DISCOVERY US 2024

BY OXFORD GLOBAL

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07 - 08 November 2024 | Boston, MA

Connecting leading experts in biology & chemistry to advance small molecule drug discovery: the exclusive forum to keep up with the latest innovations tackling the previously 'undruggable'



Content Tracks



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200+ Attendees

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45+ Industry-Leading Speakers Including...



GRAHAM DEMPSEY, Founder & Chief Scientific Officer, **Quiver Bioscience**



HONG CHENG, Vice President, Head of Research Strategy, Sanofi



PAUL SCOLA, Senior Director - Chemistry, **Bristol Myers Squibb**



FIONA MACK. Vice President & Head,



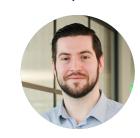
JULIE OWEN, Director of Chemistry, Recursion **Pharmaceuticals**



JULIA FOX, Director - Data & Analytics, Takeda



IVAN CORNELLA, Chief Scientific Officer, Covant **Therapeutics**



MARTIN REDHEAD, Associate Vice President. Exscientia



GIOVANNI PIEDIMONTE, Vice President for Research & Professor of Pediatrics, Biochemistry & Molecular Biology, Tulane University

WELCOME TO Discovery US 2024

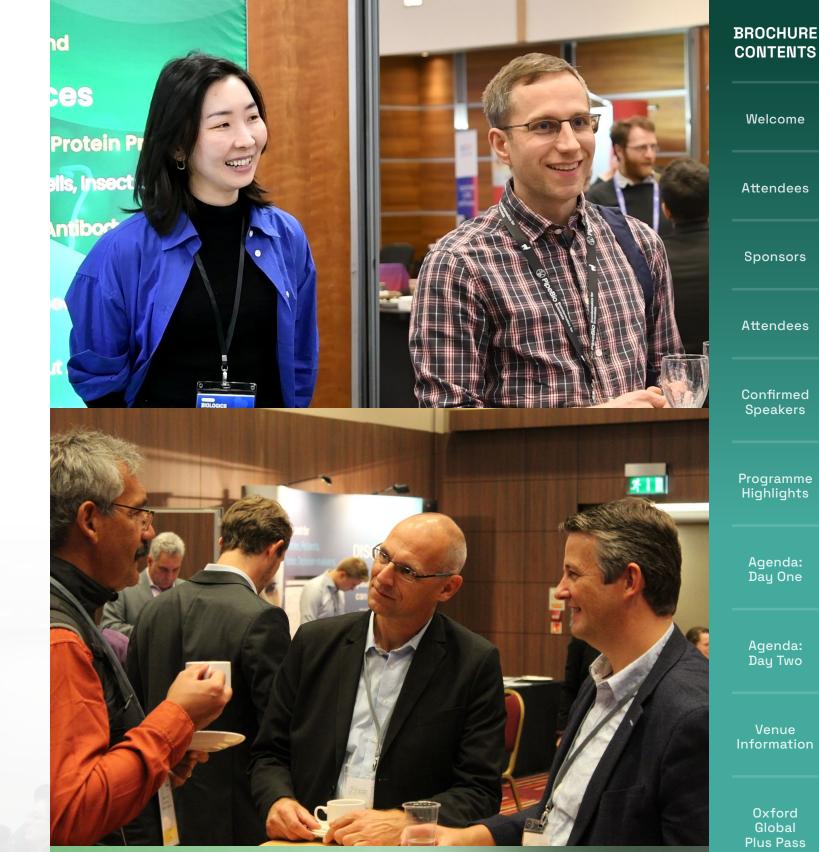
Discovering novel targets & modalities has been at the forefront of a lot of early R&D pipelines, but keeping this momentum requires the strategy to match. Collaboration across industry & academia is paramount to develop these new methods & techniques and to inspire new avenues of innovation - but the question is where do we go now?

This is central to Discovery US - regardless of stage, modality or disease area, we're here to help you outline a strategy to advance your R&D. By connecting you with VPs, Directors and relevant solution providers, we want to celebrate your innovative approaches & triumphs, ultimately to keep these small molecule

medicines in the spotlight and aid in the development of life-saving treatments for those with critical illnesses.

Jessica Thomson

Portfolio Director, Discovery & Development Oxford Global



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Why Attend?

- Benchmark against the industry leaders, thanks to our revamped program! Our new agenda will provide exclusive insights into the latest technologies, platforms & modalities transforming the industry across 45+ presentations
- Keep your R&D innovative with emerging drug targets and novel modalities, with talks on PROTACS & molecular glues through to orally available peptides & macrocycles
- Hear how to utilize Al & automation in your lab to increase productivity focusing on how Al is taking the drug discovery industry by storm and the development of machine learning & automation for efficient drug discovery processes
- Learn how to leverage computational techniques to benefit your pipeline, with a specific track to highlight advancements within medicinal & computational chemistry
- Have your burning questions answered by the key opinion leaders as part of our interactive panel & roundtable sessions & networking breaks, including spotlights on the fundamentals of Al & novel Hit identification techniques



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At Oxford Global, our mission is to curate personalized experiences that foster community and inspire innovation.

We believe in the power of networking, connection, and knowledge to deliver quality products and services that exceed expectations. Partnering with Oxford Global means having a dedicated team committed to helping you achieve your goals and navigating the industry's ever-changing landscape.

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Wat Panel & Roundtable Discussions

Feature alongside key opinion leaders to discuss current hot topics and highlight your company's expertise.

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250+ VPs, Directors & Senior Managers will be attending onsite and online, coming from leading healthcare, biotech, pharma & research institutions in the following fields & more

- Drug discovery
- Target discovery
- Disease modelling
- Artificial intelligence
- Machine learning
- ADMET
- Medicinal chemistry
- Computational chemistry
- Lead discovery
- Hit identification
- Screening
 - Drug Design Biophysics
 - Computational biology
 - Data science

Formal & informal meeting opportunities offer delegates the chance to discuss key solutions with leading service providers. Formal 1-2-1 meetings will be available to arrange prior to the event which take place during the dedicated networking breaks covering:

- Target validation
- Screening technologies
- Organoids
- Library optimization
- Small molecule discovery
- Computational platforms
- Organic synthesis
- Generative Al
- - Stem cells
- Cell-based assays
 - AI/ML
 - Data analysis tools

Attended by these companies & many more:























Exscientia

Previous Attendee Profile:

Function

Geography

Sector

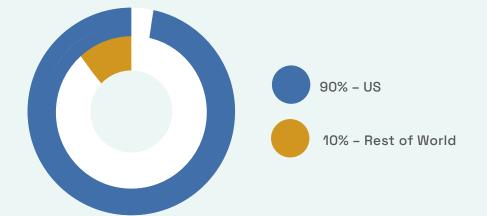
Manager/Senior - 26%

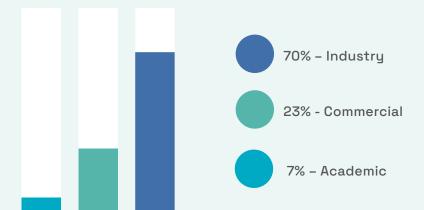
Director - 25%

Scientist - 22%

C-Level - 18%

Head/Lead - 9%





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GAIN EXPERTISE FROM THOUGHT LEADERS

Confirmed Speakers



HONG CHENG, Vice President, Head of Research Strategy, Sanofi



Day One | 09:30

MARTIN REDHEAD, Associate Vice President, Exscientia



Day One | 17:45

JULIA FOX, Director - Data & Analytics, Takeda



Day One | 9:50

IVAN CORNELLA Chief Scientific Officer, Covant Therapeutics



Day One | 12:25

FIONA MACK, Vice President & Head Co.Lab Cambridge, Bayer



GRAHAM DEMPSEY, Founder & Chief Scientific Officer, Quiver Bioscience

GRAHAM DEMPSEY

Founder & Chief Scientific Officer, Quiver Bioscience

IVAN CORNELLA

Chief Scientific Officer, Covant Therapeutics

HONG CHENG

Vice President, Head of Research Strategy, Sanofi

RICK EWING

Vice President & Head of Chemistry, Rapafusyn **Pharmaceuticals**

FIONA MACK

Vice President & Head, Cell & Gene Therapy Co.Lab Cambridge, Bayer

MARTIN REDHEAD

Associate Vice President, Exscientia

GVIDO CEBERS

Global Head of Drug Safety & Evaluation, Takeda

PAUL SCOLA

Senior Director, Discovery Sciences, Bristol Myers Squibb

NICHOLAS LARSEN

Senior Director of Lead Discovery, Kestrel Therapeutics

BOGUSLAW NOCEK

Senior Director – Structural Biology, Eli Lilly

NOEL POWELL

Senior Director - Medicinal Chemistry, **Recursion Pharmaceuticals**

AARON VAN HOOSER

Senior Director, Head of Computational Biology, Sensorium Therapeutics

IASON EKERT

Head of US Translational Technology, UCB

DIVYA KANICHAR

Director, Insitro

JULIA FOX

Director - Data & Analytics, Takeda

IONATHAN SOLOMON

Director, Novartis

ARI ALLYN-FEUER

Director, Al Product, GSK

IENNIFER BUSBY

Director - Biology, Exscientia

JULIE OWEN

Director of Chemistry, Recursion Pharmaceuticals

KIAN TAN

Director, Novartis

MELISSA FORD

Associate Director, Computational Chemistry, **Kymera Therapeutics**

CHRISTOPHER HICKEY

Associate Director, Arvinas

ANNEKE DEN HOLLANDER

Head of Functional Genomics, AbbVie

ELENA DOLGIKH

Head of Computational Chemistry, Monte Rosa Therapeutics

ABHIJAT VATSYAYAN

Head of Artificial Intelligence & Innovation, Taiho Oncology

SATYAJIT RAJAPURKAR

Investigator, GSK

SARAH WILSON

Principal Research Scientist, AbbVie

KRISTEN MARINO

Principal Scientist, Computational Chemistry, Cellarity

JUDITH RONAU

Senior Scientist II, AbbVie

NOA LIBERMAN-ISAKOV

Senior Scientist, Discovery Research, Sarepta Therapeutics

YUNHUI GE

Scientist, Alkermes

GIOVANNI PIEDIMONTE

Vice President for Research & Professor of Pediatrics, Biochemistry and Molecular Biology, **Tulane University**

IOSEPH WU

Professor and Director, Stanford Cardiovascular Institute & Co-Founder, Greenstone Biosciences

ILKAY US

Director - High Throughput Screening, Weill Cornell Medicine

PRASHANT GAHTORI

Professor of Medicinal Chemistry, Graphic Era Hill University

JAMES HICKMAN

Professor of NanoScience Technology Center, University of Central Florida

DIMA KOZAKOV

Professor, Stony Brook University

MICHAEL BREHM

Associate Professor & Associate Director, Diabetes Center of Excellence, UMass Medical School

JOSE MUNOZ

Associate Principal Scientist, LifeMine Therapeutics

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DAY ONE OVERVIEW

Thursday 07 November 2024

On Day One, key talks will enlighten you on the emerging drug targets & novel modalities gaining popularity, the utilization of complex disease models (like organoids, organ-on-chips and iPSCs) to understand disease mechanism & safety, as well as how Al & automation are revolutionizing R&D – all addressing challenges perhaps seen in traditional approaches to target discovery & drug design.



EXPLORE CURATED & INSIGHTFUL CONTENT

Agenda At A Glance

Track 1: Target Identification & Validation Of Novel Modalities

- Identification and validation of emerging drug targets, including: PROTACs, Induced Proximity, Molecular Glues, siRNAs, Orally Available Peptides, Radioligands, Macrocycles and more
- How do we assay & compute novel compounds?
- Predicting PK/PD properties
- Utilizing functional genomics & CRISPR to validate novel targets

Track 2: Novel Models For ADME-Tox Research & Disease Modelling

- Organ-on-a-chip & organoid models, including applications within neuroscience
- Using cellular technologies to understand disease mechanism & assess potential drug candidates
- In-silico predictions
- Complex models to investigate ADME-Tox properties
- iPSC-derived cells for drug discovery
- Synthetic biology for regenerative medicine

Track 3: Augmenting R&D With AI & Automation

- How can AI & automation be used to augment R&D and address challenges in target discovery, drug design and product development
- Enhanced data analytic tools to extract knowledge from data
- Generative AI for drug discovery & to improve efficiencies
- Utilizing Al to improve fast decision-making
- Overcoming sparsity of data to ensure meaningful outputs
- Lab robotic systems for drug discovery
- Maximizing R&D through cloud-based control and automation of scientific workflows
- Adoption of digital tools & technologies in labs
- Complementary use of genomic technologies with AI/ML

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DAY TWO OVERVIEW

Friday 08 November 2024

Day Two offers 2 more tracks of exclusive talks & discussions, from novel Hit identification & screening technologies and new approaches in computational chemistry to where we are with fragment & structure-based drug design.





Track 1: Innovative Technologies For Hit Identification & Screening

- Molecular Target-Based Screening: hit finding for known targets to understand function, how to modulate & how to inhibit
- Phenotypic Screening: hit finding for unknown targets, including identifying molecular targets & understanding unknown mechanisms of actions
- Affinity/binding assays for hit ID, including functional assays, mass spectrometry, biophysical approaches, DNA-encoded libraries, high content imaging & computational screening

Track 2: Computational & Medicinal Chemistry

- · New approaches in Computer-aided drug design
- Predicting & Measuring PK/PD
- Quantum mechanics in drug discovery
- Fragment & Structure based drug design, including Cryo-EM applications
- Biocatalysis for pharmaceutical synthesis & drug discovery
- Utilizing high-quality chemical probes

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07:25 **Registration Opens & Welcome Refreshments**

Oxford Global's Welcome Address

Keynote Address: A Paradigm Shift In Pharmaceutical R&D

Delegates are welcome to attend co-located sessions

• The pharmaceutical industry faces soaring R&D costs with only incremental gains in new drug launches. This talk offers a system-dynamic perspective to uncover the root causes of these productivity challenges and introduces a fresh, strategically balanced internal and external approach to enhance overall R&D productivity in pharma

HONG CHENG, Vice President, Head of Research Strategy,

Sanofi

09:00

09:25

	TRACK 1: TARGET IDENTIFICATION & VALIDATION OF NOVEL MODALITIES	TRACK 2: NOVEL MODELS FOR ADME-TOX RESEARCH & DISEASE MODELLING	TRACK 3: AUGMENTING R&D WITH AI & AUTOMATION
	Morning Track Chair: DIVYA KANICHAR, Director, Insitro	Track Chair: MICHAEL BREHM, Associate Professor & Associate Director, Diabetes Center of Excellence, UMass Medical School	Track Chair: ELENA DOLGIKH, Head of Computational Chemistry, Monte Rosa Therapeutics
00	Discovery Of A Macrocyclic Peptide Inhibitor Of Programmed Death-Ligand 1 (PD-L1) • A macrocyclic peptide was identified as an inhibitor of PD-L1 through an in vitro selection process. A co-crystal structure of this macrocycle with PD-L1 enabled rapid optimization of this series with respect to PD-L1 inhibitory activity, while also providing insight as to strategies to mitigate off-target liabilities, ultimately yielding BMS-986189. This lead macrocycle progressed to the clinic, where PK/PD was evaluated in normal healthy volunteers. Details of these discoveries will be discussed.	 Organ-On-Chip & Organoid Applications In Viral Infections Human lung organoid models that allow for the first time the exploration of the effects of vertically transmitted viruses on the cellular and molecular architecture of fetal lungs. Nerve-on-a-chip microphysiological models exploring the direct effects of viruses on peripheral nerve structure and function. Future opportunities for using these models for high-throughput screening of new antiviral therapeutics. 	 The Challenges Of Working With Al & Innovation In Pharma Al has been a prominent topic in pharma for decades, with the potential for success always within reach but not fully realized. While there have been some noteworthy achievements, the anticipated large-scale impact has yet to be seen. However, there are signs of change. This presentation will provide a candid perspective on why Al has not yet reached its potential in pharma, identify the key opportunities ahead, and outline the path to success. We will delve into why many machine learning approaches haven't worked in pharma, contrast this with the successes of deep learning in other domains, and explore the specific challenges of applying deep learning to pharmaceutical research. Additionally, we'll discuss the limitations of traditional IT engagement models in pharma, using Taiho as a case study for how innovative approaches can overcome these challenges and drive meaningful change
	PAUL SCOLA, Senior Director, Discovery Sciences, Bristol Myers Squibb	GIOVANNI PIEDIMONTE, Vice President for Research & Professor of Pediatrics, Biochemistry and Molecular Biology, Tulane University	ABHIJAT VATSYAYAN, Head of Artificial Intelligence & Innovation, Taiho Oncology

Q&A session & transition time between conference rooms

Overcoming Your Drug Metabolism Challenges Using Mechanistic In Silico Models

- In silico metabolism prediction can address critical questions to guide lead optimisation.
 Using several case studies, we demonstrate the application of these models to address design challenges involving metabolic (in)stability, the formation of reactive and/or toxic intermediates, and to mitigate the risk of genetic polymorphisms and drug-drug interations. In addition, we illustrate how these models can inform the selection of in vitro and in vivo pre-clinical experiments to avoid surprises in late-stage trials. Furthermore, accurate predictions of metabolite profiles early in the discovery process provide essential guidance for drug design. Optibrium's mechanistic metabolism models cover metabolism by P450, AOX, FMO, UGT, and SULT enzymes [1-4]. By combining these models, metabolic pathway analysis proposes the most likely metabolites with greater precision than other methods, assisting in metabolite identification studies and enabling potentially active, reactive, or toxic metabolites to be identified [5].
- [1] Mario Öeren, Peter J. Walton, James Suri, David J. Ponting, Peter A. Hunt and Matthew D. Segall, (2022) J. Med. Chem. 65(20) pp. 1406-1408
- [2] Mario Öeren, Sylvia C. Kaempf, David J. Ponting, Peter A. Hunt and Matthew D. Segall, (2023) J. Chem. Inf. Model. 63(11) pp. 3340-3349
- [3]Mario Öeren, Peter J. Walton, Peter A. Hunt, David J. Ponting and Matthew D. Segall, (2021) J. Comput.-Aided Mol. Des. 35(4) pp. 541-555
 [4] Jonathan D. Tyzack, Peter A. Hunt and Matthew D. Segall, (2016) J. Chem. Inf. Model. 56(1)
- pp. 2180-2193
 [5] Mario Öeren, Peter A. Hunt, Charlotte E. Wharrick, Hamed Tabatabaei Ghomi and Mat-
- [5] Mario Oeren, Peter A. Hunt, Charlotte E. Wharrick, Hamed Tabatabaei Ghomi and Matthew D. Segall, (2023) Xenobiotica DOI: 10.1080/00498254.2023.2284251

MATTHEW SEGALL, Chief Executive Officer, **Optibrium**



Reality of Al Drug Discovery: Revolution Or Pandora's Box

• This presentation delves into the journey of XtalPi's five-year practice of Al Drug Discovery through the sharing of case studies, aiming to present the current state of AlDD to the audience. We'll demonstrate how XtalPi utilizes Al and automation approach to drive innovation and efficiency in specific drug discovery projects, and try to address a question: is AlDD a revolution or Pandora's Box?

ZHIXIONG LIN, Head of Al Drug Discovery, **Xtalpi**



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## OF NOVEL MODALITIES & DISEASE MODELLING ### Harnessing Covalency To Target Native Disease Proteoforms ### Synthetic Biology & Programmable Organoids For Drug Discovery & An Al-Driven DMTA Loop For Drug ### Proposetive Medicine*	
Covalency is uniquely positioned to expand the druggable target space, increasing the repertoire of mechanisms of action for thousands of disease-associated proteins Covalency can help to address key challenges in drug discovery, through augmented target occupancy and selectivity O9:50 O9:50 RON WEISS, Director of Synthetic Biology Center & Professor of Biological Engineering, MARTIN REDHEAD, Associate Vice Presic	d a huge impact on the way drugs are designed, moving through clinical development. Despite the gs, this has not yet been transferred to the "make"-make-test-learn" (DMTL) loop, which underpins early POC to clinical candidate. Anchoring machine that and DMTL enables this. In order to extend the have developed a state-of-the-art automated lab to bur Al platform designs. In all synthesis platform, automated purification, eenhanced our design software to better predict ated chemical synthesis in mind. The chemistry ological testing platform, supporting biochemical latform enables fully automated lab processes that y development is fully online and the system can highly skilled scientists to focus on complex experintiation. In omnics of early discovery, allowing work to start on the enables of the process of the biological, chemical as rapidly building Al training sets for previously
IVAN CORNELLA, Chief Scientific Officer, Covant Therapeutics Massachusetts Institute of Technology Exscientia	
MORNING COFFEE & REFRESHMENTS 1-2-1 Meetings x4 Poster Displays	
• It's impossible to experimentally measure drug discovery project. Furthermore, the I mental variability and error. However, Al offer valuable insights and guide research • We will describe an Al platform, Cerella ^m , from both structure-activity relationships experimental endpoints based on sparse light high-quality compounds by 'filing in' quantitative structure-activity relationship, den opportunity acts caused by missing, unctal resources by focussing on measuring to a caused by missing, unctal resources by focussing on measuring to a form of the progression. [1] Irwin et al. Ap MATTHEW SEGALL, Chief Executive Office Optibrium	that applies deep learning imputation to learn (SAR) and directly from the relationship between edata [1]. The resulting models can proactively high- if missing data more accurately than conventional p (QSAR) models. Furthermore, it can identify hid- certain or inaccurate data, and prioritise experimenthe most valuable data to inform decisions about op. Al Lett. (2021) DOI: 10.1002/ail2.31
Q&A session & transition time between conference rooms	
Evaluation Of Human Relevant In Vitro Models Enabling Cardiac And Skeletal Phenotype Of Myotonic Dystrophy 1 Development of relevant human in vitro models: discuss the use of patient derived iPSC cells to create 2D and 3D models for studying DM1. Functional Assessments: highlight techniques for evaluating calcium handling, contractile force, and electrophysiological properties in both cardiac and skeletal models. Applications and Future Directions: emphasize the use of these models for drug screening and potential therapies. Biological Sequence Learning Is A Contractive of Review of GSK's Seneca and Exonnet models and Evaluating calcium handling, contractile force, and electrophysiological properties in both cardiac and skeletal models. Applications and Future Directions: emphasize the use of these models for drug screening and potential therapies.	dels

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	Fostering Early-Stage Innovation: Bayer Co.Lab	Stem Cells, Genomics, And Al/ML For Drug Discovery	Panel Discussion: The Fundamentals Of Al
12:25	 Bringing emerging targets & modalities into the pipeline Supporting early-stage biotechnology, startup & academic innovations Challenges & opportunities 	 Highlight the world's largest iPSC bioank with 2500+ lines. Review examples of iPSCs for disease modeling and drug screen. Develop screening assays for anti-fibrotic drug therapies. 	 The promise of AI Should we prioritize investing in LLM-based productivity and efficiency opportunities over developing deep learning models for chemistry and biology? How can we develop foundational models for biology and chemistry similar to those in other
	FIONA MACK, Vice President & Head Co. Lab Cambridge, Bayer	JOSEPH WU, Professor and Director, Stanford Cardiovascular Institute & Co-Founder, Greenstone Biosciences	fields?
	Q&A session & transition time between conference rooms		
	Utilizing CRISPR And Chemogenomics Screens With Al Tools To Validate Novel Targets	Development and Validation of a High-Throughput Drug Screening Platform Using Patient-Derived Tumor Organoids From Gastrointestinal Malignancies: Integrating Clinical And Genomic Correlations	
	Rapid validation of biological targets arising from multiple functions is made possible by Exscientia's Al tools and automated screening platform	• A diverse collection of 250+ organoid lines in our biobank	
12:50			Moderator: ABHIJAT VATSYAYAN, Head of Artificial Intelligence & Innovation, Taiho Oncology Panellists: KIAN TAN, Director, Novartis ELENA DOLGIKH, Head of Computational Chemistry, Monte Rosa Therapeutics
	JENNIFER BUSBY, Director – Biology, Exscientia	ILKAY US, Director – High Throughput Screening, Weill Cornell Medicine	ARI ALLYN-FEUER, Director, AI Product, GSK TUDOR OPREA, Chief Executive Officer, Expert Systems
13:15	LUNCH BREAK 1-2-1 Meetings x3	Poster Displays	
	Afternoon Track Chair: JENNIFER BUSBY, Director - Biology, Excientia	Track Chair: MICHAEL BREHM, Associate Professor & Associate Director, Diabetes Center of Excellence, UMass Medical School	Afternoon Track Chair: GIOVANNI PIEDIMONTE, Vice President for Research & Professor of Pediatrics, Biochemistry and Molecular Biology, Tulane University
		Navigating Target Safety With Multimodal Data And Al-Enhanced Predictions	Augmenting R&D With AI & Automation
		 Understanding target safety is crucial for avoiding costly later attrition and improving patient outcomes. However, safety assessments are typically manual and fall out of date. Meanwhile, the exponential growth of data across diverse experimental modalities presents both challenges and opportunities in biomedical research. In this talk, we share our novel approaches for predicting clinically relevant outcomes, specifically cardiotoxicity, using multiple datasets and a harmonized quantitative approach, using real examples. Our in silico prediction model demonstrates potential for increasing the reliability of early 	During the talk an overview will be given of trends in Automation and Digitization of laboratories. This will include not only automation of unit operations but also making sure the data is well protected and accessible for AI algorithms so these can suggest the next experiments
14:15	Delegates are welcome to attend co-located sessions	drug discovery discovery, bridging critical gaps between preclinical research and clinical application	
		JOSH ALMOND-THYNNE, Co-Founder Sable	JOS DE KEIJZER, Head Workflow Architect, ChemSpeed Technologies
		Sable®	CHEMSPEED

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TRACK 2: NOVEL MODELS FOR ADME-TOX RESEARCH
& DISEASE MODELLING

TRACK 1: TARGET IDENTIFICATION & VALIDATION OF NOVEL MODALITIES

			Robust Datasets For ML-Driven Drug Discovery
14:40	Delegates are welcome to attend co-located sessions	Delegates are welcome to attend co-located sessions	 The application of artificial intelligence (AI) in drug discovery is heavily dependent on the quality and reproducibility of training datasets. Robotics has emerged as a crucial enabler for generating large volumes of high-quality data to fuel machine learning (ML) algorithms. In this case study we ran for Isomorphic Labs, we present the development of a comprehensive technology platform that combines robotic assay platforms with automated analytics pipelines to streamline the data generation and analysis process for ML-driven drug discovery. The initial predicted potencies exhibited a strong correlation with the confirmed potencies, demonstrating the reliability of the generated data. We highlight the importance of assay precision and quality to fully exploit the potential of ML in drug discovery. Furthermore, we showcase the advantages of activity-based profiling, which provides immediate indications of compound activity, in contrast to affinity-based methods such as surface plasmon resonance (SPR). Activity-based profiling facilitates the identification of functionally relevant hits, enhancing the efficiency of the drug discovery process. The integration of automated analytics pipelines enables rapid data processing, rigorous statistical treatment, generation of 'gold standard' ML-ready datasets and reduces the time and effort required for data analysis. Our findings emphasise the significance of data volume, quality, and automated analytics for successful ML applications in drug discovery, and the pivotal role of robotics in achieving these requirements. By leveraging high-throughput, high-quality data generation through robotic assay platforms and automated analytics pipelines, we can accelerate the development of novel therapeutics and optimise the drug discovery workflow KINGA BERCSENYI, Chief Business Officer
			Arctoris
			ARCTORIS
		Q&A session & transition time between conference rooms	
	Targeted Protein Degradation By PROTAC Degraders	Organ-On-Chip & MPS Systems For Neurodegenerative Diseases	Al Is Not Taking Over The World, But I Still Love My Roomba: Applying Machine Learning And Automation In Drug Discovery
15:05	 Mechanisms of Targeted Protein Degradation, including PROTACs. PROTACs that co-opt the E3 ligase KLHDC2. PROTACs targeting LRRK2 as potential disease modifying therapeutics for neurodegenerative diseases 	 How neurological disease relevant models based on long term potentiation (LTP) and conduction velocity can be developed from these systems and be utilized for successful regulatory submission. How multiple organ mimics can be assembled into one platform with a recirculating serum free medium to predict therapeutic index. Clinically relevant functional readouts for electrical, mechanical and barriers can be utilized in these systems 	We will discuss the building of automation platform in Novartis to accelerate speed to data We will share how we approach data generation and machine learning in the context of library synthesis
	CHRISTOPHER HICKEY, Associate Director, Arvinas	JAMES HICKMAN, Professor of NanoScience Technology Center, University of Central Florida	KIAN TAN, Director, Novartis
	Q&A session & transition time between conference rooms		
	Beyond The Beta Turn: Discovery Of A CRBN Glue Degrader That Recruits A Novel Structural Motif	Humanized Mouse Modelling For Drug Targets	Steps Towards Building A Non-human Intelligence-Driven Drug Discovery Platform
15:30	 Discovered a CRBN molecular glue that recruits TBK1 (Tank-binding kinase) to CRBN CryoEM structures show that TBK1 recruitment to CRBN is not through a glycine beta-hairpin turn but a completely new structural degron A TBK1 degrader was identified, and we characterized its effect on the interferon pathway 	 Discuss humanized mouse models Describe the process for selection of humanized models for experiments Discuss the next generation of humanized mouse models 	
	JONATHAN SOLOMON, Director,	MICHAEL BREHM, Associate Professor & Associate Director, Diabetes Center of Excellence, UMass Medical School	
	Novartis	Old cassion & transition time between conference rooms	TUDOR OPREA, Chief Executive Officer, Expert Systems
	Q&A session & transition time between conference rooms		

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	TRACK 1: TARGET IDENTIFICATION & VALIDATION OF NOVEL MODALITIES	TRACK 2: NOVEL MODELS FOR ADME-TOX RESEARCH & DISEASE MODELLING	TRACK 3: AUGMENTING R&D WITH AI & AUTOMATION	
	Optimizing Drug Properties Of Non-Degrader Molecular Glue-Macrocyclic Peptides	Complex In Vitro Models To Investigate The Impact Of Therapeutic Intervention On Inflammation Driven Barrier Disruption In Inflammatory Bowel Disease	Developing Nature-Inspired Medicines Using Generative AI	
15:55	 The presentation will describe a macrocyclic molecular glue platform (RapaGlues) used to find hits for hard to drug targets. Large collections of molecular glues have been designed in both DELs and Array libraries that are used in screening campaigns against a disease target. The strategy to optimize hits to lead series will be describes as well as concept around building diversity in these molecular glue-macrocyclic peptides to unlock a broad range of target classes 	 Development and validation of complex in vitro models of IBD including colon-on-a-chip models Proteomics comparison across multiple complex in vitro models Applications of colon-on-a-chip models to drug discovery 	 Sensorium Therapeutics combines AI with ethnobotanical data to accelerate drug discovery and increase probability of success. SensAI identifies natural compounds with clinically rele- vant endpoints and novel mechanisms driving medicinal effects underlying human disease. With applicability across diverse disease areas, collaborators can access SensAI to initiate their own drug discovery programs 	
	RICK EWING, Vice President & Head of Chemistry, Rapafusyn Pharmaceuticals	SARAH WILSON, Principal Research Scientist AbbVie	AARON VAN HOOSER, Senior Director, Head of Computational Biology, Sensorium Therapeutics	
16:20	AFTERNOON BREAK 1-2-1 Meetings x4	AFTERNOON BREAK 1-2-1 Meetings x4 Poster Displays		
	From Genes To Therapies: Multi-Omic Approaches In Oncology Extra Cellular Target Discovery	Panel Discussion: Overcoming Challenges When Developing Disease Models Across Therapeutic Modalities	Harnessing The Power Of Genetically Encoded Small Molecule (GEM) Drug Discovery From Fungi – Convergence Of Natural Evolution And Al	
17:20	A brief overview of the utilization and integration of multi-omic data in target identification	 Optimal models for small molecules, large molecules & gene therapies Understanding toxicology & ADME and PK/PD Translation to animal models & the use of iPSCs 		
	SATYAJIT RAJAPURKAR, Investigator, GSK	Achieving regulatory acceptance	JOSE MUNOZ, Associate Principal Scientist, LifeMine Therapeutics	
	Q&A session & transition time between conference rooms		Q&A session & transition time between conference rooms	
	Genomics And Functional Genomics In Drug Discovery		More Better Data: Elevate and Deliver FAIR R&D Data for ML & AI Through Semantic Harmonization	
17:45	 Targets with genetic evidence are more likely to succeed in clinical trials. Genome-wide association studies have identified more than 500,000 variant - trait associations, but the vast majority of genetic variants have not yet been assessed in functional studies. Functional genomics approaches can help unravel causal variants, genes and disease mechanisms. A shift to functional genomics is needed to capitalize on the success of genome-wide associa- tion studies in complex disease. 		 Data drive our discoveries and are critical to deriving insight from our experiments and studies. As Data are produced in ever increasing volumes and variety, implementing an approach that leverages advanced methods for data harmonization and alignment are critical to every organization. This presentation will emphasize the importance of FAIR data and current approaches to managing data for analytics along the Drug Discovery and Development pipeline 	
		Moderator: JASON EKERT, Head of US Translational Technology, UCB Panellists: GVIDO CEBERS, Global Head of Drug Safety & Evaluation, Takeda		
	ANNEKE DEN HOLLANDER, Head of Functional Genomics, AbbVie	JAMES HICKMAN, Professor of NanoScience Technology Center, University of Central Florida MICHAEL BREHM, Associate Professor & Associate Director, Diabetes Center of Excellence, UMass Medical School	JULIA FOX, Director – Data & Analytics, Takeda	
18:10	End of Day One & Drinks Reception			

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DAY TWO: 08 NOVEMBER 2024

Keynote Address: Bridging The Gap In CNS Drug Discovery: Electrophysiology As A Classifier Of Diseases And Therapeutics

- Quiver is building the Genomic Positioning System (GPS), a foundational model for brain science and therapeutics
- We integrate a proprietary, scalable, human neuronal electrophysiology data generation platform with Al/ML computation and vast curated data sets
 - We are using the brain GPS to navigate diseases, targets, and therapeutics for the right patients

GRAHAM DEMPSEY, Founder & Chief Scientific Officer,

Quiver Bioscience

09:30

10:20

10:45

Q&A session & transition time between conference rooms

Recursion's Phenomic Map-Based Drug Discovery Approach: From Project Ideation To Lead Optimization

• Recursion's integrated operating system combines proprietary in-house data generation and advanced computational tools to generate programs. The Recursion OS platform provides a mapping and navigating approach that enables us not only to unravel the complexity of biology but also to identify chemical starting-points and drive SAR. Following this novel approach, we efficiently advance projects from initiation through different stages of pre-clinical development.

NOEL POWELL, Senior Director – Medicinal Chemistry,

Recursion Pharmaceuticals

	TRACK 1: INNOVATIVE TECHNOLOGIES FOR HIT IDENTIFICATION & SCREENING	TRACK 2: COMPUTATIONAL & MEDICINAL CHEMISTRY	
	Track Chair: ELIZABETH D'AMBROSIO, Investigator, GSK	Track Chair: NOEL POWELL, Senior Director – Medicinal Chemistry, Recursion Pharmaceuticals	
	Accelerating Drug Discovery For Hit Finding Of Novel Modalities	Finding the One - Chemical Space Exploration Problems	
	• This talk explores innovative strategies for accelerating drug discovery focused on the identification & validation of novel modalities, show the latest technological innovations in high-throughput screening can improve hit selection & pre-select better molecules for the hit lead cascade	• Discussing how Chemaxon innovates in the area of chemical space exploration, so that the industry can address the changing needs related to finding THE next compound to synthesize and test in a continuously growing virtual chemical space	
09:55	TIJMEN BOOIJ, Director HTS PivotPark Screening Centre	JEREMY MALERICH, Application Scientist, Chemaxon	
	pivotpark screeningcentre	© Chemaxon	

Q&A session & transition time between conference rooms

Targeting The Unknown: Al's Shortcut To Drug Discovery

• Al and data-driven approaches are radically improving the efficiency of drug discovery. By commanding massive experimental scale - up to millions of wet lab experiments weekly - and massive computational scale - owning and operating one of the most powerful supercomputers in the world, Recursion is uniting technology, biology and chemistry to advance the future of medicine.

Expanded Design Space For Orally Bioavailable Degraders Using Three-Dimensional Descriptors

• Targeted protein degradation (TPD) is an emerging therapeutical modality that has gained significant attention from drug developers in recent years. One key challenge in the field of TPDs has been the design of orally bioavailable molecules. Although these molecules are larger than the typical small molecules, they have been shown to achieve robust oral exposure and target coverage in humans. As many design concepts and tools to improve drug-likeliness were developed based on small molecules, their applicability in the larger, more flexible, and linear degrader molecules have been limited. Here, we will discuss Kymera's approach to designing oral degraders, redefining the drug-likeliness space through the use of 3D parameters, and how computational tools can impact the design of orally bioavailable degraders.

MELISSA FORD, Associate Director of Computational Chemistry, **Kymera Therapeutics**

JULIE OWEN, Director Of Chemistry, **Recursion Pharmaceuticals**

MORNING BREAK



1-2-1 Meetings x3



Poster Displays

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TRACK 1: INNOVATIVE TECHNOLOGIES FOR HIT TRACK 2: COMPUTATIONAL & MEDICINAL CHEMISTRY **IDENTIFICATION & SCREENING** Unlocking Plasma Discoveries: Bridging Depth, Throughput And Sensitivity • Biognosys, a leader in the proteomics field for drug discovery and development, has reached a significant milestone with the unveiling of advancements in its plasma proteomics workflows. Biognosys developed and optimized the P2 Plasma Enrichment System. Our TrueDiscovery® platform can quantify ~ 8000 PG on average and 6057 protein groups with no missing values, with 80% of protein groups quantified with a CV<20%. Biognosys remains at the forefront of proteomics research, equipping biopharma researchers with unparalleled capabilities to unravel the intricacies of the plasma proteome, thus fostering groundbreaking discoveries in drug development and clinical applications. Delegates are welcome to attend co-located sessions VALESCA ANSCHAU, Associate Scientific Director, **Biognosys ™**BIOGNOSYS Q&A session & transition time between conference rooms Innovations In DNA Encoded Libraries For Hit Discovery And Beyond **Novel Methods In Medicinal Chemistry: Dark Kinases** • Our DEL (DNA-encoded library) technologies facilitate the generation of extensive data suitable for machine learning applications. Insitro has introduced innovations in DELs for various stages of drug discovery, including hit discovery, optimization, and progression to leads. For example, DEL programming enables the creation of drug-like DELs and expedites the synthesis of second-generation DELs. These advanced • The inhibition of kinases has been pursued by the pharmaceutical industry for over 20 years. We report Dark Kinase Allostery Atlas which is a systematic collection of binding hot spots located at sites on the entire human kinome, with the focus on dark kinases. The hot spots are identified by FTMap, a computational analogue of experimental fragment screening. The ensemble is sampled by a combination of physics libraries deliver enhanced insights into medicinal chemistry, improving the speed of synthesis and validation of compounds in drug discovery. We've also developed bivalent DELs which assist in targeting difficult molecular targets. The integration of DELs with machine learning has significantly increased our confidence in identifying effective hits for complex targets. and AlphaFold-based sampling DIVYA KANICHAR, Director, Insitro DIMA KOZAKOV, Professor, Stony Brook University Q&A session & transition time between conference rooms **Using Functional Assays For Early Lead Discovery Rapid Molecular Modeling For Focused Cryptic Pocket Identification** Cryptic pocket identification is important to new target ideation in drug discovery. In this work, we explored how to use computational mode-ling tools to rapidly identify sites in target proteins to guide more advanced studies of these potential cryptic pockets. · Will discuss pros and cons of screening in silico and in situ and then provide overview of 2 hit finding campaigns for multifunctional enzymes CPS1 and WRN. 12:35 NICHOLAS LARSEN, Senior Director of Lead Discovery, YUNHUI GE, Scientist, **Kestrel Therapeutics Alkermes** Œ 13:00 LUNCH BREAK 1-2-1 Meetings x3 Poster Displays Reviving Classics: Innovative Use Of Analytical Ultracentrifugation In Degrader Ternary Complex Analysis Panel Discussion: Fragment & Structure-Based Drug Design: Where Are We Now? • Brief overview of key mechanism of action assays used in targeted protein degradation Cryo-EM applications • Development of a novel, multi-attribute assay for ternary complex formation that uses analytical ultracentrifugation, its platform enablement, • Evaluating current & future techniques to improve efficiency & resolution of drug design and the unique data that can be derived in this approach will be discussed with some example applications from other projects · Overcoming challenges through integration & optimization of drug design approaches JUDITH RONAU, Senior Scientist II, AbbVie Q&A session & transition time between conference rooms Unlocking Early Oligonucleotide Discovery - Insights On Strategies And Pitfalls • Brief overview of oligo therapeutics: key advantages and challenges • Strategies, considerations, and pitfalls in building an early oligo discovery program • Case study: early discovery program for Centronuclear Myopathy

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NOA LIBERMAN-ISAKOV, Senior Scientist, Discovery Research, Sarepta Therapeutics

Panellists:

BOGUSLAW NOCEK, Senior Director – Structural Biology, **Eli Lilly**FINITH JERNIGAN, Head of Early Discovery, **Psivant Therapeutics**MELISSA FORD, Associate Director of Computational Chemistry, **Kymera Therapeutics**KRISTEN MARINO, Principal Scientist, Computational Chemistry, **Cellarity**

DAY TWO: 08 NOVEMBER 2024

	TRACK 1: INNOVATIVE TECHNOLOGIES FOR HIT IDENTIFICATION & SCREENING	TRACK 2: COMPUTATIONAL & MEDICINAL CHEMISTRY
14:50	 Panel Discussion: Novel Platforms & Techniques To Improve Hit Identification Navigating the complexities of optimizing hit identification Balancing efficiency and minimizing false positives Overcoming challenges for Hit discovery 	Solving Centuries-Old Drug Discovery Challenges With Artificial Intelligence: Hope Versus Hype Cost-effectiveness and improving efficacy/ safety in case of novel drugs Global multifaceted collaborations CADD combined with mathematical modelling is a magic bullet Al-based model has a lot of potential to revolutionize drug R&D Hybrid CADD- and Al- powered technology in case of novel predictive medicine. PRASHANT GAHTORI, Professor of Medicinal Chemistry, Graphic Era Hill University
		Q&A session & transition time between conference rooms
15:15	Moderator: JUDITH RONAU, Senior Scientist II, AbbVie Panellists: JEREMY DISCH, Senior Director, Insitro ELIZABETH D'AMBROSIO, Investigator, GSK	Delegates are welcome to attend co-located sessions
15:40	End of Congress	

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