Australia's National
Science Agency

Program booklet

CSIRO Cutting-edge Symposium on

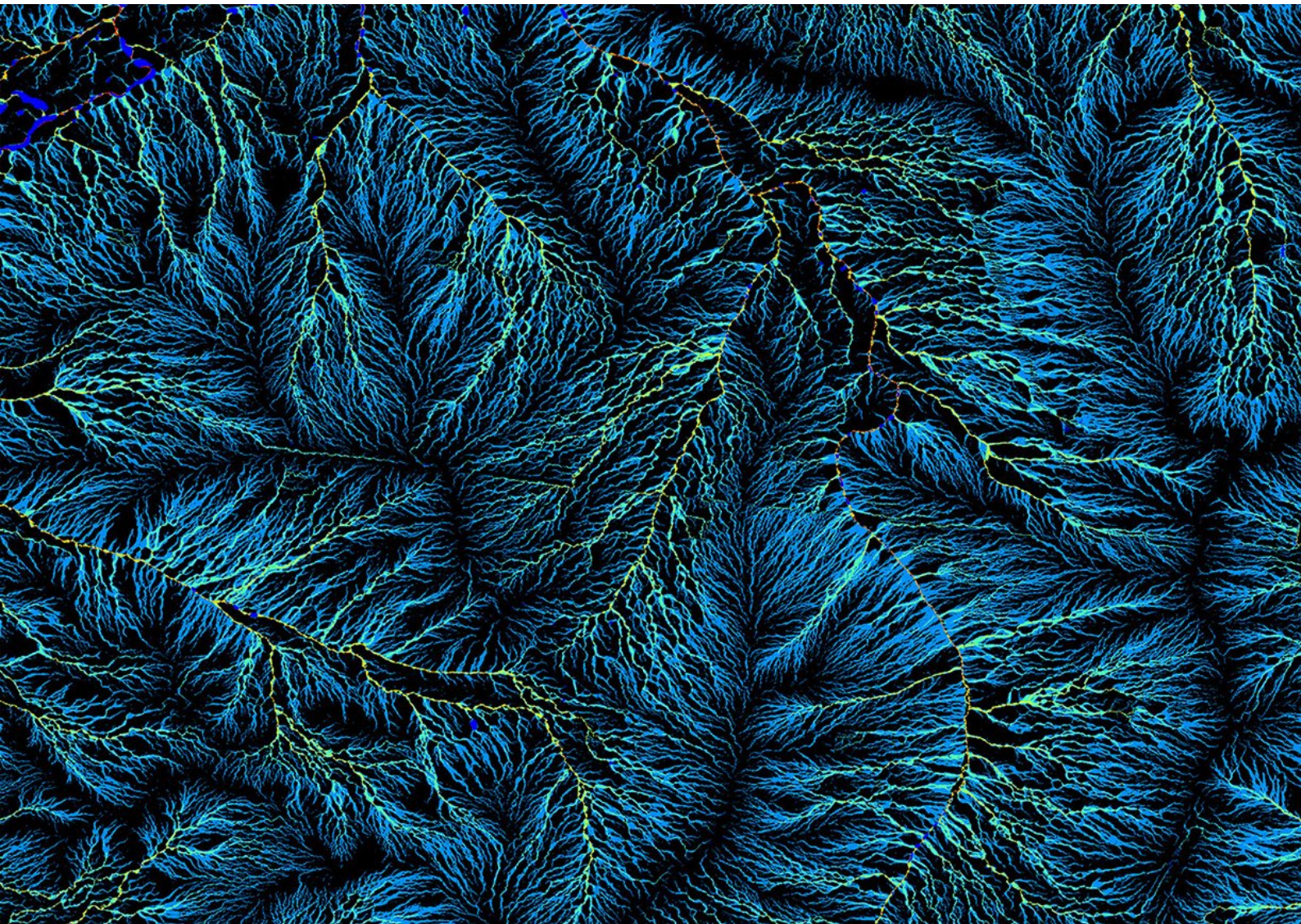
Integrated Systems Biology

Current Perspectives and Future Challenges

Wednesday 18th – Friday 20th of May 2022

Symposium venue: Brisbane Convention & Exhibition Centre, South Bank 4101, QLD

Workshop venue: Ecosciences Precinct, Dutton Park 4102, QLD.



Contents

Acknowledgments

The Integrated Systems Biology Symposium organising committee would like to acknowledge and thank the time provided by all keynote and invited speakers, and the financial support of the symposium sponsors:

Major Sponsors:

- Agilent Technologies
- Illumina
- Beckman-Coulter Life Sciences

Sessional Sponsors:

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Lastly, the organising committee would also like to acknowledge and thank the financial support provided by the CSIRO Research Office for awarding a 'Cutting-edge Symposium' grant.

Sponsors

Major Sponsors

Agilent

Agilent is a leader in life sciences, diagnostics and applied chemical markets. The company provides laboratories worldwide with instruments, services, consumables, applications and expertise, enabling customers to gain the insights they seek. Agilent's expertise and trusted collaboration give them the highest confidence in our solutions.

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Illumina is an applied genomics technology company making genomics useful for all. Our mission is to improve human health by unlocking the power of the genome. We are tirelessly working to create the leading-edge technology that enables clinicians and researchers to not only understand the genome but also fully tap its power. Now, through collaboration and innovation, we are driving genomic breakthroughs with fast, simple workflows. While the rate of progress continues to accelerate exponentially, we have only just begun to discover the true impact of genomics. What causes a cancer cell to mutate? What is the origin of a puzzling disease? Is it possible to prevent the next outbreak? Or safeguard the world's food supply?

The discoveries we know lie ahead in microbiology, agrigenomics, complex diseases, and beyond, are what inspire us to push the boundaries of our imagination, drive innovation and offer solutions across the genomic spectrum.

Advancing research and discovery is our foundation, built on an 80-year legacy of innovation. Our mission is to empower those seeking answers to life's important scientific and healthcare questions.

We are experts in:

- Centrifugation,
- Lab automation and liquid handling,
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- Genomic solutions and more.

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Session Sponsors

In Vitro Technologies Scientific Division has a long history of supporting the Australian research community reaching back to 1958 and has developed a reputation for being one of the most dynamic and successful suppliers throughout Australia and New Zealand.

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SCIEX has led the field of mass spectrometry for more than 50 years. From the launch of the first ever commercially successful triple quad in 1981, we have continued to develop ground breaking technologies and solutions for Life Science Research, Food and Beverage Testing, Environmental Testing, Forensics, Clinical Research, Pharma and BioPharma.

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PerkinElmer a leading global provider of end-to-end solutions helping scientists, researchers and clinicians better diagnose disease, discover new, more personalized drugs, monitor the safety and quality of our food, and drive environmental and applied analysis excellence. Our teams work closely with commercial, government, academic and healthcare customers to deliver reagents, assays, instruments, automation, informatics and strategic services that accelerate workflows and support improved decision making.

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Eppendorf is a leading life science manufacturer of innovative products and workflow solutions for liquid-, sample-, and cell handling. Our aim is to provide reliable services and tools to support your applications and research goals as well as being committed to proactive sustainability.

For us, that means striving for the shortest distance, the most sparing consumption of resources, the solution that produces the least waste, and the sensible reuse and recycling of materials – but also the careful use of every form of energy, whether electrical power, oil or gas. All these things are the focus of the voluntary commitments we have made to ecological and corporate sustainability.

QIAGEN is the leading global provider of Sample to Insight solutions to transform biological materials into valuable molecular insights. Our mission is to make improvements in life possible by enabling our customers to achieve outstanding success and breakthroughs in life sciences research, applied testing, pharma and molecular diagnostics.

Further information can be found at http://www.qiagen.com

We are Merck, a vibrant science and technology company.

Science is at the heart of everything we do. It drives the discoveries we make and the technologies we create.

The passion of our curious minds makes a positive difference to millions of people's lives every day.

Our Life Science experts empower scientists by developing tools and solutions that help deliver breakthroughs more quickly.

Everything we do is fuelled by a belief in science and technology as a force for good. A belief that has driven our work since 1668 and will continue to inspire us to find more joyful and sustainable ways to live.

Symposium Program

Day 1 – Wednesday 18 May 2022	
Time AEST	**Activity**
8:15 AM	Registration
8:45 AM	**Symposium opening address:** **Dr. Paul Bertsch**, Science Director, CSIRO Land & Water
9:00 AM **Machine Learning & Artificial Intelligence** Session Sponsored by **QIAGEN**	**9:00 - Prof. Jean Yang, The University of Sydney (KEYNOTE).** "Large scale single-cell multi-sample multi-condition data integration". 9:30 – **Dr. James Doecke (Virtual)**, CSIRO H&B, **"**Multi-platform analysis of genomic data for finding predictors of cancer progression: an example using TCGA data." 9:45 – **Prof. Marc Wilkins (Virtual)**, UNSW, "The cellular protein methylation network: enzymes, crosstalk, regulation, and function." 10:00 – **Ms. Manika Singh (EMCR)**, QUT, "DIA-seq: A novel, isoform-level multi-omics data analysis pipeline identifies brain-specific changes in mouse model of behaviour." 10:15 – **Dr. Ravi Kalathur**, QIAGEN (***sponsored***), "Integrated analysis of multi-omics data to identify novel players in cardiac regeneration in postnatal heart."
10:30 AM	Morning tea
11:00 AM **Environmental Sciences and Ecosystem Surveillance** Session Sponsored by **Eppendorf**	**11:00 – Dr. Elisha M Wood-Charlson, Lawrence Berkeley National Laboratory (Virtual KEYNOTE). "**Creating findable, accessible, interoperable, and reusable (FAIR) online, biological systems data platforms that support sharing and attribution beyond publications." 11:30 – **Prof. Oliver Jones**, RMIT University, "What are the metabolic effects of PFAS at environmentally relevant exposure levels?" 11:50 – **Dr. Anu Kumar**, CSIRO L&W, "Assessing ecological risk of environmental contaminants: new approaches to old challenges." 12:10 – **Dr. Erin Hahn (EMCR; Virtual)**, CSIRO NCMI, "Unlocking historical genomic data preserved in Australia's museum vaults."
12:30 PM Lunch	**Sponsor Workshop – Beckman Coulter Life Sciences.** **Mr. Brett Siddall, "Advancing Synthetic Biology and NGS Workflows: Miniaturisation and Integration".**
1:30 PM	Poster's day-1 + Lightning posters
3:00 PM	Afternoon tea
3:30 PM **Synthetic Biology** Session Sponsored by **Merck**	**3:30 – A/Prof. Esteban Marcellin, University of Queensland (KEYNOTE).** "Metabolic Engineering for Carbon Recycling." 4:00 – **Dr. Carlos Luna-Flores (EMCR)**, QUT, "Integrative metabolic analysis of high astaxanthin production in *Phaffia rhodozyma*" 4:15 – **Dr. Tim McCubbin (EMCR)**, the University of Queensland, "Discovering new metabolic potential using systems and synthetic biology." 4:30 – **Prof. Claudia Vickers**, Provectus Algae and QUT, **"**Systems and synthetic biology tools for natural product engineering in microbes."
5:00 PM	Pre-dinner free time
6:00 PM	**Conference dinner** **Agilent Keynote: A/Prof. Michelle Hill, QIMR Berghofer Medical Research Institute**, "Don't forget the fats: tools and tips for lipidomics in systems biology."

Day 2 – Thursday 19 May 2022	
Time (AEST)	**Activity**
8:15 AM	Registration
8:55 AM	**Housekeeping**
9:00 AM **Industrial Technology** Session Sponsored by **QIAGEN**	**9:00 - A/Prof. Andrew Gooley, Chief Scientific Officer, Trajan Scientific and Medical (KEYNOTE).** "Microsampling Devices for Precision Medicine - Experiences in the Translation of Research to Commercialisation." 9:30 – **Dr. Janet Reid**, CSIRO Biofoundry, "Integrated omics approach in automated synthetic biology." 9:45 – **Prof. Benjamin Schulz**, University of Queensland, "Systems biology proteomics and metabolomics to investigate beer production." 10:00 – **Dr. Martin Engel,** Inventia Life Science (***PerkinElmer Sponsored***), "Better precision medicine outcomes start at the source: an automated platform for creating phenotypical in vitro models at scale." 10:15 – **Dr. Joost Nelis (EMCR)**, CSIRO A&F, "From Smartphone to Mass spectrometer, a novel pipeline for food safety testing."
10:30 AM	Morning tea
11:00 AM **Food and Agriculture** Session Sponsored by **SCIEX**	**11:00 - Prof. Melissa Fitzgerald, University of Queensland (KEYNOTE).** "Combining metabolomics, genetics, and sensory profiling to identify compounds that affect the quality of rice." 11:30 – **Mr. Babatunde Olasege,** the University of Queensland (***MLA Sponsored***), "The tsunami of omics data will improve our phenotype predictions: can we ride it?" 11:45 – **Dr. Loan Nguyen,** the University of Queensland (***MLA Sponsored***), **"**Advances in genomic technologies for livestock production." 12:00 – **Dr. Yutao Li**, CSIRO A&F, "Using machine learning to address omics data prediction problems in livestock species: challenges and perspectives." 12:15 – **Dr. Shelby Berg (EMCR),** University of Queensland, "Microbial Crop Biostimulants for the Tropics - from Marketing to Science and Efficacy."
12:30 PM Lunch	**Sponsor Workshop – Illumina.** **Dr Anthony Beckhouse, "**More to See More to Understand - Combing Omics for Systems Biology".
1:30 PM **Food, Agriculture, and the Environment (cont.)**	1:30 – **Dr Utpal Bose (EMCR)**, CSIRO A&F, "Understanding nutritional shifts and discovering healthy barley lines through proteogenomic workflow." 1:45 – **A/Prof. Horst Schirra**, Griffith, "A front-row seat at the fashion show runway – the usefulness of model organisms in uncovering fundamental metabolism." 2:05 – **Dr. Hadi Nazem-Bokaee (EMCR)**, CSIRO NCMI, "Computational systems biology empowers knowledge on the lichen symbiosis at subcellular level." 2:20 – **Dr. Steven Melvin**, Griffith, "improving rehabilitation using metabolomics: Health, recovery, and biomarkers of mortality in sick and injured green turtles (*Chelonia mydas*)." 2:35 – **Dr. John Noel Viana (EMCR)**, ANU, "Towards an integrative and inclusive precision health future: mapping the scientific and ethical terrain."
2:50 PM	Afternoon tea (Poster Judging)
3:30 PM **Health and Precision Medicine** Session Sponsored by **In-vitro Tech.**	**3:30 - Prof. Elaine Holmes, Murdoch University (KEYNOTE). "**Developing metabolic profiling strategies for delivering personalised healthcare" 4:00 – **Dr. Maxime Francois (EMCR; Virtual)**, CSIRO H&B, "Saliva-omics as a potential tool for the molecular diagnostic of Alzheimer's disease." 4:15 – **Dr. Trung Ngo**, The University of Queensland, "Genoma.io with a VIEW: Taking the pain out of phenome- & transcriptome-wide association analytics." 4:30 – **Prof. Darren Creek, Monash University (KEYNOTE),** "Revealing drug mechanisms with multi-omics approaches."
5:30 PM	**Perkin Elmer Sponsored Cocktails & Networking** Conference close and award presentations

Symposium Venue

The Sky Room

Brisbane Convention & Exhibition Centre

Glenelg St, South Brisbane QLD 4101

When: Wednesday 18th to Thursday 19th May from 8:15 am onwards.

PUBLIC TRANSPORT

Getting to Brisbane Convention & Exhibition Centre (BCEC) via public transport is easy and efficient with bus, ferry and train options available. More information about planning your journey via public transport can be found on the 45TTransLink website.

TRAIN

South Brisbane Railway Station adjacent to the Convention Centre on Grey Street or South Bank Railway Station are the most convenient stations to the BCEC.

BUS SERVICES

The Cultural Centre Station on Melbourne Street and the South Bank Busway Station cnr of Colchester and Tribune Streets are closest to BCEC.

CITYCAT & FERRIES

The public transport ferries *CityCats* operate every day and stop at the South Bank River Terminal on the Clem Jones Promenade. The inner-city ferry travels between the CBD, North Quay and Kangaroo Point, stopping at South Bank Terminal 1 and 2 on the Clem Jones Promenade.

Venue Access

Directions to the Sky Room, Sky Level, Grey Street. The Brisbane Convention and Exhibition Centre Car Parks are accessible via Merivale Street and Grey Street. The closest Car Parks to the Sky Level are Car Park 2 and Car Park 3.

Directions to the Sky Level include:

1. Once parked please make your way towards Russell Walk.
2. Please make your way towards Grey Street via Russell Walk (towards the river).
3. Once on Grey Street please turn right and you will see the entrance to BCEC on Grey Street.
4. Once inside BCEC on Grey you will see two elevators next to the Information Desk. Please make your way to the elevator and press “S” for the Sky Level
5. The Sky Room is directly in front as you exit the lift.
6. For more information on visiting the BCEC please refer to the link https://www.bcec.com.au/visit/

Covid Information:

Only fully vaccinated persons or those with an approved medical contraindication (exemption), are currently permitted entry to the Brisbane Convention & Exhibition Centre (BCEC). Masks must be worn at all times unless when eating and drinking. Please refer to the link to view the most up to date restrictions. https://www.bcec.com.au/attending-covid-safe-events/

Workshop Program

Day 3 – Friday 20 May 2022		
Time (AEST)	**Activity**	
9:30 AM	Registration / Tea and Coffee	
10:00 AM	Workshop Introduction	
10:05 AM	**Top-Down (Gene to Metabolite) (Room 1)**	**Bottom-Up (Metabolite to Gene) (Room 2)**
	Illumina Sponsored **Chair(s):** Andrew Bissett & Amy Paten **KEYNOTE:** Dr Andrew Bissett, CSIRO Oceans & Atmosphere; and, Toni Reverter-Gomez, CSIRO Agriculture & Food. Breakout discussion	**Agilent Technologies Sponsored** **Chair(s):** David Beale & Maciej Holowko **KEYNOTE:** Professor Oliver Jones, RMIT University. Breakout discussion
12:30 PM	Lunch	
1:30 PM	**Technological Solutions (Room 1)**	**Community of Practice (Room 2)**
	Beckman Coulter Sponsored **Chair(s):** James Broadbent & Maciej Holowko **KEYNOTE: Dr** Maciej Holowko, SynBio Stack Developer, Synthetic Biology Future Science Platform. Breakout discussion	**Chair(s):** David Beale, Sharon Hook & Amy Paten **KEYNOTE:** Dr Sharon Hook, CSIRO Genomics CCC lead, CSIRO Oceans & Atmosphere. Breakout discussion
3:30 PM	Debrief and next steps	
3:45 PM	Workshop close	

Workshop Venue

When: Friday 20th May from 9:30 am to 3:45 pm

Ecosciences Precinct

41 Boggo Road, Dutton Park QLD 4102

PUBLIC TRANSPORT

Getting to Ecosciences Precinct via public transport is easy and efficient with bus and train options available. More information about planning your journey via public transport can be found on the TransLink website.

TRAIN and Bus Services

Park Road Railway and Busway is the most convenient station to the Ecosciences Precinct. They can be accessed easily from within the greater Brisbane Public Transport network.

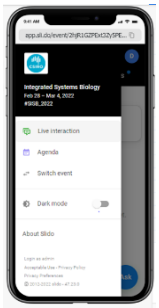
Covid Information:

Only fully vaccinated persons or those with an approved medical contraindication (exemption), are currently permitted entry to the Ecosciences Precinct. Masks must be worn at all times unless when eating and drinking.

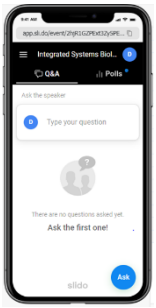
Hybrid Interactive Attendee Portal

Please Access the symposium's interactive portal at **slido.com** with **#SISB2022** (from the 16th of March onwards) by scanning this QR code below.

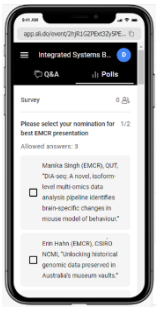
Use **Slido** to ask a question to each presenter, cast your vote for the best EMCR presentation/poster, or simply keep pace with the agenda!



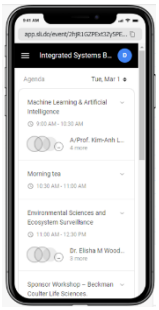
Symposium interactive portal home page.



Ask a question to each presenter.



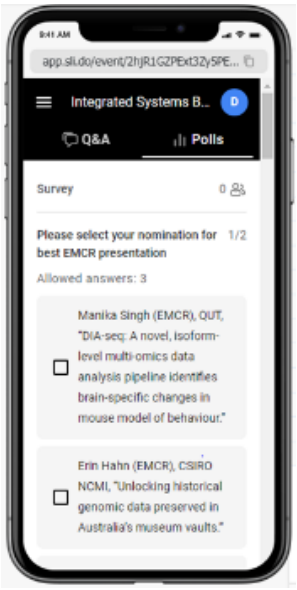
Vote for the best EMCR presentation & poster.



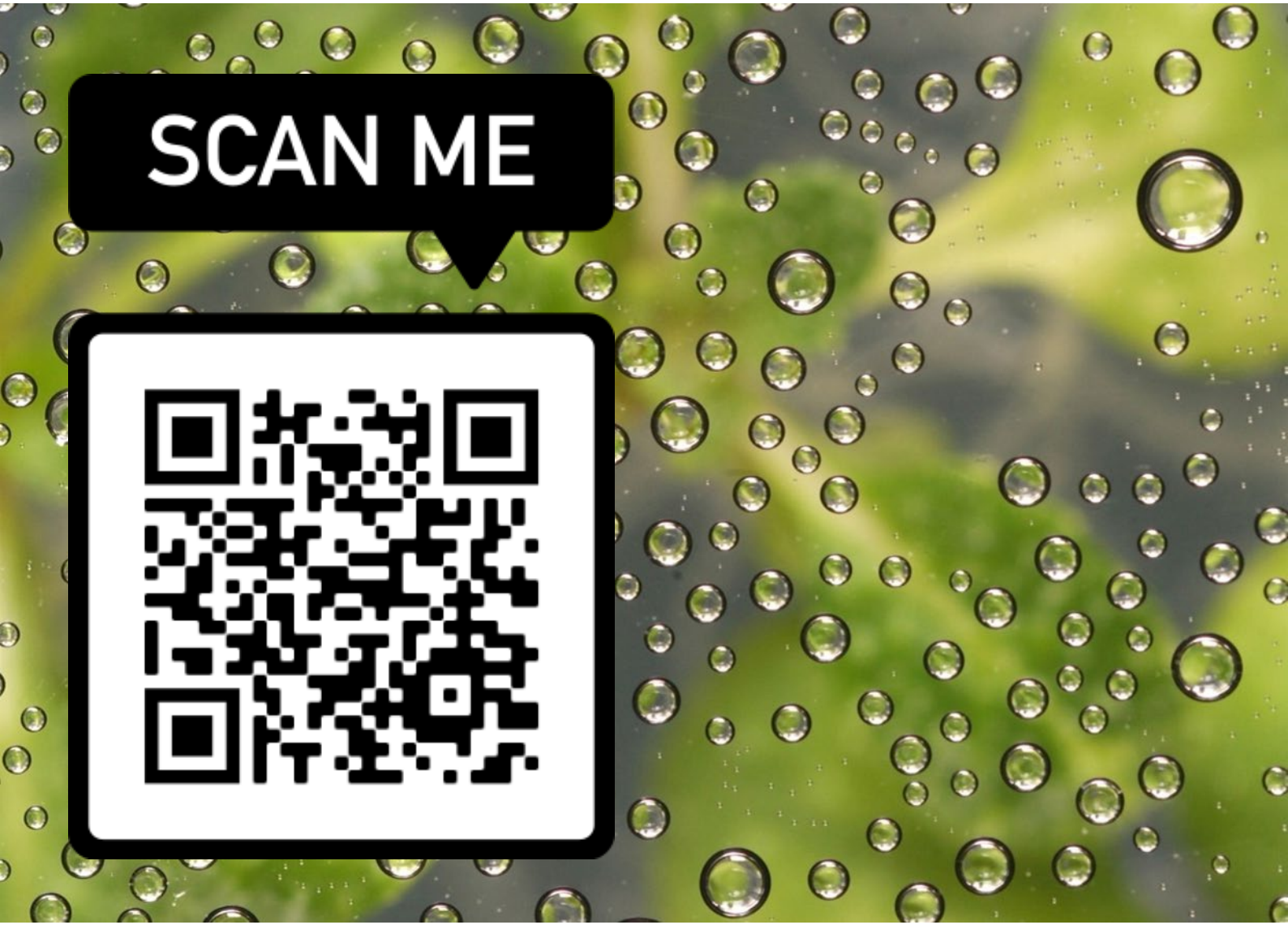
Keep pace with the daily agenda.

How to view the online poster gallery

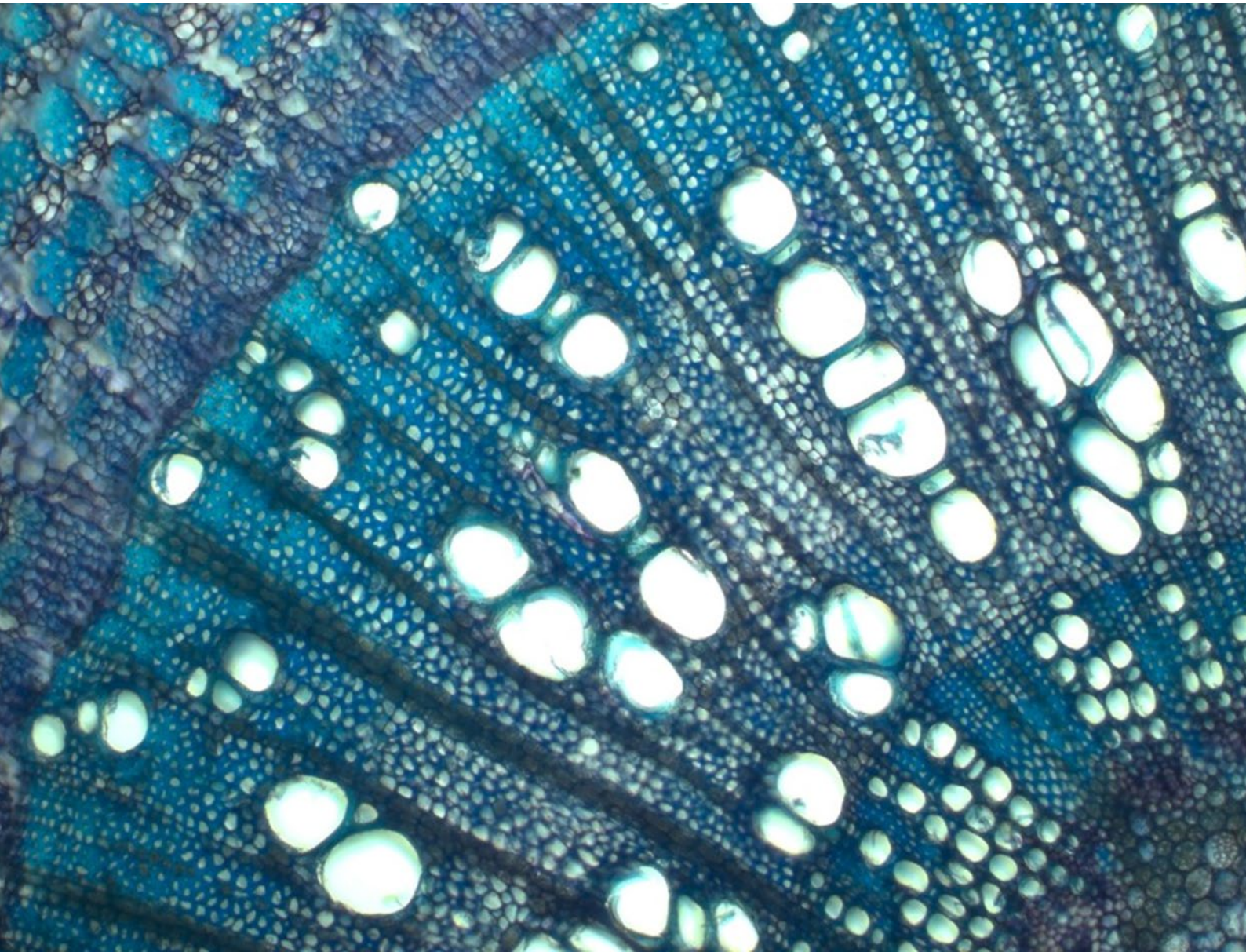
Access the symposium's online poster gallery by scanning this QR code or via your desktop at https://wp.csiro.au/sisb/posters/. Then cast your vote for the best EMCR poster (and presentation) before Thursday 19th of May at 4:30 pm (AEST) via the hybrid interactive attendee portal at slido.com with #SISB2022.



Vote for the best EMCR presentation & poster.



Part I Sponsor Workshops



1 Beckman-Coulter workshop

Title: Advancing Synthetic Biology and NGS Workflows -Miniaturisation and Integration

Speaker: Brett Siddall, Research Automation.

When: Wednesday 18th May (from 12:30pm)

Abstract: Synthetic biology and next gen sequencing workflows are characterised by high complexity, high costs and long turnaround times. In addition, some of the most-requested testing capabilities include flow cytometry, fluorescence-activated cell sorting and high-throughput micro-bioreactors. With a focus on our unique acoustic liquid dispensing technology, we present novel solutions for streamlining typical bottlenecks (for example, pooling/assembly, library creation, characterisation of synthetic promotors and cell line development), with the potential to provide walk away sample processing at a fraction of the time and cost currently experienced.

Biography: Brett Siddall is the ANZ Product Manager, Research Automation at Beckman Coulter Life Sciences, having joined Beckman Coulter in 2008. He has extensive experience in liquid handling automation sales and support since 1991.

2 Agilent Technologies Dinner Keynote

Title: Don’t forget the fats: tools and tips for lipidomics in systems biology

Speaker: Associate Professor Michelle Hill, QIMR Berghofer Medical Research Institute.

Biography: Michelle Hill obtained a PhD in biochemistry at The University of Queensland, Australia. She currently leads the Precision and Systems Biomedicine Laboratory at QIMR Berghofer Medical Research Institute, Brisbane, Australia, which aims to improve health outcomes by harnessing the power of omics and computational systems biology. Michelle has been leading her team in innovative use of mass spectrometry-based omics technologies, including the development of novel biomarker pipelines and subcellular profiling methods. Application of these methods has enabled discovery of blood biomarkers for early detection of oesophageal adenocarcinoma, and discovery of novel lipid-mediated mechanisms for extracellular vesicle cargo loading.

3 Illumina workshop

Title: More to See More to Understand | Combing Omics for Systems Biology

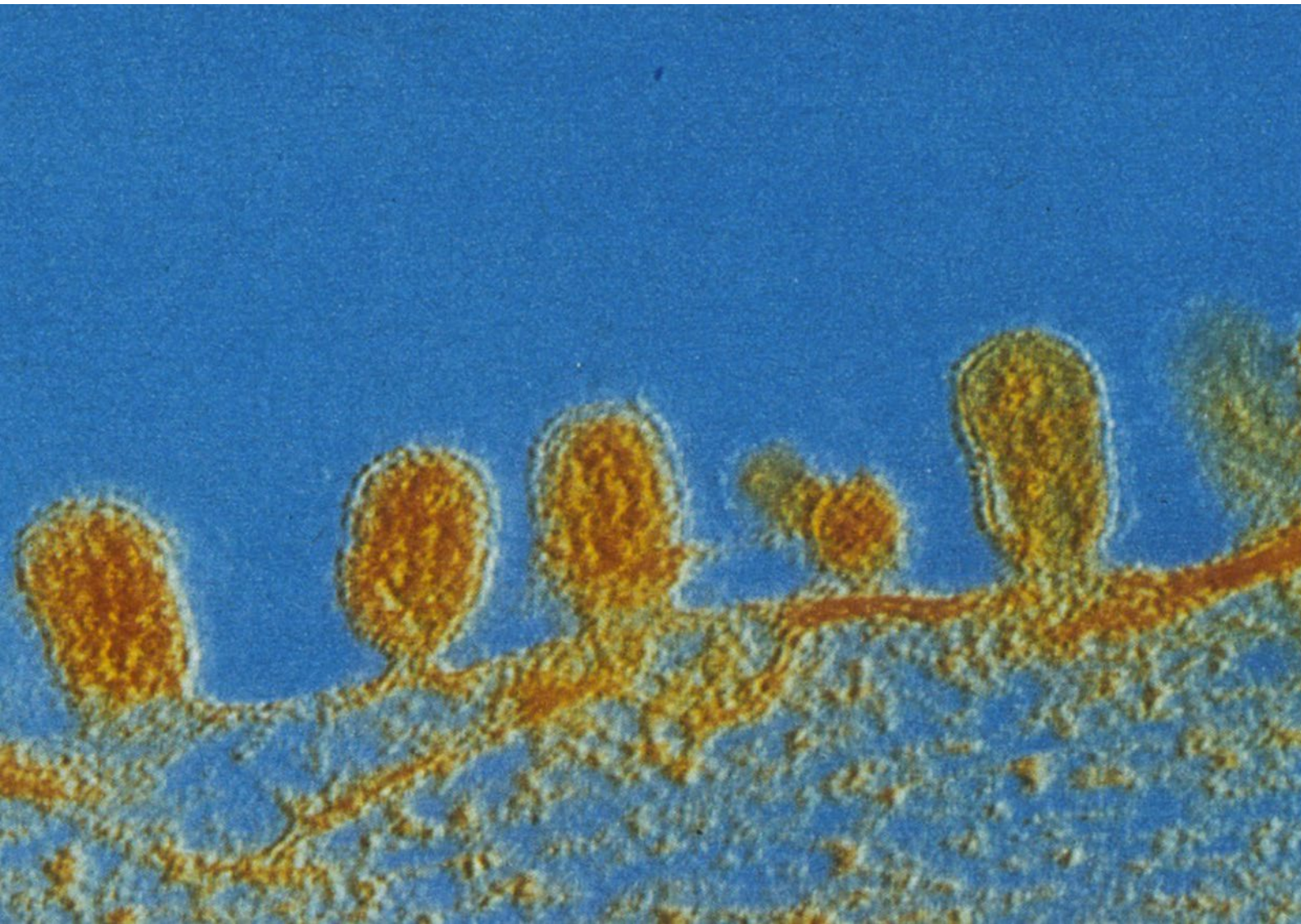
Speaker: Dr Anthony Beckhouse, Illumina (APJ)

When: Thursday 19th May (from 12:30pm)

Abstract: Systems biology provides an integrated perspective to power discovery across multiple levels of biology. Illumina NGS technology enables omics approaches across multiple modalities including genomics, transcriptomics, epigenetics, and proteomics. When combing this data together, it is now possible to measure and understand changes in genetic variation, gene expression, regulation, protein expression and the interactions of these various modalities.

Biography: After a successful seven-year academic research career, Anthony transferred his gene expression, microarray, molecular biology and library preparation skillset to biotech industries. He has now spent many years in three biotech companies supporting customers in the field to ensure they got the best quality data and analyses from their instruments. Now in Product Marketing at Illumina, he manages a large portfolio of Sequencing instruments and core consumables to keep users and internal stake holders across Asia Pacific up to date and aware of the current and future technologies. .

Part II Keynote Presentations



4 Professor Jean Yang, The University of Sydney

Title: Large scale single-cell multi-sample multi-condition data integration

Biography: Professor Jean Yang a Professor of Statistics and Data Science at the University of Sydney. She is also the Theme Leader of Integrative system and modelling at Charles Perkins Center. Her research stands at the interface between applied statistics and biology with focuses on the application of statistics to high dimensional problems in biomedical research. She was awarded the 2015 Moran Medal in statistics from the Australian Academy of Science in recognition of her work on developing methods for molecular data arising in cutting edge biomedical research. As a biomedical data scientist, she enjoys research in a collaborative environment, working closely with clinical scientific investigators from diverse backgrounds.

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5 Dr. Elisha M. Wood-Charlson, Lawrence Berkeley National Laboratory

Title: Creating findable, accessible, interoperable, and reusable (FAIR) online, biological systems data platforms that support sharing and attribution beyond publications.

Biography: Elisha M Wood-Charlson is part of the scientific community engagement teams for the US Department of Energy's Systems Biology Knowledgebase (KBase, kbase.us) and the National Microbiome Data Collaborative (NMDC, microbiomedata.org). She has a PhD and 10+ years of experience as a microbial ecologist focused on host-microbe-virus interactions in the marine environment, including a postdoctoral fellowship at the Australian Institute of Marine Science (AIMS). Since leaving the research bench, her career has focused on making data science around biological systems, microbiome data in particular, more efficient by facilitating effective collaborations, building trust in online communities, and developing shared ownership of the scientific process.

6 Associate Professor Esteban Marcellin, The University of Queensland

Title: Systems Metabolic Engineering of For Carbon Recycling.

Biography: Esteban Marcellin obtained his Chemical Engineering degree in 2004 at the Universidad Ibero (Mexico) with a specialization in biotechnology. He then worked for a polymer company in Mexico before moving to Australia for his PhD in Bioengineering in 2010 at The University of Queensland. In 2010-2012 he moved to Indianapolis to establish a systems biology pipeline for Dow Agrosciences. He is now a Group Leader at The Australian Institute for Bioengineering and Nanotechnology, the UQ Node Leader for the ARC Centre of Excellence in Synthetic Biology and co-node Leader of QMAP and the new NCRIS Synbio facility to be established at UQ this year. The Marcellin group uses systems and synthetic biology to develop microbial and mammalian cell factories to produce biopharmaceuticals, flavours, fragrances, foods and fuels.

7 Associate Professor Andrew Gooley, Trajan Scientific and Medical

Title: Microsampling Devices for Precision Medicine - Experiences in the Translation of Research to Commercialisation

Biography: Andrew is the Chief Scientific Officer for Trajan Scientific & Medical – a global business with their headquarters in Melbourne. Over the past 40 years, Andrew has experienced a career in both academia and industry. His passion is mentoring the next generation of scientists and engineers and introducing them to the opportunities that industry can provide and the diversity of careers that are possible – from R&D, Production, Project Management, Quality and Marketing. In his commercial role, he has led multi-disciplinary teams of engineers and scientists on a diversity of projects from “OMICS” development through to consumables for chromatography for the global analytical science community. He has also held an appointment as University of Melbourne Enterprise Professor in Chemistry from 2018-2021.

8 Professor Melissa Fitzgerald, The University of Queensland

Title: Combining metabolomics, genetics and sensory profiling to identify compounds that affect the quality of rice.

Biography: Melissa Fitzgerald obtained her PhD in 1998. She has changed her career every 7 years, and each career step includes rice research. She led research in rice quality at NSW Agriculture, then at the International Rice Research Institute at IRRI. Now at UQ, rice research is a key part of her work, and she has published widely on rice quality. She came to UQ in 2012, and established a metabolomics facility. She is also the Deputy Associate Dean for Research Partnerships in the Faculty of Science, and in this position, she creates opportunities for academics to engage with industry.

9 Professor Elaine Holmes, Murdoch University

Title: Developing metabolic profiling strategies for delivering personalised healthcare.

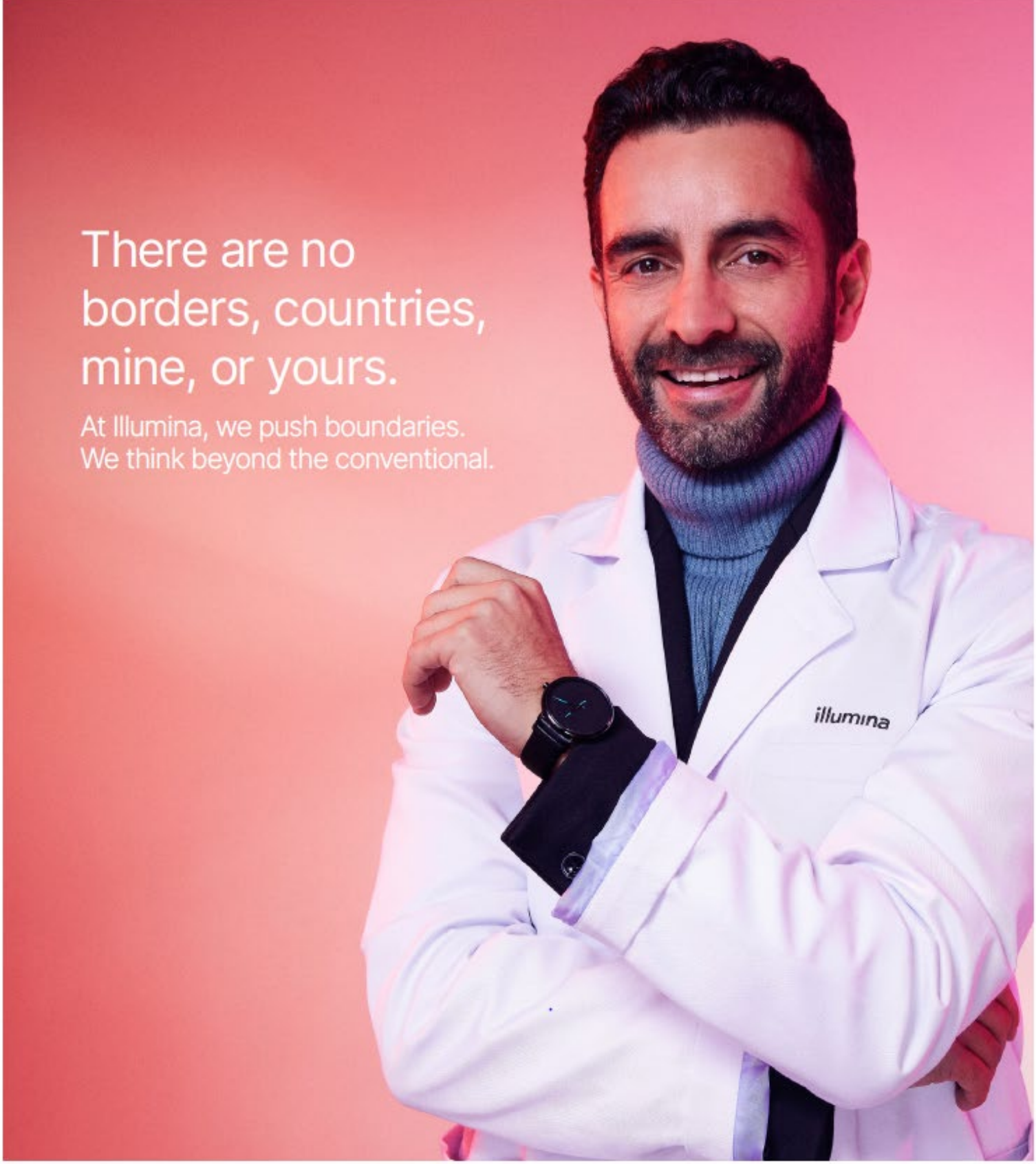
Biography: Professor Elaine Holmes is a distinguished computational biologist and a Clarivate Highly Cited Scholar. She was awarded the prestigious Australian Laureate Fellowship from the Australia Research Council (ARC) in 2020.

Elaine's main research area focuses on applying metabolic profiling and computational modelling of biofluids and tissues to understand pathological and physiological processes. She has applied the technology in several clinical and biomedical areas including Cardiovascular Disease, Diabetes, Infection, Gastrointestinal Disease, Early life environment and neurodegeneration. She co-developed the concept of the metabolome-wide association study (MWAS) and is driving new methods for the integration of metabonomic data with proteomic and transcriptomic data to gain a holistic overview of disease process. Her current work focuses on understanding the role of the gut microbiome in health and disease.

10 Professor Darren Creek, Monash University

Title: Revealing drug mechanisms with multi-omics approaches.

Biography: Associate Professor Darren Creek is coordinator of the Global Health Therapeutic Program Area at the Monash Institute of Pharmaceutical Sciences, and Director of the Parkville node of the Monash Proteomics and Metabolomics Facility. He has over 100 publications demonstrating applications of 'omics' approaches with a focus on the pharmacology and pathogenesis of infectious diseases.



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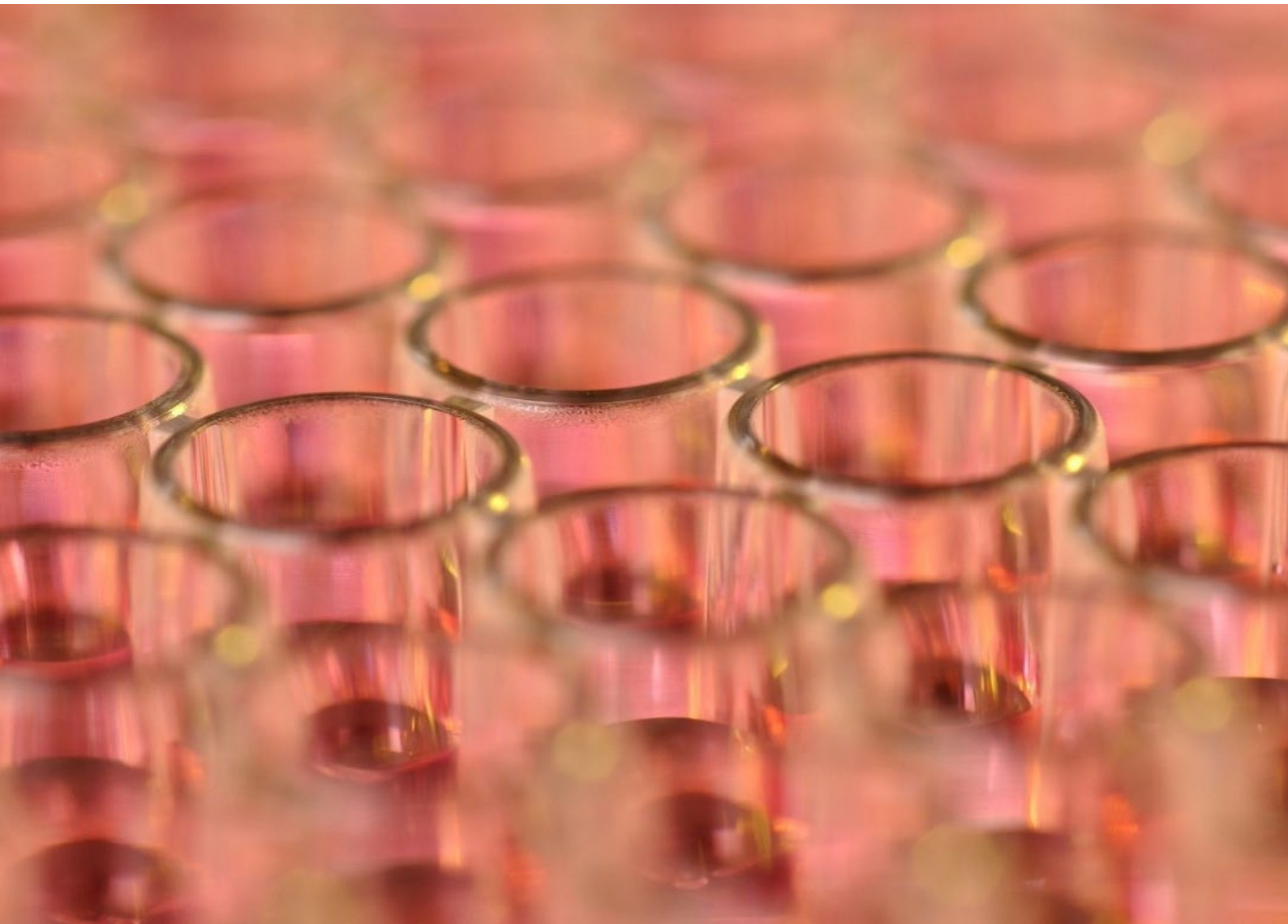
Part III Podium Presentation Abstracts



11 Machine Learning & Artificial Intelligence

Session Sponsored by: Qiagen

Keynote: Associate Professor Kim-Anh Lê Cao, The University of Melbourne

Invited Speaker: Professor Marc Wilkins, UNSW

Sponsor Speaker: Dr. Ravi Kalathur, QIAGEN

Multi-platform analysis of genomic data for finding predictors of cancer progression: an example using TCGA data

Correspondence: james.doecke@csiro.au; Tel.: (07) 3253 3697

Session Theme: *Machine learning & Artificial Intelligence.*

Doecke J.D.[1], Chekouo T.[2], Li S.[1], Do K.A.[2]

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2. Department of Biostatistics, MD Anderson Cancer Center, Houston, Texas, USA.

Analyses of large-scale genomic data sets for the identification of biomarkers predictive of cancer progression has been limited to the combination of one or two platforms simultaneously. Combining data from three or more platforms has the inherent disability of reduced sample size due to an under-representation of samples with complete data across all platforms. In the current project, we address this issue, assessing both individual and combinations of platforms to find biomarkers to predict cancer progression. Using three different classical statistical methods (Random Survival Forest, Generalised Boosted Models and LASSO) we compare top biomarker lists, and predictive capability for each biomarker set. From seven possible models, the combination of gene expression with DNA methylation information provided the highest predictive accuracy, with a C-Index of 0.75. As expected, the C-Index rose and associated error decreased with increasing sample size. Generalised Boosted Models provided the most stable and highest results compared with RF and the LASSO. Taking the intersection of markers identified via assessing genes alone, compared with analysing genes with miRNA, or genes with methylation probes, we find only a small number of genes associated with survival time, suggesting a strong association of these genes in relation to survival time, accounting for variation due to both miRNA and DNA methylation patterns. Relaxing the stringency mildly within the feature selection tuning parameters increased the number of markers found in both individual models and combinatorial models, allowing for the creation of molecular networks. Such networks are useful when comparing biomarker levels between late stage and early-stage cancer groups.

Keywords: Feature selection, prediction, modelling.

The cellular protein methylation network: enzymes, crosstalk, regulation and function

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Session Theme: *Machine learning & Artificial Intelligence.*

Abstract: Protein methylation is a widespread protein post-translational modification in the eukaryotic cell. Functionally its role is best-characterised in histone proteins, ribosomal proteins and proteins involved in RNA splicing and transport. Yet it is also found on proteins involved in other processes. Given the predominance of the modification, and its association with highly conserved processes, we asked whether methylation and its associated enzymes could be characterised and investigated as a complete system, to give insights into cellular networks and regulatory processes. Proteomics was used to discover all methylation sites on yeast proteins, creating nodes in a network, following which systematic gene knockouts were used to discover cognate protein methyltransferases. These created further network nodes and also all edges (links). The resulting network, containing 28 methyltransferases that act on 41 amino acids on 30 protein substrates is of note as it is one of the few eukaryotic networks that is likely complete. We investigated the regulation of methylation-associated processes, through examining the phosphorylation of methyltransferases and also the crosstalk between methylation and phosphorylation. This has allowed us to connect the methylation network, in part, to the cell's signalling system. The significance of our findings for synthetic biology and cellular models will be discussed.

Keywords: proteomics, post-translational modifications, network, methylation, phosphorylation, protein-protein interactions, yeast

DIA-seq: A novel, isoform-level multi-omics data analysis pipeline identifies brain-specific changes in mouse model of behaviour

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2. Data61, CSIRO, Dutton Park, QLD
3. CSIRO Agriculture and Food, St Lucia, QLD
4. School of Biomedical Sciences, Queensland University of Technology, Kelvin Grove, QLD
5. The University of Melbourne, Parkville, VIC.

Session Theme: *Machine learning & Artificial Intelligence.*

Abstract: Traditionally, proteomics research has relied on publicly accessible sequence databases for mining peptide fragmentation patterns and derive biological information. The limitation of this approach is that databases are only as good as genome annotation, and this can be incomplete, erroneous or not available for non-model organisms. Here we introduce a reference genome-independent proteomics pipeline termed DIA-seq that leverages the advancements of long-read RNA sequencing (Iso-Seq) and deep learning neural network tools for isoform-specific peptide spectra prediction and SWATH-based quantification. When applied to a known mouse model of behaviour, the pipeline allowed detection of 791 novel peptides. These corresponded to 19 exon-extension, 2 exon-skipping, 252 frameshift mutations, 2 splice junction variation, and the rest were mapped to 3', 5'-end and pseudogenes. Significant portion of novel peptides were next verified using RNA-seq and DDA datasets. Pathway analysis confirmed association of differentially abundant isoforms with known behavioural phenotype. We show that DIA-seq improves the annotation of a well-characterised model organism and suggest that it has the potential to fast-track discoveries in non-model organisms.

Keywords: SWATH-MS, Iso-seq, Mouse-model, Brain, Behaviour

Integrated analysis of multi-omics data to identify novel players in cardiac regeneration in postnatal heart

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Session Theme: *Health and Precision Medicine or Machine learning & Artificial Intelligence.*

Abstract: Post-natal heart loses its regeneration capacity and molecular mechanisms governing postnatal heart maturation is not fully understood. We performed integrated analysis of publicly available multi-omics data (RNA-seq, Proteomics and metabolomics data) from neonatal mouse heart to identify novel genes in cardiac regeneration using Ingenuity pathway analysis and omicsoft land explorer. Using analysis match we identified coactivator associated arginine methyltransferase 1 (CARM1) as a major player in cell cycle progression in post-natal heart and its expression is highly correlated with important genes involved in myocardial function or structure such as COX5B, FTX, LMNA and TUG1. The integrated analysis of multi-omics data identified molecular changes associated with the loss of cardiac regeneration and also key genes that may open up novel opportunities for the advancement of cardiac regenerative therapies.

Keywords: Cardiac regeneration; Multi-Omics data; OmicSoft

12 Environmental Sciences & Ecosystem Surveillance

Session Sponsored by: Eppendorf South Pacific

Keynote: Dr. Elisha M Wood-Charlson, Lawrence Berkeley National Laboratory

Invited Speaker: Professor Oliver Jones, RMIT University

What are the metabolic effects of PFAS at environmentally relevant exposure levels?

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Session Theme: *Environmental Sciences & Ecosystem Surveillance*

Abstract: Poly and per-fluoroalkyl substances (PFAS) are currently of high concern to environmental regulators and the public due to their widespread occurrence, resistance to degradation and reported toxicity. However, little data exists on the effects of exposure to PFAS at environmentally relevant concentrations. The development of molecular markers for PFAS exposure would be useful to better understand the environmental risks of these compounds. In this study we assessed if such markers could be developed using metabolomics. We exposed the freshwater amphipod, *Austrochiltonia subtenuis* to a range of environmentally relevant concentrations of Perfluoro-octane sulfonic acid (PFOS), Hexafluoropropylene oxide dimer acid (GenX) and Perfluorohexanesulphonic acid (PFHxS). A metabolic response was detected following PFAS exposure in all concentrations and treatments even though survival rates between treatments and controls did not differ significantly except at the highest exposure levels. All three PFAS was found to induce changes in levels of various amino acids, fatty acids and cholesterol in line with what has previously been reported. Interestingly only PFOS was found to bioaccumulate. PFHxS and GenX were quickly eliminated from the amphipods but still induced metabolic changes. This information improves our understanding of the sub-lethal effects of PFAS as well as their environmental fate and behaviour.

Keywords: Bioconcentration; Environment; Metabolomics; Monitoring; Regulation; Toxicology

Assessing ecological risk of environmental contaminants: new approaches to old challenges

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Session Theme: *Environmental Sciences & Ecosystem Surveillance,*

Abstract: Chemicals of emerging concern (CECs) are increasingly being detected at low levels in aquatic and terrestrial environments and their presence in the environment may cause undesirable effects on ecosystem and human health resulting from long-term exposures, specifically chronic toxicity, neurotoxicity and endocrine disruption. Conventional analytical approaches and/or traditional toxicity tests may not be appropriate to detecting very potent chemicals that impact specific pathways, and often are present as components of complex mixtures. A holistic risk-based approach incorporating reliable emerging technologies are required for management and mitigation of CECs and to protect wildlife and human health. To allow policy makers and regulators to carefully balance economic priorities with the need to protect vital ecosystems, equally novel, robust, reliable and coordinated scientific approaches to hazard and risk assessment are needed. The adverse outcome pathway (AOP) framework is a systematic, transparent approach used to organise existing toxicological knowledge and translate mechanistic information to adverse effects at higher levels of organisation based on causal relationships between endpoints. Strategies for developing AOPs are still evolving and depend largely on the intended use or motivation for development and data availability. We will present Australian case studies to demonstrate the application of New Approach Methodologies (NAMs) that can support current risk assessment approaches by providing more informed protection thresholds based on mechanistic understanding.

Keywords: Traditional toxicity**;** Adverse Outcome Pathway; *in-vitro*; mechanistic toxicity; case studies

Unlocking historical genomic data preserved in Australia's museum vaults

Erin E. Hahn[1,*], Marina R. Alexander[1], Alicia Grealy[1], Jiri Stiller [2], Donald M. Gardiner[2] and Clare E. Holleley[1]

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Session Theme: *Environmental Sciences & Ecosystem Surveillance*

Abstract: Museum collections house an unparalleled record of historical genomic data reflecting shifts in species distribution and adaptation trends in response to rapid environmental change over the last 150 years. While genomic analysis of frozen and dry-preserved specimens has been widely adopted, sequencing of formalin-preserved specimens has largely been regarded as intractable. Notably, for fish, reptiles and amphibians, formalin-fixation was the primary method used to preserve tissues throughout much of the 20th century. Thus, formalin preservation has impeded recovery of genome-wide data from a large proportion of older specimens and some of Australia's most biodiverse and environmentally sensitive vertebrate taxa. With a set of taxonomically diverse specimens collected between 1936 and 2015, we demonstrate an end-to-end approach of recovering whole-genome data from formalin-preserved museum specimens. We recovered complete mitochondrial genomes and up to 3X nuclear genome coverage from moderate sequencing effort of formalin-fixed archival tissues. With the assumption that formalin-preservation prohibits genomic sequencing dispelled, an enormous resource is now open to reconstruct historical species response to environmental change. We will present these results as well as avenues for extending this new capability to characterise historical community composition and species interactions.

Keywords: genomics; museum; temporal ecology; formaldehyde

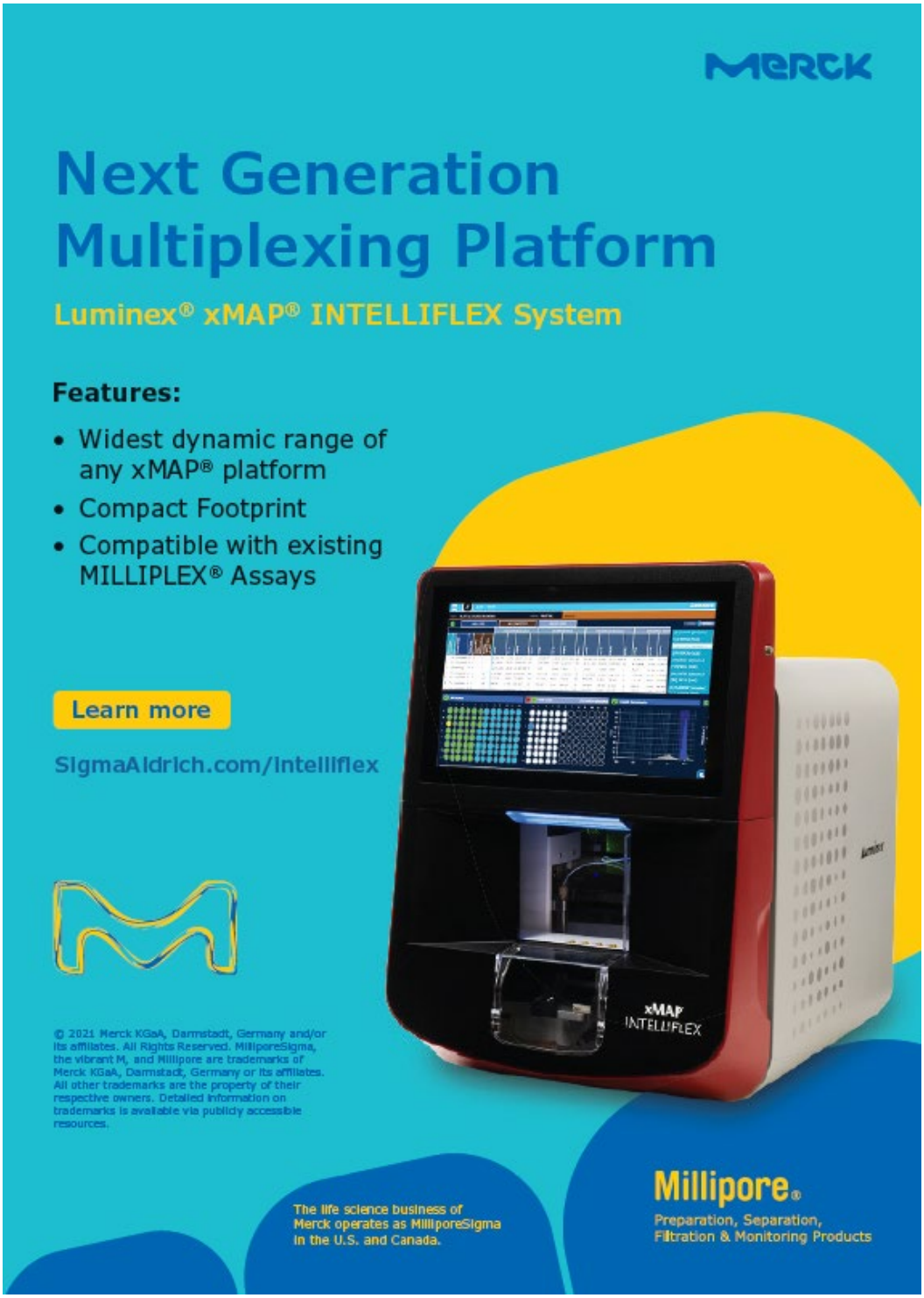
13 Synthetic Biology

Session Sponsored by: Merck

Keynote: Professor Lars Nielsen, The University of Queensland

Invited Speaker: Dr. Carlos Luna-Flores, Queensland University of Technology

Invited Speaker: Associate Professor Tim Mercer, The University of Queensland



Synthetic Biology

Design

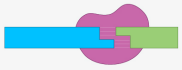
Genes of interest are identified and designed into oligonucleotides *in silico*. Plasmid backbones or fragments are selected based on downstream needs. Oligos are ordered or synthesized.

Echo 525

SPRI Genomic Reagents

EMnetik 24

Build



Plasmid fragments and oligos are pooled to construct a diverse library.

Transform plasmids into microbial cells.

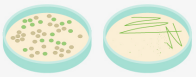
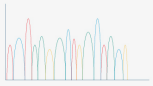


Plate and pick colonies, verifying transformation success with a selection medium.

Culture hits and extract transfection-grade plasmid for downstream use.



Validate plasmid candidates using sequencing and prepare for downstream testing.

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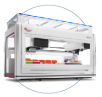

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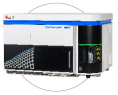

CytoFLEX SRT

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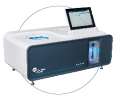
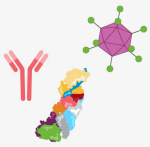


BioLector XT

Test



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Integrative metabolic analysis of high astaxanthin production in *Phaffia rhodozyma*

Carlos H. Luna-Flores[1], Alexander Wang[12], Juhani von Hellens[2], Robert Speight[1]

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Session Theme: *Industrial Technology*

Abstract: Produced mainly from unsustainable petrochemicals, astaxanthin (AX) is a potent antioxidant with commercial potential and gives salmonids their characteristics pink color. The red yeast *P. rhodozyma* naturally produces AX as its main fermentation product through carbon assimilation. The production of AX in wild-type strains does not meet the commercial metrics. To increase yields, here, we applied chemical and radiation mutagenesis and different screening methods in the wild-type *P. rhodozyma* CBS 6938. Production was maximized 50-fold in fed-batch culture. The whole genome of the wild-type and eight novel strains were sequenced and analysed finding 368 conserved mutations across the novel strains. Important mutations were found in regulators and catalysts of AX building blocks produced in the mevalonate pathway, the electron transport chain, and the electron donor of the AX synthase protein. To gain insight into metabolic changes, we grew wild-type and mutant strains in chemically defined media in instrumented fermenters and metabolomics and transcriptomic data were obtained. Metabolic data revealed an abundance of metabolites associated with the glycolysis, pentose phosphate pathway, TCA cycle, amino acid, and fatty acids metabolism. TCA cycle metabolites such as succinate, fumarate, and α-ketoglutarate were abundant across the entire fermentation course, and transcriptomics and proteomics found upregulated the electron transport chain suggesting being the main drivers for an improved AX production.

Keywords: *Phaffia rhodozyma* (also known as *Xanthophyllomyces dendrorhous*), genomics, transcriptomics, metabolomics, and proteomics.

Discovering new metabolic potential using systems and synthetic biology

Tim McCubbin [1], R. Axayacatl Gonzalez-Garcia [1], Laura Navone [1,3] , Chris Stowers [3], Lars K. Nielsen [1] and Esteban Marcellin [1]*

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Session Theme: *Synthetic Biology*

Abstract: Propionic acid is an FDA approved, generally regarded as safe (GRAS) three-carbon chemical with applications in a wide variety of industries. At present, propionate is industrially synthesized by petrochemical processes. However, recent market needs demand biological propionic acid biosynthesis as a sustainable alternative. Biological propionic acid production suffers from co-production of acetate, making the downstream purification process problematic and hindering the overall economic viability of the bioprocess. In an effort to overcome acetate production, we developed a CRISPR/CAS9 toolbox to engineer *propionibacterium* and knock out the pathway responsible for acetate production. A transient interruption of the acetate kinase gene by an in-frame green fluorescent protein insertion showed an almost lethal phenotype, which was "fixed" using adaptive laboratory evolution. The evolved strains were found to have a reduced acetate yield despite recovery of a functional acetate kinase. Using metabolomics and proteomics data, we found the stress induced by deletion of the acetate pathway lead to the induction of native alcohol dehydrogenases that resulted in the production of ethanol and propanol, products not otherwise observed from glucose catabolism. Through the transient application of a severe metabolic stress, we were able to expand the fermentation profile of *Propionibacterium*.

Keywords: Metabolic modelling; metabolic engineering; systems biology, synthetic biology, Propionibacterium, propionate

The human transcriptome or: How I learned to stop worrying and love RNA

Tim Mercer [1 *]

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Session Theme: *Synthetic Biology.*

Abstract: Upon its publication, the human genome was considered an inert sequence only sparsely populated by genes. Two decades later, we realize the human genome is pervasively transcribed into large and diverse populations of coding and non-coding RNAs. Here, we will take deep dive into the human transcriptome to discover exotic new RNA species and try to solve the codes that govern the complexity of the transcriptome. We show how this complexity is broken in fusion genes that are a major cause of cancer, and how sensitive and accurate targeted RNA sequencing is improving patient diagnosis. Most recently, we describe our design and manufacture of synthetic RNA technologies that provide new opportunities to treat human diseases. Together, this reveals the importance of RNAs in cellular biology, disease etiology and, latterly, innovative new therapies.

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14 Industrial Technologies

Keynote: Associate Professor Andrew Gooley, Chief Scientific Officer, Trajan Scientific and Medical

Invited Speaker: Professor Benjamin Schulz, The University of Queensland

Integrated omics approach in automated synthetic biology

Lisa Hartmann[1], Huw Hayman Zumpe[1], Maciej Holowko[1], Candice Jones[1], Adrian Marsh[1] and Janet Reid[1,*]

[1] Synthetic Biology FSP, Land & Water, CSIRO; synbiofoundry@csiro.au

* Presenter; Correspondence: janet.reid@csiro.au; Tel.: +61 7 3833 5704

Session Theme: *Synthetic Biology*

Abstract: Synthetic biology is undergoing a rapid change in its approach to discovery, from standard laboratory processes to automated ones, which allows for faster and more reliable strain engineering. Current methods in synthetic biology frequently use genomics, sometimes combined with one or more other omics approaches. However, this is often done without explicit integration of techniques, which can limit insight obtained from the results of genetic manipulations. Here, we envision how an automated approach to research enables tighter integration of omics methods. Key strengths of the automated approach include centralization of equipment and expertise, increased sample throughput and reproducibility of results. We recognize that the integration and automation of multiple omics techniques has challenges in resource, technical, and data management that require focused efforts to overcome. However, we also recognize the significant benefits. In such an integrated environment, pipelines involving multiple omics could be established and results from them can be collected into highly useful and insightful packages. These packages could be then analyzed with the help of data science and machine learning to enable faster, deeper analysis and prediction for future engineering.

Keywords: automation; integration; strain engineering; genomics; omics

Systems biology proteomics and metabolomics to investigate beer production

Edward Kerr [1], Christopher Caboche [1], Toan Phung [1], Cassandra Pegg [1], Mark Howes [2], Claudia Gonzalez Viejo [3], Sigfredo Fuentes [3], Kate Howell [3], Fox Glen [4], and Benjamin Schulz [1,*]

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Session Theme: *Synthetic Biology.*

Abstract: Beer is one of the most popular beverages worldwide. As a product of variable agricultural ingredients and processes, beer has high molecular complexity. We have used integrated proteomics, metabolomics, and genomics to investigate the molecular complexity and diversity throughout the beer making process. We uncovered substantial variability in barley based on variety and growth environment, and found that proteolysis during the mashing stage of beer production controls protein thermal stability and abundance in the final beer. Profiling 23 commercial Australian beers identified a very high diversity of post-translational modifications (PTMs), especially proteolysis, glycation of barley proteins, and glycosylation of yeast proteins. The key differentiator of the beer glyco/proteome was the brewery, with beer from independent breweries having a distinct profile to beer from multinational breweries. Within a given brewery, beer styles had distinct glyco/proteomes, with proteins in darker beers having low glycation and high proteolysis. Quantitative quality metrics of foam formation and stability correlated with the concentration of abundant surface-active proteins from barley and yeast. Finally, to expand the flavour and sensory profiles after fermentation we have used proteomics, genomics, and metabolomics to investigate wild yeast ferments for controlled production of diverse beer styles.

Keywords: proteomics, post-translational modifications, metabolomics, beer.

Better precision medicine outcomes start at the source: an automated platform for creating phenotypical in vitro models at scale

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Session Theme: *Industrial Technology*

Abstract: The growing recognition that disease is individual is driving a shift in drug discovery and development initiatives. The resulting development of precision discovery and personalized medicine workflows, using multifaceted data sources from small population clusters to inform drug targets and treatment choices, requires access to representative sample sources. This aspect is particularly pertinent when relying on preclinical models for genomic and proteomic insights into disease function and progression. Progress in synthetic biomaterial-based in vitro models has shown that recapitulating the structure and function of in vivo tissue at the cellular level has the potential of addressing the sample need for the new precision medicine workflows. At Inventia Life Science we are developing a platform for the effortless and scalable creation of phenotypical in vitro models which can replace traditional tissue cultures without a process change. Together with our academic and industry partners we are solving the existing adoption and implementation challenges of complex in vitro models in research, diagnostic and clinical settings to increase the predictive validity of precision medicine initiatives.

Keywords: Precision medicine; 3D Cell Culture; high throughput screening; complex in vitro models; bioprinting

From Smartphone to Mass spectrometer, a novel pipeline for food safety testing

Joost Nelis[1]*, Alisha Anderson[1], Michelle Colgrave[1], Xinlong Guan[3] and James Broadbent [1]

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Session Theme: *Food and Agriculture*

Abstract: The current food safety testing system, based on random sampling and laboratory-based LC-MS quantification, cannot keep up with the expected growth in the export market. Here we present an alternative pipeline applying a smartphone-based lateral flow assay (LFA) quantification for secure on-site testing and reporting using allergens as a case study. Additionally, the pipeline features an LC-MS method enabling direct allergen quantification from the LFA. The novel method enables direct confirmation of the rapid antigen test, allowing the detection of false positives and the confirmation that the assay was performed correctly if a negative result is returned. A ratiometric approach was applied for smartphone-based quantification resulting in excellent light-intensity variation robustness and calibration curves for peanut with R2=0.97-0.99 depending on the commercial LFA. A prediction error of 13 ± 11% was equally achieved for the best performing assay. Good performance—calibration curves (R2=0.93-0.99) and CVs (<15%)—was equally observed for the quantification of the LFAs by LC-MS. Moreover, the LOD for the LC-MS assay was 0.5 ppm, well below the LOD reported for the LFAs. This method can contribute to creating a digital, fast and more secure food safety compliance testing pipeline that will benefit the Australian export industry.

Keywords: Food Safety; Allergen quantification; Biosensors; lateral flow assay; rapid antigen test; LC-MS; food safety analyses

15 Food and Agriculture

Session Sponsored by: SCIEX

Keynote: Professor Melissa Fitzgerald, University of Queensland

MLA sponsored presentation: Dr. Marina Fortes, the University of Queensland

MLA sponsored presentation: Dr. Loan Nguyen, the University of Queensland

MLA Sponsored presentation

Will the tsunami of omics data improve our phenotype predictions?

Dr. Marina Fortes

MLA Sponsored presentation

Advances in genomic technologies for livestock production

Loan T. Nguyen[1]*, Harrison Lamb[1], Chian T. Ong[1], Ben J Hayes[1] and Elizabeth M. Ross[1]

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Session Theme: *Food and Agriculture*

Abstract: Oxford Nanopore Technologies' (ONT) portable sequencing devices have enhanced our ability to address system-level problems through the possibility to directly sequencing unmodified-DNA and RNA molecules in real-time with no limit in read length. We have used ONT data in a range of agriculturally focused research studies, including genome assembly (Ross et al 2022), epigenetic aging clock generation (predicted animal age with an accuracy of 0.71 ; Hayes et al. 2021), characterization of important structural variants related to Poll status in Brahman (Lamb et al. 2020) and coat colour in Nellore cattle (Trigo et al. 2021), and analysing metagenomes (Ong et al. 2022), parentage testing (Ross et al 2021), and even for genomic prediction of important traits (Lamb et al 2021). Lamb et al. 2021 has shown that low coverage ONT data can be used for in situ genomic predictions which are near identical to SNP array-based predictions ($r > 0.92$), suggesting the potential of on-farm genomic prediction. Our findings based on different approaches using ONT demonstrate the versatility and potential of this technology and may be of interest to researchers in different areas of science.

Keywords: Portable long read sequencing, Epigenetic clock, Parental testing, genomic prediction

Using machine learning to address omics data prediction problems in livestock species: challenges and perspectives

Yutao Li [1*], Laercio Porto-Neto[1], Russell McCulloch[1], Sean McWilliam[1], Bo Li[2], Pamela Alexandre[1], Sigrid Lehnert[1] and Antonio Reverter [1]

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Session Theme: *Machine learning & Artificial Intelligence*

Abstract: Some of the main advantages of machine learning (ML) methods over conventional statistical methods in large omics data analysis include: (1) ML can deal with "large p, small n" problems; (2) they are black-box approaches that do not require any prior knowledge about distributions of response variables; (3) they can take multiple interactions or correlations among features into account, and (4) they can provide high prediction accuracy due to both training and validation procedures built into the processes of individual algorithms, that allow ML to apply a randomly assigned cross-validation approach for prediction of individual phenotypes. However, to date, the results from applying ML for predicting phenotypes in livestock species have been mixed, depending on many factors. Some of them include the presence or absence of population structure, the additive and epistatic nature of phenotypes, ML methods, data quality, and representation of training and validation populations. Here, using four cattle and sheep datasets for different prediction purposes, namely, genomic prediction using high-density SNP information for non-ordinal multi-class reproductive traits, identification of genes for feed efficiency using multi-tissue transcriptome data, and classifying sheep behaviors using sensor data, we demonstrate both success and challenges when analyzing complex phenotypes with different ML methods.

Keywords: machine learning; phenotype prediction; omics data; cattle; sheep

Microbial Crop Biostimulants for the Tropics - from Marketing to Science and Efficacy

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Session Theme: *Food and Agriculture*

Abstract: There is much interest in green agriculture that harnesses ecological processes, reduces inputs, and manages environmental footprints. One avenue contributing to these aims is engineering the soil's biological properties to reduce the use of biocides and fertilisers. We aimed to quantify the effects of biostimulants, i.e., plant growth promoting (PGP) rhizobacteria, including isolates from sugarcane rhizospheres and commercial soil-enhancing microbial products, across several levels of experimental control from laboratory to farm. In plate assays, we found that rhizosphere microbes possess several PGP traits with some translating to benefits for crop seedlings under lab growth conditions. While we find that commercial products can alter root microbial communities in lab and farm experimentation, benefits to crops are often undetectable or inconsistent. Together the research confirms the need for product evaluation and optimisation, as well as innovative delivery practices, to realise the often-wide-ranging claims of manufacturers. This will most likely require customised and optimised biostimulants for specific crops and growth environments. We discuss the notion of 'specialist' and 'generalist' bacteria, the implications of inducible PGP traits on microbial fitness, and the need for proof-of-efficacy in tropical crops.

Keywords: Microbial biostimulants; Crop probiotics; Beneficial microbes; Root microbial communities; Soil microbial communities; Sugarcane

16 Food, Agriculture, and the Environment

Invited Speaker: Associate Professor Horst Schirra, Griffith University

Understanding nutritional shifts and discovering healthy barley lines through a proteogenomic workflow

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Session Theme: *Food and Agriculture*

Abstract: Hordeins are the major storage proteins in barley can trigger coeliac disease response. Attempts have been made to improve the nutritional quality and removing anti-nutritional storage proteins from cereal grains. Here, we studied how one of the most limiting essential amino acid lysine synthesis and accumulation regulated in mutant hordein barley lines and their pleiotropic can regulate alpha-amylase/trypsin inhibitor (ATI) protein accumulation; ATIs have role in non-coeliac gluten sensitivity is a less understood gastrointestinal-related disorder, which affects ~10% of the world population. Data-independent acquisition (DIA) mass spectrometry (MS) and targeted proteomics using MRM-MS were performed in parallel with phenotypic characterisations and bioinformatics analyses across single- double- and triple-hordein mutant lines. Balanced changes in the induced and suppressed protein abundances confirms the dual regulatory mechanisms of nutrient accumulation and energy metabolism in the mutant lines, resulting in differences both in the hordein levels and composition as well as in the lysine content of the double nulls. The MRM-MS showed that levels of ATI peptides were significantly reduced in the triple null ULG line in comparison to wild-type barley cv Sloop. This study serves as a framework for future proteomics-assisted crop development to study pleiotropic effects on safety and nutrition quality-related improvements.

Key words: Proteogenomics; SWATH-MS; MRM-MS; barley; alpha-amylase/trypsin inhibitor (ATI); non-coeliac gluten sensitivity (NCGS)

A front-row seat at the fashion show runway – the usefulness of model organisms in uncovering fundamental metabolism

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Session Theme: *Environmental Sciences & Ecosystem Surveillance.*

Abstract: We discuss three examples of NMR-based metabolomics in model organisms: Unravelling central metabolic regulation in *C. elegans*, and exploring host-symbiont interactions between *Wolbachia* and *Drosophila melanogaster* and *Aedes aegypti* : (1) Previously we discovered that the enzyme dihydrolipoamide dehydrogenase (DLD) causes phosphine resistance in *C. elegans* and is likely a metabolic master regulator [1]. Genome-scale metabolic models (GSMs) are key tools to understanding metabolism and the role of DLD in *C. elegans*, and we are now leading the international research consortium *WormJam* which aims to curate a *C. elegans* consensus GSM [2-3]. (2) *Wolbachia* infection in *D. melanogaster* depresses the insulin/insulin-like-growth factor cascade, whilst inducing the hypoxia signaling pathway [4]. This causes ROS production and ROS adaptations, and other metabolic changes that steer metabolism away from oxygen-intensive pathways and enable metabolite extraction by the symbiont and metabolite provisioning to the host. These responses signify a reprogramming of the host's mitochondrial metabolism rather than an immune response. (3) In contrast, infection with *w*MelPop in *Ae. aegypti* triggers host immune responses, including melanogenesis and ROS production. *w*MelPop is more aggressive, while *w*Mel is more likely to form stable inheritable infections. These examples show the breadth and depth of insights that can be gained through model organisms in metabolomics and systems biology.

Keywords: *Drosophila melanogaster*; *Aedes aegypti*; *Wolbachia pipientis*; *Caenorhabditis elegans*; NMR-based metabolomics; genome-scale models; host-symbiont interactions; metabolic regulation

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Computational systems biology empowers knowledge on the lichen symbiosis at subcellular level

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Session Theme: *Environmental Sciences & Ecosystem Surveillance*

Abstract: The symbiotic association of specific fungi, green algae (or cyanobacteria), and other microbes form a composite community of species known as lichens. Such diverse symbiotic community operates through the members' combined efforts ranging from C-fixation (and sometimes N-fixation), nutrient exchange and recycling, and production of unique secondary metabolites for suppressing environmental stresses and pathogens. However, little is known about these symbiotic interactions within a lichen community at molecular level. Here, we use a computational systems biology approach to predict some of the key metabolic interplays of a model lichen, *Endocarpon pusillum*. We develop a constraint-based modelling framework combining the core metabolic networks of the primary mycobiont, *E. pusillum*, and that of the primary photobiont, *Diplosphaera sp.*, encompassing over 600 metabolic reactions and 250 genes. Using this community modelling framework, we show how fixing atmospheric CO_2 into carbohydrates by the photobiont and their provision to the mycobiont fuel the coupled metabolic pathways of the symbionts. The model also predicts theoretical limits of growth for the lichen and its symbionts individually. This work provides important new insights on the lichen symbiosis paving the way for designing strategies for restoration of contaminated soils and mitigating the impact of drought on natural soils.

Keywords: Lichen; Symbiosis; Fungi; Algae; Metabolic modelling; Computational systems biology; Community network modelling

Improving rehabilitation using metabolomics: Health, recovery, and biomarkers of mortality in sick and injured green turtles (*Chelonia mydas*)

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Session Theme: *Environmental Sciences & Ecosystem Surveillance*

Abstract: Hundreds of sick and injured turtles are admitted to rehabilitation clinics annually, where recovery and release are key aspects of their conservation management. There is considerable interest in establishing biochemical markers to gauge sea turtle health, and diagnostic tools to facilitate informed decision-making about overall care and specific treatment needs during rehabilitation. We applied untargeted metabolomics to monitor the health of 28 green turtles (Chelonia mydas) admitted to a rehabilitation clinic in eastern Australia between October 2018 and April 2019. Malnutrition and ketosis were identified as major physiological manifestations in sea turtles entering the clinic. Specifically, decreased branch-chain and aromatic amino acids were observed at admission, along with increases in the ketogenic metabolite 3-hydroxybutyric acid and metabolites associated with peroxisomal disorders (pipecolic acid and beta-alanine). Comparing successfully rehabilitated animals with those that died identified a suite of metabolites that were predictive of mortality. Results show that a major cause of sea turtle mortality during rehabilitation relates to severe malnutrition that ultimately manifests as sepsis-induced metabolic failure. This showcases the strength of metabolomics for monitoring sea turtle health and informing care and management during rehabilitation and is a compelling case-study highlighting that metabolomics is well positioned to play an important role in various aspects of veterinary medicine and conservation science.

Keywords: Sea turtle; Animal rehabilitation; Metabolomics; Malnutrition; Conservation; Physiology

Towards an integrative and inclusive precision health future: mapping the scientific and ethical terrain

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Session Theme: *Health and Precision Medicine*

Abstract: Precision health aims to integrate an individual's biological, behavioural, and socio-environmental information to promote good health throughout the lifespan. With significant global funding towards precision health research, it is crucial to map the research landscape and examine how studies realise the vision of integrated, comprehensive, and personalised healthcare for all. We present the outcomes of our scoping review of 225 relevant primary studies, involving human participants, datasets, or samples and collecting health information. There is a focus on intervention development, particularly digital health promotion tools. However, only 29% of the reviewed studies used ≥4 data types for personalisation, with behavioural, sociodemographic, and clinical information the most frequently utilised. Only 16% of the articles involved a randomised controlled trial. In terms of diversity, 32% of the studies did not report participants' sex/gender, 61% did not provide participants' race/ethnicity, and only 20% included people from socio-economically disadvantaged backgrounds. More than 57% have authors from a single discipline, and only 6% were conducted in African or South American countries. These findings highlight pressing ethical concerns, particularly on social justice, beneficence, and data privacy. For equitable precision health innovation, greater interdisciplinary collaboration, data integration and protection, and inclusion efforts are urgently needed.

Keywords: precision health; equity; diversity; ethics; inclusion; scoping review; data integration; health research; interdisciplinarity; personalised medicine

17 Health and Precision Medicine

Session Sponsored by: In Vitro Technologies

Keynote: Professor Elaine Holmes, Murdoch University

Keynote: Dr. Trung Ngo, The University of Queensland

Invited Speaker: Associate Professor Horst Schirra, Griffith University

Saliva-omics as a potential tool for the molecular diagnostic of Alzheimer's disease

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Session Theme: *Health and Precision Medicine*

Abstract: To-date no simple, affordable, and non-invasive procedure is available to confirm with certainty the early diagnosis of Alzheimer's disease before the manifestation of symptoms. New simple and affordable diagnostic methods are needed to diagnose the disease early to allow for timely treatments and beneficial lifestyle changes. We analysed 80 saliva samples from individuals with mild cognitive impairment or Alzheimer's disease as well as age- and gender-matched healthy controls. Saliva proteomic and metabolomic analyses were conducted utilising mass spectrometry methods and data combined using pathway analysis. We identified several protein and metabolomic biomarkers (with area under the Receive Operator Characteristic curves >95%) and found significant alterations in multiple cellular pathways, demonstrating that at the omics level, disease progression impacts numerous cellular processes. Multivariate statistics showed that partial least squares-data analysis could be used to provide separation of the three groups. Saliva has the distinct advantage that it can be easily self-collected in a non-invasive manner. This study found significant changes in metabolites and proteins from multiple cellular pathways in saliva. These changes were associated with Alzheimer's disease, demonstrating that this approach might prove useful to identify new biomarkers to develop a diagnostic test that will have application in dementia patient's management.

Keywords: Saliva; Integrated Omics, Alzheimer's disease

Genoma.io with a VIEW: Taking the pain out of phenome- & transcriptome-wide association analytics

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Session Theme: *Health & Precision Medicine*

Abstract: The ever-increasing volume of genome-wide association study (GWAS) data being generated requires analytical tools to integrate & maximise their utility for scientific discovery, reproducibility, collaborations & translational outcomes. https://genoma.io is a freely accessible bioinformatics platform with a comprehensive toolkit for aggregating, annotating, analysing & visualising GWAS summary statistics across >1,500 traits/diseases such as height, weight & intracranial volume through to metabolites (e.g., latent causal variable analyses), infectious diseases, chronic pain, psychiatric disorders & much more. Genoma.io comprises: (I) Complex Traits Genetics-Virtual Lab (CTG-VL) — for running phenome- & transcriptome-wide association analyses; and (II) CTG-VIEW — a data aggregator for direct queries, visualisations & results storage. To date >7,000 jobs have been performed by >450 registered users so simply login and explore. For example, query any novel hypothesis not yet examined in the literature or that cannot be feasibly done — or interrogate well-established findings in your field. A live demonstration of the platform's key capabilities and open innovation utility will be presented using chronic pain as an example — https://doi.org/10.1093/brain/awab334. Its further uptake & development with the STEMM community will help to accelerate biomarker discovery, reduce research waste and advance the translational benefits of integrative systems biology for enhanced human health, performance & resilience.

Keywords: GWAS summary statistics; PheWAS; TWAS; post-GWAS downstream analyses; Genetic casual proportion; Complex traits; Neuroimaging genetics; Biomarker discovery; Precision Pain Medicine; Medical countermeasures capability

Revealing drug mechanisms with multi-omics approaches.

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Abstract: Many existing medicines, and new drug candidates, act by unknown or poorly-defined mechanisms of action. Elucidation of these drug mechanisms would enable rational optimisation of their clinical use, and would streamline the development process for new drug candidates. Multi-omics techniques (e.g. transcriptomics, proteomics and metabolomics) allow comprehensive analysis of changes to cellular biomolecules, which can provide an unbiased description of mechanism of drug action. We have applied mass spectrometry-based metabolomics and proteomics techniques to reveal mechanisms of drug action and resistance for several antimalarial drugs and drug candidates.

Metabolomics analysis of in vitro parasite cultures treated with artemisinins, the current first-line antimalarials, revealed rapid and extensive depletion of peptides derived from haemoglobin, a key nutrient source for the parasites. Proteomics analysis also detected changes to the proteolytic enzymes in the haemoglobin digestion pathway, indicating that the mode of action of artemisinin involves initial inhibition of this pathway. Additional temporal analysis of the multi-omics data revealed the downstream pathways that are inhibited due to drug action. Furthermore, multi-omics analysis of drug-resistant parasites identified mechanisms of drug resistance involving decreased haemoglobin digestion and elevated levels of glutathione, which allow the parasite to minimise artemisinin-induced damage and survive drug treatment.

Streamlining these multi-omics techniques to enable plate-based medium-throughput analyses has allowed efficient analysis of dozens of novel drug candidates. The generated metabolomic profiles enabled rapid classification of compounds that act by common mechanisms, and revealed novel mechanisms of action that can be further pursued for the discovery of novel antimalarials. Current work is combining these multi-omics studies with proteomics-based target identification tools, based on thermal stability and limited proteolysis, to identify and validate new drug targets.

Part III Poster Presentation Abstracts

18 Assigned poster presentation number

1. **David Beale**, CSIRO L&W, “A systems biology approach to investigate PFAS exposure on wild freshwater turtle populations.”
2. **Vijay Dhamale** (EMCR), Swinburne University, “Metabolic profiling to identify fundamental differences in toxic and non-toxic cyanobacterial strains.”
3. **Luke Husdell** (EMCR), The University of Queensland/Griffith University, “Metabolomic analysis of *Wolbachia*-infected *Aedes aegypti*.”
4. **Thao Nguyen** (EMCR), Auckland University of Technology, “LC-MS-based metabolomics and lipidomics investigation of abalone mortality in Cook Strait, New Zealand.”
5. **Amy Paten** (EMCR), CSIRO L&W, “Multi-omics reveals a biphasic response in honey bee larvae exposed to imidacloprid and highlights impacts on developmental signaling and metabolism.”
6. **Sophia Escobar-Correas** (EMCR), CSIRO A&F, “Proteo-genomics to explore a common weed for the presence of gluten-like proteins.”
7. **Pamela Alexandre** (EMCR), CSIRO A&F, “What can competing endogenous RNA-networks tell us about viral response in Atlantic Salmon.”
8. **Selina Fyfe** (EMCR), The University of Queensland/Griffith University, “NMR and FT-ICR-MS metabolomics of Australian native Green Plum fruit.”
9. **Alexandra Gloria** (EMCR), The University of Queensland/Griffith University, “Comparing the metabolic effects of a moderate heat load to feed restriction in *Bos taurus.”*
10. **Omar Mendoza** (EMCR), CSIRO A&F, “Using omics tools in aquaculture organisms.”
11. **Toni Reverter**, CSIRO A&F, “A perspective on systems biology applications in livestock species.”
12. **Kern Webster** (EMCR), The University of Queensland, “NMR Characterisation of Honey from Stingless Bees.”
13. **Juliana Muller Park** (EMCR), Queensland University of Technology, “Prognostic value of metabolic alterations in saliva and plasma of glioblastoma patients.”
14. **Md Zakir Hossain** (EMCR), CSIRO A&F, “CNN for Prediction of Yield Component Traits in Wheat from Transcriptome Data.”
15. **Juan Martinez** (EMCR), Queensland University of Technology, “Repurposing keratin waste as a support for biocatalysts via keratin binding fusion modules.”
16. **Jonathan Peters** (EMCR), The University of Queensland, “A flexible platform for enzymatic synthesis of mRNA.”
17. **Nizhum Rahman** (EMCR), The University of Queensland, “A mathematical model for the axonal cargo transport.”
18. **James Antoney** (EMCR), Queensland University of Technology, “Improved Cofactor F420 production in Escherichia coli”.
19. **Muzaffar-Ur-Rehman Mohammed** (EMCR), Birla Institute of Technology and Science Pilani, “Systematic down selection of FDA/TGA approved drugs for repurposing against COVID-19.”

20. **Avinash Karpe** (EMCR), CSIRO L&W, “Glycolysis and oxidative stress related redox pathway upregulation along the gut-liver axis by gut microbial perturbation and host response during giardiasis in C57BL/6J mouse model.”
21. **Brandon Mu** (EMCR), Queensland University of Technology, “Biorecycling and bioremediation of plastics and plasticizers by thermophilic enzymes from the Great Australian Artesian Basin.”

A systems biology approach to investigate PFAS exposure on wild freshwater turtle populations

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Session Theme: *Environmental Sciences & Ecosystem Surveillance.*

Abstract: Per- and polyfluoroalkyl substances (PFAS) are persistent synthetic environmental contaminants . Direct toxicity of elevated PFAS concentrations in wildlife has been studied, yet evidence of their accumulation effects on gut health, developmental impacts, and maternal offloading in aquatic egg-laying species is limited. Here, we summarise an omics-based ecosurveillance approach to investigate the impacts of PFAS pollution in freshwater turtles (*Emydura macquarii macquarii*). Turtles were collected and necropsied from an impacted waterway (n=5) downstream from a known PFAS contamination source, in addition to a suitable reference site (n=5), in Queensland, Australia. Serum PFAS (Σ30) was quantified using a standard targeted methodology. Biochemical profiles (metabolites, lipids, and proteins) were analysed using a mixture of liquid chromatography triple quadrupole (QqQ) and quadrupole time-of-flight (QToF) mass spectrometry methodologies, applied to serum, oviducal eggs, and fresh faecal samples collected from the colon. The gut microbiome was profiled using 16S rRNA gene amplicon sequencing. Serum data demonstrated significant PFAS bioaccumulation (Σ30 PFAS 990 ± 290 ng/mL) in turtles (1600 times greater than water PFAS levels), with maternal offloading into oviducal eggs 5.3 times higher than serum concentrations. Serum biochemistry suggests an inflammation response, metabolic preservation, and re-routing of central carbon metabolites. Conversely, lipid transport and binding activity were negatively correlated. Multi-omic analyses of the PFAS impacted eggs illustrated elevated purine metabolism metabolites, which is tied to potential biological dysfunctional processes. The gut microbiome was found to have a high *Firmicutes* to *Bacteroidetes* (F:B) ratio and a range of biomolecules tied to gut dysbiosis and intestinal inflammation. This data demonstrated negative mechanistic impacts possibly associated with elevated PFAS exposures on turtle metabolic health. With further research on a larger turtle cohort, omics-based data will contribute towards identifying potentially adverse outcome pathways for turtle populations exposed to PFAS mixtures. Moreover, expanding the use of ecosurveillance tools will inform mechanistic toxicological data for risk assessment and regulatory applications.

Keywords: metabolomics; lipidomics; proteomics; metagenomics; PFAS; ecosurveillance.

Metabolic profiling to identify fundamental differences in toxic and non-toxic cyanobacterial strains

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Session Theme: *Environmental Sciences & Ecosystem Surveillance*

Abstract: Cyanobacteria, commonly known as blue-green algae, pose a significant health risk to the public and animal livestock. They become problematic, in terms of management and potential health implications, when they form large blooms which are dependent on different parameters like temperature, light, nutrient loads. Some blooms produce toxins which are neurotoxic, hepatotoxins and dermatotoxic that contribute a significant risk to public health and animals. Current methods for identifying and assessing pathogen viability in water are time-consuming, expensive and possibly unreliable. There is, therefore, a strong need for rapid methods that enable the sensitive assessment of pathogens in a variety of water sources by identifying and characterizing viability and toxin production. Liquid Chromatography Mass Spectrometry (LC-MS)-based metabolomics is attractive approach to detect Cyanobacterial toxins (150-1000 g/mol). Such a mass spectrometry-based approach not only aids in the identification of metabolites, but also assists in understanding the key metabolic pathways and helps to identify biomarkers relating to the early onset of a bloom within a water body. In the current study, two toxic strains of cyanobacteria, namely Cylindrospermopsis raciborskii and Microcystis aeruginosa, and two non-toxic strains, namely Nodularia spumigena and Anabaena cylindrica, were examined using LC-MS. Significant metabolites detected in toxic cyanobacterial strains were Adenosine, D-Glucose and Uracil, whereas significant metabolites detected in non-toxic cyanobacterial strains were Xylitol, Taurocholic acid and Vanillic acid using LC-MS. Metabolite separation was observed successfully. The significant metabolites produced by these cyanobacterial strains can predict if the bloom occurring in water body will be toxic or non-toxic. Also, these signature biomarkers can be used to predict bloom events and assist in identifying toxin producing parameters and understanding of the relevant metabolic pathways.

Keywords: Cyanobacteria; toxins; metabolomics

Metabolomic analysis of *Wolbachia*-infected *Aedes aegypti*

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Session Theme: *Environmental Sciences & Ecosystem Surveillance*

Abstract: *Wolbachia* are obligate, intracellular bacterial symbionts of insects that have been proven to reduce transmission of viral diseases from insects to humans. Transfection of *Wolbachia* into the dengue mosquito, *Aedes aegypti*, has successfully reduced dengue transmission in 11 countries[1]. *Wolbachia* induces physiological changes in its hosts, but the mechanistic basis and the metabolic contributions to these host-symbiont interactions are unresolved. The *Wolbachia* genome lacks vital metabolism genes, suggesting the symbiont scavenges resources from its host. We employed ^{1}H NMR-based metabolomics and targeted UPLC metabolite quantification to identify *Wolbachia*-induced metabolic changes. We investigated the infection of two strains, *w*Mel and *w*MelPop, at two diet levels. The effects of diet overpower the metabolic changes attributed to *w*Mel but did suggest that *w*Mel participates in minor metabolic provisioning to *Ae. aegypti*. Conversely, *w*MelPop triggered immune system pathways including melanogenesis and reactive oxygen generation and management. Our research confirms that *w*MelPop is the more aggressive strain and triggers host immune responses, limiting *w*MelPop's ability to sustain infection in the field. In contrast, *w*Mel is more benign to the host and thus more likely to form a stable inheritable infection. The strains *w*Mel and *w*MelPop occupy distinct positions on the spectrum of mutualistic-parasitic symbiotic relationships that *Wolbachia* can exhibit.
1. World Mosquito Program, updated 2021, accessed February 2022, <https://www.worldmosquitoprogram.org>

Keywords: *Wolbachia*, *Aedes aegypti*, metabolomics, ^{1}H-NMR spectroscopy, melanin immune response, reactive oxygen species

LC-MS-based metabolomics and lipidomics investigation of abalone mortality in Cook Strait, New Zealand

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Session Theme: *Environmental Sciences & Ecosystem Surveillance*

Abstract: The New Zealand abalone fishery is currently being affected by mortality events associated with elevated seawater temperatures and marine heatwaves. In this study, LC-MS-based metabolomic and lipidomic approaches were employed to analyze gill and muscle tissues of healthy and perturbed abalone collected from Cook Strait, New Zealand during the heatwave event in May 2021. We identified 182 annotated metabolites of central carbon metabolites in tissues of abalone. Gills of healthy abalone differed from those of perturbed abalone in 32 metabolites, while muscle tissues of the two abalone groups were different in 40 metabolites. Most of these metabolites were higher in the perturbed abalone than healthy individuals, which suggests metabolic disturbance, mitochondrial dysfunction, cell and tissue damage, impairment in aerobic respiration and metabolic shift from aerobic to anaerobic metabolism in perturbed abalone. The lipidome of abalone comprises 412 and 407 annotated species in gills and muscle tissues, respectively, which belong to 24 lipid classes. Unlike metabolomics, lipidomics did not show a significant difference between healthy and perturbed abalone. This first omics investigation on the effects of heatwave on abalone provides insights into the effects of heatwave on abalone and perspectives for future omics applications for this event.

Keywords: omics; metabolomics; lipidomics; mass mortality; heatwaves; abalone

Multi-omics reveals a biphasic response in honey bee larvae exposed to imidacloprid and highlights impacts on developmental signaling and metabolism

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Session Theme: *Environmental Sciences & Ecosystem Surveillance*

Abstract: Here, a multi-omics approach was used to disentangle the molecular mechanisms underlying sublethal pesticide stress in honey bees. Honey bee larvae were exposed to sublethal concentrations of a commonly used neonicotinoid pesticide (Imidacloprid) and sampled over a time-series (1, 24, 48 and 72h post-exposure). The resulting molecular changes were characterised through integration of transcriptomic, proteomic and metabolomic data. An early acute response was detected 1-24h after exposure and was characterised by upregulated stress pathways, including DNA damage, and down-regulated Ca2+ signaling and developmental pathways. After a period of recovery at 48h, an additional chronic response was detected at 72h which was characterised by perturbed energy metabolism, immune, and signaling pathways. These findings provide insights into the molecular events underlying developmental and metabolic impacts of sublethal pesticide stress in honey bee larvae that may have longer term consequences for colony health.

Keywords: ecotoxicogenomics; honey bee health; pesticides

Proteo-genomics to explore a common weed for the presence of gluten-like proteins

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Abstract: Gluten proteins are the main storage proteins within cereal grains such as wheat, rye and barley. Consumption of these cereals can lead to serious digestive problems in those with Coeliac disease — an autoimmune disorder, that affects 1-2% of the global population. The only solution for these patients is adherence to a strict gluten-free diet; however, symptoms persist in about 30% of patients despite committing to this strict regimen.

Persistent symptoms may arise from the presence of gluten-containing grains from agricultural co-mingling, that is, cross-contamination occurring during cereal harvesting due to the presence of weeds. In this study, the most common weed in Australia: ryegrass, Lolium perenne was invstigated. Ryegrass, like wheat and other cultivated crop species is a member of the grass species (Poaceae) wherein the storage proteins comprise gluten-like proteins.

Herein, we use a proteogenomic approach to identify gluten-like proteins with potential immunogenic properties. Data from genomics and transcriptomic of Lolium perenne were processed and analysed using in-house developed workflows. Genome sequences alignments were used to filter gluten-like sequences and identify regions with epitope-like features and thereby potential immunogenic properties. New sequences were identified in chromosome 1, 3 and 4. A final novel database was constructed to development protein analysis.

Using proteo-genomics approaches a suite of novel gluten-like proteins were identified with LC-MS/MS across ryegrass cultivars.

Keywords: Ryegrass, gluten, Coeliac disease

What can competing endogenous RNA-networks tell us about viral response in Atlantic Salmon

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Session Theme: *Food and Agriculture*

Abstract: We know now that only a small fraction of the genome codes for proteins; the remaining fraction contains non-coding transcripts that control the expression of other genes, influencing specific pathways and, ultimately, production traits and health status. Here we used whole transcriptome sequencing data, i.e.: messager (mRNA), micro (miRNA) and long non-coding (lncRNA) RNA, to explore these gene interactions. We used gill tissue of Atlantic salmon (*Salmo salar*) infected with Pilchard orthomyxovirus (POMV) but showing no clinical signs of disease, sampled early during the challenge trial (8 to 12 days after infection) to uncover potential biomarkers of early infection, and late during the challenge trial (19 dpi) to elucidate potential markers of resistance to POMV. Based on the competing endogenous RNA (ceRNA) hypothesis, we identified a teleost-specific miR-462/miR-731 cluster strongly induced in POMV infected fish and deemed a potential biomarker of early infection. The ceRNA network also pointed to a selenoprotein (selja) downregulated in fish sampled late during the challenge, and its associated regulatory non-coding RNAs, which may be associated with viral clearance and the return to homeostasis. This study provides the basis for functional investigations to confirm the interactions presented here and their potential application at commercial level.

Keywords: RNA-sequencing; ceRNA network; orthomyxovirus

NMR and FT-ICR-MS metabolomics of Australian native Green Plum fruit

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Session Theme: Food and Agriculture.

Abstract: The green plum (*Buchanania obovata*) fruit grow in northern Australia and are a traditional food of the Aboriginal Australians that has been underutilised for its taste and nutrition. Studies show it has promising nutrition and is a good dietary source of folate and has desirable sensory flavour and texture attributes. Metabolites in the green plum have been studied using untargeted metabolomics in green plums from five stages of maturation and ripening and from four geographical locations. Individual green plum fruit were extracted in methanol and analysed using both 900 MHz nuclear magnetic resonance (NMR) spectroscopy and Fourier-transform ion cyclotron resonance mass spectrometry (FT-ICR-MS). The analysis shows that there are significant changes in the green plum through maturation and ripening, particularly between the unripe and ripe fruit. It also shows that there are metabolite differences between the fruit from the four geographical locations. This is a foundational study on the green plum and will be useful for understanding fruit metabolites, the ripening process, the composition and nutritional potential of the edible fruit and as metabolite fingerprints which could be used for fruit identification and location origin.

Keywords: metabolomics; NMR; FT-ICR-MS; green plum; *Buchanania obovata*; fruit; Australian.

Comparing the metabolic effects of a moderate heat load to feed restriction in *Bos taurus*

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Session Theme: *Food and Agriculture*

Abstract: Heat stress is an ongoing issue for animal production in the agriculture industry. Extreme heat stress causes catastrophic failures, including heat stroke, severe dehydration, and acute renal failure. Efficient body thermoregulatory systems are therefore necessary to combat the effects of increased heat load. One such system is voluntary feed intake reduction to aid in decreasing endogenous heat, but consequently reducing body mass and growth. Understanding metabolic changes occurring during heat stress will help develop methods to offset its impacts. We characterised the metabolic effects of a moderate heat challenge (maximum T_a 35°C) over several days on grain-fed *Bos taurus* steers to compare with a feed-restricted thermoneutral group. Both the feed-restricted and moderate heat stress groups experienced negative energy balance and nutrient partitioning during their respective challenge stages. Elevated levels of triglycerides during challenge relative to pre-challenge indicates fatty acid mobilisation at the onset of challenge. However, when directly comparing the challenge stage of the feed-restricted and heat-stressed groups, we found that fatty acid mobilisation is a direct consequence of feed restriction. Furthermore, heat stressed animals do not immediately recover to their pre-challenge metabolic state, suggesting that homeorhetic mechanisms are occurring. The metabolic perturbations in cattle experiencing a moderate heat load are relatively subtle in comparison to a severe heat load. The subtleties of change suggest that cattle are resilient to this level of heat stress.

Keywords: moderate heat stress; feed restriction; NEBAL; homeorhesis

Using omics tools in aquaculture organisms

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Session Theme: *Food and Agriculture*

Abstract: Aquaculture is the farming of aquatic animals and plants for commercial food production and has become the fastest growing food production sector in the last 30 years. Enhanced growth, immunity, and resilience are highly sought-after phenotypic traits in aquaculture. Omics approaches are powerful tools to unravel the effects that environmental stimuli exert upon aquaculture organisms and the relevance of this in growth immunity and resilience. Here, metabolomics and proteomics were used to identify altered molecular pathways in response to diet in prawn (haemolymph and hepatopancreas) and biomarker monitoring in liver of heat stressed Atlantic salmon. A suite of public bioinformatic resources were employed to overcome limitations of working with non-model organisms, e.g., lack of annotation and using a closely related species databases to perform joint-pathway analysis. Identified pathways indicated specific nutrient utilisation linked to diet composition. In salmon liver, markers for heat stressed were validated. Collectively, the use of omics technologies in aquaculture can enable manufacturing of advanced diets that provide specific nutrients intended to attain enhanced growth, immunity, resilience leading to increase production yield while ensuring environmental sustainability and promoting animal welfare and social license

Keywords: Aquaculture, salmon, prawn, heat stress, nutrition, omics technologies

A perspective on systems biology applications in livestock species

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Session Theme: *Food and Agriculture*

Abstract: The success of the human genome sequence project over 20 years ago signified a massive boost to other species-specific biotechnology studies, including non-model organisms such as livestock. Since then, high-throughput gene expression technologies have been a popular choice. They evolved from microarray assays in the 2000's to next-generation sequencies in the 2010's. However, soon we realized that isolated lists of differentially expressed (DE) genes which, by simply comparing genes to themselves, have the pitfall of taking molecular information out of context. The need for systems-level explanations of biological phenomena prompted us to adopt gene network approaches and to analyze rigorously the connectivity patterns within the network. Information of DNA variants (eg. SNP) associated with complex traits of interest can be overlayed in the network to assist in the interpretation. These holistic approaches allowed us to identify causal mutations and other effector molecules, such as transcription factors, irrespective of whether they themselves are DE. We present algorithms and metrics developed by our group to reverse-engineer and analyze gene networks including PCIT (partial correlation and information theory), RIF (regulatory impact factors) and AWM (association weight matrix) and provide examples within the realms of growth, reproduction, and disease resistance in livestock studies.

Keywords: RNA-sequencing; gene regulatory networks; genotypes; livestock,

NMR Characterisation of Honey from Stingless Bees

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Session Theme: *Food and Agriculture*

Abstract: Stingless bee honey has long been credited with many health benefits such as antioxidant, antimicrobial and anti-inflammatory properties. A recent study [1] has isolated the unique sugar trehalulose which is associated with the above health properties. These findings provide the motivation to characterise the composition of Stingless Bee honey in more detail which is explored in this research project using nuclear magnetic resonance spectroscopy (NMR). The spectra of 36 stingless bee honey samples from Malaysia and Australia, and from 2 different species from each country (*Tetragonula hockingsi*, *Tetragonula carbonaria* from Australia and *Heterotrigona itama*, *Geniotrigona thoracica* from Malaysia) with a total of 21 different hive locations were recorded and analysed with Multivariate Statistical Analysis (MVSA). The different stingless bee Honey samples can be characterised at a country and species level, but discrimination becomes much more difficult at a hive location level. Sugars were the largest contributing metabolites when comparing honey samples between countries and species, but when comparing hive locations low concentration aromatic and bacterial metabolic compounds have more significance in characterising the stingless bee honey. This is the first study to provide the foundation for a more detailed analysis of Stingless Bee Honey.

[1] Fletcher *et al*., *Scientific Reports* **10**, 1–8 (2020)

Keywords: Honey, Trehalulose; Nuclear Magnetic Resonance spectroscopy; Multivariate Statistical Analysis

Prognostic value of metabolic alterations in saliva and plasma of glioblastoma patients

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Session Theme: *Health and Precision Medicine*

Abstract: Glioblastoma (GBM) is the most aggressive and frequent brain cancer in adults. GBM prognosis is mainly assessed by imaging techniques which may result in misinterpretation of treatment response. There are no clinically validated biomarkers to monitor treatment response in GBM and the use of metabolomics is a promising tool to address this clinical need. Metabolomic and lipidomic profiles of saliva (unstimulated, oral rinse) and plasma were analysed using LC-QqQ-MS and LC-QTOF-MS. Samples were collected pre and post-operatively from GBM patients presenting different outcomes (progression-free survival (PFS)>9 months or PFS≤9 months, respectively). Univariate and multivariate statistical analyses were performed using MetaboAnalyst. A total of 151 and 197 statistically significant metabolites and lipids were identified across all samples, respectively. Key statistically significant metabolites in GBM patients were involved in purine and pyrimidine metabolism, and alanine/aspartate/glutamate metabolism. Across all body fluids, patients with unfavourable outcomes showed 13 and 17 metabolites differently present compared to favourable outcomes in pre and post-surgery samples, respectively. These were involved in the pentose phosphate and Warburg effect pathways. Our results suggest that salivary and plasmatic metabolic alterations in GBM have the potential to be utilised as minimally invasive prognostic biomarkers. However, studies with larger cohorts are still warranted.

Keywords: glioblastoma, biomarker, metabolites; lipids; prognosis.

CNN for Prediction of Yield Component Traits in Wheat from Transcriptome Data

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Session Theme: *Machine learning & Artificial Intelligence*

Abstract: Global food security is a critical challenge in agriculture today. Deep learning (DL) approaches have potential to provide improved avenues for accelerated genetic gain in crops and specifically wheat, which is a major source of human nutrition. Strategies to extract value from the increasing availability of 'omic data need to be identified to support production and breeding opportunities. We implemented a DL method, Convolutional Neural Network (CNN), to predict important traits (flowering time and height), which are wheat yield components, from transcriptome data collected on ~300 varieties across two controlled environments. Our CNN model, with 10-fold cross validation, achieved root mean square error (RMSE) of 0.080 and 0.067 for flowering time and height respectively, when random forest (threshold = 0.002) was applied for feature selection. In comparison, the CNN model achieved 0.115 and 0.068 RMSEs when least square linear regression was used for feature selection ($p \leq 0.01$). Considering the promising performance of our initial model, our current focus is to develop a robust DL method to predict wheat yield components from multi- 'omics data previously collected on the same panel of 300 varieties, including genome SNPs and transcriptomes, spanning multiple field experiments. These predictions will support cropping decisions and resource management on-farm.

Keywords: Deep Learning; Wheat; Multi- 'omics

Repurposing keratin waste as a support for biocatalysts via keratin binding fusion modules

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Session Theme: *Synthetic Biology.*

Abstract: Keratin is the main structural protein in nature, presented in various forms, including wool, feathers and hair. Millions of tons of keratin waste are produced every year, mostly disposed of in landfills or incinerated. Repurposing keratin waste as a support for biocatalysts is of industrial interest, adding value and reducing waste. A previously characterised keratin-based peptide reportedly binds to keratin through a cysteine-mediated disulfide-bridge. To investigate the capacity of peptides to bind to keratin, 8 peptides with 13 amino acids were designed based on the keratin type II sequence. The selection considered various regions of the keratin structure, including head, coil and tail. The peptides were fused to the fluorescent reporter mVenus-Q69M, expressed in E. coli BL21(DE3) and purified with a HisTrap column. Keratin binding assays were performed using multiple substrates, including cattle hair, feather meal, and wool blends ($n = 9$). Fusions did not bind to cattle hair or feather meal. Though, binding was observed in wool blends and pure wool ($p < 0.0001$). Head and tail-based peptides presented higher binding capacity (40-60%), whereas coil peptides did not show efficient binding (0-20%). Future work will involve new constructs, fusing the best candidates to enzymes.

Keywords: Binding domain; keratin; immobilised biocatalysts

A flexible platform for enzymatic synthesis of mRNA

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Session Theme: *Synthetic Biology*

Abstract: Synthetic nucleic-acids are rapidly becoming a key molecule for a range of therapeutic applications, from development of cells lines, production of antibodies to direct use as mRNA vaccines against viruses or for cancer treatment. One major advantage of synthetic nucleic acids is flexibility in design, providing an ideal platform for targeting different viruses, engineering proteins, or introducing sequences such as untranslated regions which improve or modify translation. BASE nucleic acid production facility is currently using these principles to establish a platform for enzymatic synthesis of high-quality mRNA for any gene or sequence of interest, providing an end-to-end service, from initial sequence design, through to scalable manufacture and final analytics. BASE, in partnership with TIA, PEF and NBF, supports the production and use of synthetic nucleic-acids for translational use, including pre-clinical and early clinical leads.

Keywords: mRNA

A mathematical model for the axonal cargo transport

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Session Theme: *Synthetic Biology*

Abstract: Axonal transport is the process where diverse cargoes deliver through the axon due to motor proteins. Actin plays a crucial role in different cellular functions, including cell motility and intracellular transport. The structures of actin are like rings wrapped around the circumference of axons. The rings are evenly spaced along axonal shafts by their nature. When the cargoes move through an axon; the spring force, viscous force and potential energy arise. We construct a physical model to compute the potential function. Finally, we get the model as an obstacle problem. The obstacle problem gives us the velocity of the cargoes. The speed of axonal cargoes is inversely correlated with their size.

Keywords: axonal transport; motor protein; actomyosin rings; mathematical model; potential energy; obstacle problem; asymptotic approximation

Improved Cofactor F_{420} production in *Escherichia coli*

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Session Theme: *Synthetic Biology,*

Abstract: The deazaflavin cofactor F_{420} is a low-potential, two-electron redox cofactor produced by some Archaea and Eubacteria that is involved in methanogenesis and methanotrophy, antibiotic biosynthesis, and xenobiotic metabolism. However, it is not produced by bacterial strains commonly used for industrial biocatalysis or recombinant protein production, such as *Escherichia coli*, limiting our ability to exploit it as an enzymatic cofactor and produce it in high yield. Here, we have utilised a genome-scale metabolic model of *E. coli* and constraint-based metabolic modelling of cofactor F_{420} biosynthesis to optimise F_{420} production in *E. coli*. This analysis identified phosphoenolpyruvate (PEP) as a limiting precursor for F_{420} biosynthesis, explaining carbon source-dependent differences in productivity. PEP availability was improved by using gluconeogenic carbon sources and overexpression of PEP synthase. By improving PEP availability, we were able to achieve a ~40-fold increase in the space-time yield of F_{420} compared with the widely used recombinant *Mycobacterium smegmatis* expression system. This study establishes *E. coli* as an industrial F_{420}-production system and will allow the recombinant *in vivo* use of F_{420}-dependent enzymes for biocatalysis and protein engineering applications.

Keywords: Cofactor F_{420}; Deazaflavin; Metabolic engineering; Cofactor biosynthesis; Biocatalysis

Systematic down selection of FDA/TGA approved drugs for repurposing against COVID-19

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Session Theme: Health and Precision Medicine

Abstract: The novel coronaviruses and its variants have shattered healthcare systems across the world claiming six million lives. Many novel antivirals have shown promising results *in vitro* yet failed in *in vivo* and human clinical trials. Development of vaccines was a silver lining in managing the pandemic, however, their efficacy against emerging variants such as Omicron is poor. This calls for a novel approach to find drugs that are safe, effective against the virus, affordable and approved by regulatory bodies such as FDA/TGA for easy availability to consumers. To achieve this, a library of 7817 drugs and their associated data were curated from various publicly available databases and literature reports. Later, sequential filters such as assay, route of administration, clinical trials, etc. were applied manually to down-select to 214 drugs based on rank scores. During this process, the library of which were then sorted An in-depth study of each class of shortlisted drugs was performed, and top 12 drugs have been selected for further confirmatory studies in various organoid/tissue models.

We will be using an 'omics-based analysis and data machine learning to measure how these drugs impact on (a) viral replication, (b) host-cell responses and (c) SARS-CoV-2 induced damage to tissues. Using systems biology-augmented, stem cell-derived, multi-tissue panel for rapid screening of approved drugs, we aim to select the three most promising therapeutic candidates to Phase II/III human clinical trials as potential COVID-19 treatments.

Keywords: antivirals; COVID-19; databases; down-selection; drugs; repurposing; SARS-CoV-2; variants, organoid models, systems biology

Glycolysis and oxidative stress related redox pathway upregulation along the gut-liver axis by gut microbial perturbation and host response during giardiasis in C57BL/6J mouse model

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Session Theme: *Health and Precision Medicine*

Abstract: Apicomplexan infections such as giardiasis and cryptosporidiosis negatively affect a considerable number of human and commercial livestock. Unlike bacterial infections, their molecular mechanism, particularly, how they affect the body beyond the intestinal tract is still not poorly understood. To highlight the biochemical interactions, we utilized integrated 16S rRNA genomics-metabolomics, and proteomics-metabolomics approaches on a C57BL/6J mouse model during giardiasis, with respect to cryptosporidiosis and Uropathogenic *E. coli* (UPEC) infection. Faeces, blood, liver tissues and luminal contents were collected 10 days post infection and subjected to proteome and metabolome analysis on liquid and gas chromatographic mass-spectrometry techniques, respectively. Proteome-metabolome analyses indicated 12 and 16 key pathways to be significantly altered across gut and liver, respectively. Energy pathways such as glycolysis along the supporting pathways such as glyoxylate and dicarboxylate metabolism and, redox pathway of glutathione metabolism as a response to oxidative stress, were upregulated particularly in small intestine and liver, during giardiasis. Metabolomics-16S rRNA genetics integration indicated the populations of 3 bacterial families, causing an upregulated glycolysis and short-chained fatty acid (SCFA) metabolism in gut. Overall, the Systems Biology approach indicated the effects of host-parasite-microbiome biochemical interactions on not only the gut ecosystem, but also on the gut-liver axis and circulatory system.

Keywords: Host-parasite Interactions; Integrated Multiomics; Giardiasis.

Biorecycling and bioremediation of plastics and plasticizers by thermophilic enzymes from the Great Australian Artesian Basin

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Session Theme: *Synthetic Biology, Environmental Sciences & Ecosystem Surveillance,*

Abstract: Plastics pose both a sustainability and environmental issue. plastics are a limited resource as they are dependent on fossil fuel reserves, and so recycling we be evermore necessary. Current methods of recycling require pure plastic feedstocks to be economically feasible. Enzymatic biorecycling would be a complimentary recycling strategy that could circumvent the sorting needed in traditional recycling. Genomes of thermophilic organisms Meiothermus ruber and a Bacillus sp. from the Great Australian Artesian Basin (GAB) were blasted against a literature of plastic degrading enzymes. Many candidates were chosen, rank ordered, codon optimized, cloned, expressed, characterized, and tested on plastics/plasticizers. Para-nitrobenzyl (PNB) esterase has the capability to hydrolyze polybutylene adipate terephthalate (PBAT) to its monomers, and hydrolyze Di-isobutyl phthalate (DiBP). PNB esterase is a promising candidate for biorecycling of (PBAT), and bioremediation of DiBP. It is a novel thermophilic enzyme that can be produced up to 1 liter scale. PNBE is a promising candidate for biorecycling PBAT and similar polymers, it also has additional bioremediation applications. With further development in its thermophily, binding, compatibility, and production, PNB esterase shows promise for developing a plastic biorecycling circular economy. Hopefully this will incentivize better landfill waste management and cleanup of plastics in ecosystems.

Keywords: Bioremediation, Biorecycling, Biodegradation, Plastics, Plasticizers, Thermophiles, Enzymes, Biotechnology, circular economy, sustainability.

The role of DLD in the toxicity and resistance mechanism of phosphine gas in *Caenorhabditis elegans*

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Session Theme: *Food and Agriculture*

Abstract: Phosphine (PH_3) fumigation is considered the most widespread method of grain pesticide control in the world. A growing number of insect species have developed a high level of resistance against PH_3, threatening global food security and grain supply. The decrease of PH_3 toxicity in resistant insect species has been traced back to variants of a key enzyme in energy metabolism, dihydrolipoamide dehydrogenase (DLD). Especially insect species, including the model organism *Caenorhabditis elegans* (*C.elegans*), carrying the *dld-1* protein variant of DLD display a high level of PH_3 resistance. Here, we show the study design to use gene expression analysis and NMR-based metabolomics to investigate the phosphine response in wild-type *C. elegans* and the phosphine-resistant CRISPR mutant strain *dld- 1(wr5)*. The objective of this study is to better understand the DLD-mediated phosphine toxicity and resistance mechanism in *C. elegans*.

Keywords: toxicology; phosphine; phosphine-resistance; *C.elegans*; dihydrolipoamide dehydrogenase; energy metabolism

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