

Project - Defining the genetic basis of barley metabolite content to improve nutrient use efficiency, crop quality and resilience with reduced inputs. PhD student George Epaku commencing September 2022

Publications

Congratulations to all members of the SMN community who recently published their research!

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Glasgow Polyomics Courses

Glasgow Polyomics are running two courses that may be of interest to the SMN community. Firstly, the Introduction to ‘Omics course aims to give attendees an understanding of the different ‘Omics, experimental design, data analysis and statistics. Secondly, the Metabolomics Data Analysis course aims to give you a grounding in LC-MS metabolomics data analysis, using the Polyomics integrated Metabolomics Pipeline (PiMP) and Metaboanalyst. This course is aimed at people who already have an understanding of the instrumentation used to generate LCMS data and wish to deepen their understanding of the data analysis.



College of Medical, Veterinary & Life Sciences

An Introduction to Omics

An online course over five half-days aimed at familiarising participants with the basis and application of various omics disciplines:

- Genomics
- Transcriptomics
- Proteomics
- Metabolomics
- Lipidomics
- Bioinformatics

By the end of the course users should understand, for each omics level: the basis of the discipline, the instrumentation used to generate high-throughput biological data, key applications, and how to visualise the resulting data using commonly used software packages.


College of Medical, Veterinary & Life Sciences

Metabolomics Data Analysis Workshop

An online course over two days where participants will learn the practical aspects of conducting a metabolomics experiment, from adopting the best study design to performing the processing, analysis and interpretation of the resulting data including statistical analysis using Metaboanalyst and biochemical analysis using KEGG.

This course is aimed at staff and students who wish to deepen their practical understanding of metabolomics experiment design and data processing.

By the end of the course, you should be comfortable processing metabolomics raw data and can begin to work on your own data sets.




SMN Equality, Diversity and Inclusivity

We are a network of people from a wide variety of backgrounds, and this makes us stronger. We value being equal champions of diversity and inclusion for everyone. Our overall purpose is to provide a channel of communication within the network and provide a forum for EDI representatives to share information and consider good EDI practices and issues.

If you would like to join the EDI group and make a difference or need support, you can confidentially contact us at sntshang@ed.ac.uk or Will.Allwood@hutton.ac.uk.

Industry news

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Current Opportunities

PhD project: Developing the new paradigm of 'meta-plant pathogens' by studying the compositional and metabolomic dynamics of a Meta-Fusarium sp. exposed to abiotic and biotic perturbations.

Host Institute: INRAE, UR 1264 MycSA (Mycology and Food Safety), Bordeaux
<https://www6.bordeauxaquitaine.inrae.fr/mycsa/>

Supervision: Florence FORGET (florence.forget@inrae.fr)

Co-supervision: Jean-Michel SAVOIE (jean-michel.savoie@inrae.fr)

Context and objectives of the PhD project:

Fusarium spp. are causal agents of Fusarium head blight (FHB), one of the most devastating fungal diseases affecting cereal crops. In addition to yield losses, some of these fungal species are responsible for grain contamination with mycotoxins that are a major health and food safety concern. Over 20 Fusarium species have been associated with FHB. The species *Fusarium graminearum*, *Fusarium culmorum*, *Fusarium avenaceum*, *Fusarium tricinctum*, *Fusarium poae*, *Fusarium sporotrichioides*, and *Fusarium langsethiae* are reported as the most common species encountered in Europe. All these Fusarium species can produce one or more mycotoxins including type A and type B trichothecenes, zearalenone, enniatins and beauvericin.

Despite intensive research over the past decades, recommended agronomic practices and current mitigation strategies are not enough to guarantee mycotoxin levels complying with European regulatory limits. Up to now, investigations aiming at providing bases for the development of mycotoxin control strategies were virtually exclusively conducted considering "one pathogen-one disease", an approach that has proved itself insufficient to reach a comprehensive understanding of the FHB disease process and mycotoxin accumulation in crops. Indeed, the blend of Fusarium species in interaction inside a shared niche is likely to result in a production of mycotoxins having its own regulation that cannot be predicted by knowing what happens in single species cultures. Taking a meta-view at Fusarium and breaking habits with the development of the innovative concept of a meta-pathogen would be a disruptive innovation in order to progress in fighting contaminations of cereals by mycotoxins.

In this context, the aim of the present PhD project is to investigate the regulation of the production of mycotoxins by what we call a Meta-Fusarium sp. The latter - comprising the seven major Fusarium species involved in FHB - will be considered in ecophysiology analyses as an individual fungus that operates as a whole. To achieve its goal, the project will be set around two main objectives:

- To characterize fungal development kinetics and evolution of secondary metabolite production profiles of Meta-Fusarium sp. under varying environmental conditions.

- To demonstrate the added value of the Meta-Fusarium sp. approach for the identification of new eco-friendly control strategies to fight against mycotoxin accumulation in cereals.

Skills expected to be acquired throughout this PhD project: The project is based on a multidisciplinary approach combining fungal microbiology, fungal DNA quantification (Taqman QPCR), metabolomics (LC et UPLC/DAD, LC/HRMS) and tests on plant organs.

Required competencies: Knowledge in fungal biology. Skills in biochemical analytical techniques, in basic molecular biology and biostatistics.

Funding: This PhD project is funded within the TEAMTOX ANR project (2022-2026). The scheduled start date is the 01/12/2022.

How to apply: You can apply until **22 August 2022**. Send your application to Dr Florence Forget (florence.forget@inrae.fr) and Dr Jean-Michel Savoie (jean-michel.savoie@inrae.fr) consisting your CV, a cover letter and a recommendation letter from the person who supervised your BSc and/or Master thesis.

Informal enquiries about the position are welcome by email to florence.forget@inrae.fr.

Associated Doctoral school: « Sciences de la Vie et de la Sante » – Bordeaux University <https://ed-svs.u-bordeaux.fr/>

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