DISCOVERY US 2024

BY OXFORD GLOBAL

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07 – 08 November 2024 | Boston, MA

Now In Its 6th Year!

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'

5 Content Tracks

50+ Hours of 1:1 Meetings

10+ Partners

250+ Attendees

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45+ Industry-Leading Speakers Including...

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

FIONA MACK, Vice President & Head, **Bayer**

JOE FRANKLIN, Senior Vice President & Head of Early Drug Discovery, **Anagenex**

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

SHELLEY ALLEN, Vice President & Head of Drug Discovery, **Nimble Therapeutics**

MARTIN REDHEAD, Associate Vice President, **Exscientia**

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

JULIA FOX, Director – Data & Analytics, **Takeda**

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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WHAT'S NEW

Benefits Of Attending

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 AI & automation in your lab to increase productivity** - focusing on how AI 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 AI & novel Hit identification techniques

WHY PARTNER WITH
OXFORD GLOBAL?

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.

- **Arrange 1-2-1 Meetings**

Benefit from guaranteed one-to-one face time with your key prospects, with detailed pre-meeting information provided to enable effective and productive conversations.

- **Speaking Opportunities**

Showcase your company's recent work to a relevant and highly engaged audience.

- **Host Panel & Roundtable Discussions**

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

- **Organise Workshops**

Demonstrate best practice within the industry in front of your peers with case studies from your clients.

- **Exhibit your Products & Solutions**

Promote your offerings and ensure delegates know where to find you with a prominent brand presence in the exhibition hall.

- **Digital Marketing & Lead Generation**

Accessing the Oxford Global database, amplify your thought leadership and branding messaging through a post-event case study e-Book.

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NETWORK & KNOWLEDGE-SHARE

Attendees

250+ VPs, Directors & Senior Managers will be attending on-site 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:

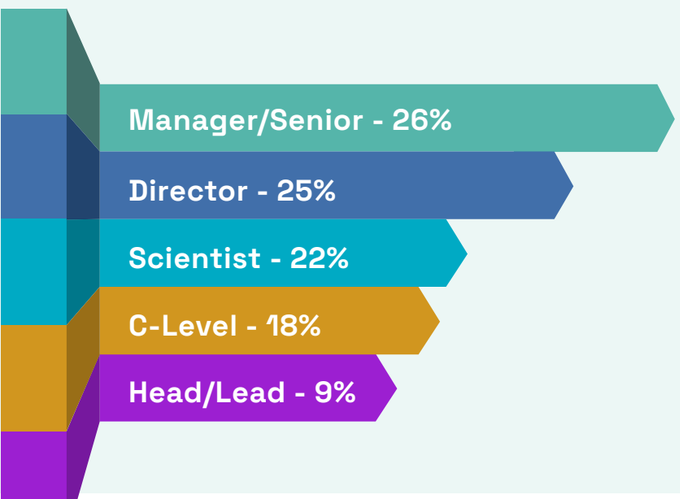
- Target validation
- Screening technologies
- Organoids
- Library optimization
- Small molecule discovery
- Computational platforms
- Organic synthesis
- Generative AI
- Cell-based assays
- Stem cells
- AI/ML
- Data analysis tools

Attended by these companies & many more:

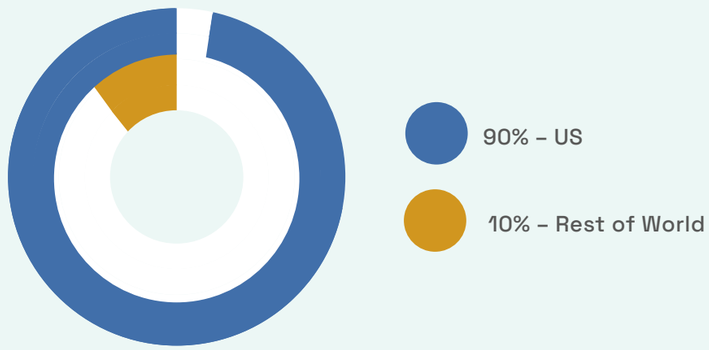
SANOFI · BAYER · Takeda · Genentech A Member of the Roche Group · Bristol Myers Squibb · ucb · Lilly · gsk · abbvie · NOVARTIS · nimble therapeutics · Exscientia DRIVEN BY KNOWLEDGE

Previous Attendee Profile:

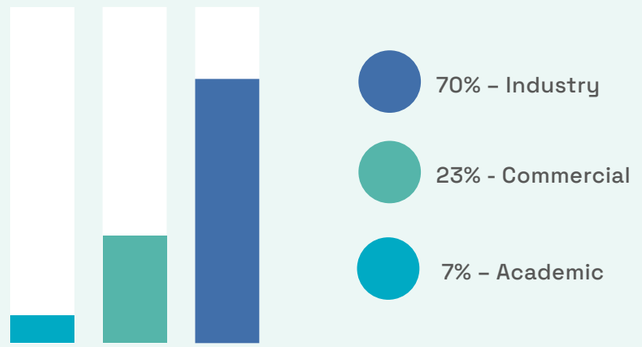
Function



Geography



Sector



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GAIN EXPERTISE FROM THOUGHT LEADERS

Confirmed Speakers

KEY SPEAKERS

Day One | 08:30

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

Day One | 09:30

MARTIN REDHEAD,
Associate Vice President, Exscientia

Day One | 11:30

SHELLEY ALLEN,
Vice President & Head of Drug Discovery, Nimble Therapeutics

Day Two | 09:30

JOE FRANKLIN,
Senior Vice President & Head of Early Drug Discovery, Anagenex

Day One | 12:25

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

Day Two | 9:00

GRAHAM DEMPSEY,
Founder & Chief Scientific Officer, Quiver Bioscience

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Founder & Chief Scientific Officer, Quiver Bioscience

IVAN CORNELLA
Chief Scientific Officer, Covant Therapeutics

JOE FRANKLIN
Senior Vice President & Head of Early Drug Discovery, Anagenex

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

SHELLEY ALLEN
Vice President & Head of Drug Discovery, Nimble Therapeutics

MARTIN REDHEAD
Associate Vice President, Exscientia

GVIDO CEBERS
Global Head of Drug Safety & Evaluation, Takeda

JODY LOGAN
Senior Director of Tech Transfer, Genentech

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

JASON EKERT
Head of US Translational Technology, UCB

DIVYA KANICHAR
Director, Insitro

JULIA FOX
Director – Data & Analytics, Takeda

JONATHAN SOLOMON
Director, Novartis

ARI ALLYN-FEUER
Director, AI Product, GSK

JENNIFER 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

JOSEPH 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

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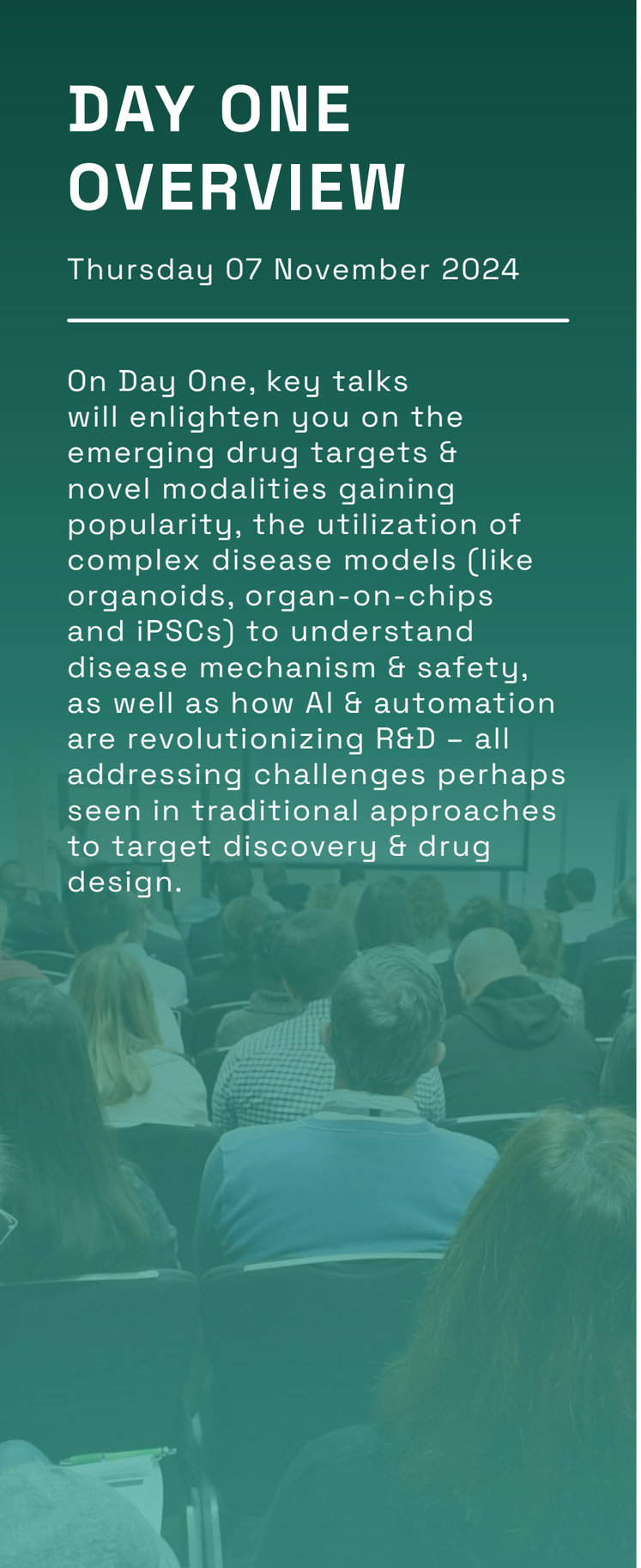
DAY ONE OVERVIEW

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 AI & 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 AI 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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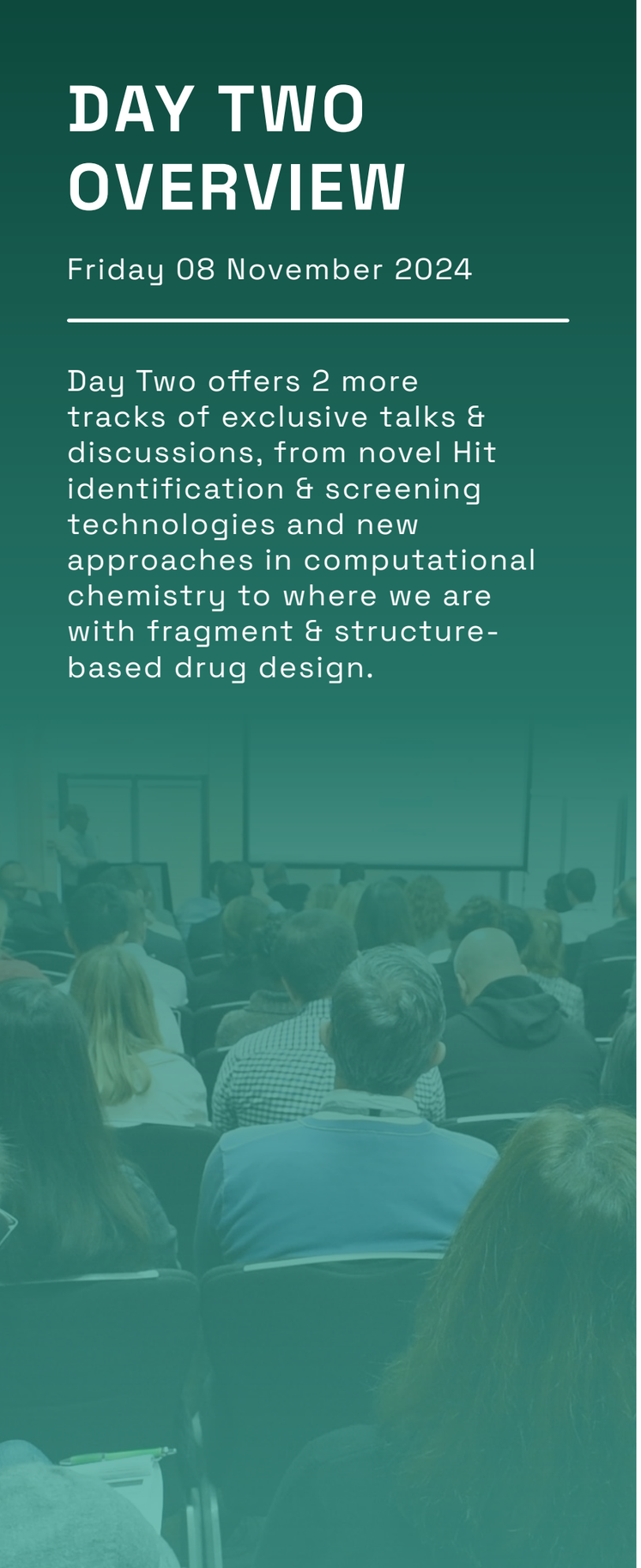
DAY TWO OVERVIEW

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.



EXPLORE CURATED & INSIGHTFUL CONTENT

Agenda At A Glance

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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DAY ONE: 07 NOVEMBER 2024

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

08:25 **Oxford Global's Welcome Address**

08:30 **Keynote Address:** The Ever-Evolving Landscape Of Drug Discovery

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

TRACK 1: TARGET IDENTIFICATION & VALIDATION OF NOVEL MODALITIES

Morning Track Chair: DIVYA KANICHAR, Director, **Insitro**

09:00 **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.

PAUL SCOLA, Senior Director, Discovery Sciences,
Bristol Myers Squibb

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

Track Chair: MICHAEL BREHM, Associate Professor & Associate Director, Diabetes Center of Excellence, **UMass Medical School**

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.

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

TRACK 3: AUGMENTING R&D WITH AI & AUTOMATION

Track Chair: Position Available

The Challenges Of Working With AI & Innovation In Pharma

- AI 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 AI 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

ABHIJAT VATSYAYAN, Head of Artificial Intelligence & Innovation,
Taiho Oncology

Q&A session & transition time between conference rooms

09:25 *Delegates are welcome to attend co-located sessions*

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 interactions. 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 Matthew D. Segall, (2023) Xenobiotica DOI: 10.1080/00498254.2023.2284251

MATTHEW SEGALL, Chief Executive Officer,
Optibrium

Silver Solution Provider Presentation

ZHIXIONG LIN, Head of AI Drug Discovery,
Xtalpi

Q&A session & transition time between conference rooms

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DAY ONE: 07 NOVEMBER 2024

TRACK 1: TARGET IDENTIFICATION & VALIDATION OF NOVEL MODALITIES

09:50

Discovery Of A Unique Covalent Modality

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

10:15

MORNING COFFEE & REFRESHMENTS | 1-2-1 Meetings x4 | Poster Displays

Morning Track Chair: DIVYA KANICHAR, Director, **Insitro**

Delegates are welcome to attend co-located sessions

11:35

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

Synthetic Biology & Programmable Organoids For Drug Discovery & Regenerative Medicine

RON WEISS, Director of Synthetic Biology Center & Professor of Biological Engineering, **Massachusetts Institute of Technology**

Track Chair: MICHAEL BREHM, Associate Professor & Associate Director, Diabetes Center of Excellence, **UMass Medical School**

Delegates are welcome to attend co-located sessions

TRACK 3: AUGMENTING R&D WITH AI & AUTOMATION

An AI-Driven DMTA Loop For Drug Discovery

- Artificial intelligence (AI) has already had a huge impact on the way drugs are designed, with tens of AI-designed drugs currently moving through clinical development. Despite the efficiency gains of AI in the design of drugs, this has not yet been transferred to the "make" and "test" phases of the iterative "design-make-test-learn" (DMTL) loop, which underpins the progression of small molecule from early POC to clinical candidate. Anchoring machine learning models to real data is important and DMTL enables this. In order to extend the limits of efficiency in drug discovery, we have developed a state-of-the-art automated lab to make and test the small molecules that our AI platform designs.
- The lab consists of an automated chemical synthesis platform, automated purification, analysis and compound storage. We have enhanced our design software to better predict synthetic routes, and design with automated chemical synthesis in mind. The chemistry synthesis platform is integrated with a biological testing platform, supporting biochemical assays and cell-based biosensors. This platform enables fully automated lab processes that don't require any manual handling. Assay development is fully online and the system can develop its own experiments, freeing up highly skilled scientists to focus on complex experimental problems such as MoA or differentiation.
- This innovative platform changes the economics of early discovery, allowing work to start on multiple projects in parallel following a genomic target discovery campaign. This means we can now select the project most likely to impact a patient in terms of the biological, chemical and pharmacological tractability, as well as rapidly building AI training sets for previously unliganded targets.

MARTIN REDHEAD, Associate Vice President, **Exscientia**

Track Chair: Position Available

Data Imputation To Augment R&D And Enhance Your Decision-Making

- It's impossible to experimentally measure all of the data we want for all compounds in a drug discovery project. Furthermore, the limited data we have are noisy because of experimental variability and error. However, AI can make sense of these 'sparse and noisy' data to offer valuable insights and guide research, saving time and money.
- We will describe an AI platform, Cerella™, that applies deep learning imputation to learn from both structure-activity relationships (SAR) and directly from the relationship between experimental endpoints based on sparse data [1]. The resulting models can proactively highlight high-quality compounds by 'filling in' missing data more accurately than conventional quantitative structure-activity relationship (QSAR) models. Furthermore, it can identify hidden opportunities caused by missing, uncertain or inaccurate data, and prioritise experimental resources by focussing on measuring the most valuable data to inform decisions about compound progression. [1] Irwin et al. App. AI Lett. (2021) DOI: 10.1002/ail2.31

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

Q&A session & transition time between conference rooms

DAY ONE: 07 NOVEMBER 2024

	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
12:00	**Discovering Oral Peptide Therapeutics At The Speed Of Light** • The Nimble platform drives the end-to-end discovery and development of oral peptide therapeutics. This presentation will detail how our proprietary platform delivers peptides at unparalleled speed and efficiency to enable lead optimization, along with how we optimize properties for oral delivery SHELLEY ALLEN, Vice President & Head of Drug Discovery, **Nimble Therapeutics**	**Computational Analysis Of Complex In Vitro Models To Uncover Neuromuscular & Inflammatory Disorders** MONICA WANG, Senior Scientist **UCB**	**Biological Sequence Learning Is A Central Part Of Drug Development** • Profundity of sequence learning applications in drug development • Review of GSK's Seneca and Exonnet models • Principles of managing experiments for AI model training ARI ALLYN-FEUER, Director, AI Product, **GSK**
	Q&A session & transition time between conference rooms		
12:25	**Fostering Early-Stage Innovation: Bayer Co.Lab** • Bringing emerging targets & modalities into the pipeline • Supporting early-stage biotechnology, startup & academic innovations • Challenges & opportunities FIONA MACK, Vice President & Head Co. Lab Cambridge, **Bayer**	**Stem Cells, Genomics, And AI/ML For Drug Discovery** • 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. JOSEPH WU, Professor and Director, Stanford Cardiovascular Institute & Co-Founder, **Greenstone Biosciences**	**Panel Discussion:** The Fundamentals Of AI • 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 fields?
	Q&A session & transition time between conference rooms		
12:50	**Utilizing CRISPR And Chemogenomics Screens With AI Tools To Validate Novel Targets** • Rapid validation of biological targets arising from multiple functions is made possible by Exscientia's AI tools and automated screening platform JENNIFER BUSBY, Director – Biology, **Exscientia**	**High Throughput Drug Screening Of Patient-Derived Tumor Organoids** ILKAY US, Director – High Throughput Screening, **Weill Cornell Medicine**	**Moderator:** ABHIJAT VATSYAYAN, Head of Artificial Intelligence & Innovation, **Taiho Oncology** **Panellists:** KIAN TAN, Director, **Novartis** ELENA DOLGIKH, Head of Computational Chemistry, **Monte Rosa Therapeutics** 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

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DAY ONE: 07 NOVEMBER 2024

	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
	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**
14:15	*Delegates are welcome to attend co-located sessions*	**Navigating Target Safety With Multimodal Data And AI-Enhanced Predictions** • 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 drug discovery discovery, bridging critical gaps between preclinical research and clinical application JOSH ALMOND-THYNNE, Co-Founder **Sable**	**Silver Solution Provider Presentation** Senior Representative, **ChemSpeed Technologies**
		Q&A session & transition time between conference rooms	
14:40	*Delegates are welcome to attend co-located sessions*	*Delegates are welcome to attend co-located sessions*	**Robust Datasets For ML-Driven Drug Discovery** • 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**
		Q&A session & transition time between conference rooms	
15:05	**Targeted Protein Degradation By PROTAC Degraders** • 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 CHRISTOPHER HICKEY, Associate Director, **Arvinas**	**Organ-On-Chip & MPS Systems 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 JAMES HICKMAN, Professor of NanoScience Technology Center, **University of Central Florida**	**AI Is Not Taking Over The World, But I Still Love My Roomba: Applying Machine Learning And Automation In Drug Discovery** • 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 KIAN TAN, Director, **Novartis**

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DAY ONE: 07 NOVEMBER 2024

	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
	Q&A session & transition time between conference rooms		
15:30	**Beyond The Beta Turn: Discovery Of A CRBN Glue Degrader That Recruits A Novel Structural Motif** • 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 JONATHAN SOLOMON, Director, **Novartis**	**Humanized Mouse Modelling For Drug Targets** • Discuss humanized mouse models • Describe the process for selection of humanized models for experiments • Discuss the next generation of humanized mouse models MICHAEL BREHM, Associate Professor & Associate Director, Diabetes Center of Excellence, **UMass Medical School**	**Digitization Of Analytical Processes** JODY LOGAN, Senior Director of Tech Transfer, **Genentech**
	Q&A session & transition time between conference rooms		
15:55	**Optimizing Drug Properties Of Non-Degrader Molecular Glue-Macrocyclic Peptides** • 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 RICK EWING, Vice President & Head of Chemistry, **Rapafusyn Pharmaceuticals**	**Complex In Vitro Models To Investigate The Impact Of Therapeutic Intervention On Inflammation Driven Barrier Disruption In Inflammatory Bowel Disease** • 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 SARAH WILSON, Principal Research Scientist **AbbVie**	**Developing Nature-Inspired Medicines Using Generative AI** • Sensorium Therapeutics combines AI with ethnobotanical data to accelerate drug discovery and increase probability of success. SensAI identifies natural compounds with clinically relevant 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 AARON VAN HOOSER, Senior Director, Head of Computational Biology, **Sensorium Therapeutics**
16:20	AFTERNOON BREAK	1-2-1 Meetings x4	Poster Displays

DAY ONE: 07 NOVEMBER 2024

	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
17:20	**From Genes To Therapies: Multi-Omic Approaches In Oncology Extra Cellular Target Discovery** • A brief overview of the utilization and integration of multi-omic data in target identification SATYAJIT RAJAPURKAR, Investigator, **GSK**	**Panel Discussion:** Overcoming Challenges When Developing Disease Models Across Therapeutic Modalities • Optimal models for small molecules, large molecules & gene therapies • Understanding toxicology & ADME • Translation to animal models & the use of iPSCs	**Harnessing The Power Of Genetically Encoded Small Molecule (GEM) Drug Discovery From Fungi – Convergence Of Natural Evolution And AI** Senior Representative, **LifeMine Therapeutics**
	Q&A session & transition time between conference rooms		*Q&A session & transition time between conference rooms*
17:45	**Genomics And Functional Genomics In Drug Discovery** • 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 association studies in complex disease. ANNEKE DEN HOLLANDER, Head of Functional Genomics, **AbbVie**	**Moderator:** JASON EKERT, Head of US Translational Technology, **UCB** **Panellists:** GVIDO CEBERS, Global Head of Drug Safety & Evaluation, **Takeda** JAMES HICKMAN, Professor of NanoScience Technology Center, **University of Central Florida** MICHAEL BREHM, Associate Professor & Associate Director, Diabetes Center of Excellence, **UMass Medical School**	**More Better Data: Elevate and Deliver FAIR R&D Data for ML & AI Through Semantic Harmonization** • 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 JULIA FOX, Director – Data & Analytics, **Takeda**
18:10	**End of Day One & Drinks Reception**		

DAY TWO: 08 NOVEMBER 2024

08:55 **Oxford Global's Welcome Address**

09:00 **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 AI/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**

	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**
09:30	**Development Of A High Throughput Synthesis And AS/MS Platform To Help Reduce The Design, Make, Test, Analyzes Cycles Associated With DEL Follow Up** • Anagenex combines DEL screening with Machine Learning to discover and advance new medicines. In this presentation we will describe the application of our high throughput synthesis platform and our AS/MS platform and how they are helping to reduce the DMTA cycle JOE FRANKLIN, Senior Vice President & Head of Early Drug Discovery, **Anagenex**	**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 novel insights to initiate and accelerate 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**
	Q&A session & transition time between conference rooms	

DAY TWO: 08 NOVEMBER 2024

TRACK 1: INNOVATIVE TECHNOLOGIES FOR HIT IDENTIFICATION & SCREENING

TRACK 2: COMPUTATIONAL & MEDICINAL CHEMISTRY

09:55

Accelerating Drug Discovery For Hit Finding Of Novel Modalities

- This talk explores innovative strategies for accelerating drug discovery focused on the identification & validation of novel modalities, showing how the latest technological innovations in high-throughput screening can improve hit selection & pre-select better molecules for the hit-to-lead cascade

TIJMEN BOOIJ, Director HTS
PivotPark Screening Centre

Finding the One – Chemical Space Exploration Problems

- 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

JEREMY MALERICH, Application Scientist,
Chemaxon

Q&A session & transition time between conference rooms

10:20

Targeting The Unknown: AI's Shortcut To Drug Discovery

- AI 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.

JULIE OWEN, Director Of Chemistry,
Recursion Pharmaceuticals

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

10:45

MORNING BREAK | 1-2-1 Meetings x3 | Poster Displays

Bronze Solution Provider Presentation

11:45

Senior Representative,
Biognosys

Delegates are welcome to attend co-located sessions

Q&A session & transition time between conference rooms

Innovations In DNA Encoded Libraries For Hit Discovery And Beyond

- 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 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.

12:10

DIVYA KANICHAR, Director,
Insitro

Novel Methods In Medicinal Chemistry: Dark Kinases

DIMA KOZAKOV, Professor, **Stony Brook University**

Q&A session & transition time between conference rooms

DAY TWO: 08 NOVEMBER 2024

TRACK 1: INNOVATIVE TECHNOLOGIES FOR HIT IDENTIFICATION & SCREENING

TRACK 2: COMPUTATIONAL & MEDICINAL CHEMISTRY

Using Functional Assays For Early Lead Discovery

- 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.

NICHOLAS LARSEN, Senior Director of Lead Discovery,
Kestrel Therapeutics

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 modeling tools to rapidly identify sites in target proteins to guide more advanced studies of these potential cryptic pockets.

YUNHUI GE, Scientist,
Alkermes

12:35

13:00 **LUNCH BREAK** | 1-2-1 Meetings x3 | Poster Displays

Reviving Classics: Innovative Use Of Analytical Ultracentrifugation In Degrader Ternary Complex Analysis

14:00

- Brief overview of key mechanism of action assays used in targeted protein degradation
- Development of a novel, multi-attribute assay for ternary complex formation that uses analytical ultracentrifugation, its platform enablement, and the unique data that can be derived in this approach will be discussed with some example applications from other projects

JUDITH RONAU, Senior Scientist II,
AbbVie

Q&A session & transition time between conference rooms

Unlocking Early Oligonucleotide Discovery – Insights On Strategies And Pitfalls

14:25

- 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

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

Panel Discussion: Fragment & Structure-Based Drug Design: Where Are We Now?

- Cryo-EM applications
- Evaluating current & future techniques to improve efficiency & resolution of drug design
- Overcoming challenges through integration & optimization of drug design approaches

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**

Panel Discussion: Novel Platforms & Techniques To Improve Hit Identification

14:50

- Navigating the complexities of optimizing hit identification
- Balancing efficiency and minimizing false positives
- Overcoming challenges for Hit discovery

Panellists:
JEREMY DISCH, Senior Director, **Insitro**
ELIZABETH D'AMBROSIO, Investigator, **GSK**

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
- AI-based model has a lot of potential to revolutionize drug R&D
- Hybrid CADD- and AI- 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

AI, Data- & Computationally-Driven Approaches For Target Identification & Validation In Drug Discovery: Quo Vadis?

15:15

Target identification and validation are rapidly evolving with support from data-intensive AI approaches

- Where are we?
- Where are we going?
- More scientific, less technical validation is needed

TUDOR OPREA, Chief Executive Officer, **Expert Systems**

15:40 **End of Congress**

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