DISCOVERY US 2023

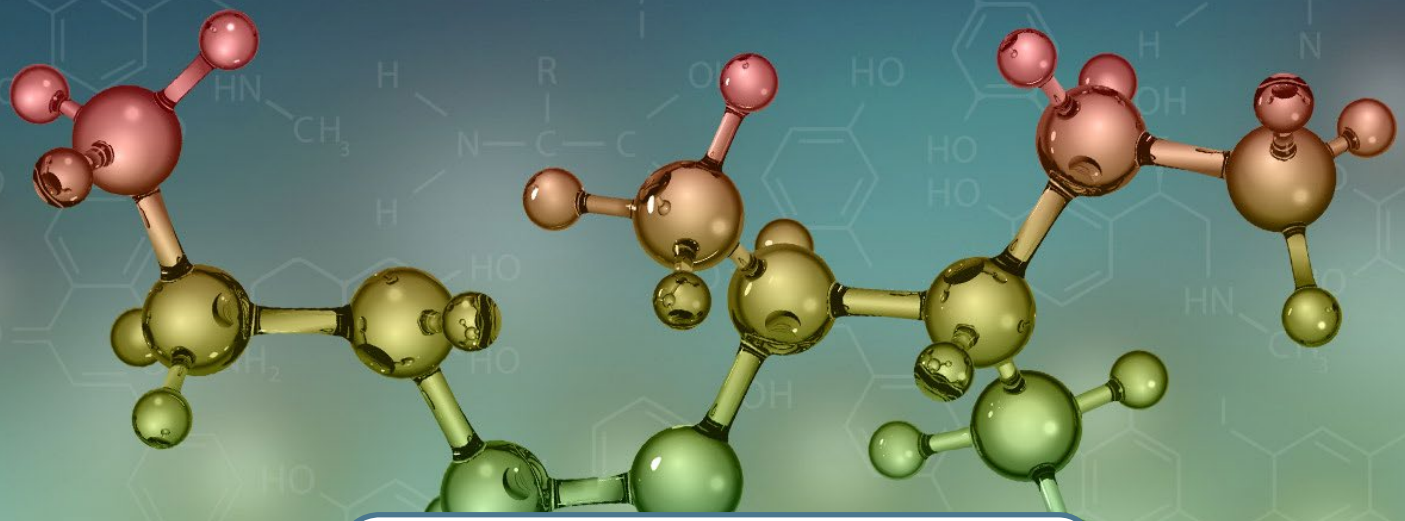
01 - 02 November 2023 | Cambridge, USA

250+
LEADING ACADEMIC, PHARMA AND BIOTECH ATTENDEES

60+
PRESENTATIONS, CASE STUDIES AND DISCUSSIONS

5
INNOVATIVE TRACKS COVERING THE LATEST DRUG DISCOVERY AND DEVELOPMENT

Conference Brochure



KEY SPEAKERS INCLUDE

Beth Hoffman
Origami Therapeutics Inc.

Nils Jakob Hansen
Vipergen ApS

Yuxin Liang
Genentech

Paul Scola
Bristol Myers Squibb

Esther Lee
AstraZeneca

John Quinn
Genentech

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OXFORD GLOBAL

BROCHURE CONTENTS

On behalf of the entire Oxford Global team, I am delighted to welcome you to Discovery US 2023. From new and exciting to the latest in products and services, our event will bring together leading companies for engaging discussions, knowledge sharing and focused networking.

The Oxford Global team look forward to meeting you over the course of the event and will be on hand to ensure your time is both productive and enjoyable.

Oxford Global Marketing Ltd. has been producing cutting edge congresses and summits for the Life Sciences Industry for over 16 years. I am pleased to let you know that we have now successfully completed a transition from an in-person event organiser to one stop shop platform for all research-critical information pertaining to the 'discovery space. We would like to invite you to visit our Discovery Content Portal to find out more about our brand-new membership offering, giving you access to the latest technology insights and research community we have been building over the last 16 years. You can register for the newsletter to get updates on upcoming activities within this series, stay up to date with industry news and more.

The event is designed to provide a comprehensive look at the current trends, challenges and developments impacting the sector. For a detailed breakdown of the areas we will discuss, please see the Session Topic Areas page, and use the Full Programme Agenda to identify which of our expert presentations are of the highest interest to you.

We want to create an environment where attendees can converse in smaller groups, so the programme will host a series of engaging discussions such as panels and workshops to encourage as much knowledge-sharing as possible.

WELCOME

We are hugely thankful to our speakers, who have given their time to provide interesting, thought-provoking presentations, and to our sponsoring companies, who have worked closely with us to provide you with unique opportunities to access the latest information on solutions and services that can directly impact and improve your research and results. Without their support this event would not be possible, so please do take some time to visit their stands in-person and featured sponsor pages on the event app (Swapcard).

Once again, welcome to the event — we hope it will prove to be both educational and enjoyable for you.

Charlotte Catley,
Sponsorship Director

On-site Health & Safety

At Oxford Global, the safety and well-being of our clients is our top priority, and we are committed to ensuring that our congresses remain safe and successful.

For more information, please see www.oxfordglobal.com/discovery-us/plan-your-visit/

WHO IS ATTENDING?

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

- Medicinal Chemistry
- Chemical Biology
- Drug Design
- Drug Discovery
- Target Discovery
- AI/ML
- Screening
- Organoid
- Organ on a chip

Previous Attendees Profile

FUNCTION

29% – Manager / Senior
24% – Director
19% – Scientist
17% – C-Level
11% – Head / Lead

SECTOR

85% – Industry
9% – Academic
6% – Commercial

GEOGRAPHY

94% – USA
4% – Rest of World
1% – Europe
1% – UK

These companies and many more:

AstraZeneca, Novartis, Bristol Myers Squibb, Origami Therapeutics, Anagenex, nimble therapeutics, Exscientia, BenevolentAI, Genentech, Theseus, AbbVie, UCB, GSK GlaxoSmithKline, Janssen, Merck

Formal and informal meeting opportunities offer delegates the chance to discuss key solutions with leading service providers:

- Protein Degradation Tools
- Medicinal Chemistry Tools
- Organoid Discovery
- Target Validation
- Contract Drug Discovery Research
- AI/ML
- Automation in Drug Discovery

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SESSION TOPIC AREAS

Discovery US 2023 features **2 days** of in-person cutting-edge presentations and knowledge-sharing, including **over 60** industry insights, sponsored presentations and think tank roundtable discussions.

DAY ONE

Track 1: Identification & Validation of Novel Targets

- New modalities & emerging drug targets in oncology, immuno-oncology and other disease areas
- AI to unblock drug discovery, drug repurposing and target validation
- Identification and validation of novel targets – genomic tools for elucidating novel targets
- Discovery of 1st class inhibitors
- Cellular and biological based drug discovery
- Digitisation & AI Approaches Featured Session

Track 2 Part 1: On Target, Phenotypic, Affinity & Virtual Based Screening

- (HTS vs Fragment vs DEL) including the use of automation of screening in in hit finding
- Fast structure-based virtual screening in readily available chemical space
- Application of CRISPR technology and screening to in vivo models of cancer immunotherapy
- Phenotypic screen in primary dendritic cells to identify new targets
- New technologies for target and phenotypic based discovery including spatial analysis
- Digitisation & AI Approaches

Part 2: Emerging Modalities: Targeted Protein Degradation

- Off-targets – Drug Repurposing
- Targeted Protein Degradation/
- Molecular Glues
- Induced proximity- RNA, Targeted
- RNA via small molecules
- Beyond rule of 5
- Discovery in targets in the noncoding genome

Track 3: Computational Drug Design and Molecular Drug Design and Medicinal Chemistry

- AI & Automation in chemical synthesis
- Measuring PK/PD and prediction of response AI in Chemical Synthesis,
- Lead Optimisation
- Predicting PK/PD and predictive cellular modelling
- Exploring the Chemical space – effective search of the space- finding the best way
- Advances in Antibodies drug design
- Quantum Based Drug Design
- Fragment & structured based drug discovery innovation including AI/ML driven drug design
- Efficient combination of machine learning and automation to accelerate DMTA cycles
- Innovating the chemistry lab bench
- Digitisation & AI Approaches Featured Session

DAY TWO

Track 1: Animal Models for Disease, Organ Modelling - Organoid Based Discovery & Organ On Chip Development

- Animal Models for Disease
- Translating breakthrough discoveries in stem cell biology and organ development
- Utilisation of 3D-model systems and organoids in phenotypic and high content screening
- Modelling protein aggregation in human iPSC
- 3D media and 3D cell culture
- Safety and efficacy considerations
- Digitisation & AI Approaches Featured Session

Track 2: Hit Finding Technologies and Advancements

- Showcase of hit-to-lead components & technologies e.g. targeted protein degradation, covalent inhibitors, DELs
- Case studies of lead generation in small and large molecules
- Enabling tools for hit-finding against difficult targets
- Applications of covalent fragments to drug lead generation
- Biophysical tools for difficult targets: building the right flow chart
- Hit identification strategy for glue degraders, deeper mechanistic understanding of TPDS
- Digitisation & AI Approaches Featured Session - Machine learning in DELs

CONFIRMED SPEAKERS – DAY ONE

MARK MURCKO
Director, Dewpoint Therapeutics

DANE CORNEIL
Director of AI Science, BenevolentAI

BETH HOFFMAN
Chief Executive Officer, Origami Therapeutics Inc.

THOMAS NITTOLI
Senior Director, Regeneron Pharmaceuticals, Inc

SHAHAR KEINAN
Chief Executive Officer, Polaris Quantum Biotech

MATTHEW PHARRIS
Senior Scientist, UCB

JOHN SANTA MARIA
Associate Director of Cheminformatics, FogPharma

ERIC MIELE
Associate Director Proteomics, AstraZeneca

SHAUN MCLOUGHLIN
Principal Research Scientist, AbbVie

ISTVAN ENYEDY
Senior Principal Scientist, UCB

LAUREN GOODRICH
Vice President, Therapeutic Discovery, Nimble Therapeutics

HASAN KHAN
Senior Scientist, AbbVie

JEFF MESSER
Director, GSK

EMMANUEL BENGIO
Senior Machine Learning Scientist, Recursion Pharmaceuticals

YUXIN LIANG
Senior Principal Scientific Manager, Genentech

JAMES HICKMAN
Professor, Nanoscience Technology Center, University of Central Florida

ERIC MARTIN
Director, Novartis

XIANG CHEN
Associate Member, St Jude Children's Research Hospital

YUAN WANG
Head, Research Analytics, UCB

NILS JAKOB HANSEN
Chief Executive Officer, Vipergen ApS

MAXIMILIAN SCHUIER
Senior Global Medical Affairs Leader Neuropsychiatry, Janssen

STEFAN PEUKERT
Associate Director, Novartis

MIKE SCHOPPERLE
Chief Executive Officer, CureMeta

For more information on our speakers,
please read the biographies available on our **event app**

CONFIRMED SPEAKERS – DAY TWO

PAUL SCOLA
Senior Scientific Director, Bristol Myers Squibb

MARTIN REDHEAD
Executive Director Primary Pharmacology, Exscientia

ANGEL GUZMAN-PEREZ
Head of Chemistry, Scorpion Therapeutics

ELLIOTT NICKBARG
Principal Scientist, Merck

JOHN QUINN
Distinguished Scientist, Biochemical and Cellular Pharmacology, Genentech

RALPH MAZITSCHEK
Assistant Professor, Harvard Medical School/Mass General Brigham

THOMAS HARTUNG
Professor and Chair, John Hopkins University

HONGWU WANG
Principal Scientist, Merck & Co., Inc

KUMAR SURESH
Vice President, Progenra Inc

AARON FRANK
Director, Head of Computational Chemistry Arrakis Therapeutics

SINA MOHAMMADI
Principal Scientist, Merck

TOMEK CIERPICKI
Professor, University of Michigan

DAVE MAUGER
Director of Data Science, Arrakis Therapeutics

TOBIAS RAABE
Research Assistant Professor, University of Pennsylvania

ABHINAV SHARMA
Translational Human Models Lead Engineer, Discovery Immunology, AbbVie

ESTHER LEE
Associate Director, AstraZeneca

KEVIN ROBBINS
Associate Principal Scientist, AstraZeneca

RAJESWARI BASU
Research Scientist, Boehringer Ingelheim

BANU PRIYA SRIDHARAN
Associate Director, GSK

JOE FRANKLIN
Senior Vice President, Anagenex

INDIA OTT
Scientist, AstraZeneca

LUCAS MASTROMATTEO
Data Analyst, GSK

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DISCOVERY US 2023

01 - 02 NOVEMBER 2023 | CAMBRIDGE, USA

DAY ONE: 01 NOVEMBER 2023

08:00 **Oxford Global Welcome Address**

TRACK 1: IDENTIFICATION & VALIDATION OF NOVEL TARGETS

Opening Keynote Address: Some Transferable Lessons In Drug Discovery

08:10

- All drug discovery programs are unique, but we tend to encounter a similar set of challenges
- Lessons gleaned from our collective experiences may be codified and utilized to help navigate future challenges

MARK MURCKO, Director,
Dewpoint Therapeutics

CONFERENCE ROOM 1: IDENTIFICATION & VALIDATION OF NOVEL TARGETS

Track Chair: NICOLA LA MONICA, Senior Director Search and Evaluation, **J&J Innovation**

Track Keynote Address: Building Explainable, Multi-Modal Language Models For Target Identification

08:40

- Identifying the right drug target is a critical challenge in drug discovery
- To address it, BenevolentAI has developed a Target-ID model based on natural language
- The model scores and ranks targets across the genome by searching an evidence database online and scoring the retrieved evidence
- The model leverages evidence across multiple modalities, such as literature and transcriptomics
- The model is explainable, using Shapley Additive exPlanations (SHAP) to illustrate how each piece of evidence impacts the prediction

DANE CORNEIL, Director of AI Science,
BenevolentAI

Targeting RNA With Small Molecules: Lessons Learned From Xist RNA

09:05

- The ability to target non-coding RNA would vastly expand the chemical space for drug development. We used a strategy based upon affinity-selection mass spectrometry to screen the noncoding XIST RNA and identified X1, a drug-like molecule that binds specifically to the RepA Q2 motif of Xist in vitro and in vivo
- Small-angle X-ray scattering analysis reveals that X1 changes the conformation of RepA in solution, which explains how it displaces interacting protein factors (PRC2 and SPEN) and inhibits X-chromosome inactivation
- These proof-of-concept experiments suggest that RNA can be systematically targeted by drug-like compounds to disrupt RNA structure and function

ELLIOTT NICKBARG, Principal Scientist,
Merck

Data Centric Approach To Discovering RNA-Targeted Small Molecules

09:30

- Arrakis has built an RNA-targeted small molecule discovery platform that is operating at scale
- Using modern informatics and data science practices allows us to extract learnings from the aggregate data
- We are currently developing machine learning models to accelerate our process

DAVE MAUGER, Director of Data Science,
Arrakis Therapeutics

09:55 **MORNING COFFEE & REFRESHMENTS**

1-2-1 Meetings x 3

Poster Displays

CONFERENCE ROOM 2: ON TARGET, PHENOTYPIC, AFFINITY AND VIRTUAL BASED SCREENING

Track Chair: GOVINDA BHISETTI, Vice President, **Cellarity**

Delegates welcome to attend co-located sessions

Joint Embeddings Of JUMP Cell Painting With Orthogonal Data Inform Hit Selection From Small Molecule Screens

- The JUMP Cell Painting data set is a public collection of phenotypic fingerprints for more than 100k small molecule perturbations. However, JUMP phenotypic fingerprints have limited separability, for example to differentiate or cluster small molecules by putative MoA
- To improve separability, we supplement JUMP data with orthogonal data, such as small molecule structure or assay data. By jointly modeling JUMP data together with these orthogonal data using AI-based methods such as variational autoencoders, we coerce separability that supports small molecule screening analytics
- We show joint models, using phenotypic data in conjunction with orthogonal data, enable hit expansion with improved confirmation rates compared to models using phenotypic or non-phenotypic data alone

MATTHEW PHARRIS, Senior Scientist,
UCB

Phenotypic Discovery Of Unique Mechanisms And Targets From Bioactivated Compounds

- Phenotypically screening large and chemically diverse compound decks can provide an abundance of unanticipated targets and mechanisms
- Bioactivation of compounds has largely been considered a nuisance characteristic of compound libraries owing to its proclivity to induce cell death through compound-mediated labeling, protein unfolding and stress
- However, selective bioactivation can lead to the identification of unique pathways and biology, opening a door to new therapeutic avenues

SHAUN MCLOUGHLIN, Principal Research Scientist,
AbbVie

CONFERENCE ROOM 3: COMPUTATIONAL DRUG DESIGN AND MOLECULAR DRUG DESIGN AND MEDICINAL CHEMISTRY

Track Chair: LEE HERMAN, Director Computational Chemistry, **Sunovion Pharmaceuticals**

Track Keynote Address: Identification Of A Novel Ultra-Potent Rifampicin Based Antibiotic

- Upon screening an anti-infective small molecule library, a trend for potent MRSA antibiotics was identified. Modifications to the lead core macrocycle followed by a SAR study yielded several potent compounds. Titrating the dose of the leads in vivo against MSRA infections identified very low amounts of the antibiotics needed to reduce the levels of the bacterium below the level of detection when concomitantly dosed with the standard of care (vancomycin). ADME and an exploratory rat toxicology study confirmed that the leads possessed the properties of a developable antibiotic for MSRA infections

THOMAS NITTOLI, Senior Director,
Regeneron Pharmaceuticals, Inc

Advances In Precision Oncology: The Discovery Of STX-478 And STX-721

- Overview of Scorpion Therapeutics approach to Precision Oncology
- The discovery of STX-721, a potent and Mutant-Selective EGFR exon 20 inhibitor with a potential best-in-class profile
- The discovery of STX-478, an allosteric, mutant-selective PI3Kα inhibitor with a best-in-class profile

ANGEL GUZMAN-PEREZ, Head of Chemistry,
Scorpion Therapeutics

In Silico Discovery Of Group II Intron RNA Splicing Inhibitors

- This presentation will discuss two key areas: Structure-based approaches as a tool to identify bioactive small molecules that target RNA, using the group II intron RNA as an example, and to uncover RNA-specific regions of chemical space

AARON FRANK, Director, Head of Computational Chemistry,
Arrakis Therapeutics

DISCOVERY US 2023

01 - 02 NOVEMBER 2023 | CAMBRIDGE, USA

	CONFERENCE ROOM 1: IDENTIFICATION & VALIDATION OF NOVEL TARGETS	CONFERENCE ROOM 2: ON TARGET, PHENOTYPIC, AFFINITY AND VIRTUAL BASED SCREENING	CONFERENCE ROOM 3: COMPUTATIONAL DRUG DESIGN AND MOLECULAR DRUG DESIGN AND MEDICINAL CHEMISTRY
10:55	**QuADD - Quantum-Aided Drug Design** • Polaris Quantum Biotech (POLARISqb), is developing QuADD (Quantum Aided Drug Design), a subscription-based SaaS product that finds your Lead-like Hits from a library of 10^30 molecules (and growing) in 1-2 days and answers the question of "When looking for new drugs, where do you start?". The output of QuADD is an enriched, diverse and superior molecular library for a specific protein target. In this presentation, we will discuss the requirements and quantum technology behind QuADD, as well as several case studies and how you can test it SHAHAR KEINAN, Chief Executive Officer, **Polaris Quantum Biotech**	**Successful Use Of Phenotypic Screening To Identify Protein Degraders For Neurodegenerative Diseases** • Considerations for phenotypic high throughput screens • Validation of hits using patient-derived cells • Deconvolution of mechanism of action for validated hits BETH HOFFMAN, Chief Executive Officer, **Origami Therapeutics, Inc.**	**Machine Learning Stapled Helical Peptide Design Principles** • Customized, interpretable, and performant ML models help us leverage diverse assay data to learn on helical peptides and prioritize synthetic designs. Analyzing feature performance in our models helps to identify residues/properties contributing to desireable activities, and analyzing performance as a function of distance to training data gives us confidence readouts for model applicability • We end by demonstrating how combining models in generative AI pipelines enables multi-objective optimization of Helicon drugs JOHN SANTA MARIA, Associate Director of Cheminformatics, **FogPharma**
11:20	**Drug Discovery At The Melting Point: Exploring And Validating Target Space With CETSA®** • The starting point for any desired biological effect is a drug-target interaction, an interaction that can be studied in a live cellular setting using the CETSA® technology. Drug hunters are now expanding the therapeutic target space to include harder to drug targets like non-enzymatic proteins, shallow protein-protein interactions, and flexible proteins like transcription factors. This focus further stresses the importance of target validation and understanding the molecular mode of action of the drugs. Because the CETSA® technology platform is label- and tag-free new targets and modalities can be studied in a physiological and therapeutically relevant way, which I will illustrate through a series of use-cases MICHAEL DABROWSKI, Chief Executive Officer, **Pelago Bioscience**	**Hit Profiler – An In-Silico Database & Text Mining Tool For Qualitative Pharmacogenomic Profiling Of Hit Series & Their Corresponding Chemical Space** • In conventional diversity-based High-Throughput Screening (HTS) workflows, the selection of the most promising compounds is mainly driven by drug-likeness and chemical tractability, and often relies on only minimal biological information generated within a screening program's assay cascade • To improve the process of selecting the best hit compounds, we have developed an in-silico tool to assess the literature for reported pharmacogenomic information that is associated with the chemical space of novel hit series. Combining this information with the actual primary, secondary and tertiary screening results, along with drug-likeness and chemical tractability assessment of the hit series facilitates and de-risks hit prioritization, expansion and hit-to-lead efforts • In this presentation we will present our fully automated ultra-High Throughput Screening workflow and show examples of how the new in-silico AI-tool helps to add value to hit discovery SAMAN HONARNEJAD, Chief Scientific Officer, **Pivot Park Screening Centre**	*Delegates welcome to attend co-located sessions*
11:50	**PRDMs - An Emerging Family Of Epigenetic Targets For Cancer** • Epigenetic modulators are valuable targets for anti-cancer therapeutics. Positive Regulatory Domain-containing Methyltransferases (PRDMs) are "Master regulators" of DNA that repress many common oncogenes (c-Myc, p53, etc) to suppress cell differentiation, proliferation, metastasis. PRDM target identification, approach to validation, and initial work with lead molecules based on on RNAi modalities will be discussed GLENN KAZO, Chief Business Officer, **ARIZ Precision Medicine**	**Myogenesis Development In Clonal Selection And Drug Resistance In Rhabdomyosarcoma** • Pediatric RMSs contain transcriptional states of developing muscle • Treatment of embryonal RMS selects for cells in a progenitor mesoderm-like state • Mesoderm-like cells are sensitive to EGFR inhibition • Treatment with both EGFR blockade and chemotherapy improves outcomes XIANG CHEN, Associate Member, **St Jude Children's Research Hospital**	**Introducing DELprint: A Dense Vector Representation Of Small Molecules Via DNA Encoded Library Selection Results And Deep Learning** • A dense vector fingerprint, pre-trained using DNA encoded library selection results is evaluated for performance in the context of virtual screening and QSAR modelling JEFF MESSER, Director, **GSK**
12:15	LUNCH BREAK & REFRESHMENTS	1-2-1 Meetings x 3 Poster Display	
	Track Chair: RUI WANG, Senior Director, **FL86**	**Track Chair:** GOVINDA BHISETTI, Vice President, **Cellarity**	**Track Chair:** LEE HERMAN, Director Computational Chemistry, **Sunovion Pharmaceuticals**

DISCOVERY US 2023

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CONFERENCE ROOM 1: IDENTIFICATION & VALIDATION OF NOVEL TARGETS

13:15

A New Era Of Single-Cell Functional Profiling For Drug Discovery

- At Lightcast we are developing a novel, programmable microfluidic platform that has the potential to both accelerate functional characterisation and shorten optimisation time in Antibody Discovery and T-Cell workflows

SIMON MARGERISON, Director of Customer Applications Support,
LightCast

13:45

Discovery Of Novel Targets – Application Of Genomic Sequencing Technologies

- Application of genomic sequencing technologies is transforming drug target discovery and therapeutics development
- Oxford Nanopore long read sequencing enables identification of patient-specific, disease relevant microbial species, facilitating understanding of disease pathobiology and development of therapeutic strategies for IBD
- Ribo-seq enables discovery of HLA-I peptides and proteins derived from novel unannotated open reading frames, facilitating novel antigen discovery for cancer immunotherapy and novel protein discovery for therapeutic targets

YUXIN LIANG, Senior Principal Scientific Manager,
Genentech

14:10

AI-Enabled Insights On Molecules Of Novel Modalities

- State-of-the-art AI models such as large language models (LLM) have demonstrated impressive performance in chatbots and related human-interfacing tasks
- In drug discovery, these models can be used for better understanding of protein structures, exemplified by recently reported folding algorithms
- They can also be used to better describe therapeutic biomolecules of novel modalities, and can enable better insights on hit-finding strategy and optimization options, which we will discuss in this talk

YUAN WANG, Head, Research Analytics,
UCB

CONFERENCE ROOM 1: IDENTIFICATION & VALIDATION OF NOVEL TARGETS

14:35

Novel Approaches To Treat Neuropsychiatric Diseases

- Major Depressive Disorder (MDD) symptoms arise from multiple underlying pathophysiological pathways
- Monoaminergic pathways are foundational to depression, however in some patients unresolved and persistent symptoms may be mediated by pathophysiology other than the monoaminergic one and will therefore best respond to add on therapy selectively targeting these pathways
- Next generation therapies selectively targeting the underlying pathophysiology of specific MMD domains should improve outcomes beyond current standard of care

MAXIMILIAN SCHUIER, Senior Global Medical Affairs Leader Neuropsychiatry,
Janssen

15:00

AFTERNOON BREAK

1-2-1 Meetings x 3

Poster Display

CONFERENCE ROOM 2: ON TARGET, PHENOTYPIC, AFFINITY AND VIRTUAL BASED SCREENING

PRCISR™ CRISPR: Vivlion's CRISPR Enabled PCR-Free Discovery Platform

- PRCISR™ CRISPR is Vivlion's CRISPR-based discovery platform, combining gene editing knowledge and our proprietary technology, to tailor uniformly distributed single and combinatorial CRISPR libraries that enable insightful CRISPR screens. PRCISR™ CRISPR PCR-free libraries maximize gene editing efficiency and hit-retention rates, while PRCISR™ CRISPR screens enable powerful parallelization and identification of combinatorial phenotypes. As such, PRCISR™ CRISPR enables the discovery of robust candidates for downstream validation, and enables genome-scale screens in hard to edit cells – for example, iPSC and primary cells

MARTIN WEGNER, Head of R&D,
Vivlion

DELs In Cells

- Screening of DNA-encode Libraries inside Living Cells (unique capability)
- Success rate higher - More physological relevant screening conditions
- Target space broader - No need for purified protein target
- TAT shorter - No need for purified protein target
- Molecular glue direct screen

NILS JAKOB HANSEN, Chief Executive Officer,
Vipergen ApS

High-Throughput Discovery And Parallel Optimization Of Peptide Therapeutics

- We developed a platform to discover peptidic molecules binding to protein targets. It uses digital micromirror devices for parallel synthesis of millions of unique peptides on a microarray. With 300+ amino acid building blocks, over 18 million peptides are synthesized in <48 hours. This technique can create linear and cyclic peptidic molecules for diverse screens. The process allows rapid evolution of high-affinity, high-specificity peptidomimetics in a reproducible, digitally controlled manner

LAUREN GOODRICH, Vice President, Therapeutic Discovery,
Nimble Therapeutics

CONFERENCE ROOM 2, PART 2: EMERGING MODALITIES: TARGETED PROTEIN DEGRADATION

Design Strategies For Optimizing PROTACs At AstraZeneca

- Exploring selectivity and oral bioavailability with VHL and CRBN E3 ligases
- Estrogen Receptor Case study

ESTHER LEE, Associate Director,
AstraZeneca

CONFERENCE ROOM 3: COMPUTATIONAL DRUG DESIGN AND MOLECULAR DRUG DESIGN AND MEDICINAL CHEMISTRY

XtalPi's Journey Into Automation: A Disruptive Force In Drug Discovery

- The field of drug discovery has long been plagued by inefficiencies and high costs, hindering the rapid development of novel therapeutics. In this talk, we will explore the journey of XtalPi, a leading AI-driven technology company to enable drug discovery, as it delves into the world of automation to disrupt the drug discovery process. We will discuss the automation technologies developed by XtalPi which have the potential to significantly accelerate the discovery and optimization of new drug candidates. XtalPi aims to reduce the time and cost associated with bringing new drugs to market, ultimately benefiting patients worldwide. We will also examine the potential disruptive impact of XtalPi's automation efforts on the broader scientific community, as well as the challenges and opportunities that lie ahead in this rapidly evolving field

SARAH TRICE, Chief Operating Officer and Head of US Operations,
XtalPi

The Use Of Molecular Dynamics To Improve Structure-Based Prediction Of hERG Inhibition

- Machine learning models are an integral part of AI platforms. These models can be very robust when the training set used to build them covers a large chemical space. When there is not enough data available target structure-based methods can be very useful. How this approach can be used to predicting hERG inhibition and how molecular dynamics can be used to improve the model will be showed

ISTVAN ENYEDY, Senior Principal Scientist,
UCB

Generative Flow Networks For Drug Discovery

- In this talk I'll introduce a new machine learning framework which we've called Generative Flow Networks, and try to convince you of its power for AI-Driven scientific discovery. I'll then showcase how we use this framework in a drug discovery context, and discuss the challenges that lie ahead

EMMANUEL BENGIO, Senior Machine Learning Scientist,
Recursion Pharmaceuticals

CONFERENCE ROOM 3: COMPUTATIONAL DRUG DESIGN AND MOLECULAR DRUG DESIGN AND MEDICINAL CHEMISTRY

Integrating HTS And DEL Hits In The Lead Generation And Optimization Of PLD2 Inhibitors

- Murine in vivo studies have shown that PLD2 deficiency significantly reduced psoriasiform inflammation in IL-23-injected ears
- Efficient and PLD2-selective hits from a high throughput screen were identified and modified to improve potency and pharmacokinetic attributes
- Structural features from hits identified in a DNA-encoded library screen were studied using in silico modeling and incorporated to improve binding kinetics. These efforts culminated in the identification of efficient in vivo active PLD2 inhibitors

(Virtual Presentation) HASAN KHAN, Senior Scientist,
AbbVie

Company Spotlights

15:10	Immunocure Discovery Solutions
15:30	Nuclera

DISCOVERY US 2023

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	CONFERENCE ROOM 1: IDENTIFICATION & VALIDATION OF NOVEL TARGETS	CONFERENCE ROOM 2, PART 2: EMERGING MODALITIES: TARGETED PROTEIN DEGRADATION	CONFERENCE ROOM 3: COMPUTATIONAL DRUG DESIGN AND MOLECULAR DRUG DESIGN AND MEDICINAL CHEMISTRY
16:00	**Panel Discussion:** The Future Of The Lead Discovery Toolbox • Comparison of fragment, virtual, and DEL screening techniques • Building a complementary toolbox, and combinations of methods • Evolution of screening strategies	**Employing Computer Aided Experimentation To Deorphan Proteins Without Cognate E3 Ligases** • Molecular glues offer a new paradigm for the modulation of biological systems compared to traditional inhibition. The search for molecular glues is hampered by a lack of data. Currently the majority of proteins do not have a cognate E3 ligase, and the majority of ligase binding motifs are unknown • The talk will detail the search for novel protein-ligase combinations and their glues by combining an understanding of the molecular pharmacology of glue systems, automation, and Exscientia's 'AI first' experimental approach MARTIN REDHEAD, Executive Director Primary Pharmacology, **Exscientia**	**Profile-QSAR Vs. Other Massively-Multitask Machine Learning Methods** • Profile-QSAR accuracy is comparable to multitask Deep Neural Networks (mtDNNs) • Profile-QSAR assesses the accuracy of final production models, mtDNNs do not • Profile-QSAR is naturally well-adapted to federated models, transfer learnings and scales well to massive datasets • However, Profile-QSAR is slower to predict a few compounds on a few models ERIC MARTIN, Director, **Novartis**
16:25	**Moderator:** JUSTYNA SIKORSKA, Associate Principal Scientist, **Merck** **Panellists:** JEFF MESSER, Director, **GSK** KINGSLEY APPIAH, Director, In Vitro Pharmacology & HTS, **Dewpoint Therapeutics**	**CoraFluor-Enabled TR-FRET Assay Strategies For Facile PROTAC Profiling** • We have developed a novel TR-FRET-based assay platform to facilitate the development of PROTACs and molecular glue degraders, including measurements of endogenous protein levels, target affinity profiling and quantitative determination of ternary complex formation and cooperativity RALPH MAZITSCHEK, Assistant Professor, **Harvard Medical School/Mass General Brigham**	**Discovery Of A Safe GIRK1/4 Inhibitor For Pharmacological Cardioversion Of Atrial Fibrillation** • Atrial fibrillation (AF) is the most common cardiac arrhythmia, and a significant risk factor for ischemic stroke and heart failure. Marketed anti-arrhythmic drugs can restore sinus rhythm, but with limited efficacy and significant toxicities, including potential to induce ventricular arrhythmia. Atrial-selective ion channel drugs are expected to restore and maintain sinus rhythm without risk of ventricular arrhythmia • One such atrial-selective channel target is GIRK1/4 (G-protein regulated inwardly rectifying potassium channel 1/4). Here we describe the discovery of a potent GIRK1/4 inhibitor developed to cardiovert AF to sinus rhythm while minimizing central nervous system exposure – an issue with preceding GIRK1/4 clinical candidates STEFAN PEUKERT, Associate Director, **Novartis**
16:50	**A Comparison Of Mass Spectrometry Based Drug Target Deconvolution Techniques For A CDK9 Inhibitor** • Mass spectrometry-based proteomics is an indispensable tool for drug discovery and development. This presentation will highlight the value of quantitative mass spectrometry approaches to drug discovery in the context of CDK9 biology • CDK9 represents one of the most studied examples of a transcriptional CDKs. Target identification and selectivity profiling in proteome wide cellular systems provide valuable information for lead candidate molecules • A comparison of classical affinity purification chemical proteomics, Kinobeads assay, compressed CEllular Thermal Shift Assay (CETSA®)-MS and Limited Proteolysis (LiP) to study the selectivity, target engagement and downstream mechanistic insights of a CDK9 tool compound will be presented ERIC MIELE, Associate Director Proteomics, **AstraZeneca**	**Targeted Protein Degradation: Beyond PROTACs** • PROTAC drug development remains a challenging endeavor and new modalities such as molecular glue degraders are emerging. Progenra has harnessed its unique expertise and UbiPro E3 discovery platform to discover novel E3 ubiquitin ligase ligands as well as molecular glue degraders of therapeutically relevant target proteins. This presentation will provide examples of harnessing E3 ligases for targeted degradation of several proteins including membrane and cytosolic proteins. This presentation will also highlight Progenra's approaches to the discovery, development, optimization, and characterization of novel E3 based small molecule degraders KUMAR SURESH, Vice President, **Progenra Inc**	**CM-09, A First-In-Class Antibody-Drug-Conjugate Specific To A Novel Embryonic Target In Pancreatic And Gastric Cancers** MIKE SCHOPPERLE, Chief Executive Officer, **CureMeta**
17:15	**Absolute Quantification Of Oncolytic Viral Proteins Using UPLC-MRM** • Development of novel analytical mass spectrometry technique for absolute quantification of viral proteins in VSV-GP • Tracking of GPC using this technique in time point VSV-GP infected HEK-293 cells *(Virtual Presentation)* RAJESWARI BASU, Research Scientist, **Boehringer Ingelheim**	*Delegates are welcome to attend co-located sessions*	**Panel Discussion:** Technologies & AI Applied To Drug Design • Using AI to optimise chemical synthesis • Designing chemical molecules • AlphaFlow: will this technology revolutionize automated synthesis • Alpha fold **Moderator:** SHAHAR KEINAN, Chief Executive Officer, **Polaris Quantum Biotech** **Panellists:** ERIC MARTIN, Director, **Novartis** ISTVAN ENYEDY, Senior Principal Scientist, **UCB** AMIR NIKOOIE, Director, **Eli Lilly and Company**
17:40	**Drinks Reception & Speed Networking**		

DISCOVERY US 2023

01 - 02 NOVEMBER 2023 | CAMBRIDGE, USA

DAY TWO: 02 NOVEMBER 2023

CONFERENCE ROOM 2: MORNING ROUNDTABLE DISCUSSIONS

Track Chair: ABHINAV SHARMA, Translational Human Models Lead Engineer, Discovery Immunology, **AbbVie**

Roundtable Discussion 1: Overcoming Challenges In Mature Tissue Organoid Modelling

- Differentiation of iPSC derived and adult tissue derived organoids
- Establishment of organoid co-cultures and organoid microfluidic systems - gene targeting of organoids
- Use of organoids in HTP screens

Moderator: TOBIAS RAABE, Research Assistant Professor, **University of Pennsylvania**

08:30

Roundtable Discussion 2: Driving Automation Efforts In Drug Discovery

- What's preventing you from using automation?
- What current hurdles face your automation efforts?
- What data/assessment do you look for before using automation for research?

Moderator: ANDREW DORAN, Principal Scientist - Automation, **Anagenex**

CONFERENCE ROOM 1: ANIMAL MODELS FOR DISEASE, ORGAN MODELLING - ORGANOID BASED DISCOVERY & ORGAN ON CHIP DEVELOPMENT

Human Derived Organoid And Organ-On-Chip Models

- Currently there is a strong unmet need to develop scale-able translational models that predict immune response for check point inhibitor efficacy in oncological preclinical platforms
- The talk with cover patient derived organoids immune coculture development and assessment through high-content assay and tool compounds response

09:00

BANU PRIYA SRIDHARAN, Associate Director,
GSK

CONFERENCE ROOM 1: ANIMAL MODELS FOR DISEASE, ORGAN MODELLING - ORGANOID BASED DISCOVERY & ORGAN ON CHIP DEVELOPMENT

Track Chair: ABHINAV SHARMA, Translational Human Models Lead Engineer, Discovery Immunology, **AbbVie**

Microphysiological Systems To Mimic Human Organ Function: Can One Size Fit All?

- Discuss an example of a commercial MPS and discuss the possibility of applying a single platform to model biological function of multiple organs
- Applying the MPS to mimic mechanism of actions relevant to human diseases that enables drug screening
- Examples of adding biological complexity in the MPS to enable the study of multi-cellular interactions

09:25

ABHINAV SHARMA, Translational Human Models Lead Engineer, Discovery Immunology,
AbbVie

Building Robust Pre-Clinical Drug Discovery Workflows With Precision Reprogrammed Human iPSC-Derived Cells

- Address the challenges of implementing hiPSC-derived cells in the drug discovery process from Target ID/Validation through to candidate selection
- Learn how a new technology is overcoming inconsistencies in human cell production to enable the generation of highly defined, rapidly maturing hiPSC-derived cells
- Discover success stories where precision reprogrammed hiPSC-derived cells have supported CRISPR screens to identify druggable targets for neurodegeneration and lead generation of antisense oligonucleotide therapeutics for genetic diseases

09:50

TIMOTHY SMITH, Associate Director of Sales,
bit.bio

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THE CELL CODING COMPANY

CONFERENCE ROOM 2: HIT FINDING TECHNOLOGIES AND MOLECULAR DRUG DESIGN

Track Chair: JEFF MESSER, Director, **GSK**

Discovery Proteomics For Investigating Interactomes

- Biotin-based LC/MS is a useful tool to examine the interactions of a protein of interest, particularly intractable targets, and has been developed beyond standard biotin ligases. It can be used for early discovery or later stage molecule testing

INDIA OTT, Scientist,
AstraZeneca

Delegates welcome to attend co-located session

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CONFERENCE ROOM 2: HIT FINDING TECHNOLOGIES AND MOLECULAR DRUG DESIGN

10:20

Comprehensive Tumor Modelling And Its Application In Discovery And Development Of Next Generation Oncology Drugs

- We present a study on comprehensively modelling of the tumor environment comprising a vascular plexus, stroma, immune cells and hepatocellular carcinoma material. We analyzed response from 8 different donors to a panel of drugs

JOS JOORE, Chief Executive Officer,
Mimetas

Delegates welcome to attend co-located session

10:50

MORNING COFFEE & REFRESHMENTS

1-2-1 Meetings x 3

Poster Displays

11:50

Discovery Of A Macrocyclic Peptide Inhibitor Of Programmed Death-Ligand 1 (PD-L1)

- Identification of a macrocyclic peptide inhibitor of PD-L1 from a selection process.
- Optimization of binding through rational drug design
- Resolution of off-target liabilities
- Further/final optimization of binding and understanding of binding kinetics
- Key studies in progression to the clinic
- Early clinical data in healthy volunteers

PAUL SCOLA, Senior Scientific Director,
Bristol Myers Squibb

Designing DNA Encoded Libraries For Success In Small Molecule Lead Identification And Machine Learning

- Combining DEL + ML: overview of Anagenex Platform
- Designing and building DEL's for success in small molecule drug discovery
- Oncology success story

JOE FRANKLIN, Senior Vice President,
Anagenex

12:15

Genome Editing In Human Organoids With Lipid Nanoparticles

- LNP mediated cell and tissue specific targeting - challenges and opportunities
- Human organoids for validation of LNP mediated cell and tissue specific targeting

TOBIAS RAABE, Research Assistant Professor,
University of Pennsylvania

Augment Diversity Screening With Machine Leaning Compound Selections

- We adopted a screening strategy of using a diverse subset of our compound collection
- We supplemented this library with specialty collections, project specific sets and post screening IFS
- This strategy yields positive outcomes for two-thirds of our HTS campaigns

HONGWU WANG, Principal Scientist,
Merck & Co., Inc

12:40

Investigations Of Neurological Diseases And Disorders Utilizing Phenotypic Human-On-A-Chip Platforms

- We have been constructing multi-organ human-on-a-chip systems for safety and efficacy with up to 5 organs and have demonstrated long-term (>28 days) evaluation of drugs and compounds, that have shown similar response to results seen from clinical data or reports in the literature
- These models utilize a pumpless platform with serum free recirculating medium, which is a low volume system that can evaluate parent compounds as well as metabolites, if the liver is included
- Sanofi has used efficacy data from our conduction velocity phenotypic model to file the first IND utilizing only MPS data for efficacy that has enabled a clinical trial (#NCT04658472) and is described in our recent joint publication

JAMES HICKMAN, Professor, Nanoscience Technology Center,
University of Central Florida

Discovery Of PRC1 E3 Ligase Inhibitors Using Fragment Based Approach

- PRC1 (Polycomb Repressive Complex 1) is an epigenetic regulator implicated in gene repression
- PRC1 plays an essential role in maintaining self-renewal and blocking differentiation of leukemia stem cells and blocking PRC1 could lead to a novel therapeutics for AML
- We employed fragment-based drug discovery approach to develop PRC1 inhibitors binding to RING1A and RING1B
- Our inhibitors block binding of PRC1 to chromatin and H2A ubiquitination
- Treatment of leukemia cells with PRC1 inhibitors results in gene de-repression, induction of cellular differentiation and block in proliferation
- PRC1 inhibitors impair leukemia burden in mice models of AML

TOMEK CIERPICKI, Professor,
University of Michigan

13:05

LUNCH BREAK & REFRESHMENTS

1-2-1 Meetings x 3

Poster Display

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14:05	**Panel Discussion:** Overcoming Challenges Of Scalability In Organoid And Organ On A Chip Modelling • Choosing the right biological inputs to increase reproducibility and robust • Considerations on the type of device and perfusion cell culture system for scalability • Integration of automation and multiple readouts • Increasing complexity and the need for efficient platforms **Moderator:** JASON EKERT, Head of US Discovery Translational Technology, **UCB** **Panellists:** JAMES HICKMAN, Professor, Nanoscience Technology Center, **University of Central Florida** BANU PRIYA SRIDHARAN, Associate Director, **GSK** ABHINAV SHARMA, Translational Human Models Lead Engineer, Discovery Immunology, **AbbVie** TIMOTHY SMITH, Associate Director of Sales, **bit.bio**	**Panel Discussion:** Integration Of Technologies For HIT Triage And Early Exploration **Moderator**: JEFF MESSER, Director, **GSK** **Panellists:** GOVINDA BHISETTI, Vice President, **Cellarity** SHAHAR KEINAN, Chief Executive Officer, **Polaris Quantum Biotech** KINGSLEY APPIAH, Director, In Vitro Pharmacology & HTS, **Dewpoint Therapeutics**
14:30		**Beyond Rule Of 5 And PROTACs Properties For Oral Bioavailability** • Property based drug design structural & dynamical parameters • Measuring free ligand drug-like descriptors for bRo5 & PROTACs • Summary and key learnings KEVIN ROBBINS, Associate Principal Scientist, **AstraZeneca**
14:55	**Development Of A High-Throughput Barrier Function Assay Using Primary Human Gut Organoids** SINA MOHAMMADI, Principal Scientist, **Merck**	**Introducing DELyte: Computational Approaches To Mitigating Sequence Specific DNA Driven Artifacts In DNA Encoded Library Selection Data** • Will discuss my work developing a computational approach to mitigating DNA driven enrichment in DNA encoded library selection experiments LUCAS MASTROMATTEO, Data Analyst, **GSK**
15:20	**End of Conference**	

Le Méridien Boston Cambridge

The nearest Subway (T) Stations are Central on the Red Line, and Kendall/MIT also on the Red Line. The nearest Bus and Train Station is Back Bay Station, which is across the Harvard Bridge or Longfellow Bridge.

Boston Logan International Airport is a 20 min taxi away from the venue. The hotel does not provide a shuttle service. Alternatively, you can take the Concord Coach to South Station and then change over to the Red Line to Central. More routes can be found on Google Maps.

The hotel does not offer on-site parking. The closest parking is 81 Green Street, Cambridge. There are 2 electric car charging stations available for a fee.

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