DISCOVERY US: In-Person

17 - 18 November 2022 | Boston, USA

200+ LEADING PHARMA, BIOTECH AND ACADEMIC DELEGATES ATTENDING ON-SITE & DIGITALLY

50+ PRESENTATIONS, CASE STUDIES AND DISCUSSIONS

6 INTERACTIVE TRACKS ON THE LATEST INNOVATIONS

Conference Brochure

KEY SPEAKERS INCLUDE

Janaky Coomaraswamy Novartis
Paul Scola Bristol Myers Squibb
Andrea Bortolato SandboxAQ
Eric Martin Novartis
Jeff Messer GSK
Paul Richardson 34|HU

Book Now: www.oxfordglobal.co.uk/discovery-us/book-now/
Join the Conversation: #RNDSeries22
On behalf of the entire Oxford Global team, I am delighted to welcome you to our Discovery US Congress. Over the next two days, the event will allow participants, both in-person and online, to engage with content and one another.

The Oxford Global team look forward to meeting you over the course of the congress and will be on hand to ensure your time is both productive and enjoyable. Oxford Global Conferences have been producing cutting edge congresses and summits for the Life Sciences Industry for over 15 years now. We annually bring together thousands of industry leaders and solution providers creating the opportunity to partner, network and knowledge share. I am pleased to let you know that we have now successfully completed a transition from an in-person event organiser to a one stop shop platform for all research-critical information pertaining to the discovery space. We also would like to invite you to visit our Discovery Series Content Portal to find out more about our brand-new membership offering giving you access to the latest advancements and technology insights within the R&D community. 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 forms part of our highly successful Discovery Series, incorporating a diverse range of topics across all stages of the drug discovery process. It will provide a comprehensive look at the current trends, challenges & developments impacting the R&D sector, providing invaluable insights on the latest innovative techniques and strategies for pharmaceutical development. With a programme full of industry-leading experts, the agenda will focus on topics addressing drug discovery in new modalities such as protein degradation, and case studies on the integration of screening approaches in phenotypic and genomics- based discovery, Organ-on-a-chip and 3D modelling. In addition to this, you will also be able to learn about key focus areas in drug design, including AI in
drug design: in chemical synthesis, target ID capabilities & lead identification/optimisation.

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 booths in-person and featured sponsor pages on the event app.

New for 2022 is the event delivery format which has been redesigned to ensure that both in-person and online delegates can access presentation recordings on-demand and interact with speakers and peers using our Swapcard platform. Swapcard serves as our content delivery tool and peer to peer networking platform for virtual delegates as well as the event app for those who are joining us in-person. You will gain access to the platform minimum three days prior the event and can enjoy access up to 7 days after the congress to catch up on any talks you have missed.

Lastly as we wanted to create an environment where in-person delegates can converse in smaller groups, all conference rooms will host a series of engaging discussions such as panels and workshops to encourage as much knowledge-sharing as possible.

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

Hayley Watson,
Senior Director, Commercial Strategy

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.co.uk/discovery-us/plan-your-visit/
**WHO IS ATTENDING?**

**200+ VPs, Directors & Senior Managers** will be attending on-site and online, 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

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**3URMHWHG$WWHQGH3UR4OH**

**These companies and many more:**

- AstraZeneca
- Novartis
- Bristol Myers Squibb
- IFM Therapeutics
- BERG
- Black Diamond Therapeutics
- Exscientia
- BenevolentAI
- Genentech
- Ipsen
- Abbvie
- Eisai
- GSK
- Janssen
- Merck

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**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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**SECTOR**

- 51% Industry
- 29% Academic
- 20% Vendor Companies

**FUNCTION**

- 59% Scientist
- 31% Directors / Managers / Professors
- 10% Commercial / Business Dev

**GEOGRAPHY**

- 90% USA
- 10% Rest of World
Who is Sponsoring?

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To view the full list of Sponsors and their profiles please visit

www.oxfordglobal.co.uk/discovery-us/sponsorship/
**Discovery US: In-Person** features 2 days of in-person cutting-edge presentations and knowledge-sharing, including over 50 industry insights, sponsored presentations and think tank roundtable discussions.

### DAY ONE - 17 NOVEMBER 2022

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<th>Track 1: Identification &amp; Validation of Novel Targets and Emerging Modalities</th>
<th>Track 2: Animal and Disease Modelling, Organoid-based Discovery, Organ On Chip Development, 3D Media</th>
<th>Track 3: Computational Drug Design</th>
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<tr>
<td>• New Modalities &amp; Emerging Drug Targets in Oncology, Immunoncology and other disease areas</td>
<td>• Translating Breakthrough Discoveries In Stem Cell Biology And Organ Development</td>
<td>• AI &amp; Automation in Chemical Synthesis, Target ID capabilities, Lead Identification, Lead Optimisation, Measuring PK/PD and prediction</td>
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<td>• Engineering The Next Generation T Cell Based Therapeutics CRISPR/Cas9</td>
<td>• Utilisation of 3D-model Systems And Organoids In Phenotypic And High Content Screening</td>
<td>• Implementation of Alpha Fold, Something Useful Or Complete Hype?</td>
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<td>• AI To Unblock Drug Discovery, Drug Repurposing And Target Validation</td>
<td>• Modelling Protein Aggregation In Human iPSC</td>
<td>• Utilisation of 3D-model Systems And Organoids In Screening For Safety And Efficacy Assessment</td>
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<td>• Discovery of 1ST Class Inhibitors</td>
<td>• 3D Media and 3D Cell Culture</td>
<td>• Target Identification and Validation</td>
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<tr>
<td>• Cellular and Biological Based Drug Discovery</td>
<td>• Cellular modelling</td>
<td>• Translational Models in Organoid and Organ on Chip</td>
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<td>• Novel Therapeutic Approaches that expand the Scope of Druggable Targets with Targeted Protein Degradation</td>
<td>• Safety and Efficacy Considerations</td>
<td>• Technologies and AI Applied To Drug Design</td>
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<td>• Small Molecule RNA based Discovery approaches</td>
<td>• Applications of Organ on a chip in disease modelling</td>
<td>• Biophysical Tools For Difficult Targets- building the right flow chart</td>
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**Afternoon Interactive Panel Sessions:**
- The Use of Alpha Fold, Something Useful Or Complete Hype?
- Utilisation of 3D-Model Systems And Organoids In Screening For Safety And Efficacy Assessment
- Target Identification and Validation
- Translational Models in Organoid and Organ on Chip
- Technologies and AI Applied To Drug Design

### DAY TWO - 18 NOVEMBER 2022

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<th>Track 1: Target and Phenotypic Based Discovery and Screening approaches</th>
<th>Track 2: Hit Finding Technologies And Advancements</th>
<th>Track 3: Molecular Drug Design and Medicinal Chemistry</th>
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<tr>
<td>(HTS vs Fragment vs DEL) Including the Use of Automation of screening in hit finding</td>
<td>Showcase of hit-to-lead components &amp; technologies e.g. Targeted Protein Degradation, covalent inhibitors, DELs</td>
<td>• Fragment &amp; Structured Based Drug Discovery Innovation including AI/ML driven Drug Design</td>
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<td>Fast Structure-Based Virtual Screening in Readily Available Chemical Space</td>
<td>Case studies of lead generation in small and large molecules</td>
<td>• Efficient Combination Of Machine Learning And Automation To Accelerate DMTA Cycles</td>
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<td>Machine Learning in DELs</td>
<td>Enabling Tools For Hit-Finding Against Difficult Targets</td>
<td>• Innovating the Chemistry Lab Bench</td>
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<td>Application of CRISPR Technology and Screening to in vivo Models of Cancer Immunotherapy</td>
<td>Applications Of Covalent Fragments To Drug Lead Generation</td>
<td>• Automation In The Organic Chemistry Laboratory- A Workflow Case Study in Accelerating:</td>
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<tr>
<td>Identification and Validation of Novel Targets – Genomic Tools For Elucidating Novel Targets</td>
<td>Biophysical Tools For Difficult Targets- building the right flow chart</td>
<td>» Generation of novel chemical space and filtering by predictive models</td>
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<td>Screening approaches in the chemical space</td>
<td>Hit Identification Strategy For Glue Degraders, Deeper Mechanistic Understanding Of TPDS</td>
<td>» Library automation</td>
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<td>» High throughput experimentation</td>
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**Afternoon Interactive Panel Sessions:**
- Phenotypic Based Discovery & Screening Approaches
- Integration Of Technologies for HIT Triage and Early Exploration
- Addressing Specific Targets And Dealing With Target Engagement
CONFIRMED SPEAKERS – DAY ONE

PAUL SCOLA
Senior Director in Drug Discovery, Bristol Myers Squibb

ERIC MARTIN
Director, Novartis

JONATHAN SOLOMON
Director, Chemical Genetics, Novartis

ANDREA BORTOLATO
Director of Drug Discovery, SandboxAQ

KUMAR SURESH
Vice President, Research and Development, Progenra

JANAKY COOMARASWAMY
Senior Principal Scientist, Novartis

SHAUN GAMBOA
Chief Executive Officer, sevenTM

SHAHAR KEINAN
Chief Executive Officer, POLARISqb

TAMARA REYES ROBLES
Associate Principal Scientist, Merck

DOMAGOJ VUCIC
Senior Fellow, Genentech

JIM CREGG
Associate Director of Medicinal Chemistry, Revolution Medicines

GRACE CHUANG
Senior Research Fellow, Cytokinetics

MINGHU SONG
Associate Research Professor, Biomedical Engineering Department, University of Connecticut

KERRIE SPENCER
Associate Principal Scientist, Chemical Biology, Merck

HENG ZHAO
Senior Scientist, AstraZeneca

THOMAS HARTUNG
Chair for Evidence-Based Toxicology, Johns Hopkins Bloomberg School of Public Health

MATTHIEU SCHAPIRA
Associate Professor, Structural Genomics Consortium, University of Toronto

AARON FRANK
Head of Computational Chemistry, Arrakis Therapeutics

ISTVAN ENYEDY
Senior Director Computational Chemistry, Theseus Pharmaceuticals

MEIHUA TU
Computational Chemist, Pfizer

GINETTE SERRERO
Chief Executive Officer, A&G Pharmaceutical

GOVINDA BHISETTI
Vice President, Computational Chemistry, Cellarity

ANDREW DORAN
Principal Scientist, Automation, Anagenex

JOSEPH RAYMAN
Associate Research Scientist, Columbia University
CONFIRMED SPEAKERS – DAY TWO

ERIC R GOEDKEN
Senior Principal Research Scientist, Dermatology, Immunology Discovery, AbbVie Bioresearch Center

RYAN MCCLURE
Senior Scientist II, AbbVie

(JOINING ONLINE)
PAUL RICHARDSON
Director, Discovery Chemistry, Pfizer Global Research & Development

JEFF MESSER
Director Analytics, GSK

PHIL COX
Research Fellow, Augmented Molecular Design, Discovery Platform Technologies AbbVie

SANJAY PANCHAL
Principal Research Scientist, AbbVie

PAUL BEROZA
Distinguished Scientist, Genentech

VICTOR HANSON-SMITH
Head of Computational Biology, Verge Genomics

HONGWU WANG
Principal Scientist, Merck

JOE FRANKLIN
Senior Vice President of Early Discovery, Anagenex

(JOINING ONLINE)
CATERINA MUSETTI
Principal Scientist, Bristol Myers Squibb

ZHENGZONG ZHU
Principal Scientist, Merck

HANS-PETER BIEMANN
Scientific Director, Sanofi

GOVINDAN SUBRAMANIAN
Senior Director, Gossamer Bio

ISRA HASSAN
Senior Scientist II, Novartis

MEGHAN LAWLER
Director, Affinity Technology, Anagenex

NATHANIEL LINTNER
Principal Scientist, Pfizer

JING YANG
Chief Scientific Officer, BaseCure Therapeutics

FLEUR KLEINPENNING
Senior Scientist Chemical Biology, Pivot Park Screening Centre

CONSTANTIN NEAGU
Senior Scientist, EMD Serono Research and Development Institute

For more information on our speakers, please read the biographies available on our event app.
# Discovery US: In-Person
## Day One: 17 November 2022 | Boston, USA

## Conference Room 1: Identification & Validation of Novel Targets, New Modalities

**Track Chair:** TAMARA REYES ROBLES, Associate Principal Scientist, Merck

**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

**Speaker:** PAUL SCOLA, Senior Director in Drug Discovery, Bristol Myers Squibb

## Conference Room 2: Animal and Disease Modelling, Organoid Based Discovery, Organ on Chip Development, 3D Media

**Track Chair:** EVA-MARIA SURMANN, Senior Product Manager, The Jackson Laboratory

**Developing Translatable Disease Biology Models In Neuroscience**
- The development of seeded aggregation models in human iPSC-derived neurons has advanced drug discovery in neuroscience:
  - Recaptulating protein misfolding in neurodegenerative disease (e.g., Parkinson's Disease)
  - Enabling the use of cell-based assays to study disease mechanisms
  - Utility for validating novel targets, and testing efficacy of compounds, related to key biological processes in vitro

**Speakers:** JANAKY COOMARASWAMY, Senior Principal Scientist, Novartis
  - ERIC MARTIN, Director, Novartis

## Conference Room 3: Computational Drug Design: AI Focus

**Track Chair:** ERIC MARTIN, Director, Novartis

**RSURYHPHQV'LYHUVH'S5OLFDWLRQV2I3UR4QH46S05DVLYHO1**

**Multitasked Modelling**
- Massively-multitask models give predictions comparable to 4-concentration IC50 experiments for 1000s of bioactivity and ADMET models
- Applications include virtual screening, off-target prediction, mechanisms-of-action, hit triaging, polypharmacology, isoform selectivity, etc
- New extensions include accuracy improvements, prediction uncertainty intervals, gene expression prediction, federated models for safe collaboration

**Speaker:** ERIC MARTIN, Director, Novartis

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## Delegates are welcome to attend co-located sessions

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## iPSC-Derived Human Cell Screening Services For A1ATD, Wilson's Disease And Other Metabolic Indications

**Speakers:** RICHARD WILLOCK, Chief Business Officer, DefiniGEN
  - FIONA LESLIE, Scientist, Newcells

**An In-Vitro High-Content Imaging Assay For The Study Of Fibroblast Activation And Matrix Deposition**
- We describe our new assay produced to meet the growing need for physiologically relevant, high-throughput assays to assist the drug development process for fibrotic respiratory disease
- The talk will cover the stages of assay optimisation and validation of an in vitro, high-content imaging assay, capable of measuring human fibroblast activation and collagen deposition
- This high-throughput assay will enable the screening of candidate compounds for their ability to alter the levels of secreted and deposited extracellular matrix

**Speakers:** RICHARD HARRISON, Chief Scientist, Causaly
  - RICHARD WILLOCK, Chief Business Officer, DefiniGEN
  - FIONA LESLIE, Scientist, Newcells

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## Delegates are welcome to attend co-located sessions

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## Morning Networking Break

**1-2-1 Meetings x 4**

**Company Spotlights**
A Structure-Based Approach To RNA-Targeted Small Molecules

AARON FRANK, Head of Computational Chemistry, Arrakis Therapeutics

Navigate Your Chemistry And Explore The Biology - Case Studies Of CETSA® Overcoming Challenges In Drug Discovery

STINA LUNDGREN, Head of Commercial Operations, Pelago Bioscience

PROTAC Mediated Degradation Of Membrane Proteins And Receptors

KUMAR SURESH, Vice President, Research and Development, Progenra
CONFERENCE ROOM 1: IDENTIFICATION & VALIDATION OF NOVEL TARGETS, NEW MODALITIES

14:10
Delegates are welcome to attend co-located sessions

14:35
TAMARA REYES ROBLES, Associate Principal Scientist, Merck

Panel Discussion: Target Identification & Validation

- What good looks like and what are realistic models
- Screening tools - application to target discovery
- Data science - integration machines learning and AI tools to target discovery
- Genomic & CRISPR techniques

Moderator: ANDREW DORAN, Principal Scientist - Automation, Anagenex
Panelists:
KUMAR SURES H, Vice President, Research and Development, Progena
VICTOR HANSON-SMITH, Head of Computational Biology, Verge Genomics
(Joining Online) GINETTE SERRERO, Chief Executive Officer, A&G Pharmaceutical

'LVFRY HU2I4FPW H6Q.SRHY H6POOOROHFXOHR Cardiac Myosin Inhibitor For The Potential Treatment Of Hypertrophic Cardiomyopathies (HCM)

GRACE CHUANG, Senior Research Fellow, Cytokinetics

Small Molecule Targeting Of Xist RNA Disrupts Repeat A Structure And X-Chromosome Inactivation

- We have developed a proof of concept study of small molecule modulation of a well-understood area of early developmental mammalian biology that relates to long non-coding RNAs (lncRNA): X-chromosome inactivation
- After screening 50,000 compounds, we discovered a series of small molecule binders to Xist that functionally active in cells by displaying the altered phenotype comparable to siRNA knockdown of Xist. The hit, X1, has drug-like properties and binds specifically to Xist's Rep6 motif biochemical and cellular assays
- This work demonstrates that RNA can be systematically targeted to yield drug-like compounds that disrupt RNA's structure and epigenetic function

KERRIE SPENCER, Associate Principal Scientist, Chemical Biology, Merck

CONFERENCE ROOM 2: ANIMAL AND DISEASE MODELLING, ORGANOID BASED DISCOVERY, ORGAN ON CHIP DEVELOPMENT, 3D MEDIA

16:25
Delegates are welcome to attend co-located sessions

Development Of Human Cell-Based Multi-Organ Microphysiological Systems (MPS)

(Joining Online) THOMAS HARTUNG, Chair for Evidence-Based Toxicology, Johns Hopkins Bloomberg School of Public Health

CONFERENCE ROOM 3: COMPUTATIONAL DRUG DESIGN: AI

16:00
Delegates are welcome to attend co-located sessions

From CPU To GPU To Quantum Computing: Machine Learning Drug Discovery Starts With The Hardware

- Machine learning drug discovery's journey over the last three decades
- Where are we now?: Serverless GPU-Based Machine Learning Drug Discovery
- What's next?: Quantum Simulation
(Joining Online) SHAHAM GAMBOA, Chief Executive Officer, sevenTM

Benchmarking Of Computational Hit-Finding Methods: Latest Developments From The CACHE Competition

- Dozens of AI and computational chemistry groups use their methods to predict hits for a predefined protein target
- Over 2000 compounds predicted for target #1 were purchased and tested experimentally. All data released on https://cache-challenge.org/
- New target announced every 4 months
MATTHIEU SCHAPIRA, Associate Professor, Structural Genomics Consortium, University of Toronto

On Decoding Strategies For Deep Molecular Generation And Chemical Space Navigation

- Few thorough studies on decoding strategies of deep molecular generation
- Current decoding approaches and their limitations when applied to the chemical space navigation
- Introduction of the concept of decoding strategies of deep molecular generation
MINGHU SONG, Associate Research Professor, Biomedical Engineering Department, University of Connecticut

Small Molecules & Quantum Computing

- Potential in improved use of Alpha-Fold
- Difficulties in generation of structures
- Current decoding approaches and their limitations when applied to the chemical space navigation
- Introduction of the concept of decoding strategies of deep molecular generation

SHAHAM KEINAN, Chief Executive Officer, POLARISqb

meal Time: 3

Company Spotlights

15:00
16:00
AFTERNOON NETWORKING BREAK
**DISCOVERY US: In-Person**

**DAY TWO: 18 NOVEMBER 2022 | BOSTON, USA**

17:15 - 17:40

**CONFERENCE ROOM 1:** IDENTIFICATION & VALIDATION OF NOVEL TARGETS, NEW MODALITIES

**Introduction To CETSA With Focus On CETSA Exploration And Compressed CETSA - Case Studies Including Application Of CETSA At Various Projects**

- Why is CETSA important for target deconvolution of small molecules?
- How CETSA helps understanding a potential therapeutics mechanism of action and safety liabilities
- How CETSA shows to be an indispensable method for unbiased, proteome-wide, chemistry free target deconvolution
- The application of CCETSA at various project stages like phenotypic HTS hit, candidate identification drug, lead optimization identification drug, literature compounds there by influencing key project decisions

*HENG ZHAO, Senior Scientist, AstraZeneca*

**CONFERENCE ROOM 2:** IDENTIFICATION & VALIDATION OF NOVEL TARGETS, NEW MODALITIES

**Leveraging Stress Granule Biology To Treat Neurodegenerative Disorders**

- Stress granules (SGs) serve an adaptive role during cellular stress
- Dysregulated SG dynamics can drive neurodegeneration
- Pharmacological targeting of SG proteins may limit pathological protein aggregation and slow neurodegenerative processes

*JOSEPH RAYMAN, Associate Research Scientist, Columbia University*

17:40 - 18:05

**Drinks Reception & End of Day One**

**CONFERENCE ROOM 3: COMPUTATIONAL DRUG DESIGN: AI FOCUS**

**Targeting KRAS* (G12C)* and Beyond**

- Tri-Complex Platform Enables Selective Targeting of Oncogenic RAS(ON) Proteins, Including KRAS* (G12C)(ON), RAS* (MULTI)(ON), KRAS* (G12D)(ON), and KRAS* (G13C)(ON)

*JIM CREGG, Associate Director of Medicinal Chemistry, Revolution Medicines*

18:05 - 20:30

**DAY TWO: 18 NOVEMBER 2022**

**CONFERENCE ROOM 1: TARGET AND PHENOTYPIC BASED DISCOVERY AND SCREENING APPROACHES**

**Track Chair:** VICTOR HANSON-SMITH, Head of Computational Biology, Verge Genomics

**The Use Of AI To Drive Target Discovery With Integrated MultiOmics**

- Industry appetite for new targets that work
- New and tractable targets can be identified by combining multi-omics data from human cohorts into a machine learning framework
- AI/ML approaches for target discovery are most powerful when embedded within a “full-stack” discovery organization that includes pre-clinical and clinical endpoints

*VICTOR HANSON-SMITH, Head of Computational Biology, Verge Genomics*

**Implementation Of A Robust In-Cell Covalent Fragment Screening Platform**

- Applying activity based protein profiling (ABBP) to proteome wide fragment screening
- Inclusion of multiple proteomics techniques to make ABBP more streamlined and more scalable
- Development of data analysis tools to improve interpretation of results.

*RYAN MCCLURE, Senior Scientist II, AbbVie*

**Panel Discussion: Phenotypic Based Discovery & Screening Approaches**

- Phenotypic Screening
- Compound Vs genetic screens
- Hit Triage and Validation
- Target Identification and Validation

**Moderator:** NATHANALE LINTNER, Principal Scientist, Pfizer

**Panelists:**
- KERRIE SPENCER, Associate Principal Scientist, Chemical Biology, Merck
- CONSTANTIN NEAGU, Senior Scientist, EMD Serono Research and Development Institute

**Label-Free Ultra-High Throughput Screening Platform: De-Risked Hit Finding And Orthogonal Triaging Through Mass Spectrometry:**

- Integration of MALDI-MS into a fully automated uHTS platform
- Development and implementation of functional and biological MS assays for high-throughput hit discovery and evaluation
- Improved uHTS hit finding workflows using label-free MS technology and early assessment of target engagement

*FEUR KLEINPENNING, Senior Scientist Chemical Biology, Pivot Park Screening Centre*

**CONFERENCE ROOM 2: HIT FINDING TECHNOLOGIES AND MOLECULAR DRUG DESIGN**

**Track Chair:** ERIC R GOEDKEN, Senior Principal Research Scientist, Dermatology, Immunology, AbbVie Bioresearch Center

**Structure-Based Drug Design Of Small Molecule Inhibitors Of Cytokines**

*ERIC GOEDKEN, Senior Principal Research Scientist, Dermatology, Immunology Discovery, AbbVie Bioresearch Center*

**Large-Scale Structure-Based Virtual Screening**

*PAUL BEROZA, Distinguished Scientist, Genentech*

**Panel Session: Addressing Specific Targets And Dealing With Target Engagement**

- AMR and Target Engagement
- Expanding the chemical space
- Need for specific targets

**Moderator:** JING YANG, Chief Scientific Officer, BaseCure Therapeutics

**Panelists:**
- GOVINDAN SUBRAMANIAN, Senior Director, Gossamer Bio
- MEGHAN LAWLER, Director, Affinity Technology, Anagenex

**CONFERENCE ROOM 3: COMPUTATIONAL DRUG DESIGN: AI FOCUS**

**Comprehensive Enumeration Of The Local Chemical Space For Tri-Complex (ON)**

- Developed a useful idea generation tool for drug design
- Provides rapid, comprehensive and unbiased exploration of local chemical space
- Implemented with chemist friendly input and convenient output for post-processing in other software

*HONGWU WANG, Principal Scientist, Merck*
**CONFERENCE ROOM 1: TARGET AND PHENOTYPIC BASED DISCOVERY AND SCREENING APPROACHES**

- **10:20**
  - High Throughput Experimentation: Expanding Scope To New Technologies
    - Examples of Implementation of Batch HTE – Benefits and Challenges
    - Expanding Chemical Space – Development of a Flow Screening Platform
    - Emerging Technologies – Proof of Concept for Photoredox Catalysis
    - Exploring Novel Reactivity and Future Directions
  - (Joining Online) PAUL RICHARDSON, Director, Discovery Chemistry, 34SU*OREDSHVHODUFK*HYHORSHPKW
  - Delegates are welcome to attend co-located sessions

**CONFERENCE ROOM 2: HIT FINDING TECHNOLOGIES AND MOLECULAR DRUG DESIGN**

- **10:20**
  - Right Target, Right Patient, Right Therapeutic Window; The *Sine Qua Non* Condition For Successful Drug Development
    - How to identify clinical target
    - How to predict clinical effect
    - How to monitor therapeutic efficacy
  - PIERRE EFTEKHARI, President & Chief Scientific Officer, QRYLYHP6FLHQL4F

**MORNING NETWORKING BREAK**

- **10:50**
  - MORNING NETWORKING BREAK
    - 1-2-1 Meetings x 3
    - Company Spotlights

**CONFERENCE ROOM 1: TARGET AND PHENOTYPIC BASED DISCOVERY AND SCREENING APPROACHES AND DEL**

- **12:15**
  - DEL & ML At GSK
    - De-risking DNA binding
    - Reducing false positives
    - Leveraging existing compounds
  - JEFF MESSER, Director Analytics, GSK

**CONFERENCE ROOM 2: HIT FINDING TECHNOLOGIES AND MOLECULAR DRUG DESIGN**

- **11:50**
  - Biophysical Tools For Challenging Targets
    - SANJAY PANCHAL, Principal Research Scientist, AbbVie

**LUNCH NETWORKING BREAK**

- **12:45**
  - LUNCH NETWORKING BREAK
    - 1-2-1 Meetings x 3

**CONFERENCE ROOM 1: TARGET AND PHENOTYPIC BASED DISCOVERY AND SCREENING APPROACHES AND DEL**

- **13:45**
  - Incorporating ASMS In Drug Discovery
    - Affinity Selection Mass Spectrometry can directly screen small molecule collections as well as focused compound sets derived from computational screens. Recent experience will be reviewed applying externalized ASMS in challenging drug target categories, including for a membrane transporter
    - JEFF MESSER, Director Analytics, GSK
    - HANS-PETER BIEMANN, Scientific Director, Sanofi

**CONFERENCE ROOM 2: HIT FINDING TECHNOLOGIES AND MOLECULAR DRUG DESIGN**

- **14:10**
  - Panel Discussion: Integration Of Technologies For HIT Triage & Early Exploration
    - Technologies in Targeted Protein Degradation, covalent inhibitors, DELs
    - Data approaches
    - High throughput chemistry
    - Massive chemical spaces
    - ADMET
    - Moderator: ZHENGRONG ZHU, Principal Scientist, Merck
    - Panellists:
      - SANJAY PANCHAL, Principal Research Scientist, AbbVie
      - ISRA HASSAN, Senior Scientist II, Novartis
      - JOE FRANKLIN, Senior Vice President of Early Discovery, Anagenex
      - (Joining Online) CATERINA MUSETTI, Principal Scientist, Bristol Myers Squibb
### Afternoon Networking Break

**Conference Room 1: Target and Phenotypic Based Discovery and Screening Approaches and DEL**

**Combining Machine Learning And Drug Discovery At Anagenexus**
- A review of some of the data Anagenex collects and uses to make high quality machine learning predictions
- The Anagenex process of iteration and how it improves machine learning outcomes
- Case studies

JOE FRANKLIN, Senior Vice President of Early Discovery,
Anagenex

**DEL And Convalent Active Compounds In Drug Discovery**

ZHENG RONG ZHU, Principal Scientist,
Merck

**Conference Room 2: Hit Finding Technologies and Molecular Drug Design**

**An MPO Approach To Compound Progressability**

PHIL COX, Research Fellow, Augmented Molecular Design, Discovery Platform Technologies
AbbVie

### 15:00

Combining Machine Learning And Drug Discovery At Anagenexus

### 15:25

DELS And Convalent Active Compounds In Drug Discovery

### 15:50

Meet BMS’s “Perseverance” Robotic Platform And Its Mission To Hit Discovery

### 16:15

End of Conference
DISCOVERY US: IN-PERSON NETWORKING DRINKS

Thursday 17th November, 18:05pm
in the Exhibition Hall

We hope to see you there
Courtyard by Marriott Boston Downtown
275 Tremont Street
Boston, Massachusetts 02116 USA

>Visit hotel website<

The nearest Bus and Train Station is South Station. After exiting the station, turn right onto Essex Street, and continue on to Boylston Street. Then turn left on to Tremont Street and the venue is on your right.

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