Save the date!

17TH ANNUAL Drug Discovery Chemistry

APRIL 18 - 21, 2022

IN-PERSON | VIRTUAL

FLEXIBLE REGISTRATION

SAN DIEGO, CA | ONLINE

CAMBRIDGE HEALTHTECH INSTITUTE'S 16TH ANNUAL

MAY 18 - 20, 2021

Drug Discovery Chemistry VIRTUAL

OPTIMIZING SMALL MOLECULES FOR TOMORROW'S THERAPEUTICS INCLUDING COVID

MAY 18 - 19, 2021

- Ubiquitin-Induced Targeted Protein Degradation
- Fragment-Based Drug Discovery
- RNA-Targeting Small Molecule Drugs
- Macrocyclics & Constrained Peptides

MAY 19 - 20, 2021

- Protein-Protein Interactions
- Artificial Intelligence for Early Drug Discovery
- Small Molecules for Immunology, Oncology & COVID
- Encoded Libraries for Small Molecule Discovery

PLENARY KEYNOTES

New Technologies for Drug Discovery

Bryan L. Roth, PhD
Distinguished Professor, Pharmacology & Psychiatry, University of North Carolina, Chapel Hill

A Brief History of Targeted Covalent Drugs: The Journey from Avoided to Essential Medicines

Juswinder Singh, PhD
Founder, Ankaa Therapeutics

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DrugDiscoveryChemistry.com

CONFERENCE AT-A-GLANCE

All times are Eastern Daylight Time

Tuesday | MAY 18	Wednesday | MAY 19	Thursday | MAY 20
Ubiquitin-Induced Targeted Protein Degradation		Protein-Protein Interactions
Fragment-Based Drug Discovery		Artificial Intelligence for Early Drug Discovery
RNA-Targeting Small Molecule Drugs		Small Molecules for Immunology, Oncology & COVID
Macrocyclics & Constrained Peptides		Encoded Libraries for Small Molecule Discovery

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PLENARY KEYNOTES

New Technologies for Drug Discovery

Bryan L. Roth, PhD, Distinguished Professor, Pharmacology & Psychiatry, University of North Carolina, Chapel Hill

In this talk I will discuss recently invented approaches to accelerate drug discovery. These include a novel approach for directed evolution to create therapeutically targeted nanobodies, new biosensors for GPCRs and ultra-large-scale docking to discover new chemical matter at druggable targets. I will also highlight how these approaches can provide insights into new approaches to target COVID-19 and related disorders.

Bryan L. Roth, MD, PhD is the Michael Hooker Distinguished Professor of Pharmacology at the University of North Carolina Chapel Hill School of Medicine. Dr. Roth was elected to the National Academy of Medicine of the National Academy of Sciences in 2014 and the American Academy of Arts and Sciences in 2019. He has published more than 450 papers, has >40 patents and has founded 2 biotech companies. He has received many honors including the Goodman and Gilman Award for Receptor Pharmacology, the PhRMA Foundation Excellence in Pharmacology Award, a NARSAD Distinguished Investigator Award and the IUPHAR Analytical Pharmacology Lectureship. Dr. Roth also given more than 20 named lectures including the 2017 Martin Rodbell Lecture and a Presidential Special Lecturer at the 2018 Society for Neurosciences meeting.

A Brief History of Targeted Covalent Drugs: The Journey from Avoided to Essential Medicines

Juswinder Singh, PhD, Founder, Ankaa Therapeutics

The past decade has witnessed remarkable progress in the field of targeted covalent drugs. Despite historical off-target toxicity concerns, covalent inhibitors have been rationally designed with high specificity leading to breakthrough therapies for cancer. Targeted covalent inhibitors are also in advanced trials for inflammatory diseases. In showing how covalent inhibitors address unmet medical needs, overcoming specific shortcomings of reversible drugs, I will highlight areas of innovation in covalent drug discovery.

Juswinder Singh, PhD is a pioneer of targeted covalent inhibitors. His work formed the basis of multiple drugs (approved and in clinical development) for the treatment of lung cancer, breast cancer, leukemia and Hepatitis C. In 2006 he founded and was CSO of Avila Therapeutics, the first company to focus on targeted covalent drugs. Using Singh's covalent discovery platform, Avila entered collaborations with Novartis, Sanofi, the Leukemia and Lymphoma Society, and Clovis Oncology. Avila advanced two drugs into clinical development and had one pre-clinical candidate when it was acquired by Celgene in 2012 for financial terms that earned the 'Exit of the Year' award from the New England Venture Capital group. Ankaa Therapeutics, the company he most recently founded, is also focused on covalent drugs. Singh earned his PhD in rational drug design from the University of London in 1988. He has worked in pharma (Parke-Davis 1991-1994) and also biotech (Biogen 1994-2005) where he pioneered computer-assisted drug design.

SHORT COURSES* | MAY 18 - 20, 2021

TUESDAY, MAY 18 1:45-3:45 PM

SC1: Emerging Chemical Tools for Phenotypic Screening and Target Deconvolution

Instructors:

Paul Brennan, PhD, Professor, Department of Medicinal Chemistry, University of Oxford

Hua Xu, PhD, Associate Director, Mechanistic Biology & Profiling, Astra Zeneca

Brent Martin, PhD, Director, Chemical Biology, Scorpion Therapeutics

This course is designed to provide an introduction as well as best practices on the use of chemical biology probes and assays that have been developed for applications in early drug discovery. Chemists and biologists working in lead generation, assay development, phenotypic screening, target discovery and deconvolution, target engagement and finding mechanism-of-action studies will all benefit from attending this course. The instructors will share their knowledge and expertise and there will be time for open discussion and exchange of ideas.

WEDNESDAY, MAY 19 2:00-4:00 PM

SC2: Targeted Protein Degradation Using PROTACs, Molecular Glues, and More

Instructors:

Alexander Statsyuk, PhD, Assistant Professor, Department of Pharmacological and Pharmaceutical Sciences, University of Houston

Stewart Fisher, PhD, CSO, C4 Therapeutics, Inc.

Targeted protein degradation using molecular glues and bifunctional small molecules, known as proteolysis-targeting chimeric molecules (PROTACs), is emerging as a useful tool for drug discovery, and as a new therapeutic modality for chasing previously "undruggable" targets. This course will cover the basic understanding of what these entities are, how they work, and how they can be applied to target and degrade specific proteins of interest. Case studies drawn from the work that the instructors have done in their labs will also be presented.

THURSDAY, MAY 20 11:15 AM-1:15 PM

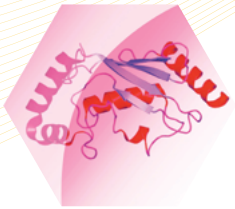
SC3: Ligand-Receptor Molecular Interactions and Drug Design

Instructor:

Maricel Torrent, PhD, Principal Research Scientist, Molecular Modeling, AbbVie Inc.

This course provides an overview of protein-ligand interactions and drug design principles. The presentation is targeted to medicinal chemists. Part 1 covers hydrophobic, H-bonding and electrostatic interactions; Part 2 covers specialized topics such as conformation analysis, pi-stack, cation-pi, halogen bonding, protein-protein interface, and covalent inhibition. Medicinal chemistry case studies are incorporated.

**All Access VIRTUAL Pricing or separate registration required*



Cambridge Healthtech Institute's 4th Annual

MAY 18-19, 2021 | ALL TIMES EASTERN DAYLIGHT (UTC-04:00)

Ubiquitin-Induced Targeted Protein Degradation

Optimizing PROTACs and Small Molecule Protein Degraders for Pursuing Undruggable Targets

TUESDAY, MAY 18

9:20 am LIVE: Greet 'n' Go Welcome Gathering

DESIGNING & OPTIMIZING PROTEIN DEGRADERS

9:30 Targeted Protein Degradation – Where Are We Going?
Adam Gilbert, PhD, Senior Director, Discovery Sciences, Design & Synthesis Sciences, Pfizer Inc.
Overview of current state of targeted protein degradation and thoughts on where the field is heading with respect to clinical candidates, new degradation targets and different degradation strategies.

10:00 *In vitro* and *in vivo* Early Proof-of-Concept Studies with Orally Bioavailable PROTACs
Dan Sherman, Senior Research Investigator, Department of Medicinal Chemistry, Arvinas Inc.
A brief presentation of some early stage work from the Arvinas oncology pipeline.

10:30 TRKing Down an Old Oncogene in a New Era of Targeted Protein Degradation
Michael Plewe, PhD, Senior Vice President, Medicinal Chemistry, Cullgen Inc.
Our research focuses on leveraging our ubiquitin-mediated, small molecule-induced protein degradation technology (uSMITE) for the treatment of cancer and other diseases. I will present the discovery and evaluation of first-in-class potent and selective degraders of tropomyosin receptor kinases (TRK) that inhibited cell growth with low nanomolar IC50 values and demonstrated sustained tumor growth inhibition in xenografted tumor models using the oral administration route.

11:00 Expanding the Targeted Protein Degradation Toolbox – Diversifying the E3scan™ Ligand Binding Assay Platform
Ksenya Cohen Katsenelson, PhD, Senior Scientist Group Leader, Research & Development, Eurofins Discovery
Eurofins Discovery is diversifying its novel E3scan™ ligand-binding platform with additional E3 ligase target assays. Here, we present assay validation data for E3scan, including for E3 ligases that have not been utilized in targeted protein degradation and for which no small molecule ligands have been previously reported. Our E3scan platform enables accelerated screening and SAR analysis, with rapid turnaround times and the largest assay panel available on a single technology platform.

11:40 LIVE: Panel Q&A with Session Speakers
Moderator: Adam Gilbert, PhD, Senior Director, Discovery Sciences, Design & Synthesis Sciences, Pfizer Inc.
Panelists:
Dan Sherman, Senior Research Investigator, Department of Medicinal Chemistry, Arvinas Inc.
Michael Plewe, PhD, Senior Vice President, Medicinal Chemistry, Cullgen Inc.
Ksenya Cohen Katsenelson, PhD, Senior Scientist Group Leader, Research & Development, Eurofins Discovery

PLENARY KEYNOTE SESSION

12:00 pm KEYNOTE PRESENTATION:
PLENARY: New Technologies for Drug Discovery
Bryan L. Roth, PhD, Distinguished Professor, Pharmacology & Psychiatry, University of North Carolina, Chapel Hill
In this talk I will discuss recently invented approaches to accelerate drug discovery. These include a novel approach for directed evolution to create therapeutically targeted nanobodies, new biosensors for GPCRs and ultra-large-scale docking to discover new chemical matter at druggable targets. I will also highlight how these approaches can provide insights into new approaches to target COVID-19 and related disorders.

12:35 LIVE: Q&A Plenary Discussion

Moderator: Phillip Schwartz, PhD, Principal Scientist, Biophysics, Frontier Medicines

Panelists:
Bryan L. Roth, PhD, Distinguished Professor, Pharmacology & Psychiatry, University of North Carolina, Chapel Hill

12:50 Session Break - View Our Virtual Exhibit Hall

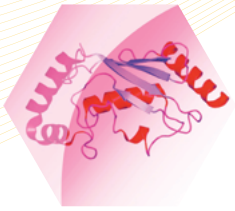
1:00 Networking Hallway Hangout with Speakers and Poster Presenters - View Our Virtual Exhibit Hall

CHARACTERIZING MECHANISM OF ACTION

1:30 Cyanopyrrolidine Inhibitors of USP7 Mediate Desulfhydration of the Active-Site Cysteine
Charlene Bashore, PhD, Principal Scientific Researcher, Genentech Inc.
We report covalent inhibitors of USP7 that unexpectedly promote a b-elimination reaction of the initial covalent adducts, thereby converting the active site cysteine residue to dehydroalanine. Unlike in conventional reversible-covalent inhibition, these compounds irreversibly destroy a catalytic residue whilst simultaneously converting the inhibitor to a non-electrophilic byproduct. This finding expands the scope of covalent inhibitor modalities and offers intriguing insights into enzyme-inhibitor dynamics in the ubiquitin-proteasome system and beyond.

Recommended Short Course* SC1: Emerging Chemical Tools for Phenotypic Screening and Target Deconvolution
All Access VIRTUAL Pricing or separate registration required. See short course page for details.

2:00 Characterization of the Recruitment of Proteins to Ligases by Molecular Glues
Charles A. Wartchow, PhD, Associate Director, Global Discovery Chemistry, Novartis Institutes for BioMedical Research
Formation of ternary complexes between a ligase, a molecular glue, and a



Ubiquitin-Induced Targeted Protein Degradation

Optimizing PROTACs and Small Molecule Protein Degraders for Pursuing Undruggable Targets

disease-modulating protein is the first step in a sequence of events leading to protein degradation. In this presentation, we present SPR methods for determining the affinities of the small molecule glue for the ligase and discuss methods for characterizing the affinities and kinetics of ternary complex formation involving the ligase, the molecular glue, and the recruited protein.

2:30 Scalable Discovery and Streamlined Characterization of Novel Molecular Glue Degraders

Matthias Brand, PhD, Co-Founder and Vice President Biology, Proxygen GmBH

Molecular glue degraders are a novel therapeutic modality and induce destabilization of proteins that would otherwise be considered undruggable due to the lack of a ligandable pocket. Their discovery however has so far been serendipitous. The Proxygen glue degrader discovery platform enables rational screening for such molecules on an industrial scale. Here, we present a case study of the subsequent chemical optimization of the resulting hit molecules.

3:00 Cellular Mechanistic Studies of Targeted Protein Degradation Compound Permeability, Ternary Complex, and Ubiquitination

Steven Edenson, Strategic Collaborations Manager, Promega Corporation

As targeted protein degradation strategies expand, understanding the impacts of compound permeability, the kinetics of ternary complex formation, and ubiquitination are critical. NanoBRET assays measure cellular compound permeability, the kinetics of complex formation and ubiquitination. Using dBET1 and dBET6 PROTACs, we demonstrate that dBET6 is more permeable than dBET1. Furthermore, dBET6 induces more complex formation and ubiquitination. These results provide insight into the difference in degradation between dBET6 and dBET1.

3:30 Small-Molecule Induced Polymerization as Novel Mechanism for Protein Degradation Therapeutics

Eric Fischer, PhD, Assistant Professor & Principal Investigator, Biological Chemistry & Molecular Pharmacology, Dana Farber Cancer Institute

Small molecules that induce protein degradation through ligase-mediated ubiquitination, have shown considerable promise as a new pharmacological modality. Thalidomide and related IMiDs provided the clinical proof of concept, while significant progress has recently been made towards chemically induced targeted protein degradation using heterobifunctional small molecule ligands. We will present recent work towards a better understanding of the molecular principles that govern neo-substrate recruitment, and other small molecule degraders.

4:00 Discovery and characterization of bifunctional degrader molecules

Dave Madge, Dr., Vice President, Research Service Division, Research Service Division, WuXi AppTec

This presentation will focus on the discovery and characterization of bifunctional molecules designed to leverage the ubiquitination pathway for degradation of a target protein. We will discuss strategies for the discovery of ligands for both the target protein and the ligase complex, determination of the kinetics of their interactions in binary and tertiary complexes, and the application of structural biology to design new ligands.

4:30 LIVE: Panel Q&A with Session Speakers

Moderator: Charles A. Wartchow, PhD, Associate Director, Global Discovery Chemistry, Novartis Institutes for BioMedical Research

Panelists:
Eric Fischer, PhD, Assistant Professor & Principal Investigator, Biological Chemistry & Molecular Pharmacology, Dana Farber Cancer Institute
Charlene Bashore, PhD, Principal Scientific Researcher, Genentech Inc.
Matthias Brand, PhD, Co-Founder and Vice President Biology, Proxygen GmBH
Steven Edenson, Strategic Collaborations Manager, Promega Corporation
Dave Madge, Dr., Vice President, Research Service Division, Research Service Division, WuXi AppTec

4:30 Drug Discovery Chemistry Connects - View Our Virtual Exhibit Hall

Explore new products and services in our Exhibit Hall, engage with poster presenters, schedule 1-on-1 meetings, and build your research community during this open networking period.

5:00 Close of Day

WEDNESDAY, MAY 19

9:30 Interactive Breakout Discussions - View Our Virtual Exhibit Hall

This group discussion is a chance for everyone to see and hear each other if they choose to turn on their cameras and microphones. Each group will have a moderator to ensure focused conversations around key issues within the conference's scope. This will be a 'now or never' session; it will not be recorded or available On Demand. **View all topics on breakouts webpage.**

CO-PRESENTATION: Topic: Designing and Optimizing Chemistry and Drug-Like Properties of Protein Degraders

Christopher Nasveschuk, PhD, Vice President, Chemistry, C4 Therapeutics, Inc.
Upendra Dahal, PhD, Principal Scientist, Pharmacokinetics and Drug Metabolism, Amgen, Inc.

- Design of protein degraders, linkers
- Kinetics of binding and degradation
- Issues surrounding PK/PD, biotransformation and bioavailability

CHASING NEW DEGRADATION TARGETS & PATHWAYS

10:00 PROTAC Drugs: Therapeutics, and Not Vaccines Will Overcome the SARS-CoV-2 Pandemic

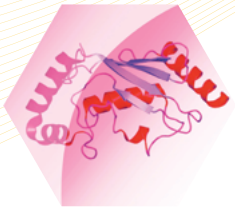
Tauseef Butt, PhD, President & CEO, Progenra, Inc.

Traditional mono-antiviral therapy has not been successful for HIV due to poor efficacy and emergence of resistance. Drugs that target viral protein for ubiquitin E3 ligase-mediated degradation can eliminate the proteins and prove to be highly efficacious. Progenra has targeted SARS-CoV-2 viral proteins with PROTAC drugs. Potent and selective PROTACs degrade viral proteins in cells and block viral growth. Discovery and development of these PROTAC drugs will be discussed.

10:30 Degrading the Undruggable–Endogenous KRAS^{G12C} Degradation by VHL-MRTX849 PROTACs

Michael Bond, Graduate Student, Laboratory of Dr. Craig Crews, Department of Pharmacology, Yale University

The discovery of covalent inhibitors of KRAS^{G12C} has reinvigorated the



Cambridge Healthtech Institute's 4th Annual

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Ubiquitin-Induced Targeted Protein Degradation

Optimizing PROTACs and Small Molecule Protein Degraders for Pursuing Undruggable Targets

field of KRAS drug discovery. While these compounds have shown promising clinic results, we wanted to explore PROTAC-mediated degradation as a complementary strategy to modulate $KRAS^{G12C}$. We report the development of LC-2, the first PROTAC capable of degrading endogenous $KRAS^{G12C}$. LC-2 induces rapid, sustained $KRAS^{G12C}$ degradation and suppresses MAPK signaling. LC-2 demonstrates that PROTAC-mediated degradation can attenuate oncogenic KRAS levels.

11:00 Harnessing DNA-Encoded Libraries and Targeted Protein Degradation for the Discovery of New Therapeutics

Daniel Robbins, PhD, Senior Scientist, Medicinal Chemistry, Nurix Therapeutics Inc.

Targeted protein degradation is mediated by Chimeric Targeting Molecules (CTMs), which bind to a target protein and an E3 ligase, resulting in target protein ubiquitylation and proteasomal destruction. This presentation will describe Nurix's DNA-encoded library (DEL) platform for the discovery of novel binders to enable CTM discovery. This presentation will also describe the discovery of orally bioavailable degraders of BTK, a clinically relevant target for oncology and immunology applications.

11:30 DNA Encoded Libraries and Their Application to Protein Degradation

Matthew Clark, PhD, CEO, X-Chem Inc.

The application of DNA-encoded library (DEL) technology to the discovery of protein degraders is increasingly appreciated among researchers in the field. The nature of the DEL selection, the structure of libraries, and flexibility of the screening experiment, lend themselves to the degradation approach. In this presentation we will examine the current state of the art of DEL design and of selection methodologies, and their application to novel degrader discovery.

12:10 pm LIVE: Panel Q&A with Session Speakers

Moderator: Tauseef Butt, PhD, President & CEO, Progenra, Inc.

Panelists:
Michael Bond, Graduate Student, Laboratory of Dr. Craig Crews, Department of Pharmacology, Yale University
Daniel Robbins, PhD, Senior Scientist, Medicinal Chemistry, Nurix Therapeutics Inc.
Matthew Clark, PhD, CEO, X-Chem Inc.

12:40 Women in Chemistry Breakout Discussion - View Our Virtual Exhibit Hall

CHI supports and promotes diversity in the life sciences. The inequities that prevent women from fully participating in this field may also deter men from participating more fully in life outside of their careers. We dedicate this session for all drug discovery community members to engage in conversation with one another around personal and professional journeys and challenges related to gender. View full info on breakouts webpage.

Women in Chemistry: The Gender Divide in Life Science Careers

Moderator: Mary Harner, PhD, Senior Manager, Oncology CI, Bristol Myers Squibb Co.

1:10 Greet 'n' Go Hallway Networker with Speakers and Poster Presenters - View Our Virtual Exhibit Hall

1:30 Close of Ubiquitin-Induced Targeted Protein Degradation Conference

Recommended Short Course* SC2: Targeted Protein Degradation Using PROTACs, Molecular Glues, and More

All Access VIRTUAL Pricing or separate registration required.
See short course page for details.

Benefits of Drug Discovery Chemistry VIRTUAL

- View more presentations at your convenience as your Virtual registration includes On-Demand access
- You have access to all concurrent talks so you no longer have to choose between multiple presentations taking place at the same time
- Reduced registration fees and no travel or hotel costs
- Connect with the right attendees based on mutual interests and expertise
- See and hear your colleagues in facilitated networking Zoom rooms
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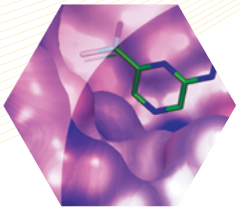

Cambridge Healthtech Institute's 16th Annual

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Fragment-Based Drug Discovery

From Small Organic Compounds to Potential Therapeutics Against Intracellular Targets

TUESDAY, MAY 18

9:20 am LIVE: Greet 'n' Go Welcome Gathering

NMR ADVANCES FOR FBDD

9:30 FEATURED PRESENTATION: Enabling Comprehensive and High-Throughput Exploration of Fragment Chemical Space by Using Broadband ^{19}F NMR-Based Screening

Andreas Lingel, PhD, Senior Principal Scientist, Global Discovery Chemistry, Novartis Institutes for Biomedical Research

Fragment-based lead discovery by 19F NMR has gained popularity owing to its high sensitivity, robustness, and ease of use. Recently, we introduced a novel broadband NMR experiment and demonstrated its application to efficient library generation, QC and screening. Resulting hits have a high degree of chemical diversity, suggesting that the method is generally applicable to obtaining tractable binders for chemistry optimization and targeting a broad range of disease-relevant biomacromolecules.

10:00 The 3F Library – Fluorinated, Fsp^3-Rich Fragments – Design, Synthesis and NMR Screening

Mads H. Clausen, PhD, Professor, Chemistry, Danish Technical University

The presentation will discuss the design, synthesis, and screening of the 3F library, which contains 115 fluorinated, Fsp^3-rich fragments that are shape diverse and natural product-like. The library is perfectly suited for rapid and efficient screening by NMR spectroscopy in a two-stage workflow of ^{19}F- followed by ^{1}H-NMR methods. Hits against four protein targets were widely distributed among the scaffolds and a 67% validation rate was achieved in secondary assays.

10:30 Session Break - View Our Virtual Exhibit Hall

11:00 Fragments with a Future – a Path Towards Tractable Chemical Series

ZOBIO

Stijn Gremmen, PhD, Head of Chemistry, ZoBio

We've previously shown the importance of designing a fragment library around the techniques used to screen it (Siegal et al, DDT, 2007). Here we will discuss further elaboration of the concept based on learnings from multiple fragment hit to lead projects. The impact of a holistic view of fragment chemistry, orthogonal biophysical techniques and structural biology for deriving novel, tractable chemical series will be illustrated.

11:40 LIVE: Panel Q&A with Session Speakers

Moderator: William C.K. Pomerantz, PhD, Associate Professor, Medicinal Chemistry, University of Minnesota Twin Cities

Panelists:

Andreas Lingel, PhD, Senior Principal Scientist, Global Discovery Chemistry, Novartis Institutes for Biomedical Research

Mads H. Clausen, PhD, Professor, Chemistry, Danish Technical University

Stijn Gremmen, PhD, Head of Chemistry, ZoBio

PLENARY KEYNOTE SESSION

12:00 pm KEYNOTE PRESENTATION: PLENARY: New Technologies for Drug Discovery

Bryan L. Roth, PhD, Distinguished Professor, Pharmacology & Psychiatry, University of North Carolina, Chapel Hill

In this talk I will discuss recently invented approaches to accelerate drug discovery. These include a novel approach for directed evolution to create therapeutically targeted nanobodies, new biosensors for GPCRs and ultra-large-scale docking to discover new chemical matter at druggable targets. I will also highlight how these approaches can provide insights into new approaches to target COVID-19 and related disorders.

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Panelists:

Bryan L. Roth, PhD, Distinguished Professor, Pharmacology & Psychiatry, University of North Carolina, Chapel Hill

12:50 Session Break - View Our Virtual Exhibit Hall

1:00 Networking Hallway Hangout with Speakers and Poster Presenters - View Our Virtual Exhibit Hall

APPROACHES FOR FBDD

1:30 CryoEM in Fragment-Based Drug Discovery

Pamela A. Williams, PhD, Director, Astex Pharmaceuticals

Advances over the last decade have led to pharmaceutical companies starting to appreciate that cryoEM can now add value to projects, despite the reduced throughput and increased expense (per structure) when compared to crystallography. The power of cryoEM may be to increase the number of targets that can be structurally enabled, but we have shown in some cases it can also be used to generate hit matter via a fragment-based campaign.

Recommended Short Course* SC1: Emerging Chemical Tools for Phenotypic Screening and Target Deconvolution

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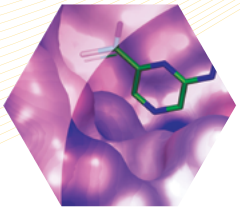

Fragment-Based Drug Discovery

From Small Organic Compounds to Potential Therapeutics Against Intracellular Targets

2:00 Structure-Free Elaboration of Fragments into Novel Allosteric MEK1 Binders

Paolo Di Fruscia, PhD, Senior Research Scientist, Medicinal Chemistry, AstraZeneca

With the aim of discovering novel allosteric MEK1 inhibitors, a fragment-based screening campaign, designed to specifically discover allosteric binders by screening with the ATP-binding site blocked, is reported. These efforts led to the identification of multiple novel allosteric MEK1 binder chemotypes, one of which, advanced in the absence of structural information, was elaborated to sub-μM affinity, with promising physicochemical and *in vitro* ADMET properties.

2:30 Hijacking Autophagy by Co-Opting LC3 with Fragment Derived Ligands

Micah Steffek, MSc, Principal Scientific Researcher, Biochemical & Cellular Pharmacology, Genentech Inc.

We used fragment-based lead discovery to identify ligands to LC3, a protein that binds and targets autophagy substrates for destruction. LC3 binding sites were determined using X-ray crystallography. Ligands were optimized using traditional SAR approaches. We used newer methods such as peptide mimetics and DNA-encoded library compounds with similar fragment-like building blocks. We aim to create a degrader-equivalent autophagy tool for targeted degradation of proteins too large for the proteosome.

3:00 Fragment Screening and Biophysical Hit validation at WuXi AppTec's HitS platform

Michael Raba, Dr., Deputy Head, Biophysics and Screening, Crelux, Research Service Division, WuXi AppTec

The HitS business unit is an integral part of the WuXi AppTec Research Services Division (RSD). We deliver customized, integrated hit finding and structure-based drug discovery solutions. By screening our proprietary fragment library by various biophysical methodologies such MST, SPR or nanoDSF we support our clients already at the early stages of their drug development projects.

3:40 LIVE: Panel Q&A with Session Speakers

Moderator: Jenny Sandmark, PhD, Associate Principal Scientist, Drug Discovery, AstraZeneca R&D
Panelists:
Pamela A. Williams, PhD, Director, Astex Pharmaceuticals
Paolo Di Fruscia, PhD, Senior Research Scientist, Medicinal Chemistry, AstraZeneca
Micah Steffek, MSc, Principal Scientific Researcher, Biochemical & Cellular Pharmacology, Genentech Inc.
Michael Raba, Dr., Deputy Head, Biophysics and Screening, Crelux, Research Service Division, WuXi AppTec

4:30 Drug Discovery Chemistry Connects - View Our Virtual Exhibit Hall

Explore new products and services in our Exhibit Hall, engage with poster presenters, schedule 1-on-1 meetings, and build your research community during this open networking period.

5:00 Close of Day

WEDNESDAY, MAY 19

9:30 Interactive Breakout Discussions - View Our Virtual Exhibit Hall

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Topic: New Horizons in FBDD

Daniel A. Erlanson, PhD, Vice President, Chemistry, Frontier Medicines Corp.

FRAGMENT-ORIGIN COMPOUNDS

10:00 Fragment-Based Discovery of Novel Non-Hydroxamate LpxC Inhibitors with Antibacterial Activity

Roderick E. Hubbard, PhD, Senior Fellow, Vernalis R&D, Ltd.

LpxC catalyzes the first committed step in the biosynthesis of Lipid A, an essential component of the cell envelope of Gram-negative bacteria. We have identified two series of compounds derived from fragments with differing modes of zinc chelation. Structure-guided design led to a compound exhibiting low nanomolar inhibition of LpxC and a minimum inhibitory concentration (MIC) of 4 μg/mL against *Pseudomonas aeruginosa*.

10:30 Utilization of a Fragment-based Approach in the Development of Orally Efficacious TNFα Inhibitors

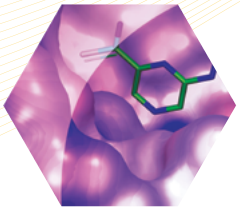
Justin Dietrich, PhD, Principal Research Scientist I, Fragment Based Drug Discovery and DNA-Encoded Library Technologies, AbbVie

TNFα and other cytokine signaling pathways have been clinically validated via macromolecular biologic drugs. However modulating these pathways with small molecules have been impeded by the challenges of a small molecule to disrupt high-affinity, protein-protein interactions. I present a fragment-based approach and lessons learned in developing orally efficacious TNFα inhibitors and broadly applied to identify starting points for other cytokines of interest.

11:00 Mimicking Nature in Drug Discovery: Enabling Good Design from Fragments to Macrocycles

Robert J. Young, PhD, Principal, Blue Burgundy Drug Discovery Consulting; formerly GSK Fellow and Scientific Leader, Medicinal Chemistry

Drug Discovery is a discipline of compromises to achieve efficacy and safety with drug molecules. The balancing of properties required to enable passage across biological membranes is considered in the context of debates over the mechanism of crossing membranes, be this via the bilayer or carrier proteins. In particular, the evolutionary consequences of the latter are explored, suggesting opportunities for better biomimetic designs in molecules large and small.



Fragment-Based Drug Discovery

From Small Organic Compounds to Potential Therapeutics Against Intracellular Targets

11:30 Accelerating Hit Expansion Using Creoptix waveRAPID® Technology

creoptix sensors

Trevor Askwith, PhD, Group Leader Assay Biology, Domainex Ltd

Being able to test newly synthesized molecules is a pivotal part of early-stage drug discovery, with the data from assays driving decisions on the next molecules to be developed. The waveRAPID technology enables testing of full kinetic parameters for up to 400 compound fragments unattended in a 24-hour period. We present how Domainex are using waveRAPID to accelerate the analogue expansion to support our fragment and virtual screening hit ID platforms.

12:10 pm LIVE: Panel Q&A with Session Speakers

Moderator: Joe Patel, PhD, Senior Director, Biochemistry Biophysics & Crystallography, C4 Therapeutics, Inc.
Panelists:
Roderick E. Hubbard, PhD, Senior Fellow, Vernalis R&D, Ltd.
Justin Dietrich, PhD, Principal Research Scientist I, Fragment Based Drug Discovery and DNA-Encoded Library Technologies, AbbVie
Robert J. Young, PhD, Principal, Blue Burgundy Drug Discovery Consulting; formerly GSK Fellow and Scientific Leader, Medicinal Chemistry
Trevor Askwith, PhD, Group Leader Assay Biology, Domainex Ltd

12:40 Women in Chemistry Breakout Discussion - View Our Virtual Exhibit Hall

CHI supports and promotes diversity in the life sciences. The inequities that prevent women from fully participating in this field may also deter men from participating more fully in life outside of their careers. We dedicate this session for all drug discovery community members to engage in conversation with one another around personal and professional journeys and challenges related to gender. View full info on breakouts webpage.

Women in Chemistry: The Gender Divide in Life Science Careers

Moderator: Mary Harner, PhD, Senior Manager, Oncology CI, Bristol Myers Squibb Co.

1:10 Greet 'n' Go Hallway Networker with Speakers and Poster Presenters - View Our Virtual Exhibit Hall

1:30 Close of Fragment-Based Drug Discovery Conference

Recommended Short Course* SC2: Targeted Protein Degradation Using PROTACs, Molecular Glues, and More

**All Access VIRTUAL Pricing or separate registration required.*
See short course page for details.

Cambridge Healthtech Institute's 2nd Annual

MAY 18-19, 2021 | ALL TIMES EASTERN DAYLIGHT (UTC-04:00)

RNA-Targeting Small Molecule Drugs

Designing and Optimizing Small Molecules to Modulate Diverse RNA Motifs and Pathways

TUESDAY, MAY 18

9:20 am LIVE: Greet 'n' Go Welcome Gathering

EXPLORING DIVERSITY OF RNA TARGETS

9:30 Targeting RNA with Small Molecules: Tools and Technologies for Medicinal Chemistry

John 'Jay' Schneekloth, Jr., PhD, Senior Investigator, Chemical Biology Laboratory; Head, Chemical Genetics Section, Center for Cancer Research, National Cancer Institute, National Institutes of Health (NIH)

The past twenty years have seen an explosion of interest in the structure and function of RNA and DNA. While some 80% of the human genome is transcribed into RNA, just ~3% of those transcripts code for protein sequences. Here, we discuss our group's efforts to target RNA and DNA with drug-like small molecules using a small-molecule microarray (SMM) screening platform and the molecular basis for these interactions.

10:00 Modulating the Conformation and Function of Viral RNA with Small Molecules

Amanda Hargrove, PhD, Assistant Professor, Department of Chemistry, Duke University

As part of our efforts to improve small molecule targeting strategies and gain fundamental insights into small molecule:RNA recognition, we have analyzed patterns in both RNA-biased small molecule chemical space and RNA topological space privileged for differentiation. We have applied these principles to functionally modulate conformations of the 3'-triple helix of the long noncoding RNA MALAT1, an enterovirus (EV71) IRES structure, and regulatory RNA in SARS-CoV-2.

10:30 Targeting mRNA Translation in a Tissue Selective and Disease-Specific Manner with Small Molecules

Iris Alroy, PhD, Vice President, R&D, Anima Biotech

Anima Biotech has developed Translation Control Therapeutics, a novel approach for the discovery of small molecules that selectively control mRNA translation against undruggable proteins. With this technology that emits light pulses from ribosomes, we visualize and analyze the kinetics of mRNA translation and identify selective translation modulators. Anima's lead compounds do not directly bind mRNA or degrade it but intervene by regulating mRNA translation in a tissue selective, disease-specific manner.

11:00 Sponsored Presentation *(Opportunity Available)*

11:40 LIVE: Panel Q&A with Session Speakers

Moderator: John 'Jay' Schneekloth, Jr., PhD, Senior Investigator, Chemical Biology Laboratory; Head, Chemical Genetics Section, Center for Cancer Research, National Cancer Institute, National Institutes of Health (NIH)
Panelists:
Amanda Hargrove, PhD, Assistant Professor, Department of Chemistry, Duke University
Iris Alroy, PhD, Vice President, R&D, Anima Biotech

PLENARY KEYNOTE SESSION

12:00 pm KEYNOTE PRESENTATION: PLENARY: New Technologies for Drug Discovery

Bryan L. Roth, PhD, Distinguished Professor, Pharmacology & Psychiatry, University of North Carolina, Chapel Hill

In this talk I will discuss recently invented approaches to accelerate drug discovery. These include a novel approach for directed evolution to create therapeutically targeted nanobodies, new biosensors for GPCRs and ultra-large-scale docking to discover new chemical matter at druggable targets. I will also highlight how these approaches can provide insights into new approaches to target COVID-19 and related disorders.

12:35 LIVE: Q&A Plenary Discussion

Moderator: Phillip Schwartz, PhD, Principal Scientist, Biophysics, Frontier Medicines

Panelists:
Bryan L. Roth, PhD, Distinguished Professor, Pharmacology & Psychiatry, University of North Carolina, Chapel Hill

12:50 Session Break - View Our Virtual Exhibit Hall

1:00 Networking Hallway Hangout with Speakers and Poster Presenters - View Our Virtual Exhibit Hall

DESIGN & OPTIMIZATION OF RNA MODULATORS

1:30 FEATURED PRESENTATION: Sequence-Based Design of Small Molecules Targeting RNA

Matthew Disney, PhD, Professor, Department of Chemistry, Scripps Research Institute

Our laboratory has targeted RNA with small molecules for sixteen years. First we define fundamental features of molecular recognition. This information is mined against the human transcriptome to identify disease-causing RNAs with motifs bound by small molecules, using an approach termed Inforna. These compounds can be selectively and potently bioactive and can be designed into molecules that facilitate RNA degradation by recruiting ribonucleases to catalytically and sub-stoichiometrically degrade disease-causing RNAs.

Recommended Short Course* SC1: Emerging Chemical Tools for Phenotypic Screening and Target Deconvolution

**All Access VIRTUAL Pricing or separate registration required. See short course page for details.*

2:30 Targeting Pre-mRNA Molecules with Small Molecules: Pharmacokinetics, Pharmacodynamics, and Efficacy in Mouse Models of Disease

Marla Weetall, PhD, Vice President, Pharmacology and Biomarkers, PTC Therapeutics

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RNA-Targeting Small Molecule Drugs

Designing and Optimizing Small Molecules to Modulate Diverse RNA Motifs and Pathways

Utilizing small molecules to modulate splicing has emerged as a successful therapeutic approach to regulating protein expression. Here, three diseases where small-molecule splicing modulators can be utilized are described: spinal muscular atrophy; familial dysautonomia; and Huntington's disease. For each of these indications, I will discuss the correlation between pharmacokinetics and pharmacodynamics, as well as the correlation between pharmacodynamics and efficacy.

3:00 Session Break - View Our Virtual Exhibit Hall

4:10 LIVE: Panel Q&A with Session Speakers
Moderator: Marla Weetall, PhD, Vice President, Pharmacology and Biomarkers, PTC Therapeutics
Panelists:
Matthew Disney, PhD, Professor, Department of Chemistry, Scripps Research Institute

4:30 Drug Discovery Chemistry Connects - View Our Virtual Exhibit Hall
Explore new products and services in our Exhibit Hall, engage with poster presenters, schedule 1-on-1 meetings, and build your research community during this open networking period.

5:00 Close of Day

WEDNESDAY, MAY 19

9:30 Interactive Breakout Discussions - View Our Virtual Exhibit Hall
This group discussion is a chance for everyone to see and hear each other if they choose to turn on their cameras and microphones. Each group will have a moderator to ensure focused conversations around key issues within the conference's scope. This will be a 'now or never' session; it will not be recorded or available On Demand. **View all topics on breakouts webpage.**

CO-PRESENTATION: Topic: Opportunities and Challenges Using Small Molecules to Target RNA
Amanda Hargrove, PhD, Assistant Professor, Department of Chemistry, Duke University
Amanda Garner, PhD, Associate Professor, College of Pharmacy, Department of Medicinal Chemistry, University of Michigan
Thomas Hermann, PhD, Professor, Department of Chemistry & Biochemistry, University of California San Diego
- Emerging techniques to study RNA structure and function
- Designing and evaluating small molecules that bind RNA
- Assays to determine if RNA binding/modulation leads to biological consequences

TOOLS TO ACCELERATE RNA DRUG DISCOVERY

10:00 Enabling Technologies for Targeting RNA-Protein Interactions
Amanda Garner, PhD, Associate Professor, College of Pharmacy, Department of Medicinal Chemistry, University of Michigan
RNAs are invariably bound to and often modified by RNA-binding proteins (RBPs), which regulate many aspects of coding and non-coding RNA biology. Disruption of this network of RNA-protein interactions (RPIs) has been implicated in a number of human diseases and targeting RPIs has arisen as a new frontier in RNA-targeted drug discovery. This talk will highlight newly developed technologies for validating and screening RPIs to enable RBP-targeted drug discovery.

10:30 Accelerated Cryo-EM-Guided Determination of Three-Dimensional RNA-Only Structures
Rhiju Das, PhD, Associate Professor, Department of Biochemistry, Stanford University School of Medicine
The discovery and design of biologically important RNA molecules is outpacing three-dimensional structural characterization. I will describe results from my and Wah Chiu's groups that demonstrate that cryo-electron microscopy can resolve maps of several kinds of RNA-only systems. These maps enable sub-nanometer-resolution coordinate estimation when complemented with multi-dimensional chemical mapping and Rosetta DRRAFTER computational modeling.

11:00 A RNA-targeting Small Molecule That Selectively Reverses Epigenetic Silencing in Fragile X Syndrome
Samie Jaffrey, MD, PhD, Professor, Department of Pharmacology, Weill Cornell Medicine; Co-Founder, Gotham Therapeutics
In fragile X syndrome a CGG trinucleotide–repeat expansion adjacent to the fragile X mental retardation 1 (FMR1) gene promoter results in its epigenetic silencing mediated by the FMR1 mRNA. Small molecules that bind the CGG-repeat RNA region can prevent FMR1 gene silencing in a model of embryonic development. Our data show that an RNA-binding small molecule can selectively control the epigenetic activation state of a single gene in the genome.

11:30 Session Break - View Our Virtual Exhibit Hall

12:10 pm LIVE: Panel Q&A with Session Speakers
Moderator: Samie Jaffrey, MD, PhD, Professor, Department of Pharmacology, Weill Cornell Medicine; Co-Founder, Gotham Therapeutics
Panelists:
Amanda Garner, PhD, Associate Professor, College of Pharmacy, Department of Medicinal Chemistry, University of Michigan
Rhiju Das, PhD, Associate Professor, Department of Biochemistry, Stanford University School of Medicine

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Moderator: Mary Harner, PhD, Senior Manager, Oncology CI, Bristol Myers Squibb Co.

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1:30 Close of RNA-Targeting Small Molecule Drugs Conference

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Cambridge Healthtech Institute's 9th Annual

Macrocyclics & Constrained Peptides

Towards Cell-Penetrating, Soluble, Middle-Sized Molecules for Oral-Based Medicines

TUESDAY, MAY 18

9:20 am LIVE: Greet 'n' Go Welcome Gathering

SYNTHETIC MACROCYCLIC PEPTIDES

9:30 Macrocyclic Peptide Drugs: An Overview

Tomi K. Sawyer, PhD, Chief Drug Hunter & President, Maestro Therapeutics

Macrocyclic peptide drug discovery has become a powerful, multidisciplinary and worldwide endeavor to advance a therapeutic modality superclass. Innovative platforms have enabled the advancement of novel molecules of varying shapes and sizes. Peptide drug hunters are engaged in this effort to address both the challenges and opportunities to exploit this macrocyclic peptide superclass to address target space, cell permeability, and drug delivery. This presentation will overview macrocyclic peptide drugs.

10:00 Synthesis of Large Macrocycle Libraries by "Mixing & Reacting" Building Blocks and HTS of Crude Products

Christian Heinis, PhD, Associate Professor, Lab of Therapeutic Proteins & Peptides, EPFL Lausanne

Our laboratory has recently developed a new method for generating ligands based on sub-kilodalton cyclic peptides (Kale, S., et al., Science Advances, 2019). In brief, we combinatorially assembled building blocks in microwell plates to obtain macrocycles at good yield and high purity, and screened the crude reactions. Omission of a purification step allowed us to generate and screen large libraries and to find binders to important targets.

10:30 Turning Linear Peptide Substrates into Macrocyclic Inhibitors

Ranganath Gopalakrishnan, PhD, Associate Principal Scientist, New Modality & Medicinal Chemistry, AstraZeneca R&D

The structural and sequence information of cellular processes involving protein interactions and modifications is a valuable starting-point for the design of novel peptide therapeutics. This work exemplifies how peptide enzyme substrates can be turned into therapeutically relevant molecules. We demonstrate how we exploit structural and sequence information on a protein mechanism and substrate specificity to convert linear peptide substrates into cyclic peptide inhibitors.

11:00 Strategies for efficient, high-throughput optimization of therapeutic cyclic peptides.

GYROS PROTEIN Technologies

Andrew Kennedy, PhD, Global Product Manager, Gyros Protein Technologies

Cyclic peptides are an important tool for development of peptide therapeutics and peptide cyclizations can be achieved several ways. Here we describe several fully automated synthesis optimization methods, some using induction heating, for therapeutically relevant peptides including APY-d4, and RFP14. Other examples in this presentation include Melanotan II, NYAD1 and Agardhipeptin A cyclic peptide sequences.

11:40 LIVE: Panel Q&A with Session Speakers

Moderator: Christian N. Cunningham, PhD, Scientist, Early Discovery Biochemistry, Genentech Inc

Panelists:

Christian Heinis, PhD, Associate Professor, Lab of Therapeutic Proteins & Peptides, EPFL Lausanne

Ranganath Gopalakrishnan, PhD, Associate Principal Scientist, New Modality & Medicinal Chemistry, AstraZeneca R&D

Tomi K. Sawyer, PhD, Chief Drug Hunter & President, Maestro Therapeutics

Andrew Kennedy, PhD, Global Product Manager, Gyros Protein Technologies

PLENARY KEYNOTE SESSION

12:00 pm KEYNOTE PRESENTATION: PLENARY: New Technologies for Drug Discovery

Bryan L. Roth, PhD, Distinguished Professor, Pharmacology & Psychiatry, University of North Carolina, Chapel Hill

In this talk I will discuss recently invented approaches to accelerate drug discovery. These include a novel approach for directed evolution to create therapeutically targeted nanobodies, new biosensors for GPCRs and ultra-large-scale docking to discover new chemical matter at druggable targets. I will also highlight how these approaches can provide insights into new approaches to target COVID-19 and related disorders.

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Panelists:

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12:50 Session Break - View Our Virtual Exhibit Hall

1:00 Networking Hallway Hangout with Speakers and Poster Presenters - View Our Virtual Exhibit Hall

TARGET-SPECIFIC CONSTRAINED PEPTIDES

1:30 Discovery and Optimization of Sulanemadlin (ALRN6924): A First-in-Class MDMX/MDM2 Dual Inhibitor Progressing in the Clinic

Vincent Guerlavais, PhD, Senior Director, Chemistry, Protagonist Therapeutics Inc.

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Stapled peptides, emerged during the past 10 years, are showing promise for addressing and solving inherent limitations of peptides, particularly their poor cell permeability. The unique drug-like properties of ALRN-6924, a stabilized cell-permeating α-helical peptide that is currently being investigated as a chemoprotective drug for patients with TP53-mutant cancers, will be discussed.

Recommended Short Course* SC1: Emerging Chemical Tools for Phenotypic Screening and Target Deconvolution
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2:00 Calcineurin-NFAT Peptidyl Inhibitor as Potential COVID-19 Treatment
Dehua Pei, PhD, Professor, Chemistry & Biochemistry, Ohio State University
The primary cause of death among COVID-19 patients is the development of acute respiratory distress syndrome (ARDS), an inflammatory disease of the lungs. We have developed a peptidyl inhibitor against the calcineurin-NFAT interaction, CNI103, which specifically blocks the activation of NFATs and the production of inflammatory cytokines (e.g., TNF-alpha and IL-6). CNI103 has demonstrated excellent efficacy for prevention of acute lung injury/ARDS in a mouse model.

2:30 Automated Design of Macrocycles for Therapeutic Applications: From Small Molecules to Peptides and Proteins
Stefan Guessregen, PhD, Principal Scientist, R&D Integrated Drug Discovery, Sanofi Germany GmbH
Macrocyclization is a promising strategy to stabilize bioactive conformations and to improve several properties for lead optimization. A general computational workflow for the recognition and evaluation of sites for macrocyclization, the identification of compatible chemical linkers, and their conformational and enthalpic scoring has been developed. The broader applicability of this approach will be demonstrated with application to different case studies, e.g., GLP1/glucagon and small molecules (TAFIa) inhibitors.

3:00 Sponsored Presentation *(Opportunity Available)*

3:30 Discovery of Oral Hepcidin Peptidomimetics
Roopa Taranath, PhD, Senior Scientist II, Discovery Biology and Translation Research, Protagonist Therapeutics
Hepcidin mimetic peptides that are orally stable and systemically active will mark a paradigm change in management of blood disorders that exhibit aberrant iron homeostasis. Protagonist Therapeutics' Rusfertide is an injectable hepcidin mimetic, currently in Phase 2 clinical studies for polycythemia vera and hereditary hemochromatosis. I will describe 2nd Gen hepcidin mimetic peptides that are orally stable, systemically absorbed, and show improvement in disease parameters in pre-clinical mouse models.

4:10 LIVE: Panel Q&A with Session Speakers
Moderator: Scott Lokey, PhD, Professor, Chemistry and Biochemistry, University of California, Santa Cruz
Panelists:
Vincent Guerlavais, PhD, Senior Director, Chemistry, Protagonist Therapeutics Inc.
Dehua Pei, PhD, Professor, Chemistry & Biochemistry, Ohio State University
Stefan Guessregen, PhD, Principal Scientist, R&D Integrated Drug Discovery, Sanofi Germany GmbH
Roopa Taranath, PhD, Senior Scientist II, Discovery Biology and Translation Research, Protagonist Therapeutics

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WEDNESDAY, MAY 19

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CO-PRESENTATION: Topic: Macrocycle Innovations
Cameron Pye, PhD, CEO and Co-Founder, Unnatural Products
Lauren G. Monovich, PhD, Director, Global Discovery Chemistry, Novartis Institutes for BioMedical Research, Inc.

MACROCYCLIC DESIGN PRINCIPLES

10:00 FEATURED PRESENTATION: Mining Natural Products for Macrocycles to Drug Difficult Targets
Jan Kihlberg, PhD, Professor, Organic Chemistry, Uppsala University
Mining of macrocyclic natural products provided sets of cores for *in silico* screening to find leads for difficult-to-drug targets. Docking of the cores led to the discovery of a structurally unique, uncharged macrocyclic inhibitor of the Keap1-Nrf2 protein-protein interaction; a particularly challenging target due to its highly polar binding site. Design of a macrocycle collection inspired by the structure of one of the cores provided submicromolar inhibitors of Leishmania infections.

10:30 New Tools for Deciphering Conformation/Property Relationships in Macrocycles
Andrei K. Yudin, PhD, Professor, Chemistry, University of Toronto
We have designed new methods for isolating unique and previously understudied conformations of macrocycles. The observation of unusual conformations was made possible by controlling their interconversion

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using dominant rotors, which represent tunable atropisomeric constituents with high rotational barriers. Evidence suggests that amino acid residues can be forced into rare turn motifs not observed in linear counterparts and homodetic rings. These findings should unlock new avenues for studying the conformation-activity relationships.

11:00 Mimicking Nature in Drug Discovery: Enabling Good Design from Fragments to Macrocycles

Robert J. Young, PhD, Principal, Blue Burgundy Drug Discovery Consulting; formerly GSK Fellow and Scientific Leader, Medicinal Chemistry

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11:40 LIVE: Panel Q&A with Session Speakers

Moderator: Adrian Whitty, PhD, Associate Professor of Chemistry, Boston University
Panelists:
Jan Kihlberg, PhD, Professor, Organic Chemistry, Uppsala University
Andrei K. Yudin, PhD, Professor, Chemistry, University of Toronto
Robert J. Young, PhD, Principal, Blue Burgundy Drug Discovery Consulting; formerly GSK Fellow and Scientific Leader, Medicinal Chemistry

12:00 pm Session Break - View Our Virtual Exhibit Hall

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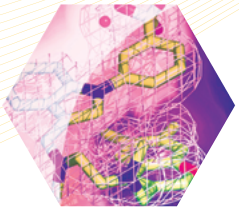

Cambridge Healthtech Institute's 14th Annual

MAY 19-20, 2021 | ALL TIMES EASTERN DAYLIGHT (UTC-04:00)

Protein-Protein Interactions

Expanding Druggable Space by Targeting Intracellular PPIs

WEDNESDAY, MAY 19

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View full info on breakouts webpage.

Women in Chemistry: The Gender Divide in Life Science Careers
Moderator: Mary Harner, PhD, Senior Manager, Oncology CI, Bristol Myers Squibb Co.

1:10 Greet 'n' Go Hallway Networker with Speakers and Poster Presenters - View Our Virtual Exhibit Hall

COVALENT INHIBITORS

1:30 Designing Potent and Selective PPI-Targeting Ligands via Combinatorial Library Screening (HTS by NMR) and Lys/Tyr Covalent Agents
Maurizio Pellecchia, PhD, Professor, Biomedical Sciences Division, University of California, Riverside
The HTS by NMR approach combines principles of positional scanning combinatorial chemistry with protein-observed NMR screening. Applied to the search of PPIs targeting ligands, the approach can be very successful. In some instances, the lengthy hit-to-lead optimization process can be facilitated by the proper design of Lys or Tyr covalent agents introducing sulfonyl-fluorides or fluoro-sulfates. I will report on these recent findings with several examples of successful applications to PPIs.

Recommended Short Course* SC2: Targeted Protein Degradation Using PROTACs, Molecular Glues, and More
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2:00 Discovery of Protein-Protein Interaction Stabilizers by Covalent Fragment-Based Screening
Markella Konstantinidou, PhD, Postdoctoral Fellow, Pharmaceutical Chemistry, University of California, San Francisco
Stabilization of protein-protein interactions remains largely underexplored, compared to inhibition. Here, we apply a site-directed fragment-based screening for the systematic discovery of stabilizers, aiming to stabilize the interaction between the hub protein 14-3-3s and client peptides using covalent fragments. Orthogonal biophysical assays were applied for fragment validation and the mechanism of stabilization was confirmed by X-ray crystallography. Aspects of selectivity for representative 14-3-3 clients were also explored.

2:30 Profiling of Covalent Inhibitors Using Biophysical Approaches
Stefan Geschwindner, Associate Director & Head of Biophysics, AstraZeneca R&D
The presentation will highlight and exemplify a range of biophysical approaches that can be utilized during the identification as well as characterization of covalent inhibitors. Those techniques and strategies aim to inform about the mechanism of inhibition by simultaneously providing data on affinity and the rate of covalent bond formation. Particular focus will be on the use of regenerable, SPR-based Biosensors as novel means for covalent inhibitor characterization.

3:00 Sponsored Presentation *(Opportunity Available)*

3:40 LIVE: Panel Q&A with Session Speakers
Moderator: Maricel Torrent, PhD, Principal Research Scientist, Molecular Modeling, AbbVie Inc.
Panelists:
Maurizio Pellecchia, PhD, Professor, Biomedical Sciences Division, University of California, Riverside
Markella Konstantinidou, PhD, Postdoctoral Fellow, Pharmaceutical Chemistry, University of California, San Francisco
Stefan Geschwindner, Associate Director & Head of Biophysics, AstraZeneca R&D

4:00 Close of Day

THURSDAY, MAY 20

PLENARY KEYNOTE SESSION

9:30 am KEYNOTE PRESENTATION: PLENARY: A Brief History of Targeted Covalent Drugs: The Journey from Avoided to Essential Medicines
Juswinder Singh, PhD, Founder and CSO, Ankaa Therapeutics
The past decade has witnessed remarkable progress in the field of targeted covalent drugs. Despite historical off-target toxicity concerns, covalent inhibitors have been rationally designed with high specificity leading to breakthrough therapies for cancer. Targeted covalent inhibitors are also in advanced trials for inflammatory diseases. In showing how covalent inhibitors address unmet medical needs, overcoming specific shortcomings of reversible drugs, I will highlight areas of innovation in covalent drug discovery.

10:05 LIVE: Q&A Plenary Discussion
Moderator: Daniel A. Erlanson, PhD, Vice President, Chemistry, Frontier Medicines Corp.
Panelists:

Juswinder Singh, PhD, Founder and CSO, Ankaa Therapeutics

10:20 Session Break - View Our Virtual Exhibit Hall

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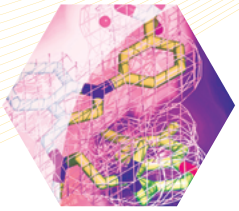
Topic: Lead Generation Against PPI Targets
Ben J Davis, PhD, Research Fellow, Biology, Vernalis R&D Ltd



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Protein-Protein Interactions

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PPI INHIBITOR CONSIDERATIONS

11:00 Determining Affinity from Irreversible Thermal Shift

Justin Hall, PhD, Principal Scientist, Structural Biology & Biophysics, Pfizer

We describe here methods and equations to fit ligand affinity from irreversible protein denaturation. Irreversible denaturation occurs for most proteins, particularly in the space of human therapeutics, but equations to fit these data have eluded investigators for many years. These results suggest the kinetic energy barrier for unfolding is similar across proteins; application of these findings should allow investigators to calculate ligand affinity from a single thermal denaturation data point.

Recommended Short Course* SC3: Ligand-Receptor Molecular Interactions and Drug Design
All Access VIRTUAL Pricing or separate registration required. See short course page for details.

11:30 Scaffold Selection for Protein-Protein Interaction Modulation: Are There Any General Principles?

Leonardo De Maria, PhD, Principal Scientist, AstraZeneca R&D

Most PPI inhibitors on the market are antibody-based because it's easier to disrupt PPIs with larger molecules. I analyzed publicly available data to compare different binding spaces between PPIs and their antibody disrupters to discern general scaffold features amenable to smaller disruptors. Focusing on binding affinities, buried surface areas and epitope characteristics, differences and similarities will be highlighted with an attempt to draw general small molecule and non-immunoglobin selection principles.

12:00 pm Discovering New Protein Interaction Partners of Gamma-Secretase with Photoaffinity Probes

Doug Johnson, PhD, Senior Director, Chemical Biology & Proteomics, Biogen

Gamma-Secretase cleaves APP to generate Abeta-42 which plays a causative role in Alzheimer's Disease. GSMs are a potential treatment for AD because they decrease Abeta-42 without affecting the processing of other critical gamma-secretase substrates. We used clickable GSM photoprobes to show that different classes of GSMs have distinct allosteric binding sites on PS1-NTF. In addition, we found that one photoprobe labeled IFITM3 and demonstrated the IFITM3 is part of gamma-secretase complex.

12:40 LIVE: Panel Q&A with Session Speakers
Moderator: Justyna Sikorska, PhD, Associate Principal Scientist, Mass Spectrometry & Biophysics, Merck
Panelists:
Justin Hall, PhD, Principal Scientist, Structural Biology & Biophysics, Pfizer
Leonardo De Maria, PhD, Principal Scientist, AstraZeneca R&D
Doug Johnson, PhD, Senior Director, Chemical Biology & Proteomics, Biogen

1:00 Session Break - View Our Virtual Exhibit Hall

INHIBITING KRAS AND OTHER PPI TARGETS

1:30 Discovery of Novel g-Secretase Modulators (GSM) for the Potential Treatment of Alzheimer's Disease

Hasane Ratni, PhD, Distinguished Scientist & Project Team Leader, Medicinal Chemistry, F. Hoffmann-La Roche AG

g-Secretase (GS) is a key target for a potential Alzheimer's disease treatment. Inhibiting GS led to serious side effects; modulating GS has greater safety potential. We report the discovery of a potent and selective gamma secretase modulator (GSM) (S)-3 (RO7185876), belonging to a novel chemical class, the triazolo-azepines demonstrating an excellent in-vitro and in-vivo DMPK profile. Furthermore, we propose a novel phenyl bioisostere with strongly improved drug-like properties.

2:00 FEATURED PRESENTATION: Translating Frontier Oncology Targets to *Outsmart Cancer*™

Jim Cregg, PhD, Senior Scientist I, Chemistry, Revolution Medicines

Revolution Medicines is developing novel RAS(ON) Inhibitors based on our proprietary tri-complex technology platform, enabling a highly differentiated approach to inhibiting the active, GTP-bound form of RAS (RAS(ON)). We will discuss a portfolio of compounds that we believe are the first and only RAS(ON) inhibitors to use this mechanism of action. RMC-6291, our inhibitor targeting $KRAS^{G12C}$/$NRAS^{G12C}$(ON), and RMC-6236, our inhibitor of multiple RAS variants (RAS^{MULTI}(ON)), are in IND-enabling preclinical development.

2:30 Evolution of BI-3406 – Getting a Foot in the Door between SOS1 and KRAS

Juergen Ramharter, PhD, Principal Scientist & Project Lead, Oncology Research, Boehringer Ingelheim RCV GmbH & Co. KG

KRAS, the most common oncogenic driver in human cancers, is controlled and signals through PPIs. Herein, we report the evolution of BI-3406, an orally available inhibitor of the SOS1-KRAS PPI. It decreases formation of GTP-KRAS, inhibits downstream signaling and limits proliferation of KRAS-driven cancers. BI-3406 served as probe for the study of SOS1 and KRAS biology and paved the way to clinical trials in combination with a MEK inhibitor.

3:00 Tools for the Discovery of KRAS Pathway Inhibitors

Ekaterina Kuznetsova, PhD, Director of Product Development, Reaction Biology

to be announced

3:40 LIVE: Panel Q&A with Session Speakers
Moderator: Matthew A. Marx, PhD, Vice President, Drug Discovery, Mirati Therapeutics, Inc.
Panelists:
Jim Cregg, PhD, Senior Scientist I, Chemistry, Revolution Medicines
Hasane Ratni, PhD, Distinguished Scientist & Project Team Leader, Medicinal Chemistry, F. Hoffmann-La Roche AG
Juergen Ramharter, PhD, Principal Scientist & Project Lead, Oncology Research, Boehringer Ingelheim RCV GmbH & Co. KG
Ekaterina Kuznetsova, PhD, Director of Product Development, Reaction Biology

4:00 Close of Conference

Cambridge Healthtech Institute's 3rd Annual

MAY 19-20, 2021 | ALL TIMES EASTERN DAYLIGHT (UTC-04:00)

Artificial Intelligence for Early Drug Discovery

Increasing Speed and Precision in Drug Design, Lead Optimization and ADMET Predictions

WEDNESDAY, MAY 19

12:40 Women in Chemistry Breakout Discussion - View Our Virtual Exhibit Hall

View full info on breakouts webpage.

Women in Chemistry: The Gender Divide in Life Science Careers

Moderator: Mary Harner, PhD, Senior Manager, Oncology CI, Bristol Myers Squibb Co.

1:10 Greet 'n' Go Hallway Networker with Speakers and Poster Presenters - View Our Virtual Exhibit Hall

AI-DRIVEN DRUG DESIGN

1:30 What Is AI Good for in Small Molecule Drug Discovery?

Jeff Blaney, Director Computational Chemistry & Cheminformatics, Computational Chemistry & Cheminformatics, Genentech, Inc.

Small molecule drug discovery is iterative. It identifies compounds and improves them through multi-parameter optimization (MPO). How can we improve upon this current approach? I'll present examples of successful applications of machine learning (ML) and more recent deep learning (DL). These include prediction of DMPK and physicochemical properties, comparison of prediction of log D, and a NNP (neural net potential) model to calculate DFT-level strain-energy for receptor-bound ligand conformation.

Recommended Short Course* SC2: Targeted Protein Degradation Using PROTACs, Molecular Glues, and More

All Access VIRTUAL Pricing or separate registration required. See short course page for details.

2:00 SYNTHIA™ Retrosynthesis Software for Practicing Chemists: Novel and *in Silico* Design at the Bench

Lindsey Rickershauser, Ph.D., Manager Sales & Marketing, Cheminformatics Technologies, MilliporeSigma

In an evolving landscape of *in silico* chemical intelligence and machine learning, computer-aided synthesis can accelerate breakthroughs in drug discovery research. SYNTHIA™ retrosynthesis software is revolutionizing the way chemists design pathways to complex targets by harnessing the power of artificial intelligence with an expert-coded database of advanced organic synthesis rules to augment chemists' expertise. Discover how this innovative cheminformatics tool is being used at the bench.

2:30 Meaningful Machine Learning Models from Fragment Screening Campaigns

Marcel Verdonk, PhD, Senior Director, Computational Chemistry & Informatics, Astex Pharmaceuticals

We derive machine learning (ML) models from over 50 fragment screening campaigns. Critically, our dataset includes true inactives as well as actives and our ML methodology produces interpretable models that we validate against expert annotations. We show that, given a high-quality training set, ML does not only generate models that separate binders from non-binders, but also accurately identifies which parts of a fragment drive its binding against the target.

3:00 Spaya and the Spaya API: AI Enhanced Retrosynthesis Planning

Quentin Perron, PhD, Co-founder and CSO, Iktos

Iktos has developed a retrosynthesis platform called Spaya, and a high-throughput API running on Spaya's algorithmic engine. Integration of the Spaya API into a molecule generator leads to the generation of synthesizable molecules without penalizing the other objectives of the generator. Integration of synthetic accessibility is an enabling step to be able to take advantage of the full potential of generative models in real life, i.e.: obtaining synthesizable optimized molecules.

3:30 An Inhibitor for Every Kinase: Using Deep Learning to Design Selective Inhibitors

John Karanicolas, PhD, Professor, Molecular Therapeutics, Fox Chase Cancer Center

Modern cancer biology leans heavily on kinase inhibitors to probe the consequences of deactivating a particular kinase, but most commonly used chemical probes are not sufficiently target-selective for robust interpretation of the observed phenotypes. Today I will sketch out a path for rapidly designing high-quality selective kinase inhibitors; these inhibitors may be used as tools for discovery, and as starting points for drug development.

4:00 Next Generation Synthesis Planning Using AI for Chemists

Abhinav Kumar, Head of Chemistry Solutions, Elsevier

Rapid navigation of increasingly complex druggable chemical space is critical for innovative drug design. However, chemical synthesis and route design is still a significant challenge. In this session, we will discuss recent development in predictive retrosynthesis. Also, we explore how Elsevier collaborated with Prof. Mark Waller to develop a 'deep learning' solution that predicts new synthesis routes with high accuracy for creating small organic drug compounds.

4:30 LIVE: Panel Q&A with Session Speakers

Moderator: Marcel Verdonk, PhD, Senior Director, Computational Chemistry & Informatics, Astex Pharmaceuticals
Panelists:
Jeff Blaney, Director Computational Chemistry & Cheminformatics, Computational Chemistry & Cheminformatics, Genentech, Inc.
John Karanicolas, PhD, Professor, Molecular Therapeutics, Fox Chase Cancer Center
Quentin Perron, PhD, Co-founder and CSO, Iktos
Lindsey Rickershauser, Ph.D., Manager Sales & Marketing, Cheminformatics Technologies, MilliporeSigma
Abhinav Kumar, Head of Chemistry Solutions, Elsevier

4:50 Close of Day

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THURSDAY, MAY 20

PLENARY KEYNOTE SESSION

9:30 am KEYNOTE PRESENTATION: PLENARY: A Brief History of Targeted Covalent Drugs: The Journey from Avoided to Essential Medicines

Juswinder Singh, PhD, Founder and CSO, Ankaa Therapeutics

The past decade has witnessed remarkable progress in the field of targeted covalent drugs. Despite historical off-target toxicity concerns, covalent inhibitors have been rationally designed with high specificity leading to breakthrough therapies for cancer. Targeted covalent inhibitors are also in advanced trials for inflammatory diseases. In showing how covalent inhibitors address unmet medical needs, overcoming specific shortcomings of reversible drugs, I will highlight areas of innovation in covalent drug discovery.

10:05 LIVE: Q&A Plenary Discussion

Moderator: Daniel A. Erlanson, PhD, Vice President, Chemistry, Frontier Medicines Corp.

Panelists:

Juswinder Singh, PhD, Founder and CSO, Ankaa Therapeutics

10:20 Session Break - View Our Virtual Exhibit Hall

10:30 Interactive Breakout Discussions - View Our Virtual Exhibit Hall

This group discussion is a chance for everyone to see and hear each other if they choose to turn on their cameras and microphones. Each group will have a moderator to ensure focused conversations around key issues within the conference's scope. This will be a 'now or never' session; it will not be recorded or available On Demand. **View all topics on breakouts webpage.**

CO-PRESENTATION: Topic: Applications of AI-Driven Drug Discovery

Arvind Rao, PhD, Associate Professor, Department of Computational Medicine and Bioinformatics, University of Michigan

Anthony Bradley, PhD, Director of Design Development, Exscientia Ltd.

Ewa Lis, PhD, Founder & CTO, Koliber Biosciences

- Types of AI models predicting individual target activities of small molecules•
- Machine-learning and structure-based approaches for ADME-Tox predictions
- Current trends for the application of AI towards pre-clinical drug discovery
- Understanding the caveats of AI-driven predictions

AI-ENABLED DECISION-MAKING FOR DRUG DISCOVERY

11:00 FEATURED PRESENTATION: The Evolution of AI-Powered Generative Chemistry 2015-2021 and Beyond

Alex Zhavoronkov, PhD, Founder & CEO, Insilico Medicine

The lecture will focus on the development and application of generative models for creating novel compounds and for generating synthetic biological data with the desired properties.

Recommended Short Course* SC3: Ligand-Receptor Molecular Interactions and Drug Design

All Access VIRTUAL Pricing or separate registration required. See short course page for details.

11:30 AI-Powered Design of Small Molecules Accelerated by Active Learning and Multimodal Constraints

Anthony Bradley, PhD, Director of Design Development, Exscientia Ltd.

In this talk we outline the breadth of generative design techniques that are involved in our AI design system. Second, we show how these generative models can incorporate multimodal 2D and 3D data to enhance their efficiency. Third, we show how a range of Active Learning capabilities are used to optimally select compounds for enhancing information gain and thus the next cycle of design.

12:00 pm Applying Machine Learning to Build a Company Pipeline

Sean Ekins, PhD, Founder & CEO, Collaborations Pharmaceuticals, Inc.

We have developed and applied machine learning software and models for various targets for rare, neglected, and common diseases which have enabled us to create a diverse portfolio of small molecules. Several of our recent published applications for infectious diseases and Alzheimer's will be described along with our exploration of approaches for *de novo* molecule design. Our goal is to progress and de-risk assets that can then be out-licensed.

12:30 Eliminating the Data Bottleneck in Surface Plasmon Resonance in Drug Discovery

cytiva

Paul Belcher, Product Strategy Manager, Biacore, Cytiva

SPR is a key tool in drug discovery due to the information rich nature of the data it provides, supporting chemistry efforts in hit to lead development. But analyzing 100s-1000s of multi-dimensional data points remains a key challenge, constrained by time and expertise. We will present a novel, AI-based prototype that overcomes the analysis bottleneck to enable greater support of chemistry efforts in hit to lead development with SPR data.

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Panelists:
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Sean Ekins, PhD, Founder & CEO, Collaborations Pharmaceuticals, Inc.
Paul Belcher, Product Strategy Manager, Biacore, Cytiva

AI PREDICTIONS FOR EFFICACY AND SAFETY

1:30 Finding Leads with Desired Multi-Target Pharmacology *in silico* and *in Vitro*
Ruben Abagyan, PhD, Professor, Department of Molecular Biology, University of California, San Diego
A large panel of AI and 3D models helps to quickly repurpose drugs to new targets or find leads with specified activity profiles composed of new or known targets. Applications to targets related to SARS-CoV-2, flaviviruses, E. Histolytica and oncology are presented.

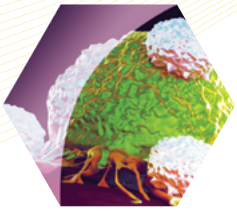
2:00 Understanding and Predicting Peptide Activity Using Artificial Intelligence Approaches
Ewa Lis, PhD, Founder & CTO, Koliber Biosciences
AI has become indispensable for drug discovery, yet the technology is not widely utilized by scientists. The core limitation of existing approaches is inability to leverage small datasets and poor interpretability. Koliber is developing an AI platform for peptide discovery that enables tuning of pre-trained models to small datasets, visualization of key features and sequence profiling to identify key sites and improved variants. This is demonstrated using examples from immunology.

2:30 AI-Driven Identification of Inhibitors of Drug Metabolizing Enzymes
Maria Miteva, PhD, Research Director, Molécules Thérapeutiques in silico (MTi), Inserm Institute
We focus on Cytochrome P450 (CYP) responsible for the metabolism of 90% drugs and on sulfotransferases (SULT), phase II conjugate drug metabolizing enzymes, acting on large number of drugs, hormones and natural compounds. We established an original *in silico* approach integrating structure-based and machine learning modeling and developed a new software DrugME to predict CYP and SULT inhibitors. This allowed the identification of new drug inhibitors and substrates of CYP2C9.

3:00 Untangling the Significance of Structural Alerts with Deep Learning
S. Joshua Swamidass, Associate Professor, Pathology & Immunology, Washington University
In developing new molecules for the clinic, we cannot avoid structural alerts in all cases. In most cases, structural alerts are only a marker of risk, and are not actually bioactivated into reactive metabolites. Machine learning, a type of artificial intelligence, is giving us new ways to understand why and when structural alerts become toxic or not.

3:40 LIVE: Panel Q&A with Session Speakers
Moderator: Ruben Abagyan, PhD, Professor, Department of Molecular Biology, University of California, San Diego
Panelists:
Ewa Lis, PhD, Founder & CTO, Koliber Biosciences
Maria Miteva, PhD, Research Director, Molécules Thérapeutiques in silico (MTi), Inserm Institute
S. Joshua Swamidass, Associate Professor, Pathology & Immunology, Washington University

4:00 Close of Conference



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Small Molecules for Immunology, Oncology & COVID

Discovering Oral-Based Therapeutics for Autoimmunity, Cancer and Infectious Diseases

WEDNESDAY, MAY 19

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Women in Chemistry: The Gender Divide in Life Science Careers
Moderator: Mary Harner, PhD, Senior Manager, Oncology CI, Bristol Myers Squibb Co.

1:10 Greet 'n' Go Hallway Networker with Speakers and Poster Presenters - View Our Virtual Exhibit Hall

INHIBITING INTRACELLULAR IMMUNOLOGY OR ONCOLOGY TARGETS

1:30 FEATURED PRESENTATION: An Orally Available Non-Nucleotide STING Agonist with Antitumor Activity: A Mechanistic Study
Gottfried Schroeder, PhD, Associate Principal Scientist, Quantitative Biosciences, Merck & Co., Inc.

Pharmacological activation of the innate immune receptor STING is a promising therapeutic strategy for cancer. MSA-2 is an orally available non-nucleotide human STING agonist. Extensive experimental analysis showed that MSA-2 exists as interconverting monomers and dimers in solution, but only dimers bind and activate STING. Extracellular acidification, mimicking the tumor microenvironment, increased MSA-2 cellular potency. These properties appear to underpin the favorable activity and tolerability profiles of systemically administered MSA-2.

March 2021 Speaker Interview with Dr. Schroeder:
Watch Interview Online

Recommended Short Course* SC2: Targeted Protein Degradation Using PROTACs, Molecular Glues, and More
**All Access VIRTUAL Pricing or separate registration required. See short course page for details.*

2:00 From Physics to Clinic: Design of a Novel Small Molecule STING Agonist (SNX281) with Excellent Drug Properties and Systemic Delivery
Woody Sherman, PhD, CSO, Silicon Therapeutics

I will show how we were able to design a new STING agonist that overcame the systemic delivery issues plaguing 1st generation agonists such as poor metabolic stability and poor physio-chemical properties. SNX281 is potent, specific, and active against all human isoforms of STING and rapidly activates downstream signaling and induces type I IFN. Our compound entered Phase1 clinical trials in November 2020.

2:30 Chemoproteomic Profiling of Covalent XPO1 Inhibitors to Assess Target Engagement and Selectivity
Jeffrey Martin, PhD, Scientist II, Drug Discovery, Biogen

Selinexor, a covalent XPO1 inhibitor, is approved in the U.S. in combination with dexamethasone for penta-refractory multiple myeloma. In this talk we will describe clickable probes based on XPO1 inhibitors selinexor and eltanexor for the labeling of XPO1 in live cells to assess target engagement and selectivity. We use mass spectrometry-based chemoproteomic workflows to profile the proteome-wide selectivity of selinexor and eltanexor and show that they are selective for XPO1.

3:00 Talk Title to be Announced
Speaker to be Announced

3:40 LIVE: Panel Q&A with Session Speakers
Moderator: Jennifer D. Venable, PhD, Senior Scientific Director, Discovery Chemistry, Janssen Pharmaceuticals, Inc.
Panelists:
Gottfried Schroeder, PhD, Associate Principal Scientist, Quantitative Biosciences, Merck & Co., Inc.
Woody Sherman, PhD, CSO, Silicon Therapeutics
Jeffrey Martin, PhD, Scientist II, Drug Discovery, Biogen
Speaker to be Announced

4:00 Close of Day

THURSDAY, MAY 20

PLENARY KEYNOTE SESSION

9:30 am KEYNOTE PRESENTATION: PLENARY: A Brief History of Targeted Covalent Drugs: The Journey from Avoided to Essential Medicines
Juswinder Singh, PhD, Founder and CSO, Ankaa Therapeutics

The past decade has witnessed remarkable progress in the field of targeted covalent drugs. Despite historical off-target toxicity concerns, covalent inhibitors have been rationally designed with high specificity leading to breakthrough therapies for cancer. Targeted covalent inhibitors are also in advanced trials for inflammatory diseases. In showing how covalent inhibitors address unmet medical needs, overcoming specific shortcomings of reversible drugs, I will highlight areas of innovation in covalent drug discovery.

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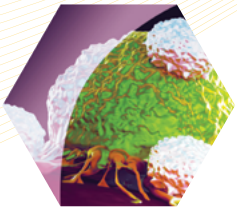
Moderator: Daniel A. Erlanson, PhD, Vice President, Chemistry, Frontier Medicines Corp.
Panelists:

Juswinder Singh, PhD, Founder and CSO, Ankaa Therapeutics

10:20 Session Break - View Our Virtual Exhibit Hall



Small Molecules for Immunology, Oncology & COVID

Discovering Oral-Based Therapeutics for Autoimmunity, Cancer and Infectious Diseases

10:30 Interactive Breakout Discussions - View Our Virtual Exhibit Hall

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Topic: New Small Molecule IO Targets
Murali Ramachandra, PhD, CEO, Aurigene Discovery Technologies, Ltd.

NEW SMALL MOLECULES AGAINST SARS-COV2 TARGETS

11:00 The COVID Moonshot: Asking the Crowd for an Antiviral

Frank von Delft, PhD, Professor, Centre for Medicines Discovery and Principal Beamline Scientist, Diamond Light Source, University of Oxford

As the pandemic was breaking, Diamond and the Weizmann Institute performed a huge crystallographic and electrophile fragment screen on Mpro of SARS-CoV-2. Data were released into the public domain and announced on Twitter, triggering a large international response that led to a fully open crowd-sourcing effort, to bring a safe, simple, oral antiviral to patients in time for this pandemic. This will be an update and prospective on the project.

Recommended Short Course* SC3: Ligand-Receptor Molecular Interactions and Drug Design
**All Access VIRTUAL Pricing or separate registration required. See short course page for details.*

11:30 Massive X-Ray Screening Reveals Two Allosteric Drug Binding Sites of SARS-CoV-2 Main Protease

Sebastian Guenther, PhD, Postdoctoral Fellow, Biomedical Research X-Rays, Deutsches Elektronen-Synchrotron DESY

In a search for drugs against COVID-19, we have performed a high-throughput X-ray crystallographic screen of two repurposing drug libraries with almost 6000 compounds against the SARS-CoV-2 main protease (M^{pro}), which is essential for viral replication. We identified 37 compounds binding to M^{pro}. In subsequent cell-based assays, five compounds showed antiviral activity at non-toxic concentrations. Additionally, we identified two allosteric binding sites representing attractive targets for drug development against SARS-CoV-2.

12:00 pm Using NMR to Discover Non-Covalent Fragment Binders against COVID Targets

Julien Orts, PhD, Assistant Professor, Physical Chemistry Lab, ETH Zurich

We will present how NMR can contribute to the global effort against the COVID-19 pandemic. In a second part, I will briefly present preliminary results on new methodologies for studying small-molecule protein complexes.

12:30 An Artificial Intelligence Drug Repurposing Approach Identifies an Oncology Medication with Antiviral Activity

Vijay Shahani, PhD, Director of Applied Science, Cyclica Inc

We used two machine learning engines to predict drug repurposing candidates for the treatment of COVID-19. A graph convolutional network using host-virus interactome data revealed potential host-antiviral targets that enabled PolypharmDB, a database of small molecule drugs and their predicted polypharmacology, to be queried for relevant putative modulators. Several of the predicted agents demonstrated antiviral activity in cell-based assays, with the oncology drug, capmatinib, demonstrating broad spectrum antiviral activity against several coronaviruses, including SARS-CoV-2.

1:10 LIVE: Panel Q&A with Session Speakers

Moderator: Samantha J. Allen, PhD, Principal Scientist, Lead Discovery & Profiling, Janssen R&D LLC
Panelists:
Frank von Delft, PhD, Professor, Centre for Medicines Discovery and Principal Beamline Scientist, Diamond Light Source, University of Oxford
Sebastian Guenther, PhD, Postdoctoral Fellow, Biomedical Research X-Rays, Deutsches Elektronen-Synchrotron DESY
Julien Orts, PhD, Assistant Professor, Physical Chemistry Lab, ETH Zurich
Vijay Shahani, PhD, Director of Applied Science, Cyclica Inc

SMALL MOLECULE INHIBITOR DISCOVERY: COVID AND BEYOND

1:30 Fragment Binding to the Nsp3 Macrodomain of SARS-CoV-2

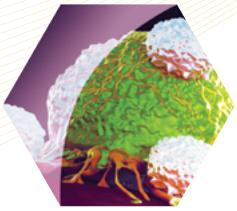
James Fraser, PhD, Assistant Professor, Bioengineering, University of California, San Francisco

Through a massive crystallographic screening and computational docking effort we identified new chemical matter primarily targeting the active site of the macrodomain of the non-structural protein 3 (Nsp3) of SARS-CoV-2. This enzyme is a promising antiviral target because catalytic mutations render viruses non-pathogenic.

2:00 Exploiting Conformational Dynamics for Drugging Pro-Apoptotic BCL-2 Proteins

Evris Gavathiotis, PhD, Professor, Biochemistry, Albert Einstein College of Medicine

Using structural similarity screening and biophysical methods, we identified that Eltrombopag, an FDA-approved drug, is a direct inhibitor of pro-apoptotic BAX. Eltrombopag binds the BAX activation site distinctly from BAX activators, preventing them from triggering BAX conformational transformation and simultaneously promoting stabilization of the inactive BAX structure. Our data demonstrate insights into a mechanism of BAX inhibition and suggest a potential use for Eltrombopag in diseases of uncontrolled cell death.



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2:30 Small Molecules for Programming Catalytic Fragment Antibodies to Control CAR Ts

Haiyong Peng, PhD, Staff Scientist, Immunology & Microbiology, Scripps Research Institute

We developed a method that endows small molecules with the ability to recruit and activate CAR Ts to kill tumor cells. It is based on a CAR-T with a generic and inert scFv that gets switched on by a catalytic Fab programmed with small molecules targeting tumor cells. In proof-of-concept studies, this switchable CAR T system mediated potent and specific eradication of cancer cells *in vitro* and *in vivo*.

3:00 Speed up Your Drug Discovery with Ready-to-Use Stable Cell Lines

GenScript
Make Research Easy

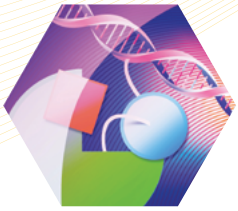
Vevian Zhang, Product Manager, GenScript Inc

Stable cell lines are critical tools of cellular assays in drug discovery and development. Over-expressing cell lines are needed to screen for hits, while functional cell lines are needed for "lead" identification. In the past couple of decades, GenScript has developed 200+ stable cell line products expressing the most popular drug targets including GPCR, FcR, immune checkpoints, and COVID19 related proteins to accelerate your drug discovery and clinical translation.

3:40 LIVE: Panel Q&A with Session Speakers

Moderator: Phillip Schwartz, PhD, Principal Scientist, Biophysics, Frontier Medicines
Panelists:
James Fraser, PhD, Assistant Professor, Bioengineering, University of California, San Francisco
Evris Gavathiotis, PhD, Professor, Biochemistry, Albert Einstein College of Medicine
Haiyong Peng, PhD, Staff Scientist, Immunology & Microbiology, Scripps Research Institute
Vevian Zhang, Product Manager, GenScript Inc

4:00 Close of Conference



Cambridge Healthtech Institute's 3rd Annual

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Encoded Libraries for Small Molecule Discovery

Expanding Chemical Space for New Drug Leads

WEDNESDAY, MAY 19

12:40 Women in Chemistry Breakout Discussion - View Our Virtual Exhibit Hall

View full info on breakouts webpage.

Women in Chemistry: The Gender Divide in Life Science Careers

Moderator: Mary Harner, PhD, Senior Manager, Oncology CI, Bristol Myers Squibb Co.

1:10 Greet 'n' Go Hallway Networker with Speakers and Poster Presenters - View Our Virtual Exhibit Hall

INNOVATIONS IN DEL TECHNOLOGIES

1:30 FEATURED PRESENTATION: Toward the Assembly and Characterization of an Encoded Library Hit Optimization Platform: Bead-Assisted Ligand Isolation for Mass Spectrometry (BALI-MS)

Anokha S. Ratnayake, PhD, Principal Scientist, Design and Synthesis Sciences, DNA Encoded Library Technology Group, Pfizer Global R&D Groton Labs

While screening DELs and proposing hits from the resultant data has proven to be a straightforward exercise, the poor conversion rate of NGS-identified hits to confirmed ligands off-DNA complicates the realization of value expected from the technology. Here we highlight our Bead-Assisted Ligand Isolation-Mass Spectrometry (BALI-MS) hit-optimization platform that enables us to efficiently interrogate features from the primary DEL screen, therefore leading to a greater percentage of viable drug leads.

Recommended Short Course* SC2: Targeted Protein Degradation Using PROTACs, Molecular Glues, and More

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2:00 Activity-Based DEL

Brian M. Paegel, PhD, Professor, Pharmaceuticals Sciences, University of California, Irvine

Solid-phase DEL technology unlocks opportunities to screen libraries using activity-based assays, from simple enzyme-substrate reactions to more complicated coupled enzymes systems (e.g. *in vitro* translation) and cells. This talk will describe new technology that we've developed for conducting activity assays directly on beads that does not require water-in-oil compartmentalization or custom droplet sorting instrumentation.

2:30 Navigating New Chemical Space of DNA-Encoded Chemical Library by Developing Novel DNA-Compatible Chemistry

Guansai Liu, Senior Director, HitGen Inc

DNA-encoded chemical libraries (DECLs) have increasingly been recognized as a powerful and economic technical tool for hit identifications. To increase successful rates of DECL selections, it's critical to develop valuable DNA-compatible reactions for constructing pharmaceutically preferred chemical structures. Here we would like to recall recent developments of on-DNA chemistry for DECL synthesis in this area and to focus on continuous endeavors of synthetic methodology exploitation at HitGen.

3:00 A New Hit ID Discovery Tool: GenScript's DNA-Encoded Chemical Library Kit

Rouba Najjar, Senior Product Manager, Catalog Products, GenScript Inc

In partnership with a leading technology expert, GenScript has developed this ready-to-use, commercially accessible GenDECL™ kit. This kit is a promising new tool for fueling drug discovery efforts, consisting of a collection of 18 sub-libraries with over 400 million drug-like chemical compounds.

3:40 LIVE: Panel Q&A with Session Speakers

Moderator: Bing Xia, PhD, Investigator, R&D Medicinal Science & Technology, GlaxoSmithKline
Panelists:
Anokha S. Ratnayake, PhD, Principal Scientist, Design and Synthesis Sciences, DNA Encoded Library Technology Group, Pfizer Global R&D Groton Labs
Brian M. Paegel, PhD, Professor, Pharmaceuticals Sciences, University of California, Irvine
Barry Morgan, CSO, HitGen Pharmaceuticals
Rouba Najjar, Senior Product Manager, Catalog Products, GenScript Inc

4:00 Close of Day

THURSDAY, MAY 20

PLENARY KEYNOTE SESSION

9:30 am KEYNOTE PRESENTATION: PLENARY: A Brief History of Targeted Covalent Drugs: The Journey from Avoided to Essential Medicines

Juswinder Singh, PhD, Founder and CSO, Ankaa Therapeutics

The past decade has witnessed remarkable progress in the field of targeted covalent drugs. Despite historical off-target toxicity concerns, covalent inhibitors have been rationally designed with high specificity leading to breakthrough therapies for cancer. Targeted covalent inhibitors are also in advanced trials for inflammatory diseases. In showing how covalent inhibitors address unmet medical needs, overcoming specific shortcomings of reversible drugs, I will highlight areas of innovation in covalent drug discovery.

Encoded Libraries for Small Molecule Discovery

Expanding Chemical Space for New Drug Leads

10:05 LIVE: Q&A Plenary Discussion
Moderator: Daniel A. Erlanson, PhD, Vice President, Chemistry, Frontier Medicines Corp.
Panelists:

Juswinder Singh, PhD, Founder and CSO, Ankaa Therapeutics

10:20 Session Break - View Our Virtual Exhibit Hall

10:30 Interactive Breakout Discussions - View Our Virtual Exhibit Hall
This group discussion is a chance for everyone to see and hear each other if they choose to turn on their cameras and microphones. Each group will have a moderator to ensure focused conversations around key issues within the conference's scope. This will be a 'now or never' session; it will not be recorded or available On Demand. **View all topics on breakouts webpage.**

CO-PRESENTATION: Topic: DNA-Encoded Library Technologies
Svetlana Belyanskaya, PhD, Vice President, Biology, Anagenex
Maria Soloveychik, PhD, Co-Founder & CEO, SyntheX

EXPANDING AND EXPLORING THE CHEMICAL SPACE OF AN ENCODED LIBRARY

11:00 Reading between Gigabytes of Lines: Decoding Chemical Reaction Information from DNA Encoded Libraries
Dennis Gillingham, PhD, Professor, Chemistry, University of Basel
The ease of writing, reading, and copying DNA information underpins DNA encoded libraries, but the information we store in DNA can be used in myriad ways. For example, I will describe how we analyze damage and mutations in DNA as a way to assess the DNA damage inflicted during encoded library synthesis. In another case, we have used indexing to keep track of and to analyze sub-library information during data analysis.

Recommended Short Course* SC3: Ligand-Receptor Molecular Interactions and Drug Design
**All Access VIRTUAL Pricing or separate registration required. See short course page for details.*

11:30 eDESIGNER: A Tool for Navigating the DNA-Encoded Libraries Chemical Space
Alfredo Martin, PhD, Senior Research Advisor, DCRT, Eli Lilly & Co.
eDESIGNER is an algorithm that comprehensively generates DNA encoded library designs, enumerates and profiles samples from each library, and evaluates them to select the libraries to be synthesized. This presentation will address the eDESIGNER concept and how we use it at Lilly to improve the chemical space coverage and compound chemical properties of our DNA encoded libraries.

12:00 pm Ring-Closing Metathesis for DNA-Encoded Libraries
Damian W. Young, PhD, Assistant Professor, Pharmacology & Chemical Biology, Baylor College of Medicine
DNA-Encoded Chemical Libraries (DECLs) have transformed modern screening against biological targets; however, chemical reactions to form DECLs must be compatible with DNA. Similarly, the ring-closing metathesis (RCM) reaction has been a staple of modern synthetic organic chemistry for ring formation owing to its wide functional group tolerance and substrate generality. We describe the development of robust conditions for performing the RCM reaction in the context of a DECL platform.

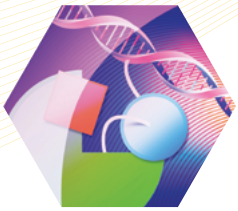
12:30 Rational Design of Di/Tri-Functionalised Scaffolds for DEL-Technology; Unlocking Stereodefined, 3D Chemical Space
Ilaria Proietti Silvestri, PhD, Head of R&D, LCC [Liverpool ChiroChem]
Drug discovery is now blessed with a wide range of high-throughput hit identification strategies that have been successfully validated in recent years, with particular success coming from DEL Screening. This talk will focus on LCC's design of novel di/tri-functionalised, 3D-rich, stereodefined building blocks for DEL technologies which can be employed to generate libraries of drug-like compounds and how recent advances in synthetic methodologies can be utilised to access these valuable scaffolds.

1:10 LIVE: Panel Q&A with Session Speakers
Moderator: Christopher B. Phelps, PhD, Vice President and Head, Early Discovery, Nurix Therapeutics Inc.
Panelists:
Dennis Gillingham, PhD, Professor, Chemistry, University of Basel
Alfredo Martin, PhD, Senior Research Advisor, DCRT, Eli Lilly & Co.
Damian W. Young, PhD, Assistant Professor, Pharmacology & Chemical Biology, Baylor College of Medicine
Ilaria Proietti Silvestri, PhD, Head of R&D, LCC [Liverpool ChiroChem]

DISCOVERY AND OPTIMIZATION OF DRUG LEADS FROM DNA-ENCODED LIBRARIES

1:30 Hit Discovery from DNA-Encoded Libraries: Past, Present and Future
Joerg Scheuermann, PhD, Senior Lecturer, Chemistry & Applied Biosciences, ETH Zurich
DEL technology, started in the early 2000s with just a handful of mostly academic groups. including mine at ETH, has developed into a valuable resource for small molecule drug discovery over the last few years. This talk will highlight the most important success stories and their respective DEL design. I will also discuss opportunities for improvement in the DEL field and the promises and limitations of different DEL architectures.

2:00 Discovery of Small Molecule Inhibitors of sEH and RIPK1 Enabled by DNA-Encoded Library Technology: Two Case Studies
Carol Mulrooney, PhD, Investigator, Cheminformatics, GlaxoSmithKline



Encoded Libraries for Small Molecule Discovery

Expanding Chemical Space for New Drug Leads

I will give a retrospective presentation about two compounds that are now progressing in clinical trials that originated from DNA-encoded Libraries. One compound is an inhibitor of expoxide hydrolases (sEH) and the other inhibits the receptor-interacting kinase (RIPK) 1.

2:30 DEL Screening Inside Living Cells

Iolanda Micco, PhD, Associate Director of Chemistry & Alliances, Vipergen

I will present 2 or 3 case studies of molecules discovered from the first successful screening of DNA-encoded library (DEL) inside a living cell: oocytes from the South-African clawed frog Xenopus Laevis. Cell-based DEL screening benefits include broader target space (no requirement for purified target protein) and lower attrition rates (screening under physiological relevant conditions).

3:00 DNA-Encoded Chemistry: Enabling the Search for Truly Novel Chemical Equity

Anthony Keefe, Senior Vice President, Innovation and Alliance Management, X-Chem Inc.

X-Chem Inc. operates a DNA-Encoded Chemistry platform and associated downstream services to support a wide range of customers in their search for novel chemical equity. This talk will introduce the platform and its achievements with a range of examples of licensed projects including oncology, infectious disease and CNS applications. Examples will demonstrate the downstream services we provide including methods to rapidly identify hits, hit-to-lead, structural biology enablement and medicinal chemistry.

3:30 Discovery of Covalent Inhibitors from DNA-Encoded Libraries

Alex Satz, Senior Director DEL Strategy and Operations, RSD, Research Service Division, WuXi AppTec

DNA-Encoded library (DEL) technology is a screening platform used throughout the pharmaceutical industry to discover novel chemical matter. Despite pharmaceutical interest in small-molecules capable of irreversibly binding to their targets, DEL technology has failed to demonstrate the ability to produce and discover covalent hit molecules. We will share recent successful covalent DEL screening efforts against Bruton's tyrosine kinase and SARS-CoV-2 main protease, including evidence of covalent interactions and potent enzymatic activity.

4:10 LIVE: Panel Q&A with Session Speakers

Moderator: Caroline Joannesse, PhD, Senior Scientist, Medicinal Chemistry, Galapagos NV

Panelists:

Joerg Scheuermann, PhD, Senior Lecturer, Chemistry & Applied Biosciences, ETH Zurich

Carol Mulrooney, PhD, Investigator, Cheminformatics, GlaxoSmithKline

Iolanda Micco, PhD, Associate Director of Chemistry & Alliances, Vipergen

Anthony Keefe, Senior Vice President, Innovation and Alliance Management, X-Chem Inc.

Alex Satz, Senior Director DEL Strategy and Operations, RSD, Research Service Division, WuXi AppTec

4:30 Close of Conference

Drug Discovery Chemistry VIRTUAL

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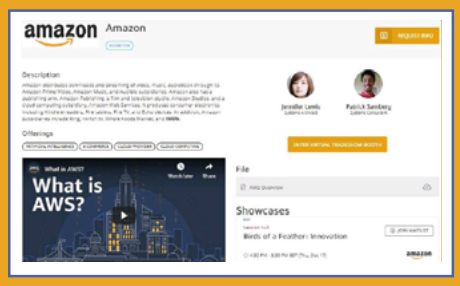

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WAYS TO CONNECT INCLUDE:

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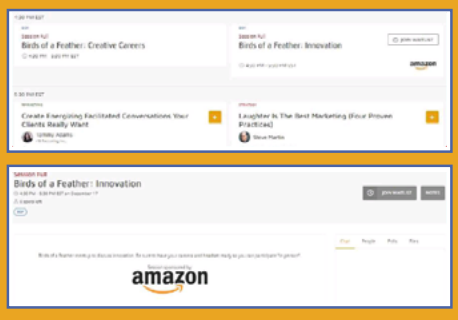

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FURTHER DETAILS WITHIN EACH AGENDA ITEM INCLUDE:

- Abstracts
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- and much MORE!

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- Post event, CHI will provide full contact information for your specific session
- Virtual Exhibit Booth Space
- and much MORE!

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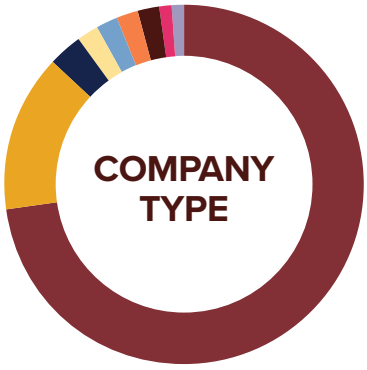
- Additional conference registrations available at a discount for your staff – limited to 5

For additional information regarding sponsorship and exhibit opportunities, please contact:

Rod Eymael | Business Development Manager
reymael@healthtech.com | 781-247-6286

2020 ATTENDEE DEMOGRAPHICS



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PRESENT A POSTER AND SAVE $50!*

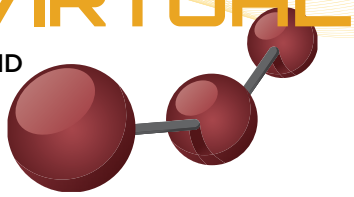
Cambridge Healthtech Institute encourages attendees to gain further exposure by presenting their work in the virtual poster sessions. To ensure your poster presentation is included in the conference materials, your full submission must be received, and your registration paid in full by April 30, 2021.

CAMBRIDGE HEALTHTECH INSTITUTE'S 16TH ANNUAL

MAY 18 - 20, 2021

Drug Discovery Chemistry VIRTUAL

OPTIMIZING SMALL MOLECULES FOR TOMORROW'S THERAPEUTICS INCLUDING COVID



PRICING & REGISTRATION INFORMATION

See website for complete details including discounts for groups and On-Demand participation

ALL ACCESS PRICING

Includes real-time access to ALL conferences, THREE short courses, virtual event benefits, plus On-Demand access for one year. You are allowed to move between virtual sessions to attend presentations taking place at the same time.

	Commercial	Academic, Government, Hospital Affiliated
Standard Rate After April 30	$1499	$899

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Includes real-time access to two conferences and virtual event benefits, plus On-Demand access for one year. You are allowed to move between virtual sessions to attend presentations taking place at the same time.

Standard Rate After April 30	$1199	$699

BASIC PRICING

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Standard Rate After April 30	$999	$599

SHORT COURSE ONLY

Includes real-time access to short course(s) only plus On-Demand access for one year.

One Short Course	$349	$149
Two Short Courses	$499	$249
Three Short Courses	$599	$299

WANT TO REGISTER BY PHONE?

Contact our Registration department at 781-972-5400 or Toll-free in the US at 888-999-6288.

CONFERENCE DISCOUNTS

Poster Submission - Discount ($50 Off*): Poster materials are due by April 30, 2021. Once your registration has been fully processed, we will send an email with a unique link and instructions for submitting your abstract and other materials. If you do not receive this email within 5 business days, please contact jring@healthtech.com. * CHI reserves the right to publish your poster title and abstract in various marketing materials and products.

**this discount does not apply to product or service providers*

Alumni Discount: Cambridge Healthtech Institute (CHI) appreciates your past participation at Drug Discovery Chemistry. As a result of the great loyalty you have shown us, we are pleased to extend to you the exclusive opportunity to save an additional 20% off the registration rate.

Group Discounts: Have your colleagues or entire team attend the virtual event. Purchase one virtual registration at full price, and participants from the same organization will receive a 50% discount when registering on the Group registration page. For more information on group rates contact Bill Mote at 781-972-5479, bmote@healthtech.com.

Concurrent Conferences *(May 18 - 19)*	**Concurrent Conferences** *(May 19 - 20)*
C1A: Ubiquitin-Induced Targeted Protein Degradation	**C1B:** Protein-Protein Interactions
C2A: Fragment-Based Drug Discovery	**C2B:** Artificial Intelligence for Early Drug Discovery
C3A: RNA-Targeting Small Molecule Drugs	**C3B:** Small Molecules for Immunology, Oncology & COVID
C4A: Macrocyclics & Constrained Peptides	**C4B:** Encoded Libraries for Small Molecule Discovery

Short Courses		
Tuesday, May 18 | *1:45 to 3:45 pm*	Wednesday, May 19 | *2:00 to 4:00 pm*	Thursday, May 20 | *11:15 am to 1:15 pm*
SC1: Emerging Chemical Tools for Phenotypic Screening and Target Deconvolution	**SC2:** Targeted Protein Degradation Using PROTACs, Molecular Glues, and More	**SC3:** Ligand-Receptor Molecular Interactions and Drug Design

How to Register: DrugDiscoveryChemistry.com

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Please use keycode **DCH V** when registering!

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