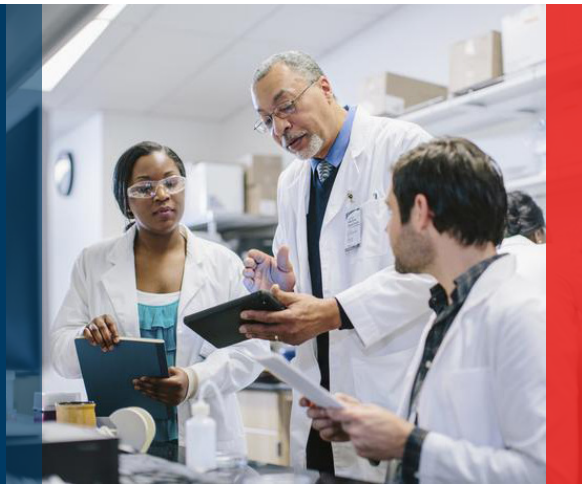
Agilent Global Partner Universities Academic Drug Discovery Virtual Symposium

On-demand



Imperial College London

NUS National University of Singapore

USC Michelson Center for Convergent Bioscience

Symposium agenda

This on-demand event is your opportunity to hear the latest on what leading researchers and labs are doing to keep pace.

Your registration gives you access to all the following sessions and exhibitions:

Development and Manufacturing of New Therapeutics

Introduction/Welcome
Mike McMullen, Chief Executive Officer and Darlene Solomon, Chief Technical Officer

Process Control in the Manufacture of Macromolecular Therapeutics
Cleo Kontoravdi, Professor, Dept. of Chemical Engineering, Imperial College London

Commercial manufacture of macromolecular therapeutics typically involves their synthesis in living cells. This introduces significant challenges in terms of our ability to obtain real-time information on the state of the system and, in turn, to exert process control. In this talk, we will present a hybrid approach that uses mathematical modeling alongside obtaining key process and cellular measurements to guide the design of optimal manufacturing strategies.

Precision Drug Delivery Through Continuous Sensing of Tissue Concentrations
Richard Wilson, Senior Healthcare Research Scientist, Centre for Antimicrobial Optimisation, Imperial College London

In this presentation, we will describe our current research on personalized antibiotic treatments through their continuous sensing in dermal interstitial fluid (ISF). Validation of the sensors is demonstrated through concomitant sampling and LC/MS analysis of both ISF and venous blood. The results show that the former tracks changes in the latter albeit at a lower concentration and with a lag in its time course.

Building O-GlcNAc-Modified Proteins to Understand the Neurodegeneration Drug Candidate MK-8719
Matthew Pratt, Professor of Chemistry, University of Southern California

MK-8719 is one of several drug candidates in development that increase the levels of the intracellular glycosylation, termed O-GlcNAc. Preclinical models of Alzheimer's and Parkinson's disease have demonstrated that increased O-GlcNAc is protective against neurodegeneration; however, the precise mechanisms explaining this observation still need to be fully understood. In this presentation, we will describe how we use synthetic protein chemistry to build homogeneous O-GlcNAc-modified proteins and what we have learned about its functions in amyloid aggregation.

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Directed Evolution of Peptide Ligands for Neurobiology and Cancer

Richard W. Roberts, Professor of Chemistry, Chemical Engineering, and Materials Science and Co-Director of Agilent Center of Excellence for Biomolecular Characterization, University of Southern California

This presentation will cover the development, synthesis, and testing of new peptide-based probes for Huntington's disease. We will cover work using mRNA display to develop peptides directed at early intermediates in huntingtin misfolding. Additionally, we will cover synthesis and biological expression of these molecules toward developing diagnostics and therapeutics.

Considerations in the Development, Characterization, and Measurements of New Approaches to Decipher Biological Pathways

Aptamers in Drug Discovery

Tony Cass, Professor of Chemistry, Department of Chemistry, Imperial College London

DNA and RNA aptamers are synthetic single stranded nucleic acids selected from large random libraries and have binding specificities and affinities comparable to antibodies whilst being much smaller molecules. They are versatile reagents with numerous applications in both the diagnosis and to a lesser extent treatment of disease. In this presentation, I will describe some of the applications that we have developed and also where they offer new opportunities in drug discovery.

Metal Complexes as Cellular Probes and Potential Therapeutic Agents

Ramon Vilar, Professor, Department of Chemistry, Imperial College London

Due to the unique properties (e.g., optical, magnetic, redox, etc.) of metal complexes, there is great interest in exploring their use in medicinal inorganic chemistry. In addition, due to the broad range of coordination geometries, metal complexes can display unique structures not easily accessible with purely organic molecules. This in turn can be used to generate unique fragments for drug discovery and the development of probes. Using the above, our group explores the interactions of metal complexes with various biomolecules including non-canonical DNA structures (e.g., quadruplexes), enzymes (e.g., phosphatases) and peptides (e.g., amyloid beta). Our aim is to exploit the properties of the metal complexes to develop novel probes and potential therapeutic agents.

Identification of Lipid Biomarkers for Risk Stratification of Vascular Conditions in the Emergency Department

Jing Kai, Graduate Student Singapore Lipidomics Incubator, National University of Singapore

In this presentation, we will talk about a prospective cohort study to be conducted on patients who visit the Emergency Department (ED) at National University Hospital (NUH), which involves the measurement and quantification of biologically significant lipids in plasma using a range of lipidomics methods on the Agilent QQQ and QTOF. Key lipidomics signatures associated with vascular and inflammatory outcomes will be determined using a series of statistical methods and may potentially be used by clinicians as biomarkers for risk stratification of vascular and inflammatory conditions in the ED.

Human Blood Plasma Lipidomics – Reference Materials and Biological Reference Ranges

Markus Wenk, Professor, Federico Torta, Research Assistant Professor, and Amaury Cazenave-Gassiot, Research Assistant Professor, National University of Singapore

Recently, members of several research groups specialized in various lipid chemistries met to find ways to better harmonize studies of the human plasma lipidome. The group settled on ceramides as the first class of molecules to be measured, as they have roles in disease and are thought to be abundant, stable, and easy to isolate. A ring trial was launched, distributing the NIST SRM 1950 plasma, and three other new reference materials, to about 30 participant labs around the world. More trials are following, with the aim of measuring absolute concentrations of other lipid classes in reference materials. After this first stage, phase two of the project will involve collecting samples from different human cohorts and measuring the same lipids, and generating reference ranges in healthy and disease conditions, to drive a transition toward the clinical use of lipidomics.

Using Systems Biology to Accelerate New Therapeutics Development

Spying on Biological Systems with New Chemistry

Valery V. Fokin, Professor of Chemistry and Co-Director of Agilent Center of Excellence for Biomolecular Characterization, University of Southern California

This presentation will focus on development and applications of biorthogonal reactions to the study of complex biological systems. Examples of selective covalent modifications of proteins, cellular and organismal imaging, and cell targeting will be highlighted.

A Resurgence in Nanoparticles: A Path Toward the Clinical Translation of New Nano-Based Imaging Strategies

Cristina Zavaleta, Assistant Professor of Biomedical Engineering, University of Southern California

In this talk, we will discuss the potential hindrances toward the clinical translation of nanoparticles and alternative strategies we are taking to accelerate their utility in the clinic. We will also highlight the ongoing research in our lab that utilizes novel imaging techniques to assess their toxicity and follow their distribution in the body post administration which will be essential for regulatory approval. With the recent success of nano-based vaccines, now is the perfect time to envision other clinical avenues for nanoparticles to improve human health.

Predicting Drug Effectiveness with Deep Phenotyping of Drug Metabolism and Biological Response

Chester Lee Drum, Assistant Professor, Department of Medicine, Yong Loo Lin School of Medicine, National University of Singapore

We are presenting a study aimed at determining the effect of plasma Atorvastatin (ATV) and its major metabolites exposure and UGT1A1 rs4148323 (211G>A) on mortality in a real-world cohort of patients on single-dose ATV (N=874). Plasma concentrations of ATV and its major metabolites (active hydroxy-acid and inactive lactone) were measured using a targeted LC/MS/MS method to detect potential quantifiable biomarkers. In conjunction with genotyping strategies, we describe how this approach may be a novel strategy to guide personalized ATV therapy.

Accelerating Cannabinoid Therapeutic Development: Non-Canonical Biochemical Definitions Realized Through the NUS-Agilent Hub

Wen Shan Yew, Associate Professor, National University of Singapore/NUS-Agilent Hub

In this presentation, we will describe the discovery of noncanonical cannabinoid synthases obtained from non-cannabis plants for the sustainable production of cannabinoids for therapeutic needs. Using the Agilent RapidFire-High-throughput-MS-System, new enzymes that can advance the molecular production of cannabinoid molecules that exist in nature, but wherein there are no known molecular tools or enzymes to biosynthesize them, can be defined. Conceptually, this work also advances the approach to biosynthesize natural products that otherwise are refractory to bioproduction due to the lack of suitably identified enzymes in various biosynthetic pathways.

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RA44573.0089699074

Published in the USA, February 16, 2022